



## Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 06:46 am BST

PDB ID : 8A3L / pdb\_00008a3l  
EMDB ID : EMD-15116  
Title : Structural insights into the binding of bS1 to the ribosome  
Authors : D'Urso, G.; Chat, S.; Gillet, R.; Giudice, E.  
Deposited on : 2022-06-08  
Resolution : 3.42 Å (reported)  
Based on initial models : 6BU8, 7NBU

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

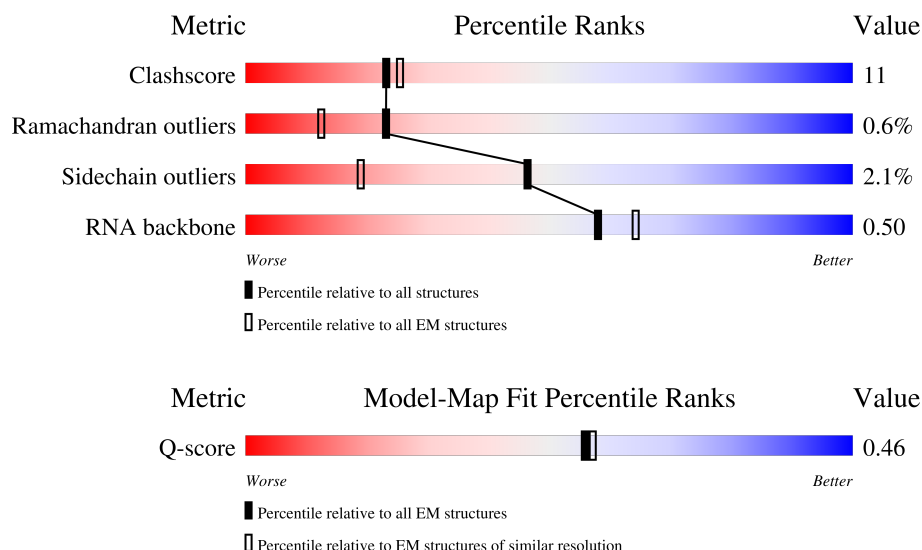
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.42 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13959 ( 2.92 - 3.92 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1539   |                  |
| 2   | B     | 224    |                  |
| 3   | C     | 206    |                  |

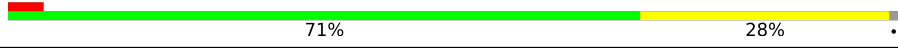
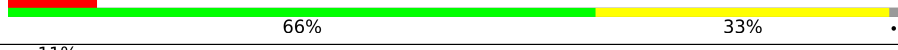
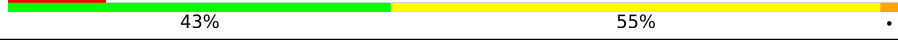
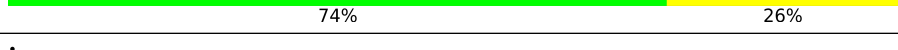
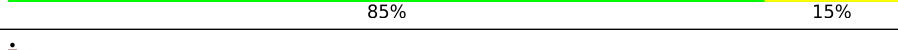
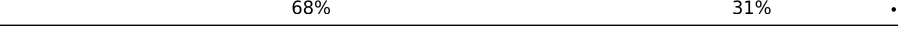
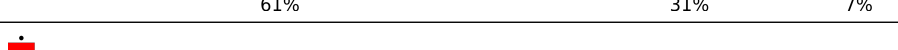
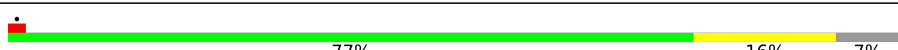
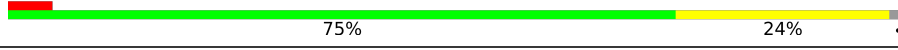
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | D     | 206    |                  |
| 5   | E     | 167    |                  |
| 6   | F     | 135    |                  |
| 7   | G     | 179    |                  |
| 8   | H     | 130    |                  |
| 9   | I     | 130    |                  |
| 10  | J     | 103    |                  |
| 11  | K     | 129    |                  |
| 12  | L     | 124    |                  |
| 13  | M     | 118    |                  |
| 14  | N     | 101    |                  |
| 15  | O     | 89     |                  |
| 16  | P     | 82     |                  |
| 17  | Q     | 84     |                  |
| 18  | R     | 75     |                  |
| 19  | S     | 92     |                  |
| 20  | T     | 87     |                  |
| 21  | U     | 71     |                  |
| 22  | V     | 77     |                  |
| 23  | W     | 77     |                  |
| 24  | X     | 38     |                  |
| 25  | Y     | 557    |                  |
| 26  | a     | 2903   |                  |
| 27  | b     | 120    |                  |
| 28  | c     | 273    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | d     | 209    |    |
| 30  | e     | 201    |    |
| 31  | f     | 179    |    |
| 32  | g     | 177    |    |
| 33  | h     | 149    |    |
| 34  | i     | 142    |    |
| 35  | j     | 123    |    |
| 36  | k     | 144    |    |
| 37  | l     | 136    |    |
| 38  | m     | 127    |    |
| 39  | n     | 117    |    |
| 40  | o     | 115    |  |
| 41  | p     | 118    |  |
| 42  | q     | 103    |  |
| 43  | r     | 110    |  |
| 44  | s     | 100    |  |
| 45  | t     | 104    |  |
| 46  | u     | 94     |  |
| 47  | v     | 85     |  |
| 48  | w     | 78     |  |
| 49  | x     | 63     |  |
| 50  | y     | 59     |  |
| 51  | z     | 57     |  |
| 52  | 0     | 55     |  |
| 53  | 1     | 46     |  |

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| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 54  | 2     | 65     | <div><div></div><div>72%</div><div>25%</div><div>••</div></div>               |
| 55  | 3     | 38     | <div><div>5%</div><div></div><div>84%</div><div>16%</div></div>               |
| 56  | 4     | 70     | <div><div>20%</div><div></div><div>54%</div><div>40%</div><div>6%</div></div> |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | A     | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33022 | 14736 | 6046 | 10702 | 1538 |         |       |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference |
|-------|---------|----------|--------|-----------|-----------|
| A     | 88      | U        | -      | insertion | GB J01859 |
| A     | 1002    | A        | G      | conflict  | GB J01859 |
| A     | 1006    | C        | G      | conflict  | GB J01859 |
| A     | 1010    | C        | U      | conflict  | GB J01859 |
| A     | 1019    | G        | A      | conflict  | GB J01859 |
| A     | 1020    | A        | G      | conflict  | GB J01859 |
| A     | 1021    | U        | A      | conflict  | GB J01859 |
| A     | 1022    | U        | A      | conflict  | GB J01859 |
| A     | 1023    | G        | U      | conflict  | GB J01859 |
| A     | 1038    | U        | C      | conflict  | GB J01859 |
| A     | 1120    | U        | C      | conflict  | GB J01859 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1753  | 1109 | 315 | 321 | 8 |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | E     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 717 | 217 | 212 | 6 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 530 | 151 | 151 | 7 |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 750 | 231 | 218 | 4 |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 552 | 179 | 157 | 3 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 403 | 127 | 112 | 1 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 641   | 406 | 120 | 112 | 3 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 18  | R     | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 345 | 102 | 96 | 1 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 427 | 127 | 112 | 2 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 21  | U     | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 351 | 123 | 94 | 1 |         |       |

- Molecule 22 is a RNA chain called P-site fMet-tRNA(fMet).

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 22  | V     | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1643  | 733 | 297 | 535 | 77 | 1 |         |       |

- Molecule 23 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | W     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |       |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 24  | X     | 6        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 136   | 60 | 30 | 40 | 6 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 25  | Y     | 172      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1332  | 840 | 230 | 262 |         |       |

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 26  | a     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62337 | 27817 | 11469 | 20148 | 2903 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| a     | 887     | A        | U      | conflict | GB NR_103073 |

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 27  | b     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2569  | 1144 | 468 | 837 | 120 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | c     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | d     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 980 | 288 | 294 | 4 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | f     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | g     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | i     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | j     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | k     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | l     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 686 | 205 | 177 | 7 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 1     | 137     | MS6      | MET    | conflict | UNP P0ADY7 |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | m     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 585 | 194 | 161 | 5 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39  | n     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | o     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 41  | p     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | q     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | r     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | s     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | t     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | u     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | v     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 634   | 391 | 129 | 113 | 1 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | w     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | x     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | y     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | z     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 52  | 0     | 51       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 417   | 269 | 76 | 72 |  |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53  | 1     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54  | 2     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | 3     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 56  | 4     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 522   | 323 | 99 | 94 | 6 |         |       |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 57  | A     | 71       | Total | Mg  | 0       |
|     |       |          | 71    | 71  |         |
| 57  | a     | 234      | Total | Mg  | 0       |
|     |       |          | 234   | 234 |         |
| 57  | b     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |

*Continued on next page...*

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 57  | c     | 3        | Total<br>3 | Mg<br>3 | 0       |
| 57  | d     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 57  | m     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 57  | z     | 1        | Total<br>1 | Mg<br>1 | 0       |

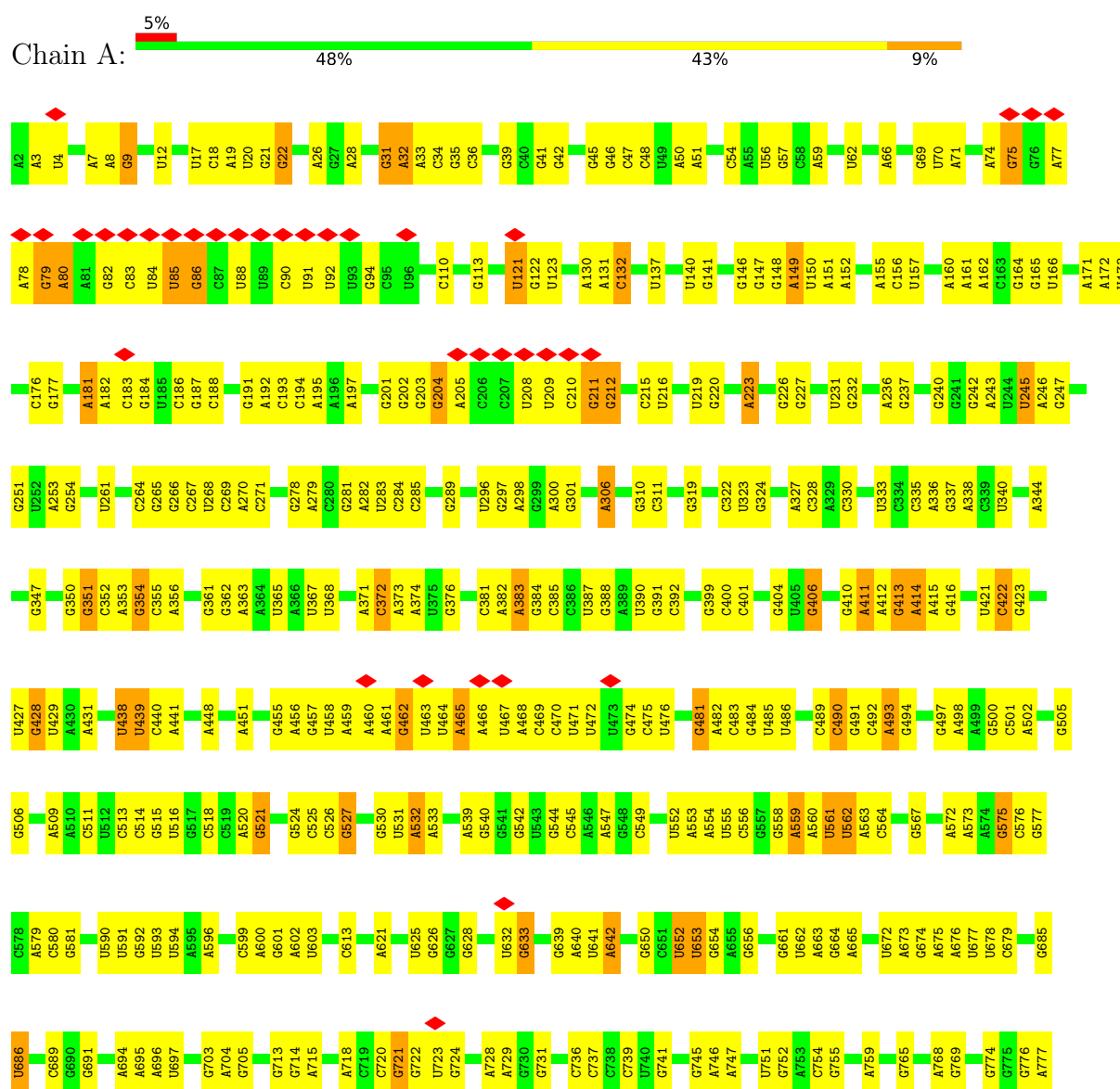
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

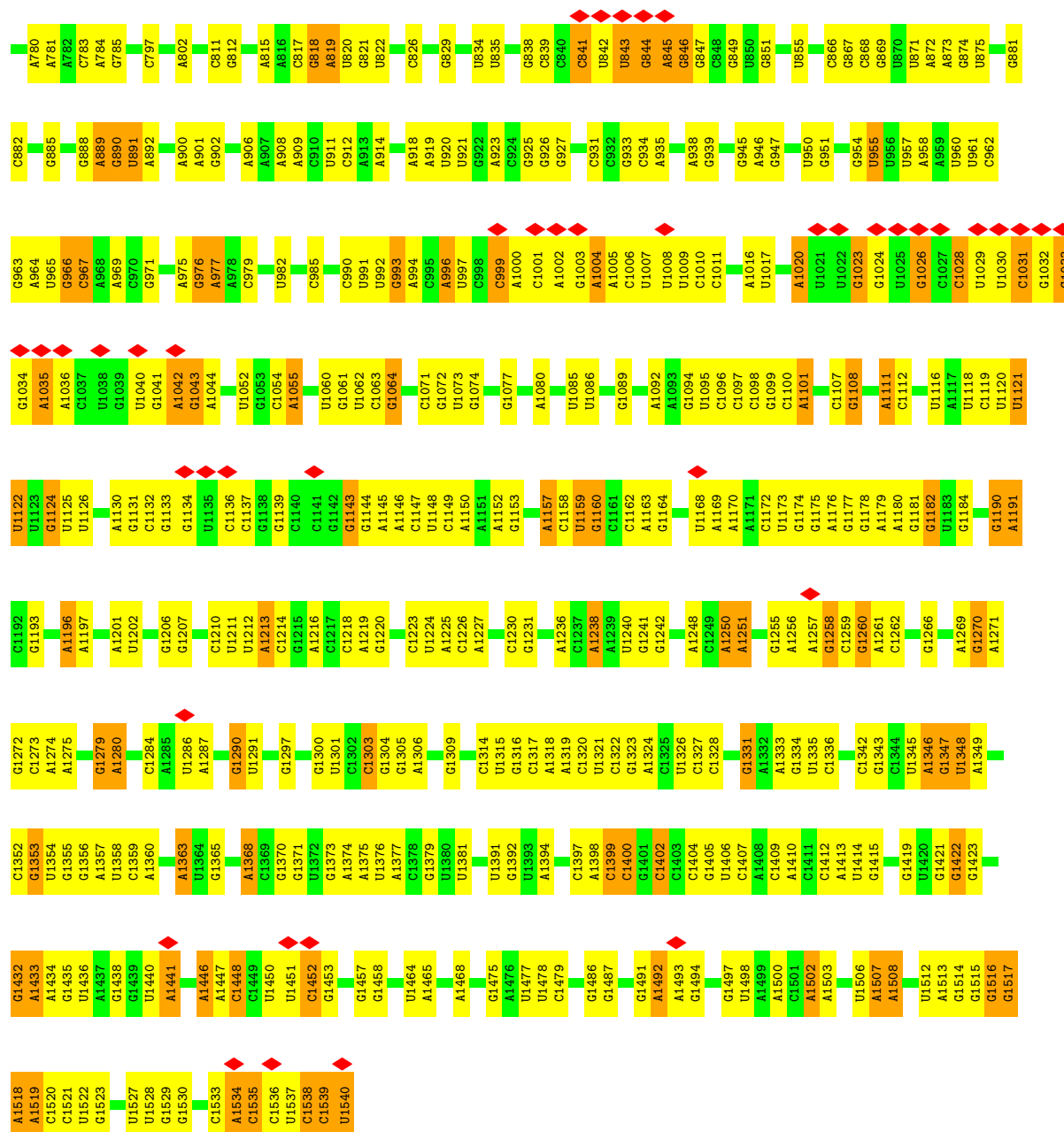
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 58  | 3     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 58  | 4     | 1        | Total<br>1 | Zn<br>1 | 0       |

### 3 Residue-property plots

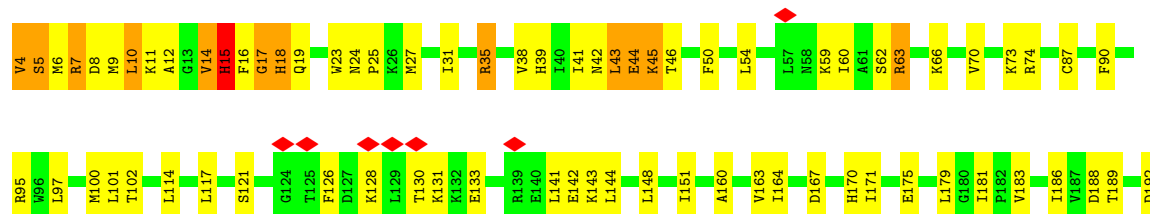
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

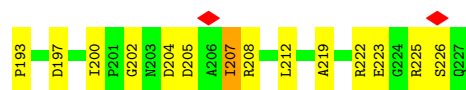
#### • Molecule 1: 16S ribosomal RNA



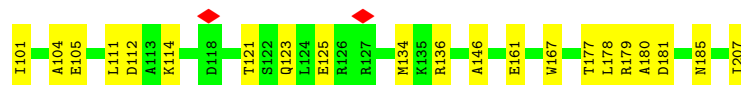
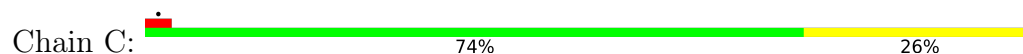


• Molecule 2: 30S ribosomal protein S2

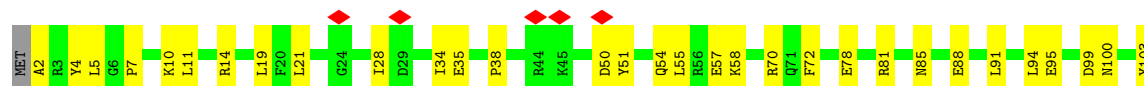




- Molecule 3: 30S ribosomal protein S3



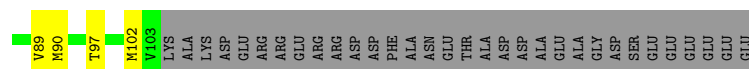
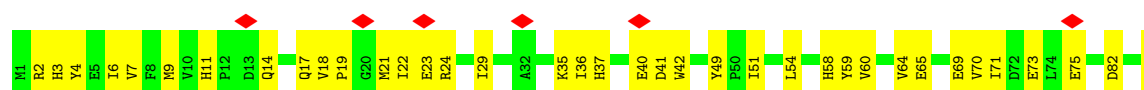
- Molecule 4: 30S ribosomal protein S4



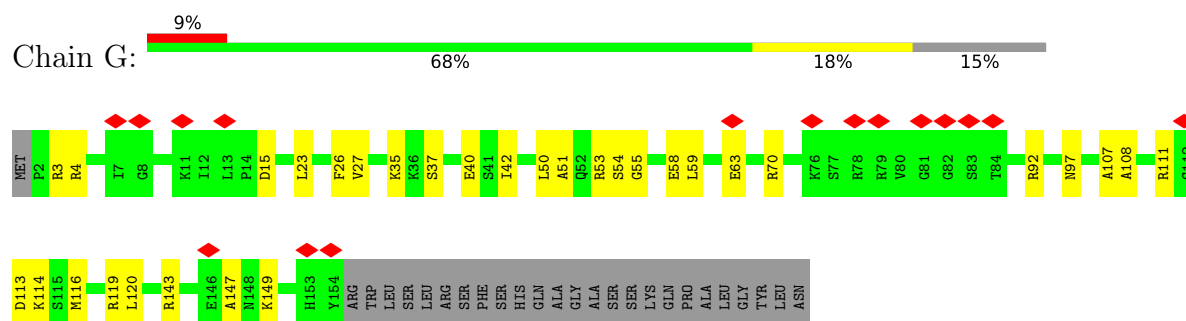
- Molecule 5: 30S ribosomal protein S5



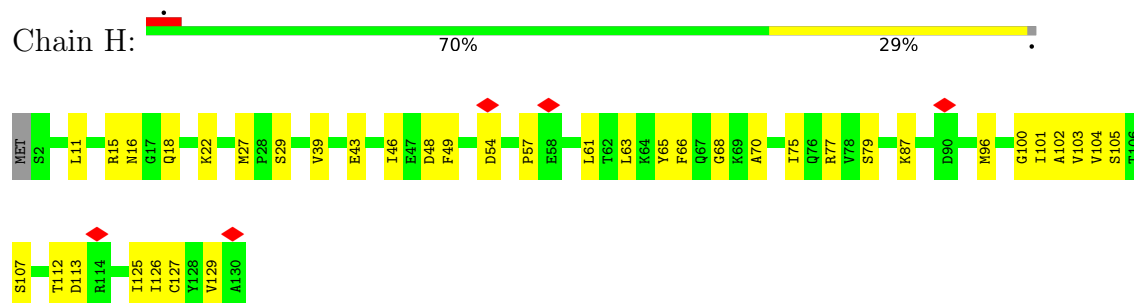
- Molecule 6: 30S ribosomal protein S6



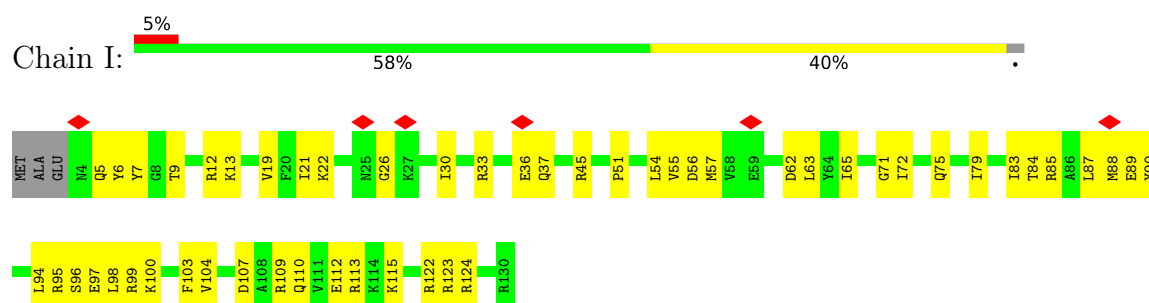
- Molecule 7: 30S ribosomal protein S7



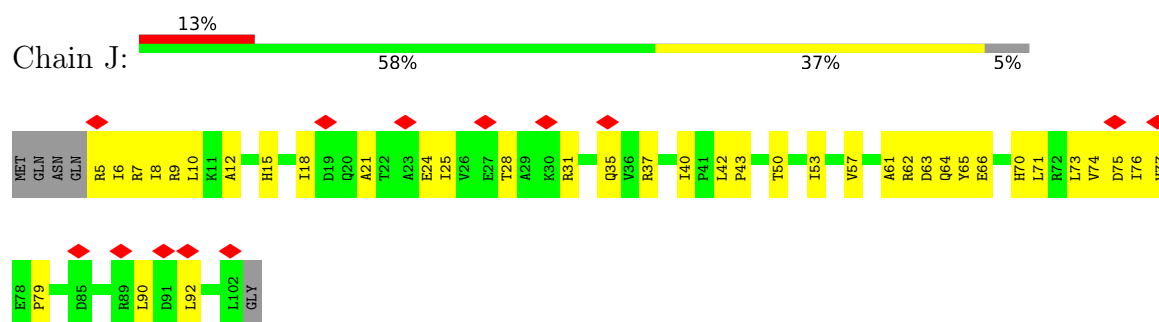
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

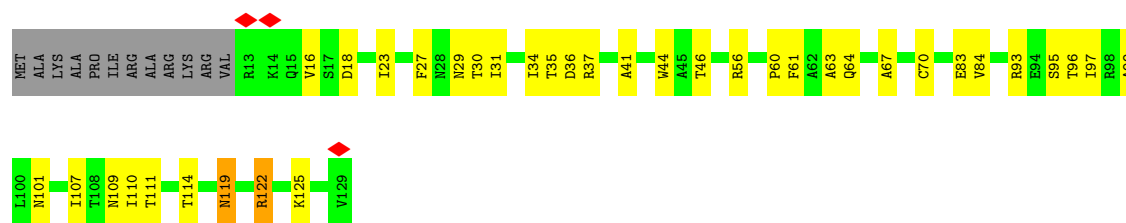


- Molecule 10: 30S ribosomal protein S10

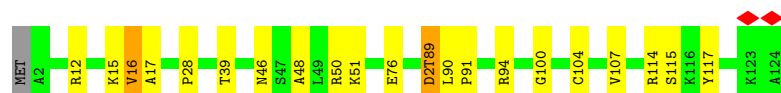
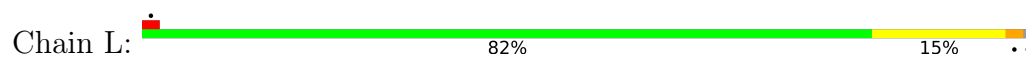


- Molecule 11: 30S ribosomal protein S11

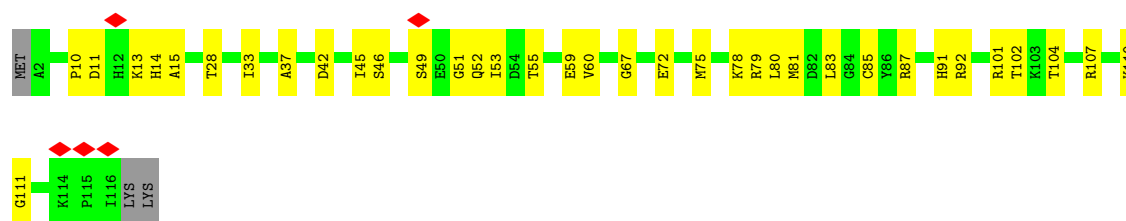




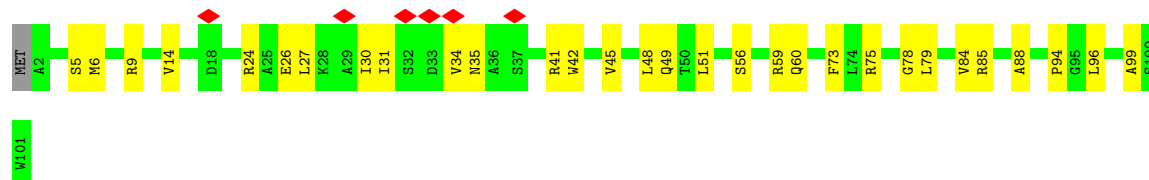
- Molecule 12: 30S ribosomal protein S12



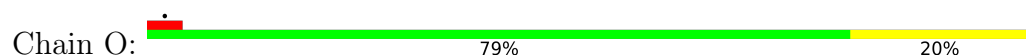
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

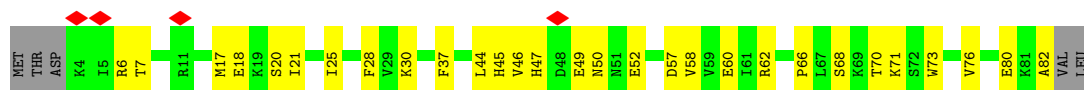


- Molecule 16: 30S ribosomal protein S16





- Molecule 17: 30S ribosomal protein S17



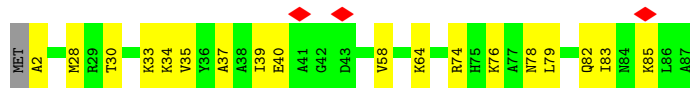
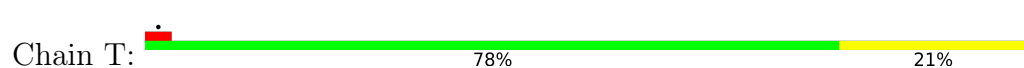
- Molecule 18: 30S ribosomal protein S18



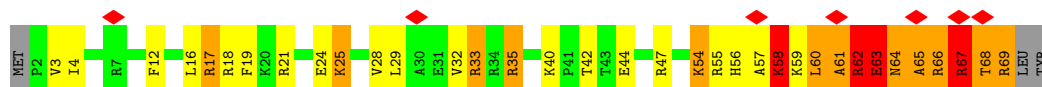
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

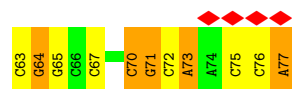
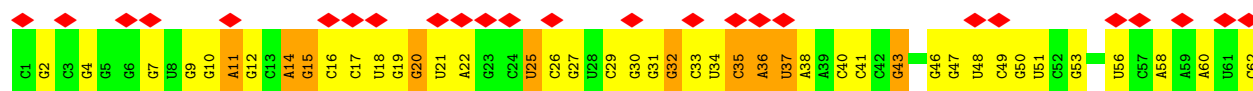


- Molecule 22: P-site fMet-tRNA(fMet)

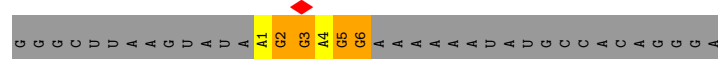




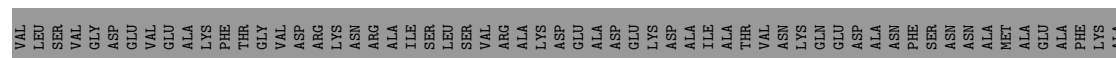
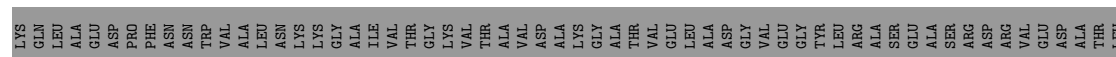
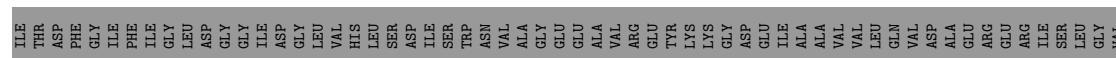
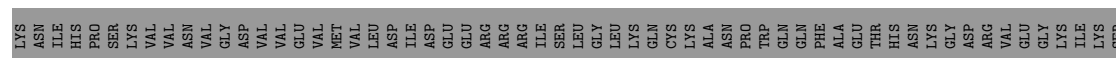
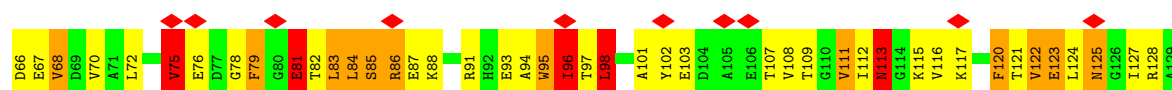
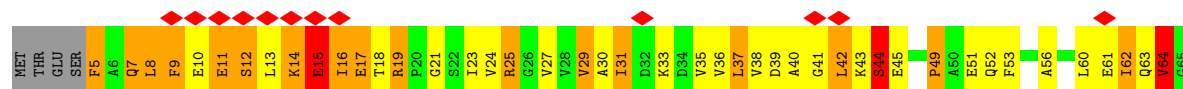
• Molecule 23: E-site tRNA



• Molecule 24: mRNA

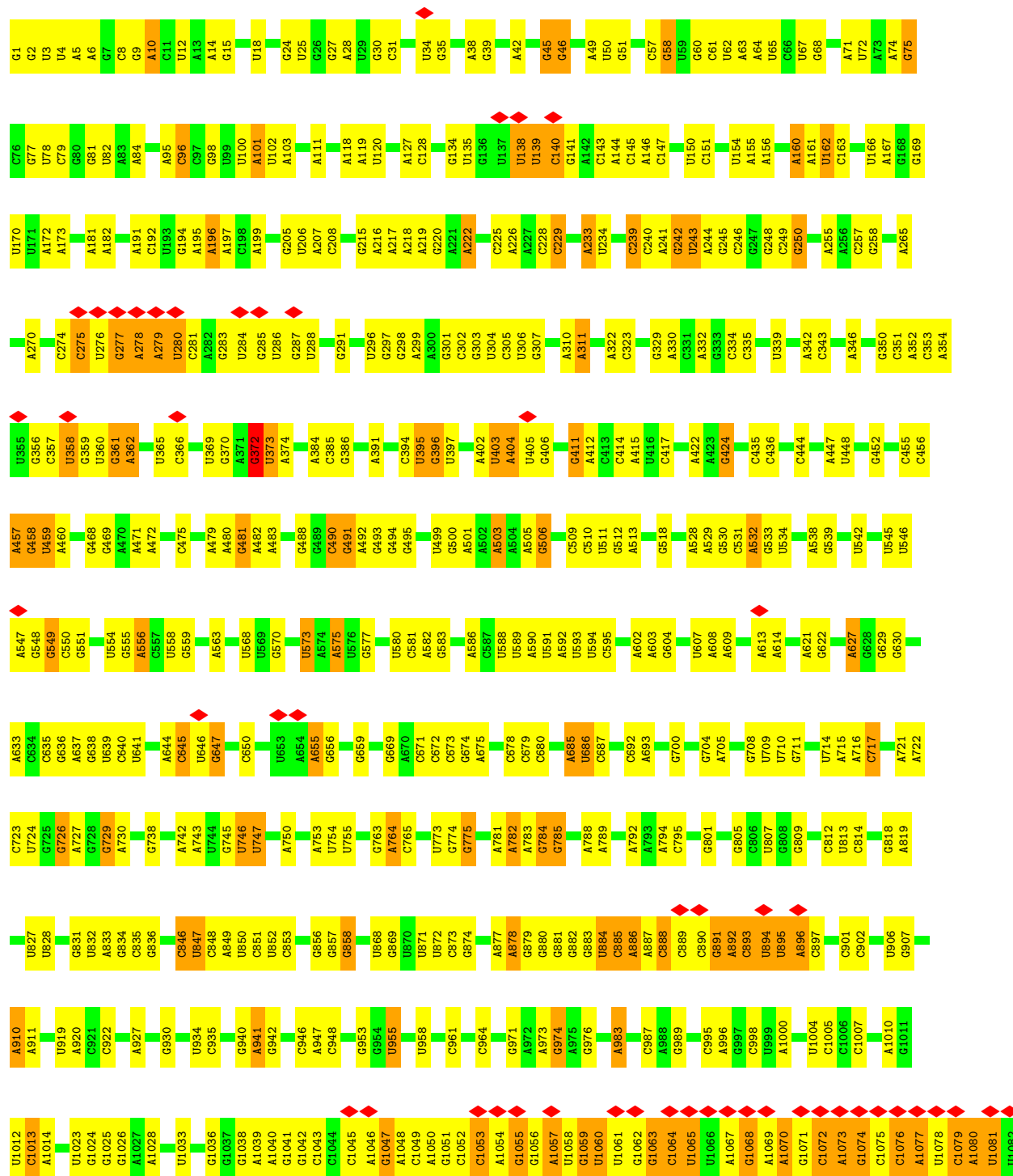


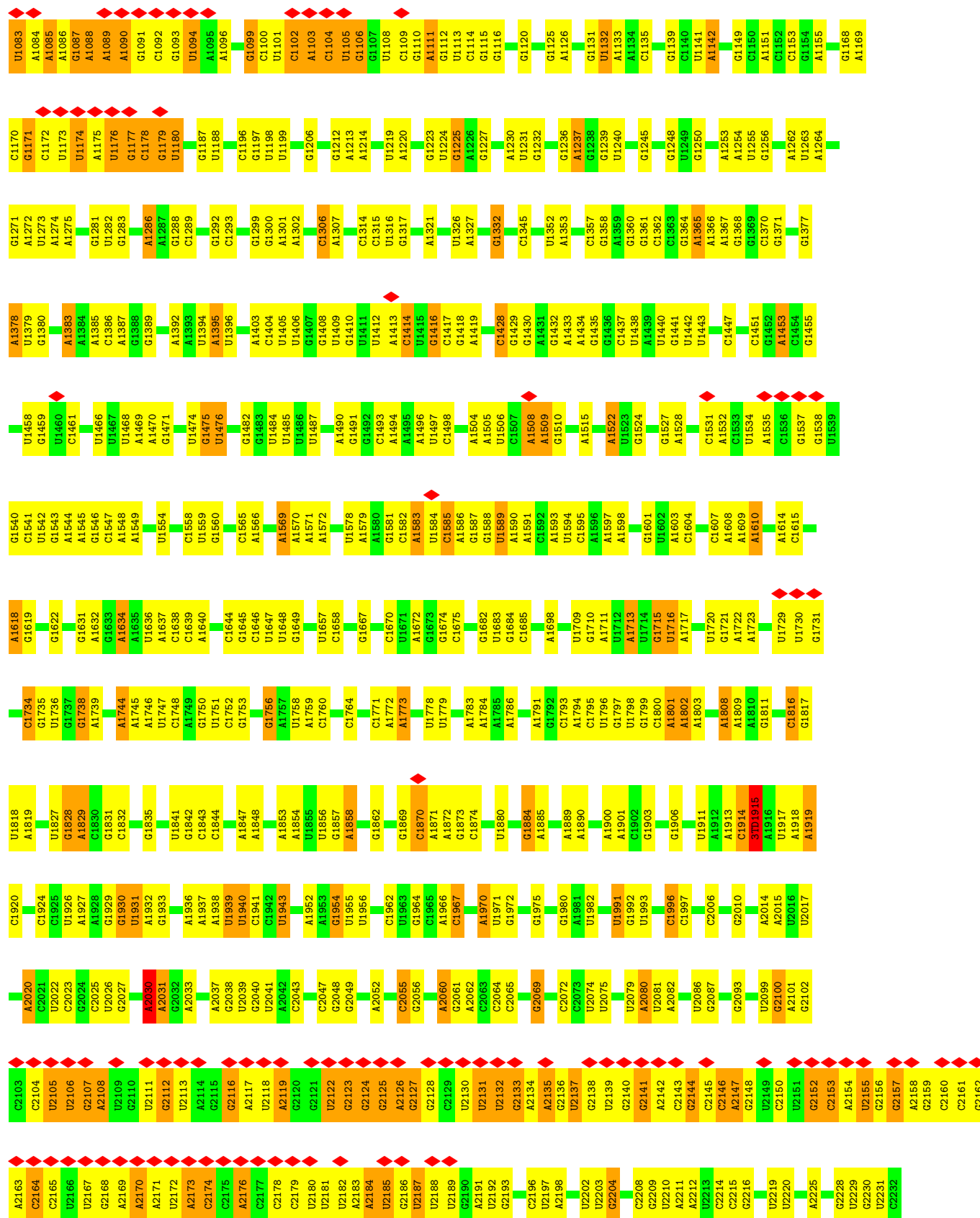
• Molecule 25: 30S ribosomal protein S1

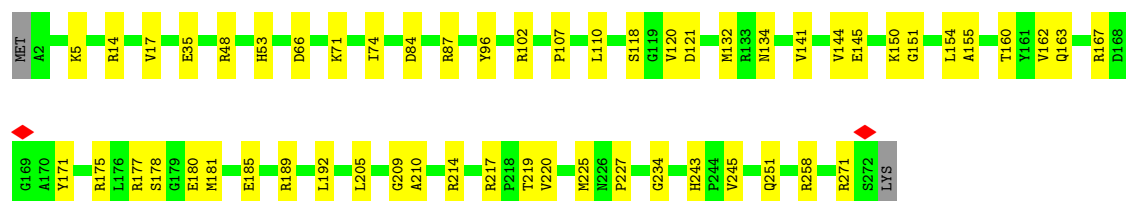


ALA  
LYS  
GLY  
GLU

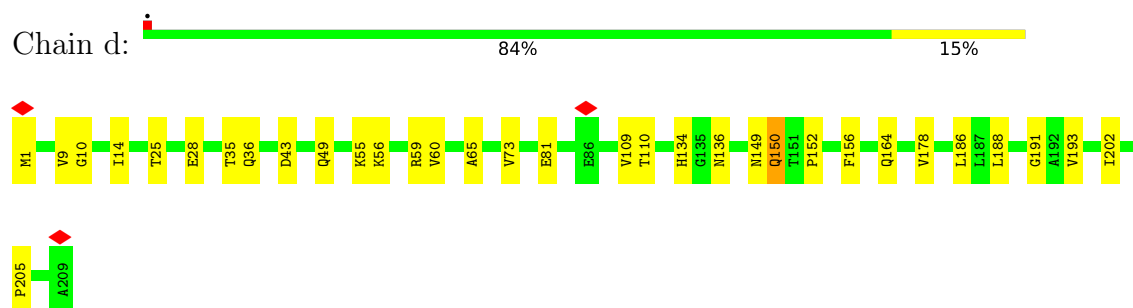
• Molecule 26: 23S ribosomal RNA



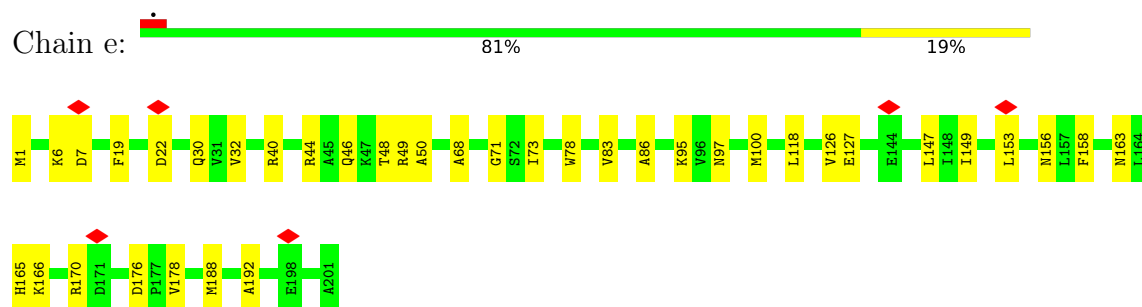




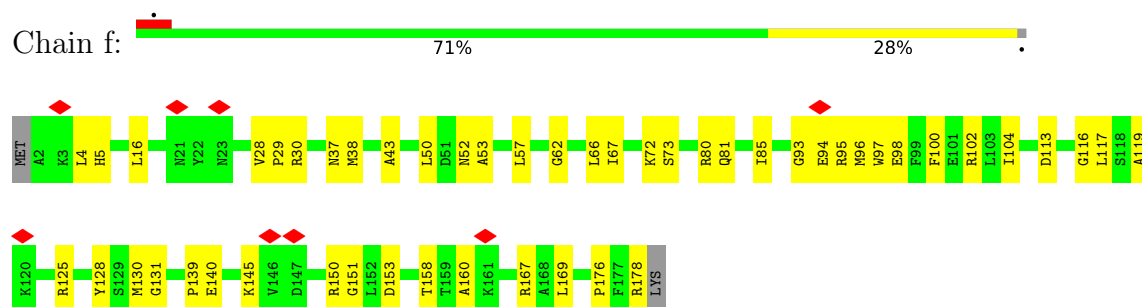
- Molecule 29: 50S ribosomal protein L3



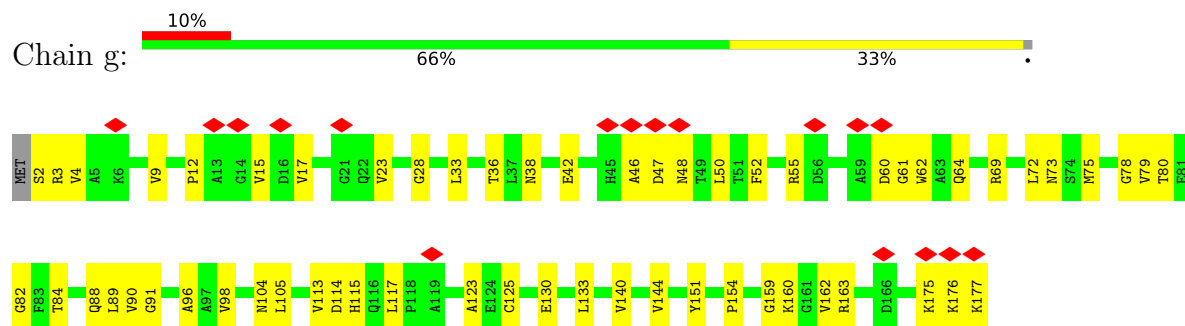
- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5

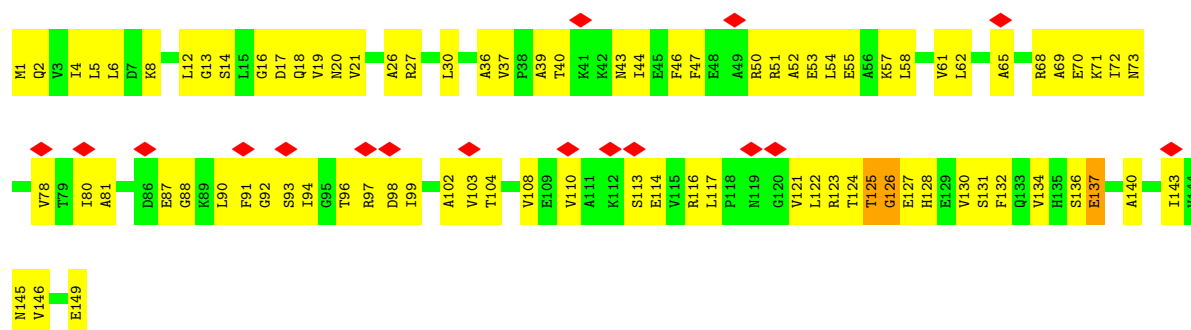


- Molecule 32: 50S ribosomal protein L6

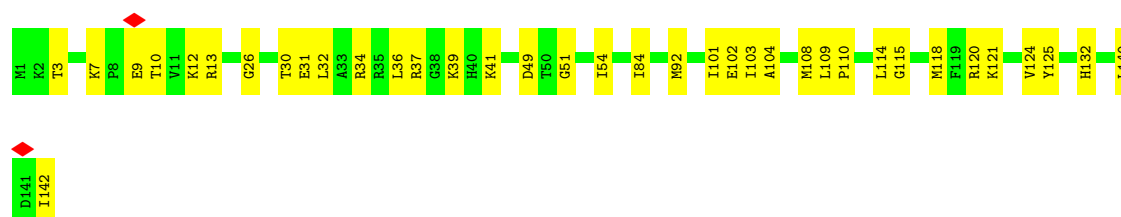


- Molecule 33: 50S ribosomal protein L9

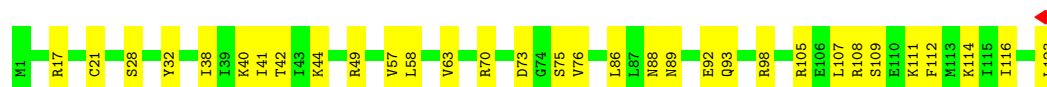




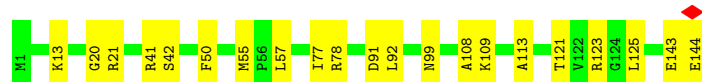
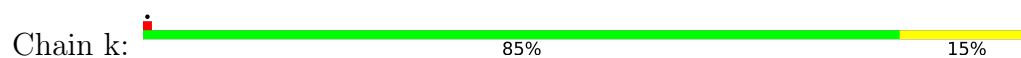
- Molecule 34: 50S ribosomal protein L13



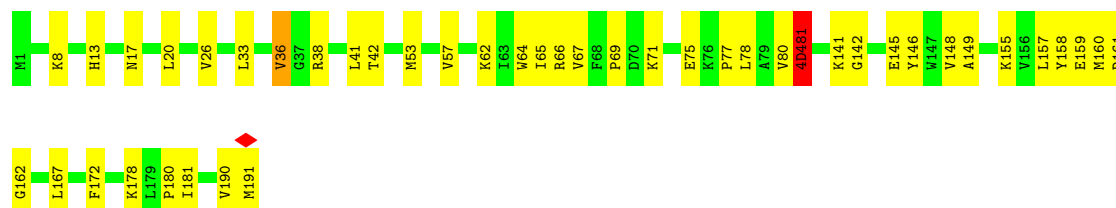
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15

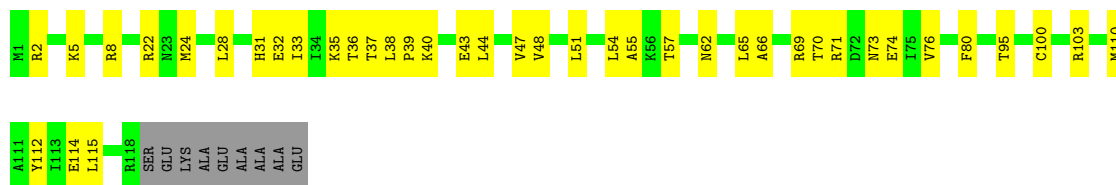


- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17

Chain m:  61% 31% 7%



- Molecule 39: 50S ribosomal protein L18

Chain n:  80% 19% .



- Molecule 40: 50S ribosomal protein L19

Chain o:  83% 16% .



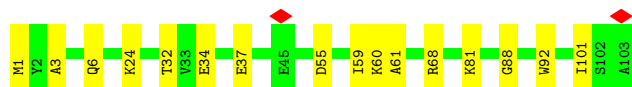
- Molecule 41: 50S ribosomal protein L20

Chain p:  82% 17% .



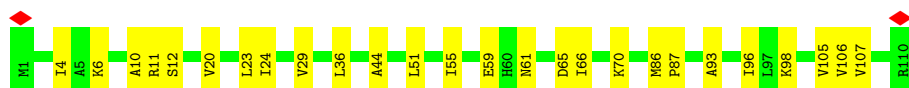
- Molecule 42: 50S ribosomal protein L21

Chain q:  84% 16%



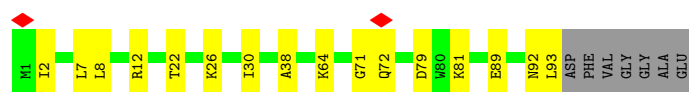
- Molecule 43: 50S ribosomal protein L22

Chain r:  76% 24%

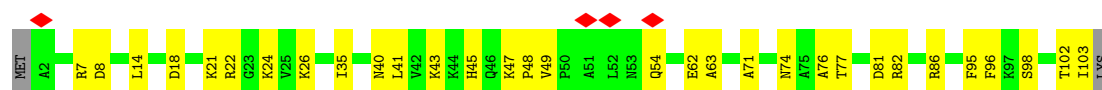


- Molecule 44: 50S ribosomal protein L23

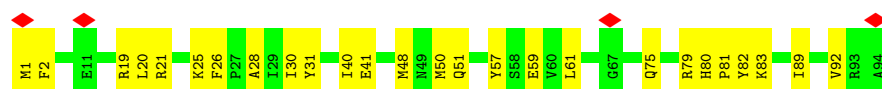
Chain s:  77% 16% 7%



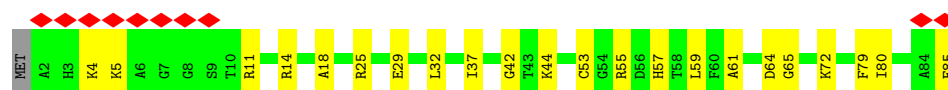
- Molecule 45: 50S ribosomal protein L24



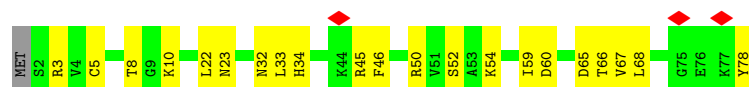
- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27



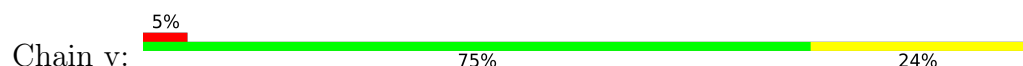
- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30



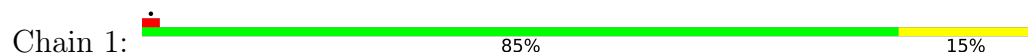
- Molecule 51: 50S ribosomal protein L32



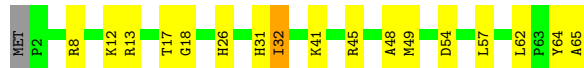
- Molecule 52: 50S ribosomal protein L33



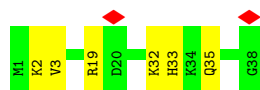
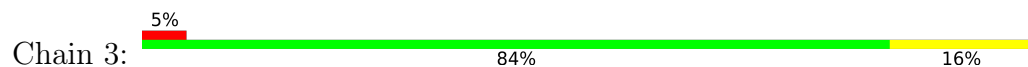
- Molecule 53: 50S ribosomal protein L34



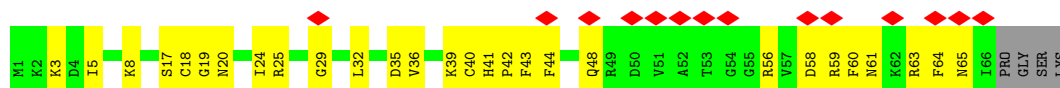
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L31



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 16381                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 35                                      | Depositor |
| Minimum defocus (nm)                 | 400                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 36000                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 29.329                                  | Depositor |
| Minimum map value                    | -18.440                                 | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 4.2                                     | Depositor |
| Map size (Å)                         | 457.216, 457.216, 457.216               | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.893, 0.893, 0.893                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, 1MG, D2T, ZN, OMC, UR3, PSU, G7M, 2MG, 2MA, 4OC, 4D4, 3TD, OMU, MS6, H2U, MA6, MEQ, MG, 6MZ, 5MC, 5MU, OMG

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.33         | 0/36690        | 0.35        | 2/57230 (0.0%)  |
| 2   | B     | 0.52         | 0/1784         | 0.87        | 8/2403 (0.3%)   |
| 3   | C     | 0.27         | 0/1651         | 0.43        | 0/2225          |
| 4   | D     | 0.34         | 0/1665         | 0.50        | 0/2227          |
| 5   | E     | 0.29         | 0/1165         | 0.38        | 0/1568          |
| 6   | F     | 0.28         | 0/858          | 0.49        | 0/1160          |
| 7   | G     | 0.23         | 0/1219         | 0.42        | 0/1635          |
| 8   | H     | 0.31         | 0/989          | 0.48        | 0/1326          |
| 9   | I     | 0.28         | 0/1034         | 0.45        | 0/1375          |
| 10  | J     | 0.27         | 0/796          | 0.49        | 0/1077          |
| 11  | K     | 0.40         | 0/893          | 0.56        | 0/1205          |
| 12  | L     | 0.29         | 0/960          | 0.46        | 0/1286          |
| 13  | M     | 0.26         | 0/900          | 0.44        | 0/1204          |
| 14  | N     | 0.29         | 0/817          | 0.40        | 0/1088          |
| 15  | O     | 0.26         | 0/722          | 0.36        | 0/964           |
| 16  | P     | 0.31         | 0/653          | 0.46        | 0/877           |
| 17  | Q     | 0.27         | 0/650          | 0.42        | 0/871           |
| 18  | R     | 0.56         | 0/553          | 0.76        | 1/742 (0.1%)    |
| 19  | S     | 0.27         | 0/685          | 0.44        | 0/922           |
| 20  | T     | 0.27         | 0/676          | 0.40        | 0/895           |
| 21  | U     | 0.63         | 0/576          | 1.18        | 6/763 (0.8%)    |
| 22  | V     | 0.27         | 0/1746         | 0.30        | 0/2721          |
| 23  | W     | 0.54         | 0/1832         | 0.81        | 1/2855 (0.0%)   |
| 24  | X     | 0.34         | 0/153          | 0.63        | 0/238           |
| 25  | Y     | 0.89         | 0/1347         | 1.28        | 9/1817 (0.5%)   |
| 26  | a     | 0.38         | 1/69244 (0.0%) | 0.37        | 4/108022 (0.0%) |
| 27  | b     | 0.30         | 0/2872         | 0.32        | 0/4478          |
| 28  | c     | 0.36         | 0/2121         | 0.42        | 0/2852          |
| 29  | d     | 0.35         | 0/1576         | 0.40        | 0/2119          |
| 30  | e     | 0.42         | 0/1571         | 0.52        | 0/2113          |
| 31  | f     | 0.27         | 0/1434         | 0.44        | 0/1926          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 32  | g     | 0.24         | 0/1343          | 0.41        | 0/1816           |
| 33  | h     | 0.40         | 0/1122          | 0.74        | 2/1515 (0.1%)    |
| 34  | i     | 0.34         | 0/1152          | 0.37        | 0/1551           |
| 35  | j     | 0.34         | 0/955           | 0.39        | 0/1279           |
| 36  | k     | 0.33         | 0/1062          | 0.42        | 0/1413           |
| 37  | l     | 0.32         | 0/1073          | 0.43        | 1/1433 (0.1%)    |
| 38  | m     | 0.35         | 0/958           | 0.45        | 0/1281           |
| 39  | n     | 0.30         | 0/902           | 0.46        | 0/1209           |
| 40  | o     | 0.32         | 0/929           | 0.43        | 0/1242           |
| 41  | p     | 0.38         | 0/960           | 0.39        | 0/1278           |
| 42  | q     | 0.33         | 0/829           | 0.47        | 0/1107           |
| 43  | r     | 0.33         | 0/864           | 0.44        | 0/1156           |
| 44  | s     | 0.31         | 0/744           | 0.45        | 0/994            |
| 45  | t     | 0.29         | 0/787           | 0.41        | 0/1051           |
| 46  | u     | 0.30         | 0/766           | 0.46        | 0/1025           |
| 47  | v     | 0.35         | 0/642           | 0.40        | 0/848            |
| 48  | w     | 0.34         | 0/635           | 0.42        | 0/848            |
| 49  | x     | 0.26         | 0/502           | 0.41        | 0/667            |
| 50  | y     | 0.35         | 0/453           | 0.46        | 0/605            |
| 51  | z     | 0.33         | 0/450           | 0.39        | 0/599            |
| 52  | 0     | 0.29         | 0/424           | 0.38        | 0/565            |
| 53  | 1     | 0.38         | 0/380           | 0.43        | 0/498            |
| 54  | 2     | 0.37         | 0/513           | 0.44        | 0/676            |
| 55  | 3     | 0.31         | 0/303           | 0.38        | 0/397            |
| 56  | 4     | 0.26         | 0/531           | 0.43        | 0/709            |
| All | All   | 0.36         | 1/159111 (0.0%) | 0.42        | 34/237946 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 37  | l     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 26  | a     | 1734 | C    | C1'-N1 | 5.09 | 1.56        | 1.48     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 21  | U     | 64   | ASN  | N-CA-C      | -12.83 | 97.66       | 113.18   |
| 2   | B     | 15   | HIS  | CA-C-N      | -12.71 | 101.03      | 122.64   |
| 2   | B     | 15   | HIS  | C-N-CA      | -12.71 | 101.03      | 122.64   |
| 25  | Y     | 12   | SER  | N-CA-C      | -11.59 | 98.52       | 112.89   |
| 25  | Y     | 7    | GLN  | N-CA-C      | -8.00  | 102.15      | 112.23   |
| 2   | B     | 43   | LEU  | N-CA-C      | -7.72  | 104.34      | 113.38   |
| 2   | B     | 45   | LYS  | N-CA-C      | -7.69  | 103.86      | 113.55   |
| 33  | h     | 125  | THR  | N-CA-C      | 7.48   | 122.52      | 107.41   |
| 2   | B     | 44   | GLU  | N-CA-C      | -7.36  | 104.81      | 114.31   |
| 21  | U     | 60   | LEU  | N-CA-C      | -7.30  | 104.23      | 113.43   |
| 25  | Y     | 10   | GLU  | N-CA-C      | -7.09  | 104.60      | 113.18   |
| 25  | Y     | 113  | ASN  | CB-CA-C     | 6.95   | 121.22      | 109.75   |
| 33  | h     | 124  | THR  | N-CA-C      | 6.85   | 119.37      | 110.53   |
| 21  | U     | 61   | ALA  | O-C-N       | 6.42   | 131.12      | 122.59   |
| 25  | Y     | 9    | PHE  | N-CA-C      | -6.26  | 105.47      | 113.23   |
| 25  | Y     | 11   | GLU  | N-CA-C      | -6.06  | 105.84      | 113.72   |
| 1   | A     | 1528 | U    | P-O3'-C3'   | 5.87   | 129.00      | 120.20   |
| 21  | U     | 58   | LYS  | N-CA-C      | -5.72  | 105.02      | 112.23   |
| 2   | B     | 14   | VAL  | O-C-N       | 5.57   | 129.35      | 122.05   |
| 26  | a     | 1100 | C    | C4'-C3'-O3' | -5.57  | 104.65      | 113.00   |
| 21  | U     | 68   | THR  | CA-C-O      | -5.57  | 114.69      | 120.70   |
| 25  | Y     | 174  | ILE  | N-CA-C      | -5.41  | 106.22      | 112.98   |
| 23  | W     | 32   | G    | C4'-C3'-C2' | -5.35  | 97.25       | 102.60   |
| 37  | l     | 36   | VAL  | N-CA-C      | -5.33  | 107.64      | 112.96   |
| 25  | Y     | 15   | GLU  | CA-C-O      | -5.26  | 115.28      | 120.70   |
| 2   | B     | 63   | ARG  | N-CA-C      | -5.25  | 106.90      | 113.15   |
| 21  | U     | 62   | ARG  | N-CA-C      | -5.20  | 99.72       | 110.80   |
| 1   | A     | 110  | C    | C3'-C2'-O2' | 5.15   | 118.42      | 110.70   |
| 18  | R     | 10   | PHE  | CB-CA-C     | 5.12   | 119.31      | 110.86   |
| 2   | B     | 17   | GLY  | CA-C-O      | -5.09  | 116.89      | 121.47   |
| 25  | Y     | 75   | VAL  | N-CA-C      | -5.07  | 105.45      | 110.62   |
| 26  | a     | 1818 | U    | C3'-C2'-O2' | 5.05   | 118.27      | 110.70   |
| 26  | a     | 372  | G    | C4'-C3'-O3' | 5.03   | 116.94      | 109.40   |
| 26  | a     | 1060 | U    | C4'-C3'-O3' | -5.01  | 105.48      | 113.00   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 37  | l     | 81  | 4D4  | Mainchain |

## 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   | A     | 33022 | 0        | 16643    | 607     | 0            |
| 2   | B     | 1753  | 0        | 1780     | 74      | 0            |
| 3   | C     | 1624  | 0        | 1696     | 35      | 0            |
| 4   | D     | 1643  | 0        | 1707     | 52      | 0            |
| 5   | E     | 1152  | 0        | 1196     | 28      | 0            |
| 6   | F     | 839   | 0        | 833      | 38      | 0            |
| 7   | G     | 1203  | 0        | 1254     | 25      | 0            |
| 8   | H     | 979   | 0        | 1031     | 28      | 0            |
| 9   | I     | 1022  | 0        | 1070     | 46      | 0            |
| 10  | J     | 786   | 0        | 828      | 31      | 0            |
| 11  | K     | 877   | 0        | 887      | 35      | 0            |
| 12  | L     | 957   | 0        | 1017     | 18      | 0            |
| 13  | M     | 891   | 0        | 952      | 32      | 0            |
| 14  | N     | 805   | 0        | 844      | 25      | 0            |
| 15  | O     | 714   | 0        | 734      | 13      | 0            |
| 16  | P     | 643   | 0        | 661      | 19      | 0            |
| 17  | Q     | 641   | 0        | 682      | 23      | 0            |
| 18  | R     | 544   | 0        | 565      | 50      | 0            |
| 19  | S     | 668   | 0        | 693      | 32      | 0            |
| 20  | T     | 670   | 0        | 719      | 14      | 0            |
| 21  | U     | 569   | 0        | 609      | 45      | 0            |
| 22  | V     | 1643  | 0        | 840      | 25      | 0            |
| 23  | W     | 1640  | 0        | 837      | 16      | 0            |
| 24  | X     | 136   | 0        | 67       | 23      | 0            |
| 25  | Y     | 1332  | 0        | 1356     | 100     | 0            |
| 26  | a     | 62337 | 0        | 31370    | 936     | 0            |
| 27  | b     | 2569  | 0        | 1301     | 28      | 0            |
| 28  | c     | 2082  | 0        | 2154     | 53      | 0            |
| 29  | d     | 1566  | 0        | 1618     | 24      | 0            |
| 30  | e     | 1552  | 0        | 1619     | 27      | 0            |
| 31  | f     | 1410  | 0        | 1444     | 38      | 0            |
| 32  | g     | 1323  | 0        | 1371     | 40      | 0            |
| 33  | h     | 1111  | 0        | 1148     | 99      | 0            |
| 34  | i     | 1129  | 0        | 1162     | 24      | 0            |
| 35  | j     | 946   | 0        | 1023     | 27      | 0            |
| 36  | k     | 1053  | 0        | 1129     | 18      | 0            |
| 37  | l     | 1075  | 0        | 1145     | 31      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | m     | 945    | 0        | 989      | 28      | 0            |
| 39  | n     | 892    | 0        | 923      | 13      | 0            |
| 40  | o     | 917    | 0        | 962      | 18      | 0            |
| 41  | p     | 947    | 0        | 1019     | 17      | 0            |
| 42  | q     | 816    | 0        | 839      | 11      | 0            |
| 43  | r     | 857    | 0        | 922      | 16      | 0            |
| 44  | s     | 738    | 0        | 807      | 11      | 0            |
| 45  | t     | 779    | 0        | 831      | 22      | 0            |
| 46  | u     | 753    | 0        | 780      | 20      | 0            |
| 47  | v     | 634    | 0        | 653      | 18      | 0            |
| 48  | w     | 625    | 0        | 652      | 16      | 0            |
| 49  | x     | 501    | 0        | 531      | 15      | 0            |
| 50  | y     | 449    | 0        | 488      | 10      | 0            |
| 51  | z     | 444    | 0        | 458      | 12      | 0            |
| 52  | 0     | 417    | 0        | 451      | 12      | 0            |
| 53  | 1     | 377    | 0        | 418      | 5       | 0            |
| 54  | 2     | 504    | 0        | 572      | 17      | 0            |
| 55  | 3     | 302    | 0        | 340      | 4       | 0            |
| 56  | 4     | 522    | 0        | 520      | 22      | 0            |
| 57  | A     | 71     | 0        | 0        | 0       | 0            |
| 57  | a     | 234    | 0        | 0        | 0       | 0            |
| 57  | b     | 2      | 0        | 0        | 0       | 0            |
| 57  | c     | 3      | 0        | 0        | 0       | 0            |
| 57  | d     | 1      | 0        | 0        | 0       | 0            |
| 57  | m     | 1      | 0        | 0        | 0       | 0            |
| 57  | z     | 1      | 0        | 0        | 0       | 0            |
| 58  | 3     | 1      | 0        | 0        | 0       | 0            |
| 58  | 4     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 147640 | 0        | 99140    | 2672    | 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 11.

All (2672) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 28:c:121:ASP:HB3 | 33:h:91:PHE:CE1 | 1.32                     | 1.57              |
| 1:A:1540:U:O2    | 24:X:1:A:C2     | 1.81                     | 1.34              |
| 28:c:121:ASP:CB  | 33:h:91:PHE:CE1 | 2.14                     | 1.30              |
| 1:A:845:A:C2'    | 18:R:9:LYS:HZ1  | 1.41                     | 1.29              |
| 28:c:121:ASP:HB3 | 33:h:91:PHE:CZ  | 1.66                     | 1.29              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:845:A:C2'    | 18:R:9:LYS:NZ     | 1.96                     | 1.28              |
| 33:h:136:SER:O   | 33:h:137:GLU:CD   | 1.81                     | 1.22              |
| 1:A:1098:C:OP2   | 2:B:143:LYS:NZ    | 1.76                     | 1.18              |
| 1:A:845:A:H2'    | 18:R:9:LYS:NZ     | 1.60                     | 1.13              |
| 4:D:95:GLU:HG2   | 4:D:186:PRO:HG3   | 1.33                     | 1.10              |
| 28:c:121:ASP:CA  | 33:h:91:PHE:HE1   | 1.67                     | 1.07              |
| 1:A:845:A:C1'    | 18:R:9:LYS:HZ1    | 1.66                     | 1.07              |
| 1:A:1540:U:O2    | 24:X:1:A:N1       | 1.87                     | 1.07              |
| 11:K:27:PHE:CE1  | 21:U:33:ARG:NH2   | 2.25                     | 1.05              |
| 1:A:845:A:H2'    | 18:R:9:LYS:HZ1    | 1.14                     | 1.03              |
| 1:A:736:C:OP1    | 18:R:61:ARG:NH1   | 1.91                     | 1.02              |
| 1:A:845:A:H1'    | 18:R:15:ALA:HB2   | 1.42                     | 1.02              |
| 33:h:90:LEU:HD12 | 33:h:125:THR:HG22 | 1.38                     | 1.01              |
| 28:c:121:ASP:CB  | 33:h:91:PHE:CZ    | 2.39                     | 0.99              |
| 21:U:61:ALA:O    | 21:U:63:GLU:N     | 1.95                     | 0.98              |
| 1:A:845:A:C8     | 18:R:9:LYS:HE3    | 1.98                     | 0.98              |
| 25:Y:79:PHE:N    | 25:Y:79:PHE:HD1   | 1.62                     | 0.97              |
| 1:A:1535:C:H42   | 24:X:6:G:N2       | 1.64                     | 0.96              |
| 1:A:1535:C:N4    | 24:X:6:G:N2       | 2.15                     | 0.94              |
| 25:Y:18:THR:HG21 | 25:Y:24:VAL:HG22  | 1.49                     | 0.94              |
| 26:a:1847:A:HO2' | 26:a:1848:A:H8    | 1.00                     | 0.94              |
| 32:g:90:VAL:O    | 32:g:160:LYS:HA   | 1.68                     | 0.94              |
| 33:h:136:SER:C   | 33:h:137:GLU:CD   | 2.36                     | 0.94              |
| 33:h:136:SER:O   | 33:h:137:GLU:CG   | 2.15                     | 0.93              |
| 26:a:883:G:H1    | 26:a:894:U:H3     | 1.16                     | 0.93              |
| 9:I:5:GLN:HE21   | 9:I:22:LYS:HE3    | 1.33                     | 0.93              |
| 6:F:90:MET:HE1   | 18:R:61:ARG:NH1   | 1.85                     | 0.92              |
| 33:h:136:SER:C   | 33:h:137:GLU:OE1  | 2.13                     | 0.91              |
| 25:Y:18:THR:H    | 25:Y:25:ARG:HH21  | 1.15                     | 0.91              |
| 13:M:78:LYS:NZ   | 26:a:889:C:C5     | 2.40                     | 0.90              |
| 9:I:99:ARG:HG2   | 9:I:104:VAL:HG21  | 1.54                     | 0.89              |
| 54:2:17:THR:HG21 | 54:2:49:MET:HE1   | 1.55                     | 0.89              |
| 11:K:97:ILE:HG22 | 21:U:12:PHE:HZ    | 1.39                     | 0.87              |
| 25:Y:24:VAL:HG11 | 25:Y:41:GLY:HA2   | 1.56                     | 0.87              |
| 28:c:121:ASP:CG  | 33:h:91:PHE:HZ    | 1.81                     | 0.87              |
| 25:Y:79:PHE:N    | 25:Y:79:PHE:CD1   | 2.37                     | 0.87              |
| 1:A:1538:C:H42   | 21:U:17:ARG:HH12  | 1.18                     | 0.87              |
| 28:c:121:ASP:CB  | 33:h:91:PHE:HE1   | 1.67                     | 0.85              |
| 18:R:34:THR:HG23 | 21:U:25:LYS:NZ    | 1.92                     | 0.85              |
| 1:A:1540:U:C2    | 24:X:1:A:N1       | 2.44                     | 0.85              |
| 1:A:1120:U:H3    | 1:A:1153:G:H1     | 1.25                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:Y:18:THR:H     | 25:Y:25:ARG:NH2   | 1.74                     | 0.85              |
| 19:S:50:ALA:HB1   | 19:S:57:HIS:HB3   | 1.60                     | 0.84              |
| 38:m:35:LYS:NZ    | 38:m:100:CYS:SG   | 2.50                     | 0.84              |
| 28:c:121:ASP:CG   | 33:h:91:PHE:CZ    | 2.56                     | 0.84              |
| 21:U:17:ARG:NH1   | 21:U:21:ARG:HE    | 1.76                     | 0.83              |
| 21:U:60:LEU:O     | 21:U:63:GLU:HB2   | 1.80                     | 0.82              |
| 1:A:1538:C:O2     | 24:X:3:G:N1       | 2.11                     | 0.82              |
| 1:A:1539:C:O2     | 24:X:2:G:O6       | 1.97                     | 0.82              |
| 26:a:495:G:N3     | 43:r:61:ASN:ND2   | 2.28                     | 0.81              |
| 26:a:881:G:N2     | 26:a:895:U:O2     | 2.12                     | 0.81              |
| 27:b:30:C:H1'     | 27:b:57:A:H61     | 1.45                     | 0.81              |
| 33:h:4:ILE:HB     | 33:h:39:ALA:HB2   | 1.63                     | 0.81              |
| 1:A:845:A:H8      | 18:R:9:LYS:HE3    | 1.38                     | 0.81              |
| 33:h:81:ALA:HB1   | 33:h:149:GLU:HA   | 1.61                     | 0.81              |
| 26:a:542:U:H3     | 26:a:551:G:H1     | 1.23                     | 0.80              |
| 2:B:8:ASP:HB3     | 2:B:212:LEU:HD11  | 1.64                     | 0.79              |
| 11:K:97:ILE:HG22  | 21:U:12:PHE:CZ    | 2.17                     | 0.79              |
| 28:c:120:VAL:HG13 | 33:h:91:PHE:CE1   | 2.17                     | 0.79              |
| 25:Y:140:PRO:HB3  | 25:Y:173:VAL:HG11 | 1.62                     | 0.79              |
| 13:M:78:LYS:NZ    | 26:a:889:C:H5     | 1.77                     | 0.79              |
| 26:a:2682:A:H61   | 26:a:2728:U:H1'   | 1.47                     | 0.79              |
| 1:A:845:A:C1'     | 18:R:9:LYS:NZ     | 2.34                     | 0.79              |
| 2:B:17:GLY:O      | 2:B:38:VAL:HG13   | 1.82                     | 0.79              |
| 38:m:37:THR:HG22  | 38:m:39:PRO:HD2   | 1.65                     | 0.79              |
| 26:a:884:U:N3     | 26:a:893:C:O2     | 2.15                     | 0.78              |
| 26:a:1115:G:H2'   | 26:a:1116:G:H8    | 1.47                     | 0.78              |
| 1:A:1538:C:O2     | 24:X:3:G:C6       | 2.36                     | 0.78              |
| 25:Y:18:THR:N     | 25:Y:25:ARG:HH21  | 1.81                     | 0.78              |
| 26:a:2126:A:N6    | 26:a:2163:A:N3    | 2.31                     | 0.78              |
| 25:Y:88:LYS:HD3   | 25:Y:91:ARG:HH21  | 1.49                     | 0.78              |
| 1:A:1540:U:C2     | 24:X:1:A:C2       | 2.73                     | 0.77              |
| 1:A:845:A:C2'     | 18:R:9:LYS:HZ3    | 1.92                     | 0.77              |
| 46:u:51:GLN:OE1   | 46:u:57:TYR:OH    | 2.02                     | 0.77              |
| 33:h:65:ALA:O     | 33:h:68:ARG:N     | 2.12                     | 0.77              |
| 1:A:845:A:O2'     | 18:R:9:LYS:NZ     | 2.18                     | 0.77              |
| 4:D:95:GLU:CD     | 4:D:100:ASN:HD21  | 1.93                     | 0.77              |
| 1:A:458:U:H2'     | 1:A:459:A:H8      | 1.49                     | 0.76              |
| 26:a:881:G:O6     | 26:a:895:U:O4     | 2.03                     | 0.76              |
| 26:a:1042:G:H1    | 26:a:1113:U:H3    | 1.34                     | 0.76              |
| 26:a:1053:C:N4    | 26:a:1054:A:N6    | 2.34                     | 0.76              |
| 26:a:884:U:O4     | 26:a:893:C:N3     | 2.18                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1356:G:H2'   | 1:A:1357:A:C8     | 2.21                     | 0.76              |
| 1:A:1538:C:O2    | 24:X:3:G:O6       | 2.04                     | 0.76              |
| 2:B:97:LEU:HD22  | 2:B:148:LEU:HD21  | 1.68                     | 0.76              |
| 4:D:91:LEU:HD12  | 4:D:188:ARG:HD3   | 1.68                     | 0.75              |
| 21:U:56:HIS:O    | 21:U:58:LYS:N     | 2.19                     | 0.75              |
| 1:A:1538:C:O2'   | 1:A:1539:C:C5     | 2.38                     | 0.75              |
| 1:A:1100:C:OP2   | 2:B:95:ARG:HD3    | 1.86                     | 0.75              |
| 9:I:88:MET:HE3   | 9:I:98:LEU:HD12   | 1.68                     | 0.75              |
| 33:h:47:PHE:CE1  | 33:h:51:ARG:HD2   | 2.22                     | 0.75              |
| 1:A:673:A:H2'    | 1:A:674:G:C8      | 2.21                     | 0.75              |
| 25:Y:98:LEU:HB2  | 25:Y:166:VAL:HG13 | 1.67                     | 0.75              |
| 1:A:845:A:C8     | 18:R:9:LYS:CE     | 2.69                     | 0.75              |
| 26:a:856:G:H2'   | 26:a:857:G:C8     | 2.21                     | 0.75              |
| 13:M:92:ARG:NH1  | 26:a:887:A:H5'    | 2.02                     | 0.74              |
| 54:2:62:LEU:HG   | 54:2:65:ALA:HB2   | 1.69                     | 0.74              |
| 4:D:145:ILE:HD13 | 4:D:178:MET:HB3   | 1.69                     | 0.74              |
| 33:h:136:SER:O   | 33:h:137:GLU:HG3  | 1.86                     | 0.74              |
| 1:A:1305:G:HO2'  | 1:A:1306:A:H8     | 1.35                     | 0.74              |
| 1:A:1540:U:O4'   | 24:X:1:A:H2       | 1.70                     | 0.74              |
| 26:a:545:U:O2    | 26:a:548:G:O6     | 2.05                     | 0.74              |
| 1:A:846:G:H2'    | 1:A:847:G:C8      | 2.23                     | 0.74              |
| 33:h:132:PHE:HB2 | 33:h:140:ALA:HB3  | 1.70                     | 0.74              |
| 5:E:142:ASP:OD1  | 5:E:146:ASN:ND2   | 2.21                     | 0.74              |
| 1:A:736:C:H5''   | 6:F:90:MET:HE3    | 1.69                     | 0.73              |
| 1:A:1347:G:O6    | 9:I:12:ARG:NH2    | 2.20                     | 0.73              |
| 1:A:113:G:H1'    | 1:A:354:G:H5'     | 1.71                     | 0.73              |
| 4:D:187:GLU:HG3  | 4:D:189:SER:H     | 1.53                     | 0.73              |
| 6:F:17:GLN:NE2   | 33:h:87:GLU:HA    | 2.03                     | 0.73              |
| 10:J:6:ILE:HB    | 10:J:76:ILE:HB    | 1.68                     | 0.73              |
| 25:Y:25:ARG:C    | 25:Y:67:GLU:OE2   | 2.31                     | 0.73              |
| 28:c:144:VAL:HB  | 28:c:154:LEU:HB2  | 1.69                     | 0.73              |
| 1:A:1538:C:N4    | 21:U:17:ARG:HH12  | 1.87                     | 0.72              |
| 3:C:19:ASN:O     | 3:C:40:ARG:NH2    | 2.23                     | 0.72              |
| 26:a:976:G:HO2'  | 26:a:1155:A:HO2'  | 1.34                     | 0.72              |
| 1:A:1539:C:C2    | 24:X:2:G:O6       | 2.42                     | 0.72              |
| 2:B:70:VAL:HB    | 2:B:163:VAL:HG12  | 1.72                     | 0.72              |
| 4:D:95:GLU:HG2   | 4:D:186:PRO:CG    | 2.17                     | 0.72              |
| 12:L:15:LYS:O    | 12:L:17:ALA:N     | 2.23                     | 0.72              |
| 1:A:1005:A:N6    | 1:A:1024:G:O2'    | 2.21                     | 0.72              |
| 1:A:1377:A:OP1   | 7:G:92:ARG:NH2    | 2.23                     | 0.72              |
| 10:J:66:GLU:HB2  | 14:N:99:ALA:HB2   | 1.72                     | 0.72              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:686:U:H1'      | 11:K:44:TRP:HE1   | 1.53                     | 0.72              |
| 26:a:2127:G:H2'    | 26:a:2128:G:C8    | 2.24                     | 0.72              |
| 28:c:121:ASP:N     | 33:h:91:PHE:HE1   | 1.88                     | 0.72              |
| 1:A:845:A:H2'      | 18:R:9:LYS:HZ3    | 1.50                     | 0.72              |
| 26:a:2107:G:O6     | 26:a:2183:A:N6    | 2.23                     | 0.72              |
| 32:g:46:ALA:O      | 32:g:48:ASN:N     | 2.23                     | 0.72              |
| 37:l:161:ASP:OD1   | 37:l:162:GLY:N    | 2.23                     | 0.72              |
| 26:a:539:G:H1      | 26:a:554:U:H3     | 1.38                     | 0.71              |
| 26:a:1063:G:N2     | 26:a:1079:C:OP2   | 2.23                     | 0.71              |
| 26:a:2141:G:N7     | 26:a:2143:C:N4    | 2.37                     | 0.71              |
| 1:A:493:A:H2'      | 1:A:494:G:C8      | 2.25                     | 0.71              |
| 26:a:1248:G:OP1    | 30:e:44:ARG:NH2   | 2.22                     | 0.71              |
| 34:i:92:MET:HE1    | 34:i:103:ILE:HD12 | 1.71                     | 0.71              |
| 26:a:2498:OMC:HM22 | 26:a:2499:C:H5'   | 1.71                     | 0.71              |
| 28:c:210:ALA:O     | 28:c:214:ARG:NH1  | 2.24                     | 0.71              |
| 56:4:58:ASP:OD1    | 56:4:59:ARG:N     | 2.23                     | 0.71              |
| 1:A:718:A:H2       | 18:R:38:LYS:HZ2   | 1.39                     | 0.71              |
| 26:a:1858:A:N6     | 26:a:1884:G:O2'   | 2.23                     | 0.71              |
| 1:A:674:G:H2'      | 1:A:675:A:H8      | 1.56                     | 0.71              |
| 29:d:14:ILE:HD11   | 29:d:188:LEU:HD23 | 1.73                     | 0.71              |
| 33:h:57:LYS:O      | 33:h:61:VAL:HG22  | 1.91                     | 0.71              |
| 33:h:93:SER:OG     | 33:h:123:ARG:NH2  | 2.23                     | 0.71              |
| 33:h:113:SER:O     | 33:h:116:ARG:NH1  | 2.24                     | 0.70              |
| 52:0:5:ILE:HG22    | 52:0:28:ARG:HH21  | 1.56                     | 0.70              |
| 2:B:183:VAL:N      | 2:B:197:ASP:OD2   | 2.25                     | 0.70              |
| 26:a:655:A:H4'     | 26:a:656:G:H5'    | 1.73                     | 0.70              |
| 36:k:78:ARG:HG2    | 36:k:113:ALA:HB3  | 1.74                     | 0.70              |
| 25:Y:120:PHE:HA    | 25:Y:128:ARG:HH21 | 1.57                     | 0.70              |
| 6:F:9:MET:HE2      | 6:F:85:ILE:HD11   | 1.71                     | 0.70              |
| 25:Y:27:VAL:HA     | 25:Y:67:GLU:OE1   | 1.91                     | 0.70              |
| 26:a:2406:A:OP2    | 26:a:2411:A:N6    | 2.23                     | 0.70              |
| 26:a:500:G:H22     | 26:a:503:A:H5'    | 1.57                     | 0.70              |
| 5:E:76:LEU:HD21    | 5:E:120:VAL:HG22  | 1.74                     | 0.70              |
| 1:A:1535:C:N4      | 24:X:6:G:H22      | 1.84                     | 0.70              |
| 12:L:100:GLY:N     | 12:L:104:CYS:O    | 2.22                     | 0.70              |
| 26:a:1753:G:N2     | 26:a:1756:G:OP2   | 2.25                     | 0.70              |
| 26:a:72:U:O4       | 49:x:58:ASN:ND2   | 2.25                     | 0.69              |
| 26:a:2144:G:N2     | 26:a:2146:C:O2'   | 2.24                     | 0.69              |
| 1:A:340:U:OP2      | 35:j:98:ARG:NH2   | 2.25                     | 0.69              |
| 1:A:1346:A:OP1     | 9:I:122:ARG:NH1   | 2.25                     | 0.69              |
| 26:a:1063:G:O6     | 26:a:1075:C:N4    | 2.25                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:2867:G:HO2' | 26:a:2868:A:H8    | 1.40                     | 0.69              |
| 35:j:42:THR:HG22 | 35:j:57:VAL:HG22  | 1.74                     | 0.69              |
| 1:A:539:A:H2'    | 1:A:540:G:C8      | 2.27                     | 0.69              |
| 9:I:36:GLU:O     | 9:I:45:ARG:NH2    | 2.26                     | 0.69              |
| 26:a:1508:A:O2'  | 26:a:1509:A:O4'   | 2.07                     | 0.69              |
| 26:a:1607:C:N4   | 26:a:1622:G:OP2   | 2.21                     | 0.69              |
| 1:A:19:A:H5''    | 5:E:91:GLY:HA3    | 1.75                     | 0.69              |
| 2:B:10:LEU:HD13  | 25:Y:11:GLU:HB3   | 1.73                     | 0.69              |
| 26:a:1075:C:OP2  | 26:a:1076:C:N4    | 2.26                     | 0.69              |
| 1:A:1175:G:H2'   | 1:A:1176:A:H8     | 1.58                     | 0.69              |
| 11:K:27:PHE:CZ   | 21:U:33:ARG:NH2   | 2.61                     | 0.69              |
| 28:c:66:ASP:OD2  | 28:c:102:ARG:NH1  | 2.25                     | 0.68              |
| 1:A:422:C:O2'    | 1:A:423:G:N2      | 2.25                     | 0.68              |
| 25:Y:91:ARG:HD2  | 25:Y:95:TRP:HA    | 1.75                     | 0.68              |
| 26:a:197:A:H62   | 26:a:2430:A:H2'   | 1.58                     | 0.68              |
| 7:G:147:ALA:O    | 11:K:56:ARG:NH2   | 2.27                     | 0.68              |
| 10:J:10:LEU:HB3  | 10:J:18:ILE:HD11  | 1.74                     | 0.68              |
| 26:a:1801:A:OP2  | 28:c:150:LYS:NZ   | 2.20                     | 0.68              |
| 26:a:2883:A:OP2  | 51:z:50:ARG:NH1   | 2.27                     | 0.68              |
| 1:A:74:A:OP2     | 1:A:75:G:N2       | 2.27                     | 0.68              |
| 4:D:150:LYS:O    | 4:D:156:LYS:NZ    | 2.27                     | 0.68              |
| 26:a:2124:G:OP1  | 26:a:2176:A:N6    | 2.27                     | 0.68              |
| 35:j:105:ARG:NH2 | 35:j:123:LEU:O    | 2.27                     | 0.68              |
| 25:Y:25:ARG:O    | 25:Y:67:GLU:HG3   | 1.93                     | 0.68              |
| 26:a:307:G:N1    | 26:a:310:A:OP2    | 2.25                     | 0.68              |
| 26:a:2154:A:H5'' | 26:a:2155:U:H5'   | 1.76                     | 0.68              |
| 38:m:28:LEU:HD23 | 38:m:48:VAL:HG21  | 1.76                     | 0.68              |
| 26:a:627:A:OP1   | 36:k:78:ARG:NH2   | 2.21                     | 0.68              |
| 1:A:552:U:H2'    | 1:A:553:A:H8      | 1.59                     | 0.68              |
| 2:B:87:CYS:O     | 2:B:225:ARG:NH2   | 2.27                     | 0.68              |
| 25:Y:8:LEU:HA    | 25:Y:11:GLU:HG2   | 1.75                     | 0.68              |
| 26:a:1386:C:H2'  | 26:a:1387:A:H8    | 1.59                     | 0.68              |
| 1:A:501:C:OP1    | 12:L:114:ARG:NH2  | 2.22                     | 0.68              |
| 1:A:1033:G:H2'   | 1:A:1034:G:C8     | 2.28                     | 0.68              |
| 6:F:90:MET:CE    | 18:R:61:ARG:NH1   | 2.56                     | 0.68              |
| 26:a:358:U:N3    | 26:a:359:G:O6     | 2.27                     | 0.68              |
| 33:h:90:LEU:HB2  | 33:h:125:THR:HG23 | 1.76                     | 0.68              |
| 11:K:110:ILE:O   | 21:U:4:ILE:HG22   | 1.93                     | 0.67              |
| 20:T:79:LEU:O    | 20:T:83:ILE:HG12  | 1.94                     | 0.67              |
| 26:a:279:A:N6    | 26:a:361:G:O2'    | 2.26                     | 0.67              |
| 1:A:532:A:N6     | 1:A:1206:G:O2'    | 2.26                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:5:GLN:HE21   | 9:I:22:LYS:CE    | 2.05                     | 0.67              |
| 9:I:75:GLN:O     | 9:I:79:ILE:HG12  | 1.93                     | 0.67              |
| 26:a:2328:A:H2'  | 26:a:2329:U:C6   | 2.30                     | 0.67              |
| 13:M:85:CYS:HB2  | 19:S:73:GLU:HG2  | 1.76                     | 0.67              |
| 25:Y:98:LEU:HD22 | 25:Y:167:VAL:H   | 1.59                     | 0.67              |
| 1:A:539:A:H2'    | 1:A:540:G:H8     | 1.59                     | 0.67              |
| 1:A:1043:G:H2'   | 1:A:1044:A:C8    | 2.29                     | 0.67              |
| 40:o:33:VAL:HG22 | 40:o:38:LYS:HG3  | 1.77                     | 0.67              |
| 33:h:46:PHE:HE1  | 33:h:50:ARG:HE   | 1.42                     | 0.67              |
| 1:A:1323:G:H2'   | 1:A:1324:A:C8    | 2.29                     | 0.67              |
| 3:C:20:SER:HG    | 3:C:40:ARG:HH22  | 1.43                     | 0.67              |
| 19:S:12:ASP:OD2  | 19:S:14:HIS:NE2  | 2.27                     | 0.67              |
| 26:a:2391:G:H2'  | 26:a:2424:C:H41  | 1.59                     | 0.67              |
| 16:P:55:ASP:OD1  | 16:P:56:ARG:N    | 2.28                     | 0.67              |
| 33:h:5:LEU:HD13  | 33:h:13:GLY:HA2  | 1.77                     | 0.67              |
| 1:A:85:U:O2      | 1:A:86:G:N2      | 2.28                     | 0.67              |
| 1:A:1098:C:P     | 2:B:143:LYS:HZ1  | 2.12                     | 0.67              |
| 4:D:172:GLU:O    | 4:D:180:GLY:HA2  | 1.95                     | 0.67              |
| 21:U:54:LYS:C    | 21:U:56:HIS:H    | 2.02                     | 0.67              |
| 1:A:888:G:H3'    | 1:A:889:A:H5''   | 1.76                     | 0.66              |
| 1:A:1040:U:H2'   | 1:A:1041:G:H8    | 1.59                     | 0.66              |
| 31:f:62:GLY:O    | 31:f:95:ARG:NH1  | 2.27                     | 0.66              |
| 33:h:72:ILE:HG22 | 33:h:108:VAL:HB  | 1.78                     | 0.66              |
| 1:A:1347:G:O2'   | 1:A:1348:U:OP2   | 2.13                     | 0.66              |
| 26:a:880:G:H2'   | 26:a:881:G:C8    | 2.30                     | 0.66              |
| 26:a:1584:U:H3'  | 26:a:1585:C:H5'  | 1.75                     | 0.66              |
| 33:h:90:LEU:HD12 | 33:h:125:THR:CG2 | 2.21                     | 0.66              |
| 2:B:23:TRP:CZ3   | 2:B:25:PRO:HA    | 2.31                     | 0.66              |
| 11:K:35:THR:HG22 | 11:K:41:ALA:HA   | 1.76                     | 0.66              |
| 25:Y:16:ILE:O    | 25:Y:17:GLU:C    | 2.38                     | 0.66              |
| 25:Y:18:THR:CG2  | 25:Y:24:VAL:HG22 | 2.23                     | 0.66              |
| 26:a:2144:G:H1'  | 26:a:2147:A:H61  | 1.61                     | 0.66              |
| 30:e:126:VAL:O   | 30:e:156:ASN:ND2 | 2.27                     | 0.66              |
| 2:B:50:PHE:HD1   | 2:B:200:ILE:HD12 | 1.60                     | 0.66              |
| 26:a:1802:A:H2'  | 26:a:1803:A:C8   | 2.31                     | 0.66              |
| 26:a:2657:A:O2'  | 32:g:160:LYS:NZ  | 2.27                     | 0.66              |
| 2:B:27:MET:HE3   | 2:B:193:PRO:HD3  | 1.78                     | 0.66              |
| 22:V:51:U:H2'    | 22:V:52:C:C6     | 2.31                     | 0.66              |
| 1:A:841:C:O2     | 1:A:846:G:N2     | 2.27                     | 0.66              |
| 13:M:83:LEU:HD11 | 19:S:65:GLU:HG3  | 1.78                     | 0.66              |
| 26:a:270:A:N1    | 26:a:369:U:O2'   | 2.29                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:1590:A:H2'  | 26:a:1591:A:H8    | 1.59                     | 0.66              |
| 26:a:2107:G:H2'  | 26:a:2108:A:H4'   | 1.78                     | 0.66              |
| 26:a:2333:A:H5'  | 26:a:2335:A:H1'   | 1.78                     | 0.66              |
| 1:A:1507:A:H2'   | 1:A:1508:A:C8     | 2.30                     | 0.66              |
| 9:I:87:LEU:HB3   | 9:I:94:LEU:HD11   | 1.77                     | 0.66              |
| 16:P:69:ASP:OD1  | 16:P:70:ARG:N     | 2.28                     | 0.66              |
| 33:h:78:VAL:HG21 | 33:h:103:VAL:HG22 | 1.77                     | 0.66              |
| 14:N:6:MET:SD    | 14:N:9:ARG:NH1    | 2.69                     | 0.66              |
| 15:O:88:ARG:NH2  | 26:a:715:A:OP2    | 2.29                     | 0.66              |
| 32:g:2:SER:OG    | 32:g:3:ARG:N      | 2.26                     | 0.66              |
| 1:A:1133:G:H2'   | 1:A:1134:G:C8     | 2.30                     | 0.65              |
| 2:B:27:MET:HA    | 2:B:27:MET:HE2    | 1.78                     | 0.65              |
| 19:S:11:ILE:HD12 | 19:S:38:SER:HB3   | 1.78                     | 0.65              |
| 25:Y:9:PHE:HA    | 25:Y:12:SER:HB2   | 1.78                     | 0.65              |
| 25:Y:93:GLU:HB3  | 25:Y:124:LEU:HD13 | 1.78                     | 0.65              |
| 26:a:807:U:OP2   | 36:k:41:ARG:NH1   | 2.29                     | 0.65              |
| 1:A:845:A:H8     | 18:R:9:LYS:CE     | 2.07                     | 0.65              |
| 1:A:1317:C:H5'   | 14:N:24:ARG:HH21  | 1.60                     | 0.65              |
| 26:a:848:C:H2'   | 26:a:849:A:H8     | 1.61                     | 0.65              |
| 26:a:1570:A:H2'  | 26:a:1571:A:C8    | 2.31                     | 0.65              |
| 26:a:1936:A:H2   | 26:a:1943:U:H3    | 1.43                     | 0.65              |
| 1:A:826:C:O2     | 8:H:16:ASN:ND2    | 2.29                     | 0.65              |
| 1:A:1043:G:H2'   | 1:A:1044:A:H8     | 1.61                     | 0.65              |
| 2:B:164:ILE:HA   | 2:B:186:ILE:HG22  | 1.77                     | 0.65              |
| 4:D:95:GLU:CD    | 4:D:100:ASN:ND2   | 2.54                     | 0.65              |
| 25:Y:79:PHE:HD1  | 25:Y:79:PHE:H     | 1.40                     | 0.65              |
| 36:k:108:ALA:HB3 | 36:k:125:LEU:HD22 | 1.77                     | 0.65              |
| 45:t:74:ASN:O    | 45:t:76:ALA:N     | 2.28                     | 0.65              |
| 1:A:458:U:H2'    | 1:A:459:A:C8      | 2.30                     | 0.65              |
| 1:A:946:A:H2'    | 1:A:947:G:C8      | 2.31                     | 0.65              |
| 26:a:1469:A:H2'  | 26:a:1470:A:C8    | 2.32                     | 0.65              |
| 1:A:147:G:H2'    | 1:A:148:G:C8      | 2.32                     | 0.65              |
| 1:A:1004:A:O4'   | 1:A:1026:G:N2     | 2.28                     | 0.65              |
| 2:B:73:LYS:HE2   | 2:B:205:ASP:HB2   | 1.77                     | 0.65              |
| 14:N:88:ALA:HB1  | 14:N:96:LEU:HD22  | 1.79                     | 0.65              |
| 18:R:34:THR:HG23 | 21:U:25:LYS:HZ2   | 1.62                     | 0.65              |
| 21:U:56:HIS:O    | 21:U:59:LYS:N     | 2.22                     | 0.65              |
| 26:a:475:C:O2    | 26:a:479:A:N6     | 2.26                     | 0.65              |
| 33:h:47:PHE:HE1  | 33:h:51:ARG:HD2   | 1.60                     | 0.65              |
| 26:a:500:G:N1    | 26:a:503:A:OP2    | 2.25                     | 0.64              |
| 26:a:639:U:H2'   | 26:a:640:C:C6     | 2.33                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:1597:A:H5''  | 26:a:1598:A:H5'   | 1.78                     | 0.64              |
| 26:a:1054:A:N1    | 26:a:1106:G:C6    | 2.65                     | 0.64              |
| 26:a:1590:A:H2'   | 26:a:1591:A:C8    | 2.32                     | 0.64              |
| 28:c:121:ASP:N    | 33:h:91:PHE:CE1   | 2.65                     | 0.64              |
| 28:c:163:GLN:OE1  | 28:c:175:ARG:NH1  | 2.31                     | 0.64              |
| 19:S:25:SER:O     | 19:S:28:LYS:NZ    | 2.28                     | 0.64              |
| 12:L:46:ASN:ND2   | 12:L:89:D2T:SB    | 2.70                     | 0.64              |
| 26:a:2287:A:O2'   | 26:a:2288:A:H2'   | 1.97                     | 0.64              |
| 1:A:1368:A:OP1    | 10:J:64:GLN:NE2   | 2.29                     | 0.64              |
| 15:O:18:ASP:OD1   | 15:O:19:ALA:N     | 2.30                     | 0.64              |
| 26:a:1047:G:O2'   | 26:a:1111:A:N6    | 2.31                     | 0.64              |
| 1:A:269:C:H2'     | 1:A:270:A:C8      | 2.32                     | 0.64              |
| 1:A:514:C:H2'     | 1:A:515:G:H8      | 1.62                     | 0.64              |
| 26:a:353:C:H2'    | 26:a:354:A:H8     | 1.63                     | 0.64              |
| 43:r:29:VAL:HB    | 43:r:55:ILE:HD11  | 1.79                     | 0.64              |
| 1:A:176:C:OP2     | 20:T:64:LYS:NZ    | 2.30                     | 0.64              |
| 10:J:21:ALA:O     | 10:J:25:ILE:HG12  | 1.98                     | 0.64              |
| 4:D:116:GLN:OE1   | 4:D:154:ARG:NH1   | 2.30                     | 0.64              |
| 9:I:30:ILE:HD13   | 9:I:65:ILE:HB     | 1.80                     | 0.64              |
| 26:a:2751:G:OP2   | 32:g:3:ARG:NH1    | 2.31                     | 0.64              |
| 26:a:1429:G:H2'   | 26:a:1430:G:H8    | 1.62                     | 0.64              |
| 31:f:158:THR:HG22 | 31:f:160:ALA:H    | 1.63                     | 0.64              |
| 32:g:42:GLU:HB2   | 32:g:55:ARG:HE    | 1.63                     | 0.64              |
| 1:A:56:U:H2'      | 1:A:57:G:C8       | 2.33                     | 0.64              |
| 11:K:67:ALA:HB2   | 11:K:96:THR:HG23  | 1.80                     | 0.64              |
| 28:c:53:HIS:CE1   | 28:c:219:THR:HA   | 2.33                     | 0.64              |
| 28:c:120:VAL:HG13 | 33:h:91:PHE:CZ    | 2.32                     | 0.64              |
| 38:m:24:MET:HE2   | 38:m:44:LEU:HD22  | 1.80                     | 0.64              |
| 48:w:32:ASN:OD1   | 48:w:34:HIS:NE2   | 2.30                     | 0.64              |
| 2:B:10:LEU:C      | 2:B:12:ALA:H      | 2.05                     | 0.63              |
| 15:O:88:ARG:NH1   | 26:a:714:U:OP2    | 2.31                     | 0.63              |
| 19:S:63:THR:HG22  | 19:S:66:MET:HE3   | 1.79                     | 0.63              |
| 26:a:894:U:O2'    | 26:a:895:U:H6     | 1.80                     | 0.63              |
| 1:A:652:U:O2'     | 1:A:653:U:O5'     | 2.15                     | 0.63              |
| 31:f:29:PRO:HB2   | 31:f:169:LEU:HD22 | 1.80                     | 0.63              |
| 1:A:1144:G:N2     | 1:A:1146:A:H62    | 1.96                     | 0.63              |
| 26:a:239:C:HO2'   | 26:a:622:G:HO2'   | 1.43                     | 0.63              |
| 26:a:1174:U:OP1   | 26:a:1177:G:N2    | 2.31                     | 0.63              |
| 26:a:1808:A:H3'   | 26:a:1809:A:C8    | 2.33                     | 0.63              |
| 2:B:128:LYS:O     | 2:B:131:LYS:NZ    | 2.32                     | 0.63              |
| 26:a:2683:C:OP1   | 40:o:51:ARG:NH2   | 2.27                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:u:57:TYR:OH   | 46:u:79:ARG:NH2  | 2.31                     | 0.63              |
| 26:a:700:G:O2'   | 26:a:1632:A:N3   | 2.30                     | 0.63              |
| 1:A:204:G:H3'    | 1:A:205:A:H8     | 1.64                     | 0.63              |
| 1:A:1028:C:H2'   | 1:A:1029:U:O4'   | 1.99                     | 0.63              |
| 26:a:1263:U:OP1  | 51:z:13:ARG:NH1  | 2.30                     | 0.63              |
| 1:A:979:C:O2     | 14:N:59:ARG:NH1  | 2.32                     | 0.63              |
| 6:F:7:VAL:HG11   | 18:R:65:LEU:HD21 | 1.80                     | 0.63              |
| 18:R:9:LYS:HA    | 18:R:46:GLY:HA3  | 1.80                     | 0.63              |
| 26:a:45:G:H5'    | 26:a:46:G:H5'    | 1.80                     | 0.63              |
| 3:C:43:LEU:HD13  | 3:C:68:ILE:HD11  | 1.81                     | 0.63              |
| 21:U:62:ARG:HG2  | 21:U:62:ARG:O    | 1.98                     | 0.63              |
| 26:a:2758:A:O2'  | 32:g:38:ASN:ND2  | 2.31                     | 0.63              |
| 32:g:60:ASP:O    | 32:g:62:TRP:N    | 2.32                     | 0.63              |
| 37:l:66:ARG:NH1  | 37:l:159:GLU:OE2 | 2.31                     | 0.63              |
| 1:A:1447:A:H5''  | 1:A:1448:C:H5    | 1.64                     | 0.62              |
| 9:I:123:ARG:NH1  | 9:I:124:ARG:O    | 2.32                     | 0.62              |
| 13:M:78:LYS:HZ1  | 26:a:889:C:H5    | 1.46                     | 0.62              |
| 14:N:26:GLU:O    | 14:N:30:ILE:HD12 | 1.98                     | 0.62              |
| 17:Q:20:SER:HB2  | 17:Q:71:LYS:NZ   | 2.14                     | 0.62              |
| 3:C:24:ALA:HB1   | 3:C:28:GLU:HB2   | 1.81                     | 0.62              |
| 24:X:3:G:C8      | 24:X:4:A:H1'     | 2.34                     | 0.62              |
| 26:a:181:A:H2'   | 26:a:182:A:C8    | 2.33                     | 0.62              |
| 29:d:35:THR:HG22 | 29:d:73:VAL:HG21 | 1.81                     | 0.62              |
| 1:A:390:U:H2'    | 1:A:391:G:H8     | 1.64                     | 0.62              |
| 1:A:411:A:H4'    | 1:A:412:A:H5'    | 1.81                     | 0.62              |
| 26:a:1288:G:OP2  | 26:a:1288:G:N2   | 2.29                     | 0.62              |
| 33:h:26:ALA:HA   | 33:h:30:LEU:HB2  | 1.82                     | 0.62              |
| 45:t:74:ASN:HB3  | 45:t:77:THR:HG22 | 1.81                     | 0.62              |
| 1:A:79:G:N2      | 1:A:91:U:O4      | 2.32                     | 0.62              |
| 1:A:269:C:H2'    | 1:A:270:A:H8     | 1.64                     | 0.62              |
| 1:A:297:G:N2     | 1:A:300:A:OP2    | 2.30                     | 0.62              |
| 3:C:111:LEU:HD22 | 3:C:146:ALA:HB2  | 1.81                     | 0.62              |
| 26:a:630:G:N2    | 26:a:633:A:OP2   | 2.30                     | 0.62              |
| 26:a:1223:G:OP1  | 42:q:68:ARG:NH2  | 2.33                     | 0.62              |
| 47:v:4:LYS:HD3   | 47:v:5:LYS:HG2   | 1.80                     | 0.62              |
| 18:R:9:LYS:HD3   | 18:R:14:THR:HB   | 1.81                     | 0.62              |
| 25:Y:23:ILE:HD11 | 25:Y:95:TRP:HH2  | 1.63                     | 0.62              |
| 26:a:481:G:H1'   | 26:a:506:G:N2    | 2.15                     | 0.62              |
| 26:a:1799:G:OP1  | 28:c:258:ARG:NH1 | 2.30                     | 0.62              |
| 26:a:1869:G:N2   | 26:a:1872:A:OP2  | 2.28                     | 0.62              |
| 26:a:2128:G:O2'  | 26:a:2174:C:OP2  | 2.16                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:2848:G:O2'   | 26:a:2868:A:N6    | 2.33                     | 0.62              |
| 45:t:40:ASN:O     | 45:t:63:ALA:N     | 2.32                     | 0.62              |
| 26:a:310:A:O2'    | 26:a:311:A:O5'    | 2.18                     | 0.62              |
| 4:D:188:ARG:NH2   | 4:D:195:ILE:O     | 2.31                     | 0.62              |
| 1:A:1539:C:N3     | 24:X:2:G:O6       | 2.32                     | 0.62              |
| 26:a:172:A:H2'    | 26:a:173:A:H8     | 1.65                     | 0.62              |
| 1:A:215:C:H2'     | 1:A:216:U:C6      | 2.34                     | 0.62              |
| 1:A:1422:G:O3'    | 35:j:49:ARG:NH1   | 2.32                     | 0.62              |
| 26:a:2788:C:O2'   | 26:a:2809:A:N3    | 2.28                     | 0.62              |
| 33:h:18:GLN:HE22  | 33:h:44:ILE:HG12  | 1.65                     | 0.62              |
| 1:A:362:G:N2      | 1:A:365:U:OP2     | 2.30                     | 0.61              |
| 1:A:613:C:OP1     | 4:D:81:ARG:NH2    | 2.27                     | 0.61              |
| 26:a:545:U:O2     | 26:a:548:G:C6     | 2.53                     | 0.61              |
| 26:a:2483:C:N3    | 37:l:178:LYS:NZ   | 2.45                     | 0.61              |
| 10:J:42:LEU:HB2   | 10:J:71:LEU:HD22  | 1.82                     | 0.61              |
| 23:W:14:A:H61     | 23:W:22:A:H2      | 1.49                     | 0.61              |
| 26:a:833:A:H2'    | 26:a:834:G:H8     | 1.64                     | 0.61              |
| 26:a:2006:C:O2'   | 26:a:2823:A:N3    | 2.32                     | 0.61              |
| 26:a:2816:G:N3    | 26:a:2883:A:O2'   | 2.31                     | 0.61              |
| 25:Y:98:LEU:HD21  | 25:Y:156:VAL:HG13 | 1.82                     | 0.61              |
| 28:c:245:VAL:HG12 | 28:c:251:GLN:HA   | 1.80                     | 0.61              |
| 40:o:31:TRP:NE1   | 40:o:82:ASP:OD2   | 2.32                     | 0.61              |
| 1:A:542:G:OP1     | 4:D:10:LYS:NZ     | 2.28                     | 0.61              |
| 2:B:24:ASN:ND2    | 2:B:192:ASP:HB3   | 2.14                     | 0.61              |
| 2:B:90:PHE:HB3    | 2:B:151:ILE:HG22  | 1.82                     | 0.61              |
| 6:F:3:HIS:ND1     | 6:F:65:GLU:OE1    | 2.33                     | 0.61              |
| 26:a:1779:U:OP2   | 26:a:1784:A:N6    | 2.32                     | 0.61              |
| 1:A:811:C:O2'     | 1:A:901:A:N1      | 2.33                     | 0.61              |
| 26:a:782:A:N7     | 28:c:220:VAL:HG21 | 2.16                     | 0.61              |
| 1:A:376:G:H5''    | 16:P:5:ARG:HB2    | 1.83                     | 0.61              |
| 18:R:14:THR:HG23  | 18:R:48:ARG:HD2   | 1.83                     | 0.61              |
| 26:a:1527:G:N1    | 26:a:1544:A:OP2   | 2.25                     | 0.61              |
| 37:l:57:VAL:HA    | 37:l:167:LEU:HD21 | 1.83                     | 0.61              |
| 26:a:444:C:OP1    | 30:e:40:ARG:NH2   | 2.33                     | 0.61              |
| 26:a:650:C:H4'    | 54:2:49:MET:HE3   | 1.81                     | 0.61              |
| 26:a:930:G:H1'    | 50:y:25:LEU:HD21  | 1.82                     | 0.61              |
| 26:a:2247:A:H2'   | 26:a:2248:C:H6    | 1.65                     | 0.61              |
| 11:K:27:PHE:CZ    | 21:U:33:ARG:CZ    | 2.84                     | 0.61              |
| 17:Q:25:ILE:HD12  | 17:Q:44:LEU:HD12  | 1.83                     | 0.61              |
| 11:K:111:THR:HG23 | 21:U:3:VAL:HG12   | 1.82                     | 0.61              |
| 26:a:2134:A:H62   | 26:a:2157:G:H5''  | 1.66                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 33:h:27:ARG:NH1  | 48:w:60:ASP:OD2   | 2.33                     | 0.61              |
| 6:F:18:VAL:O     | 6:F:22:ILE:HG13   | 2.00                     | 0.61              |
| 8:H:77:ARG:NH1   | 8:H:79:SER:O      | 2.34                     | 0.61              |
| 20:T:35:VAL:O    | 20:T:39:ILE:HD12  | 2.00                     | 0.61              |
| 26:a:883:G:O2'   | 26:a:884:U:H5''   | 2.01                     | 0.61              |
| 31:f:52:ASN:HB2  | 31:f:150:ARG:HH22 | 1.66                     | 0.61              |
| 17:Q:45:HIS:ND1  | 17:Q:70:THR:OG1   | 2.29                     | 0.60              |
| 26:a:639:U:H2'   | 26:a:640:C:H6     | 1.66                     | 0.60              |
| 26:a:1589:U:H2'  | 26:a:1590:A:H8    | 1.66                     | 0.60              |
| 26:a:2279:G:N7   | 47:v:14:ARG:NH1   | 2.47                     | 0.60              |
| 26:a:2557:G:H2'  | 26:a:2558:C:C6    | 2.36                     | 0.60              |
| 6:F:90:MET:SD    | 18:R:61:ARG:HD3   | 2.41                     | 0.60              |
| 26:a:181:A:H2'   | 26:a:182:A:H8     | 1.65                     | 0.60              |
| 26:a:1141:U:H4'  | 26:a:1142:A:O4'   | 2.01                     | 0.60              |
| 26:a:2469:A:N6   | 26:a:2481:G:O2'   | 2.33                     | 0.60              |
| 13:M:92:ARG:HH12 | 26:a:887:A:H5'    | 1.63                     | 0.60              |
| 25:Y:8:LEU:HG    | 25:Y:11:GLU:HB2   | 1.83                     | 0.60              |
| 1:A:845:A:H1'    | 18:R:15:ALA:CB    | 2.25                     | 0.60              |
| 4:D:188:ARG:HE   | 4:D:197:GLU:CD    | 2.09                     | 0.60              |
| 11:K:27:PHE:CE1  | 21:U:33:ARG:CZ    | 2.84                     | 0.60              |
| 33:h:5:LEU:HB2   | 33:h:16:GLY:H     | 1.66                     | 0.60              |
| 37:l:77:PRO:HG2  | 37:l:80:VAL:HG21  | 1.83                     | 0.60              |
| 41:p:50:ARG:O    | 41:p:54:LYS:NZ    | 2.33                     | 0.60              |
| 1:A:1054:C:O2    | 1:A:1196:A:N6     | 2.35                     | 0.60              |
| 2:B:97:LEU:H     | 2:B:100:MET:HE3   | 1.66                     | 0.60              |
| 4:D:103:TYR:OH   | 4:D:165:ARG:NH1   | 2.34                     | 0.60              |
| 8:H:48:ASP:OD1   | 8:H:49:PHE:N      | 2.33                     | 0.60              |
| 22:V:63:C:H2'    | 22:V:64:G:C8      | 2.36                     | 0.60              |
| 26:a:191:A:H2'   | 26:a:192:C:H6     | 1.66                     | 0.60              |
| 26:a:468:G:N7    | 53:l:39:ARG:NH2   | 2.45                     | 0.60              |
| 54:2:31:HIS:CD2  | 54:2:32:ILE:HD12  | 2.35                     | 0.60              |
| 1:A:1534:A:H2'   | 1:A:1535:C:H5''   | 1.83                     | 0.60              |
| 17:Q:57:ASP:OD2  | 17:Q:82:ALA:N     | 2.26                     | 0.60              |
| 31:f:98:GLU:OE2  | 56:4:25:ARG:NH1   | 2.35                     | 0.60              |
| 1:A:390:U:H2'    | 1:A:391:G:C8      | 2.37                     | 0.60              |
| 1:A:1464:U:H2'   | 1:A:1465:A:H8     | 1.65                     | 0.60              |
| 25:Y:43:LYS:HG2  | 25:Y:79:PHE:HA    | 1.84                     | 0.60              |
| 48:w:65:ASP:OD1  | 48:w:66:THR:N     | 2.35                     | 0.60              |
| 3:C:77:ILE:HA    | 3:C:84:VAL:HG13   | 1.84                     | 0.60              |
| 4:D:14:ARG:HD2   | 4:D:38:PRO:HD2    | 1.84                     | 0.60              |
| 21:U:61:ALA:C    | 21:U:63:GLU:N     | 2.59                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:2646:C:OP2  | 26:a:2732:G:O2'   | 2.20                     | 0.60              |
| 47:v:59:LEU:HD12 | 47:v:80:ILE:HD12  | 1.82                     | 0.60              |
| 2:B:130:THR:O    | 2:B:133:GLU:N     | 2.23                     | 0.60              |
| 26:a:1171:G:C6   | 26:a:1178:C:H2'   | 2.37                     | 0.60              |
| 33:h:96:THR:HA   | 33:h:99:ILE:HG22  | 1.83                     | 0.60              |
| 39:n:39:VAL:HB   | 39:n:49:VAL:HG22  | 1.82                     | 0.60              |
| 56:4:56:ARG:NH1  | 56:4:59:ARG:HH22  | 1.98                     | 0.60              |
| 1:A:1157:A:N7    | 1:A:1180:A:N6     | 2.50                     | 0.60              |
| 26:a:460:A:OP1   | 53:1:41:ARG:NH1   | 2.32                     | 0.60              |
| 26:a:2141:G:H2'  | 26:a:2142:A:H8    | 1.67                     | 0.60              |
| 31:f:128:TYR:HE1 | 31:f:130:MET:HB3  | 1.67                     | 0.60              |
| 33:h:127:GLU:OE1 | 33:h:143:ILE:HG12 | 2.02                     | 0.60              |
| 1:A:201:G:H1     | 1:A:216:U:H3      | 1.48                     | 0.59              |
| 1:A:1000:A:H2'   | 1:A:1001:C:C6     | 2.36                     | 0.59              |
| 7:G:27:VAL:HG11  | 7:G:40:GLU:HG3    | 1.83                     | 0.59              |
| 26:a:1588:G:H2'  | 26:a:1589:U:H6    | 1.65                     | 0.59              |
| 26:a:2349:G:OP1  | 54:2:45:ARG:NH2   | 2.35                     | 0.59              |
| 35:j:63:VAL:HG12 | 35:j:107:LEU:HD11 | 1.83                     | 0.59              |
| 1:A:845:A:C8     | 18:R:9:LYS:NZ     | 2.70                     | 0.59              |
| 1:A:1527:U:OP2   | 21:U:42:THR:OG1   | 2.19                     | 0.59              |
| 6:F:35:LYS:NZ    | 6:F:36:ILE:O      | 2.27                     | 0.59              |
| 10:J:25:ILE:HD11 | 10:J:92:LEU:HD21  | 1.84                     | 0.59              |
| 26:a:1469:A:H2'  | 26:a:1470:A:H8    | 1.67                     | 0.59              |
| 1:A:713:G:H2'    | 1:A:714:G:C8      | 2.38                     | 0.59              |
| 1:A:1539:C:H1'   | 1:A:1540:U:O5'    | 2.03                     | 0.59              |
| 13:M:101:ARG:HE  | 13:M:104:THR:HG22 | 1.67                     | 0.59              |
| 16:P:52:LEU:HD12 | 16:P:57:ILE:HD11  | 1.84                     | 0.59              |
| 26:a:882:G:N2    | 26:a:895:U:O4'    | 2.35                     | 0.59              |
| 26:a:1601:G:OP1  | 44:s:64:LYS:NZ    | 2.30                     | 0.59              |
| 26:a:1715:G:HO2' | 26:a:1716:U:H6    | 1.48                     | 0.59              |
| 28:c:160:THR:HB  | 28:c:177:ARG:HG3  | 1.82                     | 0.59              |
| 1:A:451:A:OP2    | 16:P:70:ARG:NH2   | 2.30                     | 0.59              |
| 1:A:1391:U:H2'   | 1:A:1392:G:C8     | 2.37                     | 0.59              |
| 4:D:50:ASP:OD1   | 4:D:51:TYR:N      | 2.35                     | 0.59              |
| 26:a:228:C:N4    | 26:a:2407:A:N3    | 2.51                     | 0.59              |
| 1:A:264:C:O2'    | 17:Q:66:PRO:O     | 2.20                     | 0.59              |
| 1:A:465:A:H3'    | 1:A:466:A:H8      | 1.67                     | 0.59              |
| 26:a:5:A:H2'     | 26:a:6:A:C8       | 2.38                     | 0.59              |
| 26:a:373:U:H2'   | 26:a:374:A:H8     | 1.66                     | 0.59              |
| 31:f:116:GLY:O   | 31:f:178:ARG:NH1  | 2.30                     | 0.59              |
| 1:A:500:G:H2'    | 1:A:501:C:C6      | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1347:G:HO2'   | 1:A:1373:G:H1     | 1.49                     | 0.59              |
| 49:x:32:ALA:HB2   | 49:x:37:LEU:HD23  | 1.85                     | 0.59              |
| 1:A:1086:U:H3     | 1:A:1099:G:H22    | 1.48                     | 0.59              |
| 1:A:1355:G:H2'    | 1:A:1356:G:H8     | 1.68                     | 0.59              |
| 26:a:1040:A:H61   | 26:a:1115:G:H1    | 1.49                     | 0.59              |
| 33:h:30:LEU:HB3   | 33:h:36:ALA:HB3   | 1.84                     | 0.59              |
| 33:h:99:ILE:HD11  | 33:h:130:VAL:HG21 | 1.85                     | 0.59              |
| 33:h:128:HIS:CE1  | 33:h:146:VAL:HB   | 2.38                     | 0.59              |
| 1:A:481:G:O2'     | 1:A:483:C:N4      | 2.36                     | 0.59              |
| 1:A:1360:A:OP2    | 14:N:75:ARG:NH2   | 2.33                     | 0.59              |
| 2:B:35:ARG:HH12   | 25:Y:15:GLU:CD    | 2.11                     | 0.59              |
| 4:D:110:THR:HG23  | 4:D:113:GLU:H     | 1.68                     | 0.59              |
| 19:S:31:LEU:HB2   | 19:S:49:ILE:HG12  | 1.83                     | 0.59              |
| 39:n:51:ALA:HB3   | 39:n:78:VAL:HB    | 1.84                     | 0.59              |
| 52:0:5:ILE:O      | 52:0:28:ARG:NH2   | 2.36                     | 0.59              |
| 26:a:1042:G:N2    | 26:a:1113:U:O2    | 2.28                     | 0.59              |
| 26:a:2557:G:H2'   | 26:a:2558:C:H6    | 1.67                     | 0.59              |
| 1:A:1071:C:H2'    | 1:A:1072:G:H8     | 1.68                     | 0.58              |
| 18:R:34:THR:HG23  | 21:U:25:LYS:HZ3   | 1.66                     | 0.58              |
| 32:g:17:VAL:HG11  | 32:g:50:LEU:HD11  | 1.85                     | 0.58              |
| 32:g:159:GLY:O    | 32:g:163:ARG:NH1  | 2.34                     | 0.58              |
| 33:h:94:ILE:HD11  | 33:h:122:LEU:HB2  | 1.85                     | 0.58              |
| 40:o:5:ILE:O      | 40:o:9:GLU:HG2    | 2.02                     | 0.58              |
| 1:A:21:G:H2'      | 1:A:22:G:C8       | 2.39                     | 0.58              |
| 1:A:32:A:H2'      | 1:A:33:A:C8       | 2.38                     | 0.58              |
| 1:A:1210:C:HO2'   | 1:A:1213:A:HO2'   | 1.51                     | 0.58              |
| 22:V:4:G:H2'      | 22:V:5:G:O4'      | 2.03                     | 0.58              |
| 38:m:35:LYS:HE3   | 38:m:110:MET:HE3  | 1.86                     | 0.58              |
| 25:Y:52:GLN:NE2   | 25:Y:87:GLU:OE1   | 2.33                     | 0.58              |
| 25:Y:135:LEU:HD13 | 25:Y:139:ARG:CZ   | 2.33                     | 0.58              |
| 26:a:881:G:H1     | 26:a:895:U:H3     | 0.64                     | 0.58              |
| 26:a:1721:G:O2'   | 26:a:1739:A:N6    | 2.36                     | 0.58              |
| 26:a:1779:U:H5    | 26:a:1784:A:N7    | 2.01                     | 0.58              |
| 1:A:41:G:H2'      | 1:A:42:G:H8       | 1.68                     | 0.58              |
| 1:A:373:A:O2'     | 1:A:451:A:N7      | 2.36                     | 0.58              |
| 6:F:42:TRP:HB2    | 6:F:59:TYR:HB2    | 1.86                     | 0.58              |
| 25:Y:134:SER:HA   | 25:Y:142:ARG:HD2  | 1.85                     | 0.58              |
| 26:a:1636:U:H2'   | 26:a:1637:A:C8    | 2.38                     | 0.58              |
| 1:A:718:A:H2      | 18:R:38:LYS:NZ    | 2.00                     | 0.58              |
| 1:A:1280:A:OP2    | 10:J:9:ARG:NH2    | 2.31                     | 0.58              |
| 9:I:19:VAL:HG22   | 9:I:65:ILE:HG12   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:1236:G:HO2'  | 26:a:1237:A:P     | 2.25                     | 0.58              |
| 26:a:2514:U:H2'   | 26:a:2515:C:C6    | 2.39                     | 0.58              |
| 29:d:149:ASN:OD1  | 29:d:150:MEQ:N    | 2.37                     | 0.58              |
| 1:A:741:G:OP1     | 15:O:2:SER:N      | 2.37                     | 0.58              |
| 47:v:65:GLY:HA2   | 47:v:85:GLU:HB3   | 1.86                     | 0.58              |
| 1:A:505:G:H2'     | 1:A:506:G:H8      | 1.68                     | 0.58              |
| 1:A:945:G:C2      | 1:A:946:A:C8      | 2.91                     | 0.58              |
| 1:A:1452:C:O2'    | 1:A:1453:G:N2     | 2.37                     | 0.58              |
| 11:K:37:ARG:NE    | 11:K:83:GLU:OE2   | 2.36                     | 0.58              |
| 13:M:11:ASP:HB3   | 13:M:46:SER:HB3   | 1.86                     | 0.58              |
| 26:a:2698:U:H2'   | 26:a:2699:C:C6    | 2.39                     | 0.58              |
| 1:A:261:U:OP2     | 20:T:74:ARG:NH1   | 2.30                     | 0.58              |
| 2:B:121:SER:HA    | 2:B:126:PHE:CD1   | 2.38                     | 0.58              |
| 25:Y:112:ILE:HG22 | 25:Y:145:LEU:HD13 | 1.86                     | 0.58              |
| 26:a:2683:C:O2    | 35:j:70:ARG:NH1   | 2.30                     | 0.58              |
| 9:I:7:TYR:OH      | 9:I:9:THR:OG1     | 2.22                     | 0.58              |
| 26:a:242:G:H4'    | 26:a:243:U:O5'    | 2.04                     | 0.58              |
| 26:a:1187:G:N2    | 26:a:1188:U:O4    | 2.37                     | 0.58              |
| 26:a:2125:G:N2    | 26:a:2171:A:OP1   | 2.37                     | 0.58              |
| 26:a:2146:C:O2'   | 26:a:2147:A:N7    | 2.35                     | 0.58              |
| 26:a:2291:U:H2'   | 26:a:2292:U:C6    | 2.38                     | 0.58              |
| 26:a:2867:G:O2'   | 26:a:2868:A:H8    | 1.85                     | 0.58              |
| 1:A:1040:U:H2'    | 1:A:1041:G:C8     | 2.38                     | 0.57              |
| 1:A:1539:C:N3     | 24:X:2:G:C6       | 2.72                     | 0.57              |
| 17:Q:6:ARG:C      | 17:Q:7:THR:HG23   | 2.29                     | 0.57              |
| 26:a:1219:U:H2'   | 26:a:1220:A:C8    | 2.39                     | 0.57              |
| 26:a:1283:G:N2    | 26:a:1286:A:OP2   | 2.37                     | 0.57              |
| 1:A:958:A:N3      | 1:A:985:C:O2'     | 2.30                     | 0.57              |
| 1:A:1218:C:H2'    | 1:A:1219:A:C8     | 2.39                     | 0.57              |
| 26:a:833:A:H2'    | 26:a:834:G:C8     | 2.39                     | 0.57              |
| 26:a:1645:G:H5''  | 26:a:1646:C:H5'   | 1.86                     | 0.57              |
| 26:a:2183:A:H2'   | 26:a:2184:A:H4'   | 1.85                     | 0.57              |
| 26:a:2532:G:N2    | 26:a:2663:G:O2'   | 2.37                     | 0.57              |
| 26:a:2566:A:N1    | 35:j:28:SER:OG    | 2.33                     | 0.57              |
| 32:g:52:PHE:HE2   | 32:g:72:LEU:HD12  | 1.69                     | 0.57              |
| 1:A:664:G:H22     | 1:A:741:G:H1      | 1.52                     | 0.57              |
| 1:A:1291:U:OP1    | 7:G:37:SER:OG     | 2.20                     | 0.57              |
| 13:M:33:ILE:HD13  | 13:M:60:VAL:HG22  | 1.87                     | 0.57              |
| 21:U:61:ALA:O     | 21:U:64:ASN:N     | 2.35                     | 0.57              |
| 26:a:365:U:H2'    | 26:a:366:C:C6     | 2.39                     | 0.57              |
| 26:a:1636:U:H2'   | 26:a:1637:A:H8    | 1.68                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 43:r:20:VAL:HG11 | 43:r:44:ALA:HA   | 1.86                     | 0.57              |
| 1:A:505:G:H2'    | 1:A:506:G:C8     | 2.39                     | 0.57              |
| 9:I:65:ILE:HG21  | 9:I:79:ILE:HD12  | 1.85                     | 0.57              |
| 26:a:704:G:H1'   | 26:a:727:A:H61   | 1.68                     | 0.57              |
| 26:a:1796:U:H2'  | 26:a:1797:G:H8   | 1.69                     | 0.57              |
| 1:A:1130:A:H2'   | 1:A:1131:G:H8    | 1.70                     | 0.57              |
| 1:A:1359:C:OP2   | 14:N:75:ARG:NE   | 2.37                     | 0.57              |
| 2:B:24:ASN:HD21  | 2:B:192:ASP:HB3  | 1.68                     | 0.57              |
| 16:P:18:GLN:OE1  | 16:P:35:ARG:NE   | 2.37                     | 0.57              |
| 18:R:34:THR:CG2  | 21:U:25:LYS:HZ2  | 2.18                     | 0.57              |
| 22:V:6:G:H2'     | 22:V:7:G:C8      | 2.40                     | 0.57              |
| 27:b:51:G:OP2    | 39:n:67:ASN:ND2  | 2.37                     | 0.57              |
| 56:4:18:CYS:SG   | 56:4:40:CYS:HB3  | 2.44                     | 0.57              |
| 26:a:1571:A:H2'  | 26:a:1572:A:C8   | 2.40                     | 0.57              |
| 26:a:2169:A:C5   | 26:a:2170:A:H1'  | 2.39                     | 0.57              |
| 49:x:13:GLU:HA   | 49:x:16:THR:HG22 | 1.85                     | 0.57              |
| 56:4:63:ARG:HG3  | 56:4:64:PHE:CD2  | 2.39                     | 0.57              |
| 15:O:3:LEU:HG    | 15:O:35:GLN:HE21 | 1.70                     | 0.57              |
| 21:U:28:VAL:HG23 | 21:U:29:LEU:HD12 | 1.87                     | 0.57              |
| 26:a:1565:C:O2'  | 26:a:1566:A:H2'  | 2.05                     | 0.57              |
| 34:i:125:TYR:OH  | 34:i:132:HIS:NE2 | 2.33                     | 0.57              |
| 36:k:57:LEU:HD22 | 54:2:54:ASP:HB3  | 1.86                     | 0.57              |
| 3:C:123:GLN:OE1  | 3:C:136:ARG:NH2  | 2.34                     | 0.57              |
| 25:Y:27:VAL:HG12 | 25:Y:29:VAL:HG22 | 1.87                     | 0.57              |
| 26:a:2305:U:H5'' | 31:f:131:GLY:HA3 | 1.87                     | 0.57              |
| 32:g:52:PHE:CE2  | 32:g:72:LEU:HD12 | 2.39                     | 0.57              |
| 1:A:464:U:H2'    | 1:A:465:A:H5''   | 1.87                     | 0.57              |
| 1:A:784:A:H2'    | 1:A:785:G:H8     | 1.70                     | 0.57              |
| 26:a:1085:A:H3'  | 26:a:1086:A:H2   | 1.70                     | 0.57              |
| 1:A:1440:U:O2'   | 1:A:1441:A:H5'   | 2.05                     | 0.56              |
| 8:H:11:LEU:HD22  | 8:H:75:ILE:HD11  | 1.87                     | 0.56              |
| 25:Y:42:LEU:HD22 | 25:Y:75:VAL:HG23 | 1.87                     | 0.56              |
| 26:a:1386:C:H2'  | 26:a:1387:A:C8   | 2.40                     | 0.56              |
| 26:a:1734:C:H2'  | 26:a:1735:G:H8   | 1.70                     | 0.56              |
| 31:f:93:GLY:O    | 31:f:96:MET:HB3  | 2.05                     | 0.56              |
| 2:B:222:ARG:O    | 2:B:226:SER:N    | 2.31                     | 0.56              |
| 13:M:79:ARG:O    | 13:M:83:LEU:HD23 | 2.04                     | 0.56              |
| 1:A:337:G:H2'    | 1:A:338:A:H8     | 1.68                     | 0.56              |
| 1:A:714:G:H2'    | 1:A:715:A:C8     | 2.40                     | 0.56              |
| 1:A:1005:A:H3'   | 1:A:1006:C:H6    | 1.70                     | 0.56              |
| 2:B:101:LEU:HB3  | 2:B:179:LEU:HD12 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:85:ASN:HB3    | 4:D:88:GLU:HG2    | 1.87                     | 0.56              |
| 25:Y:27:VAL:H     | 25:Y:40:ALA:HB3   | 1.71                     | 0.56              |
| 26:a:75:G:H22     | 26:a:111:A:H2     | 1.51                     | 0.56              |
| 26:a:299:A:N1     | 26:a:322:A:O2'    | 2.34                     | 0.56              |
| 26:a:589:U:H2'    | 26:a:590:A:H8     | 1.70                     | 0.56              |
| 26:a:673:C:OP1    | 30:e:49:ARG:NH1   | 2.36                     | 0.56              |
| 26:a:886:A:H62    | 26:a:890:C:N4     | 2.03                     | 0.56              |
| 27:b:30:C:O2'     | 27:b:57:A:N1      | 2.35                     | 0.56              |
| 3:C:114:LYS:HB2   | 3:C:185:ASN:HD22  | 1.70                     | 0.56              |
| 25:Y:170:ARG:O    | 25:Y:171:ARG:HD2  | 2.06                     | 0.56              |
| 26:a:1219:U:H2'   | 26:a:1220:A:H8    | 1.70                     | 0.56              |
| 26:a:2229:U:H2'   | 26:a:2230:G:H8    | 1.70                     | 0.56              |
| 28:c:141:VAL:HG12 | 28:c:192:LEU:HD23 | 1.87                     | 0.56              |
| 46:u:20:LEU:HD22  | 46:u:25:LYS:HB2   | 1.87                     | 0.56              |
| 1:A:1124:G:O5'    | 10:J:37:ARG:NH1   | 2.39                     | 0.56              |
| 26:a:191:A:H2'    | 26:a:192:C:C6     | 2.41                     | 0.56              |
| 26:a:774:G:O2'    | 26:a:775:G:O5'    | 2.23                     | 0.56              |
| 26:a:1125:G:OP2   | 26:a:1126:A:O2'   | 2.18                     | 0.56              |
| 26:a:1213:A:N6    | 26:a:1236:G:H1'   | 2.20                     | 0.56              |
| 26:a:1587:G:H2'   | 26:a:1588:G:H8    | 1.71                     | 0.56              |
| 26:a:1588:G:H2'   | 26:a:1589:U:C6    | 2.41                     | 0.56              |
| 4:D:129:VAL:HG22  | 4:D:146:ARG:HD3   | 1.86                     | 0.56              |
| 8:H:96:MET:HB2    | 8:H:100:GLY:H     | 1.70                     | 0.56              |
| 9:I:94:LEU:HD23   | 9:I:94:LEU:H      | 1.71                     | 0.56              |
| 26:a:357:C:O2'    | 26:a:358:U:OP1    | 2.23                     | 0.56              |
| 26:a:1108:U:H2'   | 26:a:1109:C:C6    | 2.41                     | 0.56              |
| 26:a:2297:A:N1    | 26:a:2321:U:H5    | 2.03                     | 0.56              |
| 26:a:2636:C:H5'   | 29:d:81:GLU:HB2   | 1.88                     | 0.56              |
| 1:A:501:C:H2'     | 1:A:502:A:C8      | 2.39                     | 0.56              |
| 25:Y:31:ILE:HD11  | 25:Y:62:ILE:HG23  | 1.86                     | 0.56              |
| 26:a:573:U:N3     | 26:a:2031:A:OP1   | 2.39                     | 0.56              |
| 26:a:172:A:H2'    | 26:a:173:A:C8     | 2.40                     | 0.56              |
| 26:a:2419:U:H4'   | 52:0:22:THR:HG21  | 1.88                     | 0.56              |
| 49:x:55:THR:O     | 49:x:59:GLU:HG3   | 2.06                     | 0.56              |
| 26:a:672:C:OP2    | 36:k:42:SER:OG    | 2.23                     | 0.56              |
| 36:k:123:ARG:HA   | 36:k:143:GLU:HB3  | 1.88                     | 0.56              |
| 43:r:11:ARG:NH2   | 43:r:98:LYS:HD3   | 2.21                     | 0.56              |
| 45:t:8:ASP:OD1    | 45:t:24:LYS:NZ    | 2.39                     | 0.56              |
| 49:x:49:ASP:OD1   | 49:x:52:ARG:NH2   | 2.38                     | 0.56              |
| 1:A:769:G:H4'     | 1:A:1513:A:H4'    | 1.88                     | 0.56              |
| 26:a:2725:A:O2'   | 26:a:2726:A:O5'   | 2.24                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:a:277:G:H4'    | 26:a:278:A:C5    | 2.41                     | 0.55              |
| 26:a:310:A:O2'    | 26:a:311:A:H2'   | 2.06                     | 0.55              |
| 26:a:1175:A:H5''  | 26:a:1176:U:H1'  | 1.87                     | 0.55              |
| 26:a:2626:C:H2'   | 26:a:2627:G:H8   | 1.72                     | 0.55              |
| 38:m:8:ARG:HD2    | 38:m:43:GLU:HG2  | 1.86                     | 0.55              |
| 11:K:29:ASN:OD1   | 11:K:30:THR:N    | 2.38                     | 0.55              |
| 26:a:141:G:OP2    | 26:a:141:G:N2    | 2.31                     | 0.55              |
| 26:a:2340:A:OP1   | 27:b:41:G:N2     | 2.39                     | 0.55              |
| 1:A:62:U:OP1      | 1:A:385:C:O2'    | 2.23                     | 0.55              |
| 1:A:524:G:H2'     | 1:A:525:C:C6     | 2.42                     | 0.55              |
| 1:A:1060:U:H2'    | 1:A:1061:G:H8    | 1.71                     | 0.55              |
| 9:I:5:GLN:NE2     | 9:I:22:LYS:HE3   | 2.14                     | 0.55              |
| 26:a:1794:A:H2'   | 26:a:1795:C:C6   | 2.40                     | 0.55              |
| 26:a:2141:G:H2'   | 26:a:2142:A:C8   | 2.41                     | 0.55              |
| 28:c:120:VAL:HG21 | 33:h:91:PHE:O    | 2.06                     | 0.55              |
| 31:f:73:SER:OG    | 31:f:81:GLN:N    | 2.37                     | 0.55              |
| 37:l:141:LYS:HG2  | 37:l:142:GLY:H   | 1.71                     | 0.55              |
| 11:K:93:ARG:CZ    | 21:U:29:LEU:HD11 | 2.36                     | 0.55              |
| 26:a:704:G:H1'    | 26:a:727:A:N6    | 2.21                     | 0.55              |
| 26:a:1013:C:H2'   | 26:a:1014:A:H8   | 1.71                     | 0.55              |
| 1:A:718:A:H5'     | 11:K:119:ASN:HB2 | 1.87                     | 0.55              |
| 26:a:891:G:H1     | 26:a:892:A:N6    | 2.03                     | 0.55              |
| 26:a:922:C:O2'    | 47:v:29:GLU:OE2  | 2.22                     | 0.55              |
| 1:A:736:C:H2'     | 1:A:737:C:H6     | 1.70                     | 0.55              |
| 26:a:1102:C:OP2   | 26:a:1104:C:N4   | 2.39                     | 0.55              |
| 26:a:1710:G:H2'   | 26:a:1711:A:C8   | 2.40                     | 0.55              |
| 49:x:19:LEU:HB3   | 49:x:23:ARG:HH12 | 1.72                     | 0.55              |
| 1:A:12:U:H4'      | 1:A:526:C:H4'    | 1.88                     | 0.55              |
| 1:A:28:A:O2'      | 1:A:296:U:OP1    | 2.24                     | 0.55              |
| 2:B:10:LEU:HD22   | 25:Y:11:GLU:HG3  | 1.89                     | 0.55              |
| 8:H:18:GLN:NE2    | 8:H:63:LEU:HB3   | 2.22                     | 0.55              |
| 13:M:10:PRO:HG3   | 13:M:13:LYS:HE2  | 1.87                     | 0.55              |
| 25:Y:142:ARG:NH1  | 25:Y:143:ASP:HB2 | 2.22                     | 0.55              |
| 26:a:750:A:OP1    | 26:a:1615:C:N4   | 2.39                     | 0.55              |
| 1:A:231:U:H2'     | 1:A:232:G:H8     | 1.72                     | 0.55              |
| 4:D:91:LEU:HD12   | 4:D:188:ARG:CD   | 2.34                     | 0.55              |
| 10:J:35:GLN:NE2   | 10:J:77:VAL:HB   | 2.21                     | 0.55              |
| 18:R:34:THR:CG2   | 21:U:25:LYS:NZ   | 2.68                     | 0.55              |
| 25:Y:88:LYS:HD3   | 25:Y:91:ARG:NH2  | 2.20                     | 0.55              |
| 1:A:845:A:H1'     | 18:R:9:LYS:NZ    | 2.18                     | 0.55              |
| 1:A:1004:A:N6     | 1:A:1026:G:O2'   | 2.39                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1406:U:O2     | 1:A:1517:G:N2    | 2.35                     | 0.55              |
| 2:B:17:GLY:O      | 2:B:38:VAL:CG1   | 2.53                     | 0.55              |
| 3:C:73:PRO:HA     | 3:C:76:VAL:HG12  | 1.89                     | 0.55              |
| 9:I:21:ILE:HG22   | 9:I:63:LEU:HD13  | 1.89                     | 0.55              |
| 11:K:23:ILE:HG12  | 11:K:96:THR:HG21 | 1.88                     | 0.55              |
| 26:a:2099:U:H2'   | 26:a:2100:G:C8   | 2.42                     | 0.55              |
| 1:A:662:U:H2'     | 1:A:663:A:C8     | 2.42                     | 0.55              |
| 1:A:746:A:H2'     | 1:A:747:A:C8     | 2.41                     | 0.55              |
| 1:A:1316:G:N2     | 1:A:1319:A:OP2   | 2.34                     | 0.55              |
| 4:D:78:GLU:OE2    | 4:D:81:ARG:NH1   | 2.31                     | 0.55              |
| 5:E:148:ASN:HB2   | 8:H:96:MET:HE1   | 1.89                     | 0.55              |
| 45:t:81:ASP:OD1   | 45:t:82:ARG:N    | 2.40                     | 0.55              |
| 1:A:674:G:H2'     | 1:A:675:A:C8     | 2.40                     | 0.54              |
| 17:Q:20:SER:HB2   | 17:Q:71:LYS:HZ2  | 1.70                     | 0.54              |
| 25:Y:137:ASP:OD1  | 25:Y:138:VAL:N   | 2.37                     | 0.54              |
| 26:a:353:C:H2'    | 26:a:354:A:C8    | 2.42                     | 0.54              |
| 30:e:153:LEU:HD21 | 30:e:158:PHE:HB2 | 1.89                     | 0.54              |
| 1:A:933:G:O6      | 7:G:3:ARG:NH2    | 2.41                     | 0.54              |
| 26:a:2847:U:H2'   | 26:a:2848:G:O4'  | 2.07                     | 0.54              |
| 27:b:5:U:H2'      | 27:b:6:G:H8      | 1.72                     | 0.54              |
| 34:i:114:LEU:HG   | 34:i:118:MET:HE3 | 1.89                     | 0.54              |
| 1:A:406:G:H5'     | 4:D:5:LEU:HD13   | 1.89                     | 0.54              |
| 26:a:2313:C:O4'   | 31:f:37:ASN:ND2  | 2.40                     | 0.54              |
| 30:e:147:LEU:HD11 | 30:e:170:ARG:HB2 | 1.90                     | 0.54              |
| 1:A:157:U:O2      | 1:A:164:G:O6     | 2.26                     | 0.54              |
| 1:A:1450:U:N3     | 1:A:1452:C:O2    | 2.40                     | 0.54              |
| 2:B:188:ASP:CG    | 2:B:189:THR:H    | 2.14                     | 0.54              |
| 26:a:1231:U:H2'   | 26:a:1232:G:H8   | 1.73                     | 0.54              |
| 26:a:2233:U:H2'   | 26:a:2234:G:H8   | 1.72                     | 0.54              |
| 33:h:127:GLU:OE2  | 33:h:127:GLU:HA  | 2.07                     | 0.54              |
| 50:y:24:LEU:HD11  | 50:y:54:MET:SD   | 2.47                     | 0.54              |
| 3:C:69:HIS:HA     | 3:C:104:ALA:HB3  | 1.88                     | 0.54              |
| 3:C:85:GLU:OE2    | 3:C:89:LYS:NZ    | 2.36                     | 0.54              |
| 6:F:41:ASP:OD2    | 6:F:58:HIS:NE2   | 2.28                     | 0.54              |
| 10:J:63:ASP:OD2   | 14:N:85:ARG:NE   | 2.33                     | 0.54              |
| 26:a:356:G:H2'    | 26:a:357:C:C6    | 2.42                     | 0.54              |
| 26:a:2135:A:H5''  | 26:a:2156:G:H1   | 1.72                     | 0.54              |
| 1:A:401:C:O2'     | 1:A:621:A:N3     | 2.37                     | 0.54              |
| 2:B:9:MET:HB3     | 2:B:43:LEU:HD13  | 1.88                     | 0.54              |
| 26:a:1113:U:H2'   | 26:a:1114:C:H6   | 1.73                     | 0.54              |
| 26:a:1816:C:N4    | 28:c:35:GLU:OE1  | 2.31                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:2125:G:O2'  | 26:a:2126:A:O4'   | 2.25                     | 0.54              |
| 26:a:2246:G:H2'  | 26:a:2247:A:H8    | 1.73                     | 0.54              |
| 43:r:51:LEU:HD13 | 43:r:105:VAL:HG11 | 1.89                     | 0.54              |
| 44:s:12:ARG:HD3  | 49:x:29:ARG:HD2   | 1.89                     | 0.54              |
| 1:A:160:A:H1'    | 1:A:344:A:N7      | 2.21                     | 0.54              |
| 3:C:47:LEU:HD21  | 3:C:87:LEU:HD11   | 1.89                     | 0.54              |
| 17:Q:6:ARG:O     | 17:Q:7:THR:HG23   | 2.08                     | 0.54              |
| 26:a:134:G:H2'   | 26:a:135:U:C6     | 2.42                     | 0.54              |
| 26:a:1088:A:H4'  | 26:a:1089:A:N7    | 2.22                     | 0.54              |
| 31:f:102:ARG:HG2 | 56:4:24:ILE:HD12  | 1.89                     | 0.54              |
| 47:v:37:ILE:HD11 | 47:v:61:ALA:HB2   | 1.89                     | 0.54              |
| 1:A:559:A:H4'    | 1:A:560:A:H3'     | 1.90                     | 0.54              |
| 1:A:1517:G:N3    | 26:a:1919:A:O2'   | 2.40                     | 0.54              |
| 6:F:6:ILE:HG12   | 6:F:89:VAL:HG22   | 1.90                     | 0.54              |
| 9:I:88:MET:HE1   | 9:I:95:ARG:HA     | 1.90                     | 0.54              |
| 11:K:84:VAL:N    | 11:K:109:ASN:O    | 2.39                     | 0.54              |
| 16:P:40:ASN:HB3  | 16:P:43:ALA:HB2   | 1.90                     | 0.54              |
| 17:Q:47:HIS:NE2  | 17:Q:49:GLU:OE2   | 2.34                     | 0.54              |
| 19:S:64:ASP:OD1  | 19:S:65:GLU:N     | 2.40                     | 0.54              |
| 26:a:589:U:H2'   | 26:a:590:A:C8     | 2.42                     | 0.54              |
| 26:a:2636:C:H2'  | 26:a:2637:U:C6    | 2.42                     | 0.54              |
| 27:b:89:U:H5''   | 27:b:90:C:C6      | 2.43                     | 0.54              |
| 42:q:24:LYS:HD3  | 42:q:92:TRP:HB3   | 1.89                     | 0.54              |
| 1:A:337:G:H2'    | 1:A:338:A:C8      | 2.42                     | 0.54              |
| 1:A:1121:U:C2    | 1:A:1122:U:C5     | 2.96                     | 0.54              |
| 6:F:17:GLN:HG2   | 33:h:87:GLU:HB2   | 1.90                     | 0.54              |
| 8:H:18:GLN:HG2   | 8:H:63:LEU:HD13   | 1.90                     | 0.54              |
| 26:a:155:A:H2'   | 26:a:156:A:H8     | 1.73                     | 0.54              |
| 26:a:781:A:OP1   | 28:c:217:ARG:NH2  | 2.39                     | 0.54              |
| 26:a:1716:U:H2'  | 26:a:1717:A:H8    | 1.73                     | 0.54              |
| 26:a:2074:U:H2'  | 26:a:2075:U:C6    | 2.43                     | 0.54              |
| 26:a:2233:U:H2'  | 26:a:2234:G:C8    | 2.43                     | 0.54              |
| 28:c:121:ASP:CA  | 33:h:91:PHE:CE1   | 2.57                     | 0.54              |
| 1:A:191:G:H2'    | 1:A:192:A:H8      | 1.73                     | 0.54              |
| 1:A:1328:C:H5''  | 13:M:28:THR:HG21  | 1.89                     | 0.54              |
| 3:C:20:SER:HG    | 3:C:40:ARG:NH2    | 2.04                     | 0.54              |
| 11:K:34:ILE:HG12 | 11:K:70:CYS:SG    | 2.48                     | 0.54              |
| 25:Y:142:ARG:CZ  | 25:Y:143:ASP:HB2  | 2.38                     | 0.54              |
| 26:a:1385:A:O2'  | 26:a:1396:U:O2    | 2.26                     | 0.54              |
| 26:a:2595:G:N2   | 26:a:2598:A:OP2   | 2.35                     | 0.54              |
| 26:a:2804:U:H2'  | 26:a:2805:C:C6    | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:o:31:TRP:HE3   | 40:o:38:LYS:HG2   | 1.73                     | 0.54              |
| 1:A:18:C:OP1      | 5:E:132:ASN:ND2   | 2.40                     | 0.53              |
| 1:A:69:G:H2'      | 1:A:70:U:C6       | 2.44                     | 0.53              |
| 1:A:131:A:H2'     | 1:A:132:C:C6      | 2.44                     | 0.53              |
| 7:G:70:ARG:NH1    | 7:G:97:ASN:OD1    | 2.41                     | 0.53              |
| 26:a:987:C:O2'    | 26:a:1000:A:N3    | 2.35                     | 0.53              |
| 1:A:1004:A:H2'    | 1:A:1005:A:O4'    | 2.09                     | 0.53              |
| 1:A:1507:A:H2'    | 1:A:1508:A:H8     | 1.72                     | 0.53              |
| 16:P:45:GLU:O     | 16:P:46:LYS:HB2   | 2.09                     | 0.53              |
| 25:Y:171:ARG:HH11 | 25:Y:171:ARG:HG3  | 1.72                     | 0.53              |
| 26:a:675:A:N3     | 26:a:2443:C:O2'   | 2.39                     | 0.53              |
| 28:c:71:LYS:HE3   | 28:c:74:ILE:HD12  | 1.91                     | 0.53              |
| 34:i:49:ASP:OD1   | 34:i:121:LYS:NZ   | 2.40                     | 0.53              |
| 44:s:8:LEU:O      | 49:x:29:ARG:NH1   | 2.41                     | 0.53              |
| 1:A:1399:C:O2     | 1:A:1502:A:N6     | 2.41                     | 0.53              |
| 2:B:10:LEU:C      | 2:B:12:ALA:N      | 2.65                     | 0.53              |
| 2:B:208:ARG:HH21  | 25:Y:44:SER:HA    | 1.72                     | 0.53              |
| 10:J:8:ILE:HB     | 10:J:74:VAL:HB    | 1.89                     | 0.53              |
| 22:V:64:G:H5''    | 47:v:11:ARG:HH12  | 1.73                     | 0.53              |
| 25:Y:70:VAL:HG13  | 25:Y:85:SER:HA    | 1.90                     | 0.53              |
| 26:a:1332:G:N7    | 26:a:1609:A:O2'   | 2.34                     | 0.53              |
| 26:a:2243:U:H2'   | 26:a:2244:U:C6    | 2.43                     | 0.53              |
| 26:a:2830:C:H5''  | 29:d:56:LYS:HE2   | 1.90                     | 0.53              |
| 33:h:88:GLY:HA2   | 33:h:125:THR:OG1  | 2.08                     | 0.53              |
| 52:0:7:GLU:HB2    | 52:0:27:LYS:NZ    | 2.23                     | 0.53              |
| 1:A:460:A:H2'     | 1:A:461:A:O4'     | 2.09                     | 0.53              |
| 1:A:996:A:H2'     | 1:A:997:U:C6      | 2.43                     | 0.53              |
| 8:H:101:ILE:HG12  | 8:H:129:VAL:HB    | 1.88                     | 0.53              |
| 26:a:351:C:H2'    | 26:a:352:A:C8     | 2.44                     | 0.53              |
| 34:i:31:GLU:OE2   | 34:i:34:ARG:NH1   | 2.41                     | 0.53              |
| 39:n:33:ARG:O     | 39:n:65:THR:OG1   | 2.25                     | 0.53              |
| 1:A:554:A:H2'     | 1:A:555:U:C6      | 2.44                     | 0.53              |
| 1:A:1477:U:H2'    | 1:A:1478:U:C6     | 2.44                     | 0.53              |
| 20:T:37:ALA:HA    | 20:T:40:GLU:HG3   | 1.90                     | 0.53              |
| 25:Y:138:VAL:O    | 25:Y:140:PRO:HD2  | 2.08                     | 0.53              |
| 38:m:32:GLU:HG2   | 38:m:115:LEU:HD12 | 1.90                     | 0.53              |
| 45:t:86:ARG:HG3   | 45:t:95:PHE:CD1   | 2.44                     | 0.53              |
| 1:A:736:C:H2'     | 1:A:737:C:C6      | 2.43                     | 0.53              |
| 1:A:1144:G:H21    | 1:A:1146:A:H62    | 1.55                     | 0.53              |
| 17:Q:30:LYS:HB2   | 17:Q:37:PHE:CE1   | 2.44                     | 0.53              |
| 21:U:65:ALA:O     | 21:U:67:ARG:N     | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:a:481:G:H1'   | 26:a:506:G:H21   | 1.73                     | 0.53              |
| 26:a:848:C:H2'   | 26:a:849:A:C8    | 2.43                     | 0.53              |
| 26:a:1453:A:N6   | 38:m:74:GLU:HG2  | 2.24                     | 0.53              |
| 26:a:1980:G:O2'  | 26:a:1982:U:OP2  | 2.25                     | 0.53              |
| 26:a:2804:U:H2'  | 26:a:2805:C:H6   | 1.72                     | 0.53              |
| 27:b:1:U:H2'     | 27:b:2:G:H8      | 1.73                     | 0.53              |
| 33:h:58:LEU:HD12 | 33:h:58:LEU:H    | 1.72                     | 0.53              |
| 39:n:80:GLU:O    | 39:n:84:GLU:HG2  | 2.07                     | 0.53              |
| 1:A:1001:C:H2'   | 1:A:1002:A:H8    | 1.73                     | 0.53              |
| 26:a:78:U:H2'    | 26:a:79:C:C6     | 2.44                     | 0.53              |
| 56:4:41:HIS:CE1  | 56:4:43:PHE:HB3  | 2.43                     | 0.53              |
| 1:A:1423:G:P     | 35:j:49:ARG:HH12 | 2.31                     | 0.53              |
| 4:D:170:TRP:CE2  | 4:D:186:PRO:HB3  | 2.44                     | 0.53              |
| 13:M:15:ALA:HA   | 13:M:45:ILE:HD11 | 1.90                     | 0.53              |
| 26:a:1589:U:H2'  | 26:a:1590:A:C8   | 2.42                     | 0.53              |
| 26:a:1992:G:N2   | 26:a:1996:C:O2'  | 2.42                     | 0.53              |
| 1:A:181:A:H2'    | 1:A:182:A:C8     | 2.44                     | 0.53              |
| 1:A:600:A:H2'    | 1:A:601:G:H8     | 1.74                     | 0.53              |
| 26:a:834:G:H5'   | 54:2:57:LEU:HD21 | 1.90                     | 0.53              |
| 26:a:1565:C:HO2' | 26:a:1566:A:H2'  | 1.72                     | 0.53              |
| 26:a:1571:A:H2'  | 26:a:1572:A:H8   | 1.73                     | 0.53              |
| 26:a:1746:A:H2'  | 26:a:1747:U:C6   | 2.44                     | 0.53              |
| 29:d:36:GLN:OE1  | 29:d:49:GLN:NE2  | 2.42                     | 0.53              |
| 1:A:35:G:H2'     | 1:A:36:C:C6      | 2.44                     | 0.53              |
| 1:A:641:U:H5''   | 1:A:642:A:OP1    | 2.09                     | 0.53              |
| 1:A:1491:G:H2'   | 1:A:1492:A:C8    | 2.44                     | 0.53              |
| 1:A:1538:C:O2'   | 24:X:3:G:O6      | 2.27                     | 0.53              |
| 3:C:58:GLU:OE2   | 3:C:65:ARG:NH1   | 2.42                     | 0.53              |
| 25:Y:153:GLU:O   | 25:Y:170:ARG:HB3 | 2.08                     | 0.53              |
| 27:b:42:C:C6     | 31:f:66:LEU:HB2  | 2.45                     | 0.53              |
| 39:n:57:ALA:O    | 39:n:61:GLN:NE2  | 2.42                     | 0.53              |
| 39:n:76:LYS:HD3  | 39:n:113:ALA:HB2 | 1.90                     | 0.53              |
| 1:A:438:U:O2'    | 1:A:439:U:O5'    | 2.25                     | 0.52              |
| 1:A:501:C:H2'    | 1:A:502:A:H8     | 1.73                     | 0.52              |
| 1:A:1001:C:H2'   | 1:A:1002:A:C8    | 2.45                     | 0.52              |
| 1:A:1355:G:H2'   | 1:A:1356:G:C8    | 2.44                     | 0.52              |
| 26:a:296:U:H2'   | 26:a:297:G:H8    | 1.73                     | 0.52              |
| 26:a:396:G:OP2   | 48:w:10:LYS:NZ   | 2.42                     | 0.52              |
| 26:a:1796:U:H2'  | 26:a:1797:G:C8   | 2.44                     | 0.52              |
| 26:a:2249:U:O2'  | 26:a:2252:G:OP2  | 2.23                     | 0.52              |
| 28:c:5:LYS:NZ    | 28:c:14:ARG:O    | 2.41                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:g:88:GLN:HG3  | 32:g:130:GLU:HG2  | 1.91                     | 0.52              |
| 50:y:11:ARG:HB2  | 50:y:54:MET:HB2   | 1.91                     | 0.52              |
| 1:A:845:A:H5''   | 1:A:846:G:C8      | 2.44                     | 0.52              |
| 1:A:977:A:O2'    | 1:A:979:C:OP2     | 2.23                     | 0.52              |
| 1:A:1029:U:H2'   | 1:A:1031:C:H5'    | 1.90                     | 0.52              |
| 1:A:1335:U:H5''  | 1:A:1336:C:H5'    | 1.91                     | 0.52              |
| 3:C:177:THR:HG22 | 3:C:180:ALA:H     | 1.74                     | 0.52              |
| 17:Q:6:ARG:O     | 17:Q:7:THR:CG2    | 2.56                     | 0.52              |
| 26:a:303:G:H2'   | 26:a:304:U:C6     | 2.44                     | 0.52              |
| 26:a:1224:U:H2'  | 26:a:1225:G:C8    | 2.44                     | 0.52              |
| 33:h:70:GLU:OE1  | 33:h:140:ALA:HA   | 2.09                     | 0.52              |
| 2:B:117:LEU:HD23 | 2:B:141:LEU:HB2   | 1.91                     | 0.52              |
| 3:C:20:SER:OG    | 3:C:40:ARG:NH2    | 2.34                     | 0.52              |
| 19:S:11:ILE:HD11 | 19:S:15:LEU:HD22  | 1.90                     | 0.52              |
| 21:U:17:ARG:HH12 | 21:U:21:ARG:HE    | 1.55                     | 0.52              |
| 26:a:219:A:N3    | 26:a:234:U:O2'    | 2.32                     | 0.52              |
| 26:a:2290:G:H2'  | 26:a:2291:U:C6    | 2.44                     | 0.52              |
| 38:m:65:LEU:HD22 | 38:m:69:ARG:HH22  | 1.75                     | 0.52              |
| 39:n:2:ASP:OD1   | 39:n:3:LYS:N      | 2.42                     | 0.52              |
| 1:A:1120:U:H2'   | 1:A:1121:U:H6     | 1.75                     | 0.52              |
| 2:B:66:LYS:HG2   | 2:B:90:PHE:HE2    | 1.74                     | 0.52              |
| 8:H:18:GLN:OE1   | 8:H:70:ALA:HB1    | 2.09                     | 0.52              |
| 26:a:244:A:OP2   | 54:2:8:ARG:NH2    | 2.32                     | 0.52              |
| 26:a:721:A:H2'   | 26:a:722:A:C8     | 2.44                     | 0.52              |
| 26:a:1103:A:H2'  | 26:a:1104:C:C2    | 2.43                     | 0.52              |
| 26:a:1315:C:O2'  | 26:a:1392:A:N3    | 2.41                     | 0.52              |
| 26:a:1670:C:O2   | 29:d:134:HIS:NE2  | 2.34                     | 0.52              |
| 26:a:2079:U:O2'  | 48:w:23:ASN:OD1   | 2.26                     | 0.52              |
| 1:A:976:G:OP2    | 1:A:1358:U:O2'    | 2.27                     | 0.52              |
| 1:A:1248:A:H2    | 9:I:72:ILE:HD11   | 1.75                     | 0.52              |
| 8:H:29:SER:HB3   | 8:H:57:PRO:HB2    | 1.92                     | 0.52              |
| 11:K:101:ASN:HB2 | 11:K:107:ILE:HD12 | 1.91                     | 0.52              |
| 18:R:13:PHE:CE2  | 18:R:55:LEU:HD13  | 2.44                     | 0.52              |
| 22:V:16:C:H1'    | 22:V:60:A:H2      | 1.73                     | 0.52              |
| 26:a:370:G:O2'   | 26:a:424:G:OP1    | 2.24                     | 0.52              |
| 26:a:1715:G:O2'  | 26:a:1716:U:H6    | 1.93                     | 0.52              |
| 26:a:2286:G:H4'  | 26:a:2287:A:O5'   | 2.09                     | 0.52              |
| 26:a:2751:G:H4'  | 32:g:4:VAL:HG23   | 1.90                     | 0.52              |
| 33:h:126:GLY:H   | 33:h:128:HIS:HE1  | 1.56                     | 0.52              |
| 46:u:20:LEU:HD21 | 46:u:41:GLU:OE2   | 2.10                     | 0.52              |
| 1:A:155:A:H2'    | 1:A:156:C:C6      | 2.44                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:13:GLU:OE1    | 5:E:39:VAL:HG12  | 2.09                     | 0.52              |
| 26:a:716:A:H2'    | 26:a:717:C:O4'   | 2.10                     | 0.52              |
| 26:a:764:A:H5''   | 28:c:209:GLY:CA  | 2.40                     | 0.52              |
| 26:a:1857:G:H1'   | 26:a:1885:A:N6   | 2.25                     | 0.52              |
| 26:a:2515:C:H2'   | 26:a:2516:A:H8   | 1.73                     | 0.52              |
| 45:t:86:ARG:NH1   | 45:t:102:THR:OG1 | 2.42                     | 0.52              |
| 1:A:461:A:H2      | 1:A:471:U:H3     | 1.56                     | 0.52              |
| 1:A:656:G:O2'     | 15:O:28:GLN:OE1  | 2.27                     | 0.52              |
| 1:A:1226:C:OP2    | 13:M:102:THR:OG1 | 2.21                     | 0.52              |
| 6:F:19:PRO:O      | 6:F:23:GLU:HG3   | 2.09                     | 0.52              |
| 26:a:5:A:H2'      | 26:a:6:A:H8      | 1.73                     | 0.52              |
| 26:a:154:U:H2'    | 26:a:155:A:H8    | 1.74                     | 0.52              |
| 26:a:1010:A:OP1   | 41:p:66:ASN:ND2  | 2.34                     | 0.52              |
| 26:a:1292:G:H2'   | 26:a:1293:C:C6   | 2.45                     | 0.52              |
| 26:a:2286:G:H4'   | 26:a:2287:A:O4'  | 2.09                     | 0.52              |
| 26:a:2637:U:H2'   | 26:a:2638:G:O4'  | 2.10                     | 0.52              |
| 26:a:2822:G:OP1   | 29:d:164:GLN:NE2 | 2.36                     | 0.52              |
| 40:o:31:TRP:CE3   | 40:o:38:LYS:HG2  | 2.44                     | 0.52              |
| 1:A:676:A:H2'     | 1:A:677:U:H6     | 1.74                     | 0.52              |
| 2:B:60:ILE:HG21   | 2:B:160:ALA:HB2  | 1.91                     | 0.52              |
| 22:V:22:A:H61     | 22:V:47:A:H2'    | 1.75                     | 0.52              |
| 25:Y:159:LEU:HD23 | 25:Y:165:ASN:HB2 | 1.92                     | 0.52              |
| 26:a:871:U:H2'    | 26:a:872:U:C6    | 2.44                     | 0.52              |
| 30:e:97:ASN:HB2   | 30:e:100:MET:HG3 | 1.90                     | 0.52              |
| 32:g:38:ASN:ND2   | 32:g:64:GLN:OE1  | 2.43                     | 0.52              |
| 35:j:73:ASP:OD2   | 35:j:75:SER:OG   | 2.28                     | 0.52              |
| 38:m:54:LEU:HD23  | 38:m:66:ALA:HB2  | 1.92                     | 0.52              |
| 1:A:1095:U:H2'    | 1:A:1096:C:C6    | 2.44                     | 0.52              |
| 1:A:1111:A:N1     | 3:C:177:THR:OG1  | 2.42                     | 0.52              |
| 3:C:16:LYS:NZ     | 3:C:181:ASP:OD1  | 2.34                     | 0.52              |
| 4:D:138:SER:N     | 4:D:141:ASP:OD2  | 2.42                     | 0.52              |
| 4:D:186:PRO:HB2   | 4:D:191:LEU:HD21 | 1.91                     | 0.52              |
| 26:a:1437:C:H2'   | 26:a:1438:U:C6   | 2.45                     | 0.52              |
| 26:a:2845:U:H5''  | 40:o:52:ASN:O    | 2.09                     | 0.52              |
| 36:k:91:ASP:OD1   | 36:k:92:LEU:N    | 2.42                     | 0.52              |
| 40:o:31:TRP:CD1   | 40:o:82:ASP:HB2  | 2.44                     | 0.52              |
| 2:B:50:PHE:HA     | 2:B:200:ILE:HD12 | 1.92                     | 0.52              |
| 3:C:54:ARG:HB3    | 3:C:69:HIS:HB2   | 1.90                     | 0.52              |
| 26:a:335:C:OP2    | 45:t:82:ARG:NH1  | 2.43                     | 0.52              |
| 26:a:910:A:C5     | 37:l:13:HIS:CD2  | 2.97                     | 0.52              |
| 26:a:1028:A:N6    | 26:a:1125:G:H2'  | 2.25                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:1263:U:O2'  | 51:z:8:PRO:HD2    | 2.10                     | 0.52              |
| 26:a:1900:A:H1'  | 26:a:1970:A:H2'   | 1.91                     | 0.52              |
| 26:a:2184:A:H8   | 26:a:2185:U:H5    | 1.58                     | 0.52              |
| 32:g:104:ASN:ND2 | 32:g:114:ASP:OD1  | 2.43                     | 0.52              |
| 34:i:12:LYS:O    | 34:i:41:LYS:NZ    | 2.43                     | 0.52              |
| 37:l:75:GLU:OE1  | 37:l:146:TYR:HE1  | 1.93                     | 0.52              |
| 45:t:18:ASP:HB3  | 45:t:21:LYS:HD2   | 1.91                     | 0.52              |
| 1:A:600:A:H2'    | 1:A:601:G:C8      | 2.44                     | 0.51              |
| 2:B:60:ILE:HD13  | 2:B:160:ALA:HB2   | 1.91                     | 0.51              |
| 7:G:50:LEU:HA    | 7:G:53:ARG:HG2    | 1.92                     | 0.51              |
| 19:S:55:ARG:HG3  | 19:S:56:GLN:HG2   | 1.92                     | 0.51              |
| 26:a:588:U:H2'   | 26:a:589:U:C6     | 2.45                     | 0.51              |
| 26:a:1058:U:H2'  | 26:a:1059:G:C8    | 2.45                     | 0.51              |
| 26:a:1274:A:N1   | 26:a:1644:C:O2'   | 2.36                     | 0.51              |
| 26:a:2086:U:H2'  | 26:a:2087:G:C8    | 2.45                     | 0.51              |
| 35:j:107:LEU:O   | 35:j:109:SER:N    | 2.42                     | 0.51              |
| 1:A:938:A:N3     | 1:A:1376:U:O2'    | 2.39                     | 0.51              |
| 4:D:174:ASP:OD1  | 4:D:175:ALA:N     | 2.44                     | 0.51              |
| 22:V:44:A:H2'    | 22:V:45:A:C8      | 2.45                     | 0.51              |
| 26:a:483:A:C8    | 45:t:45:HIS:HD2   | 2.28                     | 0.51              |
| 26:a:490:C:O2'   | 26:a:491:G:OP1    | 2.27                     | 0.51              |
| 26:a:594:U:H2'   | 26:a:595:C:C6     | 2.46                     | 0.51              |
| 26:a:2345:G:N3   | 26:a:2381:A:H2'   | 2.25                     | 0.51              |
| 26:a:2861:U:H2'  | 26:a:2862:G:H8    | 1.76                     | 0.51              |
| 33:h:121:VAL:O   | 33:h:121:VAL:HG12 | 2.10                     | 0.51              |
| 33:h:127:GLU:OE2 | 33:h:145:ASN:HA   | 2.10                     | 0.51              |
| 33:h:136:SER:C   | 33:h:137:GLU:CG   | 2.77                     | 0.51              |
| 45:t:41:LEU:HA   | 45:t:62:GLU:HA    | 1.92                     | 0.51              |
| 1:A:253:A:H2'    | 1:A:254:G:H8      | 1.75                     | 0.51              |
| 1:A:784:A:H2'    | 1:A:785:G:C8      | 2.45                     | 0.51              |
| 1:A:1009:U:H3    | 1:A:1020:A:H61    | 1.57                     | 0.51              |
| 26:a:493:G:H2'   | 26:a:494:G:O4'    | 2.10                     | 0.51              |
| 26:a:1548:A:H2'  | 26:a:1549:A:C8    | 2.45                     | 0.51              |
| 26:a:2133:G:C5   | 26:a:2157:G:H1'   | 2.45                     | 0.51              |
| 26:a:2299:U:OP1  | 31:f:72:LYS:NZ    | 2.38                     | 0.51              |
| 26:a:2834:G:H2'  | 26:a:2879:A:H61   | 1.75                     | 0.51              |
| 26:a:2898:U:H2'  | 26:a:2899:A:H8    | 1.74                     | 0.51              |
| 42:q:6:GLN:HB3   | 42:q:37:GLU:HG3   | 1.92                     | 0.51              |
| 12:L:50:ARG:NH2  | 12:L:89:D2T:OD2   | 2.38                     | 0.51              |
| 26:a:243:U:OP1   | 54:2:8:ARG:NH1    | 2.44                     | 0.51              |
| 26:a:1058:U:N3   | 26:a:1059:G:O6    | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:a:1089:A:H2   | 26:a:1090:A:H62  | 1.53                     | 0.51              |
| 26:a:1791:A:N6   | 26:a:1828:G:O2'  | 2.41                     | 0.51              |
| 26:a:2014:A:H2'  | 26:a:2015:A:C8   | 2.46                     | 0.51              |
| 26:a:2147:A:H2'  | 26:a:2148:G:O4'  | 2.10                     | 0.51              |
| 35:j:41:ILE:HD11 | 35:j:86:LEU:HD22 | 1.92                     | 0.51              |
| 43:r:86:MET:HE2  | 43:r:96:ILE:HD11 | 1.93                     | 0.51              |
| 26:a:1682:G:H2'  | 26:a:1683:U:C6   | 2.45                     | 0.51              |
| 26:a:2152:G:OP2  | 26:a:2153:C:N4   | 2.42                     | 0.51              |
| 26:a:2162:G:H2'  | 26:a:2163:A:C8   | 2.46                     | 0.51              |
| 1:A:561:U:O2'    | 1:A:562:U:OP1    | 2.25                     | 0.51              |
| 1:A:996:A:H2'    | 1:A:997:U:H6     | 1.76                     | 0.51              |
| 1:A:1375:A:H2'   | 1:A:1376:U:O4'   | 2.11                     | 0.51              |
| 1:A:1535:C:C4    | 24:X:6:G:N2      | 2.69                     | 0.51              |
| 14:N:34:VAL:O    | 14:N:41:ARG:NH2  | 2.44                     | 0.51              |
| 18:R:47:THR:O    | 18:R:48:ARG:C    | 2.54                     | 0.51              |
| 25:Y:52:GLN:NE2  | 25:Y:86:ARG:O    | 2.43                     | 0.51              |
| 26:a:361:G:O2'   | 26:a:362:A:O5'   | 2.24                     | 0.51              |
| 26:a:1447:C:O2'  | 26:a:1544:A:N3   | 2.36                     | 0.51              |
| 26:a:1585:C:H2'  | 26:a:1586:A:O4'  | 2.11                     | 0.51              |
| 26:a:1964:G:O2'  | 26:a:1967:C:OP2  | 2.28                     | 0.51              |
| 31:f:38:MET:HE3  | 31:f:57:LEU:HB2  | 1.93                     | 0.51              |
| 51:z:33:THR:HG22 | 51:z:51:GLY:HA2  | 1.93                     | 0.51              |
| 1:A:149:A:H1'    | 1:A:1446:A:H2    | 1.76                     | 0.51              |
| 1:A:1006:C:H42   | 1:A:1023:G:H1    | 1.59                     | 0.51              |
| 1:A:1320:C:H2'   | 1:A:1321:U:C6    | 2.46                     | 0.51              |
| 14:N:31:ILE:HD12 | 14:N:45:VAL:HG23 | 1.93                     | 0.51              |
| 26:a:1064:C:H2'  | 26:a:1065:U:C6   | 2.46                     | 0.51              |
| 26:a:2626:C:H2'  | 26:a:2627:G:C8   | 2.46                     | 0.51              |
| 1:A:8:A:N6       | 4:D:206:LYS:HB2  | 2.26                     | 0.51              |
| 1:A:335:C:O2'    | 1:A:1433:A:N3    | 2.40                     | 0.51              |
| 1:A:457:G:H2'    | 1:A:458:U:H6     | 1.76                     | 0.51              |
| 26:a:146:A:H2'   | 26:a:147:C:C6    | 2.46                     | 0.51              |
| 26:a:154:U:H2'   | 26:a:155:A:C8    | 2.45                     | 0.51              |
| 26:a:636:G:OP2   | 36:k:109:LYS:NZ  | 2.33                     | 0.51              |
| 26:a:644:A:H2'   | 26:a:645:C:O4'   | 2.11                     | 0.51              |
| 26:a:1534:U:H1'  | 26:a:1537:G:H1   | 1.76                     | 0.51              |
| 26:a:2159:G:O2'  | 26:a:2160:C:O4'  | 2.26                     | 0.51              |
| 26:a:2554:U:H2'  | 26:a:2555:U:C6   | 2.46                     | 0.51              |
| 26:a:2898:U:H2'  | 26:a:2899:A:C8   | 2.46                     | 0.51              |
| 38:m:73:ASN:HA   | 38:m:76:VAL:HG12 | 1.93                     | 0.51              |
| 43:r:23:LEU:HD22 | 51:z:24:ALA:HB2  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:12:ALA:HB2  | 10:J:18:ILE:HD13 | 1.93                     | 0.51              |
| 26:a:2312:U:H5'  | 31:f:85:ILE:HD11 | 1.92                     | 0.51              |
| 26:a:2355:G:OP1  | 47:v:25:ARG:NH2  | 2.43                     | 0.51              |
| 26:a:2866:U:H4'  | 26:a:2867:G:H4'  | 1.93                     | 0.51              |
| 28:c:5:LYS:HD2   | 28:c:17:VAL:HG22 | 1.93                     | 0.51              |
| 29:d:56:LYS:HB2  | 29:d:59:ARG:HB2  | 1.93                     | 0.51              |
| 32:g:154:PRO:HA  | 32:g:160:LYS:O   | 2.11                     | 0.51              |
| 50:y:16:ARG:HG3  | 50:y:54:MET:HE1  | 1.92                     | 0.51              |
| 1:A:381:C:H2'    | 1:A:382:A:O4'    | 2.11                     | 0.51              |
| 1:A:514:C:H2'    | 1:A:515:G:C8     | 2.44                     | 0.51              |
| 1:A:1238:A:OP1   | 1:A:1335:U:O2'   | 2.22                     | 0.51              |
| 4:D:95:GLU:OE1   | 4:D:100:ASN:ND2  | 2.44                     | 0.51              |
| 23:W:25:U:H2'    | 23:W:26:C:C6     | 2.46                     | 0.51              |
| 26:a:139:U:H2'   | 26:a:140:C:H5    | 1.76                     | 0.51              |
| 26:a:586:A:N1    | 26:a:809:G:O2'   | 2.38                     | 0.51              |
| 26:a:2687:U:H2'  | 26:a:2688:G:O4'  | 2.10                     | 0.51              |
| 32:g:9:VAL:HG22  | 32:g:50:LEU:HB2  | 1.92                     | 0.51              |
| 33:h:5:LEU:HD11  | 33:h:12:LEU:HD12 | 1.93                     | 0.51              |
| 33:h:50:ARG:NH1  | 33:h:51:ARG:HG2  | 2.26                     | 0.51              |
| 45:t:35:ILE:HD12 | 45:t:62:GLU:OE2  | 2.11                     | 0.51              |
| 1:A:590:U:H2'    | 1:A:591:U:C6     | 2.46                     | 0.50              |
| 1:A:867:G:O2'    | 1:A:873:A:N1     | 2.33                     | 0.50              |
| 1:A:1092:A:H5''  | 7:G:4:ARG:HH22   | 1.76                     | 0.50              |
| 1:A:1354:U:H2'   | 1:A:1355:G:H8    | 1.76                     | 0.50              |
| 5:E:57:PRO:O     | 5:E:61:GLN:HG2   | 2.12                     | 0.50              |
| 9:I:112:GLU:OE1  | 9:I:115:LYS:NZ   | 2.30                     | 0.50              |
| 10:J:7:ARG:HD2   | 10:J:73:LEU:HD11 | 1.93                     | 0.50              |
| 26:a:868:U:O2    | 37:l:8:LYS:NZ    | 2.43                     | 0.50              |
| 26:a:1223:G:C6   | 26:a:1227:G:C6   | 2.99                     | 0.50              |
| 26:a:1614:A:C6   | 43:r:87:PRO:HB3  | 2.46                     | 0.50              |
| 27:b:5:U:OP1     | 27:b:61:G:O2'    | 2.25                     | 0.50              |
| 33:h:98:ASP:O    | 33:h:102:ALA:N   | 2.43                     | 0.50              |
| 38:m:22:ARG:HG3  | 38:m:70:THR:HA   | 1.93                     | 0.50              |
| 13:M:72:GLU:HA   | 13:M:75:MET:HE2  | 1.93                     | 0.50              |
| 26:a:2064:C:H2'  | 26:a:2065:C:C6   | 2.46                     | 0.50              |
| 26:a:2391:G:O2'  | 26:a:2429:G:N2   | 2.45                     | 0.50              |
| 26:a:2756:U:H4'  | 26:a:2757:A:H5'  | 1.93                     | 0.50              |
| 42:q:55:ASP:OD1  | 42:q:55:ASP:N    | 2.44                     | 0.50              |
| 1:A:41:G:H2'     | 1:A:42:G:C8      | 2.44                     | 0.50              |
| 1:A:310:G:H5''   | 16:P:31:ARG:HB2  | 1.94                     | 0.50              |
| 1:A:555:U:H2'    | 1:A:556:C:C6     | 2.46                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1004:A:C5    | 1:A:1026:G:H1'    | 2.46                     | 0.50              |
| 9:I:79:ILE:O     | 9:I:83:ILE:HD12   | 2.11                     | 0.50              |
| 26:a:155:A:H2'   | 26:a:156:A:C8     | 2.45                     | 0.50              |
| 26:a:404:A:H1'   | 26:a:406:G:C4     | 2.46                     | 0.50              |
| 26:a:575:A:OP2   | 26:a:2055:C:N4    | 2.44                     | 0.50              |
| 26:a:873:C:O2'   | 37:l:64:TRP:NE1   | 2.44                     | 0.50              |
| 26:a:1007:C:OP1  | 34:i:37:ARG:NH2   | 2.43                     | 0.50              |
| 26:a:2857:G:N2   | 26:a:2860:A:OP2   | 2.34                     | 0.50              |
| 46:u:26:PHE:HE2  | 46:u:89:ILE:HG12  | 1.76                     | 0.50              |
| 1:A:521:G:OP2    | 12:L:51:LYS:NZ    | 2.41                     | 0.50              |
| 1:A:1539:C:C4'   | 1:A:1540:U:OP1    | 2.60                     | 0.50              |
| 26:a:483:A:H5''  | 45:t:47:LYS:HD2   | 1.93                     | 0.50              |
| 26:a:704:G:H2'   | 26:a:726:G:H22    | 1.76                     | 0.50              |
| 26:a:882:G:O2'   | 26:a:883:G:O5'    | 2.27                     | 0.50              |
| 26:a:2319:G:HO2' | 26:a:2320:U:H6    | 1.59                     | 0.50              |
| 26:a:2419:U:OP1  | 54:2:41:LYS:NZ    | 2.36                     | 0.50              |
| 26:a:2467:C:H2'  | 26:a:2468:A:O4'   | 2.10                     | 0.50              |
| 29:d:1:MET:HG2   | 29:d:205:PRO:HG2  | 1.94                     | 0.50              |
| 33:h:1:MET:N     | 33:h:21:VAL:O     | 2.45                     | 0.50              |
| 38:m:57:THR:O    | 38:m:62:ASN:ND2   | 2.37                     | 0.50              |
| 1:A:74:A:N6      | 1:A:75:G:N7       | 2.60                     | 0.50              |
| 1:A:1000:A:H2'   | 1:A:1001:C:H6     | 1.77                     | 0.50              |
| 1:A:1042:A:H2'   | 1:A:1043:G:O4'    | 2.11                     | 0.50              |
| 1:A:1432:G:H1'   | 1:A:1468:A:H62    | 1.77                     | 0.50              |
| 26:a:296:U:H2'   | 26:a:297:G:C8     | 2.47                     | 0.50              |
| 26:a:581:C:H2'   | 26:a:582:A:C8     | 2.46                     | 0.50              |
| 26:a:671:C:H2'   | 26:a:672:C:C6     | 2.47                     | 0.50              |
| 26:a:1171:G:N2   | 26:a:1179:G:OP2   | 2.44                     | 0.50              |
| 26:a:1198:U:H2'  | 26:a:1199:U:C6    | 2.46                     | 0.50              |
| 26:a:2591:C:H2'  | 26:a:2592:G:C8    | 2.46                     | 0.50              |
| 34:i:140:LEU:HG  | 34:i:142:ILE:HG13 | 1.92                     | 0.50              |
| 42:q:34:GLU:OE1  | 42:q:60:LYS:HG2   | 2.10                     | 0.50              |
| 1:A:254:G:O2'    | 17:Q:18:GLU:O     | 2.30                     | 0.50              |
| 1:A:1112:C:O2    | 3:C:178:LEU:HB2   | 2.11                     | 0.50              |
| 2:B:46:THR:O     | 2:B:50:PHE:N      | 2.26                     | 0.50              |
| 4:D:54:GLN:HB3   | 4:D:203:LEU:HB2   | 1.94                     | 0.50              |
| 23:W:37:U:H2'    | 23:W:38:A:C8      | 2.47                     | 0.50              |
| 26:a:1039:A:H2   | 26:a:1116:G:H22   | 1.59                     | 0.50              |
| 26:a:1484:U:H2'  | 26:a:1485:U:C6    | 2.46                     | 0.50              |
| 26:a:1594:U:H2'  | 26:a:1595:C:C6    | 2.47                     | 0.50              |
| 1:A:384:G:H2'    | 1:A:385:C:C6      | 2.46                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:841:C:O2'    | 1:A:843:U:O5'     | 2.29                     | 0.50              |
| 1:A:1323:G:H2'   | 1:A:1324:A:H8     | 1.73                     | 0.50              |
| 1:A:1438:G:OP1   | 20:T:33:LYS:NZ    | 2.33                     | 0.50              |
| 24:X:4:A:H5''    | 24:X:6:G:O2'      | 2.12                     | 0.50              |
| 25:Y:140:PRO:HD3 | 25:Y:173:VAL:HG21 | 1.94                     | 0.50              |
| 26:a:1:G:H2'     | 26:a:2:G:C8       | 2.46                     | 0.50              |
| 26:a:196:A:C2    | 36:k:50:PHE:HZ    | 2.30                     | 0.50              |
| 26:a:1412:U:H2'  | 26:a:1413:A:C8    | 2.46                     | 0.50              |
| 26:a:2285:C:OP2  | 52:0:6:ARG:NH1    | 2.39                     | 0.50              |
| 26:a:2491:U:H4'  | 26:a:2492:U:OP1   | 2.12                     | 0.50              |
| 26:a:2865:U:OP2  | 26:a:2866:U:O2'   | 2.16                     | 0.50              |
| 1:A:9:G:OP2      | 5:E:126:LYS:NZ    | 2.35                     | 0.50              |
| 1:A:1190:G:H4'   | 1:A:1191:A:OP2    | 2.12                     | 0.50              |
| 8:H:39:VAL:HG11  | 8:H:103:VAL:HG22  | 1.93                     | 0.50              |
| 26:a:1418:G:N2   | 26:a:1579:A:C8    | 2.80                     | 0.50              |
| 26:a:2146:C:H4'  | 26:a:2147:A:C4    | 2.46                     | 0.50              |
| 28:c:132:MET:O   | 28:c:167:ARG:NH1  | 2.40                     | 0.50              |
| 37:l:13:HIS:O    | 37:l:71:LYS:NZ    | 2.42                     | 0.50              |
| 1:A:592:G:H2'    | 1:A:593:U:C6      | 2.47                     | 0.50              |
| 1:A:1074:G:O2'   | 1:A:1101:A:N1     | 2.44                     | 0.50              |
| 1:A:1169:A:H2'   | 1:A:1170:A:C8     | 2.47                     | 0.50              |
| 2:B:35:ARG:NH1   | 25:Y:15:GLU:HG3   | 2.26                     | 0.50              |
| 17:Q:60:GLU:OE1  | 17:Q:76:VAL:HB    | 2.11                     | 0.50              |
| 26:a:499:U:H5''  | 45:t:43:LYS:HD2   | 1.94                     | 0.50              |
| 26:a:2246:G:H2'  | 26:a:2247:A:C8    | 2.46                     | 0.50              |
| 31:f:30:ARG:O    | 31:f:158:THR:HG23 | 2.12                     | 0.50              |
| 34:i:34:ARG:HG3  | 34:i:39:LYS:HB2   | 1.94                     | 0.50              |
| 1:A:834:U:H2'    | 1:A:835:U:C6      | 2.47                     | 0.49              |
| 1:A:1225:A:H2'   | 1:A:1225:A:N3     | 2.27                     | 0.49              |
| 26:a:1102:C:H5   | 26:a:1103:A:N7    | 2.10                     | 0.49              |
| 26:a:1113:U:H2'  | 26:a:1114:C:C6    | 2.46                     | 0.49              |
| 26:a:2107:G:H1   | 26:a:2182:U:H3    | 1.60                     | 0.49              |
| 26:a:2327:A:H2'  | 26:a:2328:A:C8    | 2.47                     | 0.49              |
| 26:a:2625:G:H2'  | 26:a:2626:C:C6    | 2.47                     | 0.49              |
| 1:A:455:G:H2'    | 1:A:456:A:H8      | 1.77                     | 0.49              |
| 19:S:67:VAL:O    | 56:4:56:ARG:NH2   | 2.37                     | 0.49              |
| 26:a:1083:U:H1'  | 26:a:1086:A:H61   | 1.75                     | 0.49              |
| 26:a:1720:U:H2'  | 26:a:1721:G:O4'   | 2.11                     | 0.49              |
| 26:a:2655:G:H4'  | 26:a:2656:U:O5'   | 2.11                     | 0.49              |
| 28:c:155:ALA:HB2 | 28:c:162:VAL:HG23 | 1.94                     | 0.49              |
| 32:g:28:GLY:HA3  | 32:g:79:VAL:HB    | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:296:U:O2'    | 1:A:556:C:O2     | 2.29                     | 0.49              |
| 1:A:1191:A:OP2   | 1:A:1191:A:H8    | 1.94                     | 0.49              |
| 1:A:1515:G:H2'   | 1:A:1516:2MG:C8  | 2.47                     | 0.49              |
| 26:a:1709:U:H2'  | 26:a:1710:G:H8   | 1.77                     | 0.49              |
| 26:a:1853:A:H2'  | 26:a:1854:A:C8   | 2.47                     | 0.49              |
| 26:a:2686:G:H2'  | 26:a:2687:U:C6   | 2.48                     | 0.49              |
| 26:a:2705:A:O2'  | 26:a:2852:G:OP1  | 2.29                     | 0.49              |
| 31:f:128:TYR:CE1 | 31:f:130:MET:HB3 | 2.46                     | 0.49              |
| 44:s:22:THR:HG22 | 44:s:26:LYS:HE3  | 1.93                     | 0.49              |
| 1:A:414:A:H2'    | 1:A:415:A:H8     | 1.76                     | 0.49              |
| 1:A:652:U:O4     | 1:A:752:G:O2'    | 2.22                     | 0.49              |
| 1:A:918:A:H2'    | 1:A:919:A:C8     | 2.47                     | 0.49              |
| 18:R:70:TYR:HB2  | 18:R:74:HIS:NE2  | 2.28                     | 0.49              |
| 26:a:456:C:H5''  | 26:a:457:A:OP1   | 2.13                     | 0.49              |
| 26:a:1053:C:H42  | 26:a:1054:A:N6   | 2.11                     | 0.49              |
| 26:a:1429:G:H2'  | 26:a:1430:G:C8   | 2.45                     | 0.49              |
| 26:a:1721:G:H22  | 26:a:1738:G:H2'  | 1.76                     | 0.49              |
| 26:a:1952:A:OP1  | 35:j:44:LYS:NZ   | 2.32                     | 0.49              |
| 33:h:116:ARG:O   | 33:h:131:SER:OG  | 2.31                     | 0.49              |
| 51:z:38:HIS:ND1  | 51:z:42:HIS:O    | 2.41                     | 0.49              |
| 1:A:35:G:H2'     | 1:A:36:C:H6      | 1.77                     | 0.49              |
| 1:A:1363:A:O2'   | 1:A:1365:G:N7    | 2.34                     | 0.49              |
| 25:Y:66:ASP:OD1  | 25:Y:67:GLU:N    | 2.45                     | 0.49              |
| 26:a:2300:C:H2'  | 26:a:2301:C:H6   | 1.77                     | 0.49              |
| 1:A:335:C:H2'    | 1:A:336:A:C8     | 2.47                     | 0.49              |
| 1:A:440:C:C2     | 1:A:441:A:C8     | 3.00                     | 0.49              |
| 1:A:490:C:H2'    | 1:A:491:G:H8     | 1.77                     | 0.49              |
| 1:A:993:G:O2'    | 1:A:994:A:N7     | 2.44                     | 0.49              |
| 1:A:1536:C:H2'   | 1:A:1537:U:H6    | 1.76                     | 0.49              |
| 14:N:49:GLN:NE2  | 19:S:11:ILE:O    | 2.34                     | 0.49              |
| 26:a:24:G:H2'    | 26:a:25:U:H6     | 1.78                     | 0.49              |
| 26:a:832:U:H2'   | 26:a:833:A:H8    | 1.77                     | 0.49              |
| 26:a:1080:A:H1'  | 26:a:1081:U:H3   | 1.77                     | 0.49              |
| 26:a:1432:G:H2'  | 26:a:1433:A:C8   | 2.47                     | 0.49              |
| 26:a:1715:G:O2'  | 26:a:1716:U:O5'  | 2.30                     | 0.49              |
| 26:a:1747:U:H2'  | 26:a:1748:C:C6   | 2.47                     | 0.49              |
| 43:r:59:GLU:OE2  | 43:r:66:ILE:HB   | 2.12                     | 0.49              |
| 46:u:2:PHE:HB3   | 46:u:50:MET:HE2  | 1.93                     | 0.49              |
| 48:w:33:LEU:HD23 | 48:w:52:SER:HB3  | 1.94                     | 0.49              |
| 49:x:13:GLU:OE2  | 49:x:13:GLU:N    | 2.36                     | 0.49              |
| 1:A:324:G:N1     | 1:A:327:A:OP2    | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1224:U:O2'    | 1:A:1322:C:OP1    | 2.24                     | 0.49              |
| 9:I:6:TYR:HB3     | 9:I:89:GLU:OE2    | 2.11                     | 0.49              |
| 14:N:48:LEU:HD12  | 14:N:51:LEU:HD12  | 1.95                     | 0.49              |
| 24:X:2:G:H2'      | 24:X:3:G:O4'      | 2.13                     | 0.49              |
| 25:Y:135:LEU:HD13 | 25:Y:139:ARG:NH2  | 2.28                     | 0.49              |
| 26:a:458:G:O2'    | 26:a:459:U:P      | 2.71                     | 0.49              |
| 26:a:1036:G:C6    | 26:a:1120:G:C6    | 3.01                     | 0.49              |
| 26:a:1264:A:OP1   | 51:z:16:ARG:NH1   | 2.36                     | 0.49              |
| 26:a:2105:U:O2'   | 26:a:2107:G:N7    | 2.30                     | 0.49              |
| 26:a:2250:G:O2'   | 26:a:2496:C:OP1   | 2.26                     | 0.49              |
| 27:b:103:U:O2'    | 46:u:31:TYR:OH    | 2.30                     | 0.49              |
| 28:c:107:PRO:HD2  | 28:c:110:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:1241:G:H2'    | 1:A:1242:G:H8     | 1.77                     | 0.49              |
| 7:G:15:ASP:OD2    | 7:G:23:LEU:HD23   | 2.12                     | 0.49              |
| 9:I:33:ARG:HB3    | 9:I:37:GLN:HE22   | 1.77                     | 0.49              |
| 11:K:16:VAL:O     | 11:K:18:ASP:N     | 2.44                     | 0.49              |
| 22:V:65:G:OP1     | 47:v:11:ARG:NH1   | 2.45                     | 0.49              |
| 26:a:250:G:OP2    | 54:2:13:ARG:NH2   | 2.41                     | 0.49              |
| 26:a:849:A:H2'    | 26:a:850:U:C6     | 2.48                     | 0.49              |
| 28:c:84:ASP:OD2   | 28:c:87:ARG:NE    | 2.23                     | 0.49              |
| 44:s:71:GLY:O     | 44:s:72:GLN:HG2   | 2.13                     | 0.49              |
| 49:x:18:LEU:HB2   | 49:x:53:VAL:HG11  | 1.94                     | 0.49              |
| 1:A:1118:U:H4'    | 9:I:85:ARG:HH22   | 1.77                     | 0.49              |
| 1:A:1306:A:N6     | 1:A:1331:G:O2'    | 2.46                     | 0.49              |
| 9:I:56:ASP:O      | 9:I:57:MET:HE2    | 2.11                     | 0.49              |
| 25:Y:24:VAL:HG12  | 25:Y:25:ARG:N     | 2.27                     | 0.49              |
| 26:a:207:A:H2'    | 26:a:208:C:O4'    | 2.13                     | 0.49              |
| 26:a:687:C:H5''   | 53:1:2:LYS:HE3    | 1.94                     | 0.49              |
| 26:a:1283:G:H22   | 26:a:1286:A:H5'   | 1.78                     | 0.49              |
| 26:a:1475:G:O2'   | 26:a:1476:U:H6    | 1.96                     | 0.49              |
| 26:a:2774:C:H2'   | 26:a:2775:G:O4'   | 2.13                     | 0.49              |
| 36:k:77:ILE:CD1   | 36:k:108:ALA:HB1  | 2.43                     | 0.49              |
| 37:l:20:LEU:HD13  | 46:u:81:PRO:HG2   | 1.95                     | 0.49              |
| 46:u:2:PHE:HB2    | 46:u:61:LEU:HD13  | 1.94                     | 0.49              |
| 1:A:560:A:H5''    | 1:A:561:U:H3'     | 1.95                     | 0.49              |
| 1:A:1270:G:H2'    | 1:A:1271:A:H8     | 1.78                     | 0.49              |
| 1:A:1356:G:H2'    | 1:A:1357:A:H8     | 1.75                     | 0.49              |
| 4:D:95:GLU:OE2    | 4:D:104:ARG:HG3   | 2.13                     | 0.49              |
| 4:D:99:ASP:OD1    | 4:D:100:ASN:N     | 2.46                     | 0.49              |
| 7:G:149:LYS:HE3   | 11:K:61:PHE:CZ    | 2.48                     | 0.49              |
| 26:a:414:C:H2'    | 26:a:415:A:C8     | 2.48                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:1076:C:H4'  | 26:a:1077:A:OP1   | 2.12                     | 0.49              |
| 46:u:2:PHE:HB2   | 46:u:61:LEU:CD1   | 2.43                     | 0.49              |
| 1:A:203:G:O2'    | 1:A:465:A:N6      | 2.46                     | 0.48              |
| 1:A:1147:C:O3'   | 9:I:7:TYR:OH      | 2.30                     | 0.48              |
| 1:A:1290:G:OP1   | 7:G:35:LYS:NZ     | 2.43                     | 0.48              |
| 3:C:11:ARG:NH2   | 3:C:177:THR:O     | 2.40                     | 0.48              |
| 6:F:29:ILE:HD13  | 6:F:64:VAL:HG11   | 1.95                     | 0.48              |
| 25:Y:93:GLU:OE1  | 25:Y:125:ASN:N    | 2.46                     | 0.48              |
| 27:b:94:A:OP1    | 46:u:19:ARG:NH1   | 2.45                     | 0.48              |
| 32:g:15:VAL:HG12 | 32:g:28:GLY:HA2   | 1.95                     | 0.48              |
| 56:4:56:ARG:HH11 | 56:4:59:ARG:HH22  | 1.60                     | 0.48              |
| 13:M:37:ALA:HB2  | 13:M:59:GLU:HG3   | 1.94                     | 0.48              |
| 21:U:63:GLU:C    | 21:U:65:ALA:N     | 2.67                     | 0.48              |
| 26:a:857:G:H2'   | 26:a:858:G:O4'    | 2.13                     | 0.48              |
| 26:a:2292:U:H2'  | 26:a:2293:G:H8    | 1.77                     | 0.48              |
| 27:b:31:C:H1'    | 27:b:53:A:H61     | 1.78                     | 0.48              |
| 34:i:9:GLU:HG2   | 34:i:10:THR:HG23  | 1.94                     | 0.48              |
| 1:A:500:G:H2'    | 1:A:501:C:H6      | 1.78                     | 0.48              |
| 1:A:561:U:HO2'   | 1:A:562:U:P       | 2.35                     | 0.48              |
| 1:A:695:A:H2'    | 1:A:696:A:C8      | 2.47                     | 0.48              |
| 1:A:838:G:H2'    | 1:A:839:C:C6      | 2.48                     | 0.48              |
| 1:A:1077:G:N2    | 1:A:1080:A:OP2    | 2.43                     | 0.48              |
| 1:A:1126:U:N3    | 1:A:1280:A:OP1    | 2.43                     | 0.48              |
| 1:A:1178:G:N7    | 9:I:99:ARG:NH2    | 2.62                     | 0.48              |
| 1:A:1347:G:O2'   | 1:A:1348:U:P      | 2.71                     | 0.48              |
| 1:A:1534:A:C2'   | 1:A:1535:C:H5''   | 2.43                     | 0.48              |
| 19:S:42:PRO:HD3  | 56:4:60:PHE:CE1   | 2.49                     | 0.48              |
| 26:a:280:U:H2'   | 26:a:281:C:C6     | 2.49                     | 0.48              |
| 26:a:1442:U:H2'  | 26:a:1443:U:C6    | 2.48                     | 0.48              |
| 26:a:2155:U:H2'  | 26:a:2156:G:H5'   | 1.95                     | 0.48              |
| 26:a:2579:C:O2'  | 29:d:136:ASN:OD1  | 2.30                     | 0.48              |
| 32:g:91:GLY:HA2  | 32:g:160:LYS:HG2  | 1.95                     | 0.48              |
| 33:h:96:THR:HG22 | 33:h:117:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:575:G:O2'    | 1:A:821:G:H5'     | 2.14                     | 0.48              |
| 1:A:890:G:H2'    | 1:A:906:A:H61     | 1.79                     | 0.48              |
| 1:A:1486:G:H2'   | 1:A:1487:G:O4'    | 2.13                     | 0.48              |
| 1:A:1539:C:N4    | 24:X:2:G:H1       | 2.11                     | 0.48              |
| 6:F:40:GLU:OE1   | 6:F:42:TRP:HD1    | 1.97                     | 0.48              |
| 18:R:13:PHE:O    | 18:R:14:THR:C     | 2.56                     | 0.48              |
| 26:a:2300:C:H2'  | 26:a:2301:C:C6    | 2.48                     | 0.48              |
| 1:A:676:A:H2'    | 1:A:677:U:C6      | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:990:C:H2'     | 1:A:991:U:O4'     | 2.13                     | 0.48              |
| 2:B:10:LEU:HG     | 2:B:11:LYS:N      | 2.27                     | 0.48              |
| 2:B:23:TRP:CG     | 2:B:39:HIS:HE2    | 2.32                     | 0.48              |
| 4:D:57:GLU:HG2    | 4:D:199:LEU:HB2   | 1.95                     | 0.48              |
| 13:M:107:ARG:NH2  | 13:M:111:GLY:O    | 2.47                     | 0.48              |
| 23:W:35:C:H2'     | 23:W:36:A:C8      | 2.48                     | 0.48              |
| 26:a:302:C:H2'    | 26:a:303:G:H8     | 1.78                     | 0.48              |
| 26:a:1087:G:H22   | 26:a:1102:C:N4    | 2.11                     | 0.48              |
| 26:a:1115:G:H2'   | 26:a:1116:G:C8    | 2.38                     | 0.48              |
| 33:h:103:VAL:HB   | 33:h:110:VAL:HG11 | 1.96                     | 0.48              |
| 37:l:157:LEU:HD11 | 37:l:181:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:254:G:OP1     | 17:Q:68:SER:OG    | 2.30                     | 0.48              |
| 1:A:350:G:H2'     | 1:A:351:G:C8      | 2.49                     | 0.48              |
| 2:B:4:VAL:HG23    | 2:B:5:SER:H       | 1.78                     | 0.48              |
| 25:Y:25:ARG:CB    | 25:Y:67:GLU:OE2   | 2.62                     | 0.48              |
| 25:Y:72:LEU:HA    | 25:Y:82:THR:HB    | 1.95                     | 0.48              |
| 25:Y:113:ASN:HB3  | 25:Y:121:THR:HG23 | 1.94                     | 0.48              |
| 26:a:30:G:H2'     | 26:a:31:C:C6      | 2.49                     | 0.48              |
| 26:a:100:U:H4'    | 26:a:101:A:O4'    | 2.13                     | 0.48              |
| 26:a:1475:G:HO2'  | 26:a:1476:U:H6    | 1.62                     | 0.48              |
| 5:E:108:GLY:O     | 5:E:112:ARG:HB2   | 2.13                     | 0.48              |
| 8:H:105:SER:HB2   | 8:H:126:ILE:HD11  | 1.95                     | 0.48              |
| 14:N:27:LEU:O     | 14:N:31:ILE:HG12  | 2.13                     | 0.48              |
| 26:a:306:U:H2'    | 26:a:307:G:O4'    | 2.13                     | 0.48              |
| 26:a:358:U:H2'    | 26:a:359:G:C8     | 2.48                     | 0.48              |
| 26:a:878:A:H5'    | 26:a:879:G:N7     | 2.29                     | 0.48              |
| 26:a:1365:A:OP1   | 48:w:3:ARG:NH2    | 2.44                     | 0.48              |
| 26:a:1466:U:O3'   | 26:a:1546:G:O2'   | 2.31                     | 0.48              |
| 26:a:1545:A:H2'   | 26:a:1546:G:O4'   | 2.13                     | 0.48              |
| 26:a:2245:U:H5''  | 26:a:2246:G:H5'   | 1.95                     | 0.48              |
| 26:a:2329:U:H2'   | 26:a:2330:G:C8    | 2.49                     | 0.48              |
| 26:a:2591:C:N4    | 26:a:2592:G:O6    | 2.47                     | 0.48              |
| 28:c:145:GLU:HG2  | 28:c:151:GLY:C    | 2.39                     | 0.48              |
| 1:A:554:A:H2'     | 1:A:555:U:H6      | 1.78                     | 0.48              |
| 1:A:728:A:H2'     | 1:A:729:A:C8      | 2.49                     | 0.48              |
| 1:A:776:G:N2      | 1:A:802:A:OP2     | 2.47                     | 0.48              |
| 7:G:42:ILE:HD13   | 7:G:116:MET:HB3   | 1.95                     | 0.48              |
| 26:a:75:G:N3      | 26:a:75:G:H2'     | 2.29                     | 0.48              |
| 26:a:194:G:H2'    | 26:a:195:A:O4'    | 2.13                     | 0.48              |
| 26:a:549:G:H2'    | 26:a:550:C:C6     | 2.48                     | 0.48              |
| 26:a:1085:A:H3'   | 26:a:1086:A:C2    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:1638:C:O3'   | 26:a:2709:G:N2    | 2.46                     | 0.48              |
| 26:a:2803:G:H2'   | 26:a:2804:U:C6    | 2.49                     | 0.48              |
| 30:e:1:MET:HE1    | 30:e:19:PHE:O     | 2.13                     | 0.48              |
| 1:A:492:C:H2'     | 1:A:493:A:C8      | 2.49                     | 0.48              |
| 1:A:1063:C:OP2    | 1:A:1064:G:O2'    | 2.30                     | 0.48              |
| 1:A:1316:G:N2     | 1:A:1318:A:H3'    | 2.29                     | 0.48              |
| 1:A:1368:A:OP1    | 9:I:113:ARG:NH2   | 2.47                     | 0.48              |
| 11:K:31:ILE:HG12  | 11:K:46:THR:HG22  | 1.96                     | 0.48              |
| 16:P:6:LEU:HB3    | 16:P:17:TYR:HB3   | 1.94                     | 0.48              |
| 17:Q:58:VAL:HB    | 17:Q:80:GLU:HG3   | 1.95                     | 0.48              |
| 26:a:161:A:H3'    | 26:a:162:U:H5''   | 1.95                     | 0.48              |
| 26:a:1413:A:H2'   | 26:a:1414:C:O4'   | 2.13                     | 0.48              |
| 26:a:1856:U:H2'   | 26:a:1857:G:O4'   | 2.13                     | 0.48              |
| 26:a:2370:G:H4'   | 52:0:44:ARG:HH11  | 1.79                     | 0.48              |
| 29:d:14:ILE:HD12  | 29:d:178:VAL:HG11 | 1.95                     | 0.48              |
| 29:d:55:LYS:HD3   | 29:d:60:VAL:HG22  | 1.96                     | 0.48              |
| 31:f:37:ASN:HB3   | 31:f:153:ASP:OD1  | 2.14                     | 0.48              |
| 39:n:77:ALA:O     | 39:n:80:GLU:HG2   | 2.14                     | 0.48              |
| 46:u:48:MET:O     | 46:u:51:GLN:HG3   | 2.13                     | 0.48              |
| 1:A:32:A:H2'      | 1:A:33:A:H8       | 1.79                     | 0.48              |
| 1:A:721:G:H4'     | 1:A:722:G:O4'     | 2.14                     | 0.48              |
| 2:B:59:LYS:HE2    | 2:B:59:LYS:HA     | 1.96                     | 0.48              |
| 4:D:72:PHE:HE1    | 4:D:94:LEU:HD11   | 1.79                     | 0.48              |
| 9:I:54:LEU:HD13   | 9:I:103:PHE:CE2   | 2.49                     | 0.48              |
| 21:U:67:ARG:HD3   | 21:U:67:ARG:HA    | 1.54                     | 0.48              |
| 23:W:35:C:H2'     | 23:W:36:A:H8      | 1.78                     | 0.48              |
| 26:a:64:A:H2'     | 26:a:65:U:C6      | 2.49                     | 0.48              |
| 26:a:359:G:H2'    | 26:a:360:U:O4'    | 2.13                     | 0.48              |
| 26:a:2808:G:O2'   | 26:a:2809:A:H8    | 1.97                     | 0.48              |
| 33:h:40:THR:O     | 33:h:44:ILE:N     | 2.43                     | 0.48              |
| 33:h:110:VAL:HG23 | 33:h:114:GLU:OE2  | 2.14                     | 0.48              |
| 37:l:75:GLU:HB2   | 37:l:145:GLU:HG3  | 1.96                     | 0.48              |
| 1:A:253:A:H2'     | 1:A:254:G:C8      | 2.49                     | 0.47              |
| 1:A:1306:A:H61    | 1:A:1331:G:H1'    | 1.78                     | 0.47              |
| 2:B:35:ARG:NH1    | 25:Y:15:GLU:CG    | 2.76                     | 0.47              |
| 9:I:107:ASP:OD1   | 9:I:109:ARG:HG3   | 2.14                     | 0.47              |
| 26:a:1169:A:H2'   | 26:a:1170:C:O4'   | 2.14                     | 0.47              |
| 26:a:1589:U:C2    | 26:a:1590:A:C8    | 3.02                     | 0.47              |
| 26:a:2127:G:H1'   | 26:a:2173:A:C2    | 2.49                     | 0.47              |
| 26:a:2803:G:H2'   | 26:a:2804:U:H6    | 1.79                     | 0.47              |
| 34:i:13:ARG:NH1   | 34:i:49:ASP:O     | 2.47                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:y:5:ILE:HG22  | 50:y:59:GLU:HA    | 1.95                     | 0.47              |
| 1:A:845:A:C1'    | 18:R:15:ALA:HB2   | 2.31                     | 0.47              |
| 1:A:1175:G:H2'   | 1:A:1176:A:C8     | 2.43                     | 0.47              |
| 2:B:167:ASP:O    | 2:B:170:HIS:ND1   | 2.46                     | 0.47              |
| 22:V:19:G:H1'    | 22:V:59:A:C2      | 2.48                     | 0.47              |
| 23:W:29:C:H2'    | 23:W:30:G:C8      | 2.49                     | 0.47              |
| 26:a:874:G:OP1   | 37:l:62:LYS:HE2   | 2.14                     | 0.47              |
| 33:h:5:LEU:C     | 33:h:6:LEU:HD12   | 2.39                     | 0.47              |
| 1:A:34:C:H2'     | 1:A:35:G:H8       | 1.78                     | 0.47              |
| 1:A:1029:U:H2'   | 1:A:1031:C:H4'    | 1.96                     | 0.47              |
| 1:A:1297:G:N2    | 7:G:114:LYS:HB3   | 2.29                     | 0.47              |
| 1:A:1414:U:H2'   | 1:A:1415:G:H8     | 1.79                     | 0.47              |
| 2:B:219:ALA:O    | 2:B:222:ARG:N     | 2.48                     | 0.47              |
| 5:E:110:ALA:HB1  | 5:E:137:VAL:HG23  | 1.96                     | 0.47              |
| 25:Y:66:ASP:OD1  | 25:Y:68:VAL:HG12  | 2.15                     | 0.47              |
| 26:a:67:U:C2     | 26:a:68:G:C8      | 3.02                     | 0.47              |
| 26:a:291:G:C6    | 26:a:350:G:C6     | 3.02                     | 0.47              |
| 26:a:2031:A:N3   | 26:a:2455:G:O2'   | 2.37                     | 0.47              |
| 26:a:2287:A:HO2' | 26:a:2288:A:H2'   | 1.79                     | 0.47              |
| 30:e:32:VAL:HG13 | 30:e:178:VAL:HG22 | 1.96                     | 0.47              |
| 49:x:12:GLU:HG2  | 49:x:13:GLU:N     | 2.28                     | 0.47              |
| 1:A:457:G:H2'    | 1:A:458:U:C6      | 2.49                     | 0.47              |
| 1:A:1250:A:H2'   | 1:A:1251:A:C8     | 2.48                     | 0.47              |
| 7:G:113:ASP:HB2  | 7:G:119:ARG:HG3   | 1.95                     | 0.47              |
| 10:J:40:ILE:HB   | 10:J:73:LEU:HB3   | 1.96                     | 0.47              |
| 26:a:581:C:H2'   | 26:a:582:A:H8     | 1.77                     | 0.47              |
| 26:a:813:U:H2'   | 26:a:814:C:H6     | 1.79                     | 0.47              |
| 46:u:1:MET:N     | 46:u:59:GLU:OE1   | 2.48                     | 0.47              |
| 1:A:383:A:C5     | 1:A:384:G:H1'     | 2.50                     | 0.47              |
| 1:A:460:A:C8     | 1:A:461:A:C8      | 3.02                     | 0.47              |
| 1:A:745:G:H2'    | 1:A:746:A:H8      | 1.79                     | 0.47              |
| 1:A:1060:U:H4'   | 10:J:53:ILE:HG13  | 1.95                     | 0.47              |
| 1:A:1100:C:P     | 2:B:95:ARG:HD3    | 2.54                     | 0.47              |
| 1:A:1512:U:H2'   | 1:A:1513:A:C8     | 2.49                     | 0.47              |
| 9:I:13:LYS:O     | 9:I:110:GLN:NE2   | 2.38                     | 0.47              |
| 10:J:5:ARG:NH1   | 10:J:7:ARG:HH21   | 2.13                     | 0.47              |
| 24:X:5:G:H3'     | 24:X:6:G:H2'      | 1.97                     | 0.47              |
| 26:a:140:C:H2'   | 26:a:141:G:H5'    | 1.95                     | 0.47              |
| 26:a:511:U:O4    | 26:a:512:G:N1     | 2.48                     | 0.47              |
| 26:a:1064:C:N4   | 26:a:1070:A:OP1   | 2.32                     | 0.47              |
| 26:a:2047:C:H2'  | 26:a:2048:G:H8    | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:e:118:LEU:HD11 | 30:e:188:MET:HE2  | 1.95                     | 0.47              |
| 1:A:335:C:H2'     | 1:A:336:A:H8      | 1.79                     | 0.47              |
| 6:F:71:ILE:O      | 6:F:75:GLU:HG2    | 2.15                     | 0.47              |
| 6:F:82:ASP:OD1    | 6:F:82:ASP:N      | 2.47                     | 0.47              |
| 10:J:6:ILE:HG12   | 10:J:79:PRO:HB3   | 1.96                     | 0.47              |
| 11:K:114:THR:HG21 | 21:U:32:VAL:HG21  | 1.95                     | 0.47              |
| 25:Y:49:PRO:HB2   | 25:Y:84:LEU:HD12  | 1.95                     | 0.47              |
| 26:a:100:U:H1'    | 26:a:101:A:C4     | 2.49                     | 0.47              |
| 26:a:568:U:O4     | 42:q:81:LYS:NZ    | 2.48                     | 0.47              |
| 26:a:1385:A:H1'   | 26:a:1386:C:C6    | 2.50                     | 0.47              |
| 26:a:2159:G:H2'   | 26:a:2160:C:C6    | 2.50                     | 0.47              |
| 26:a:2230:G:H2'   | 26:a:2231:U:C6    | 2.48                     | 0.47              |
| 31:f:37:ASN:OD1   | 31:f:38:MET:N     | 2.48                     | 0.47              |
| 35:j:107:LEU:HB2  | 35:j:116:ILE:HD11 | 1.95                     | 0.47              |
| 50:y:57:VAL:HG12  | 50:y:59:GLU:HG3   | 1.97                     | 0.47              |
| 1:A:270:A:H2'     | 1:A:271:C:C6      | 2.50                     | 0.47              |
| 1:A:890:G:O2'     | 1:A:891:U:O5'     | 2.32                     | 0.47              |
| 1:A:1272:G:H2'    | 1:A:1273:C:C6     | 2.50                     | 0.47              |
| 1:A:1342:C:H2'    | 1:A:1343:G:C8     | 2.49                     | 0.47              |
| 1:A:1404:C:H2'    | 1:A:1405:G:C8     | 2.50                     | 0.47              |
| 1:A:1457:G:OP1    | 20:T:34:LYS:NZ    | 2.37                     | 0.47              |
| 9:I:84:THR:HG23   | 9:I:98:LEU:HD13   | 1.97                     | 0.47              |
| 18:R:14:THR:HG23  | 18:R:48:ARG:CD    | 2.43                     | 0.47              |
| 25:Y:21:GLY:HA2   | 25:Y:72:LEU:HB3   | 1.96                     | 0.47              |
| 26:a:287:G:H2'    | 26:a:288:U:C6     | 2.50                     | 0.47              |
| 26:a:394:C:H2'    | 26:a:395:U:O4'    | 2.15                     | 0.47              |
| 26:a:532:A:N1     | 26:a:2020:A:H1'   | 2.30                     | 0.47              |
| 26:a:1040:A:N6    | 26:a:1115:G:H1    | 2.12                     | 0.47              |
| 26:a:1245:G:OP1   | 36:k:13:LYS:HE2   | 2.15                     | 0.47              |
| 26:a:1409:U:H2'   | 26:a:1410:G:H8    | 1.79                     | 0.47              |
| 26:a:1496:A:H2'   | 26:a:1498:C:C5    | 2.49                     | 0.47              |
| 26:a:1709:U:C2    | 26:a:1750:G:N2    | 2.83                     | 0.47              |
| 26:a:1713:A:N6    | 26:a:1746:A:N1    | 2.62                     | 0.47              |
| 26:a:1722:A:H2'   | 26:a:1723:A:C8    | 2.50                     | 0.47              |
| 26:a:1722:A:H2'   | 26:a:1723:A:H8    | 1.78                     | 0.47              |
| 26:a:1744:A:H3'   | 26:a:1745:A:H8    | 1.80                     | 0.47              |
| 26:a:1889:A:H2'   | 26:a:1890:A:C8    | 2.50                     | 0.47              |
| 26:a:1930:G:O2'   | 26:a:1931:U:P     | 2.73                     | 0.47              |
| 26:a:1996:C:H5    | 35:j:32:TYR:OH    | 1.97                     | 0.47              |
| 26:a:2039:U:H2'   | 26:a:2040:G:C8    | 2.50                     | 0.47              |
| 26:a:2316:G:O2'   | 31:f:125:ARG:NH2  | 2.47                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:a:2537:U:H2'   | 26:a:2538:C:C6   | 2.49                     | 0.47              |
| 26:a:2897:U:H2'   | 26:a:2898:U:C6   | 2.50                     | 0.47              |
| 27:b:111:U:H2'    | 27:b:112:G:H8    | 1.79                     | 0.47              |
| 29:d:186:LEU:HD21 | 40:o:4:ILE:HG21  | 1.96                     | 0.47              |
| 32:g:23:VAL:HG22  | 32:g:36:THR:HG22 | 1.97                     | 0.47              |
| 37:l:67:VAL:HG12  | 37:l:155:LYS:HE3 | 1.96                     | 0.47              |
| 39:n:83:LEU:HD11  | 39:n:114:GLY:HA3 | 1.97                     | 0.47              |
| 1:A:427:U:OP2     | 1:A:428:G:O2'    | 2.27                     | 0.47              |
| 1:A:461:A:H2'     | 1:A:462:G:C8     | 2.49                     | 0.47              |
| 1:A:685:G:H2'     | 1:A:686:U:C6     | 2.50                     | 0.47              |
| 1:A:954:G:H2'     | 1:A:955:U:C6     | 2.50                     | 0.47              |
| 1:A:1097:C:H2'    | 1:A:1098:C:C6    | 2.50                     | 0.47              |
| 21:U:4:ILE:HD11   | 21:U:18:ARG:NH1  | 2.30                     | 0.47              |
| 22:V:24:C:H2'     | 22:V:25:U:C6     | 2.50                     | 0.47              |
| 26:a:197:A:N6     | 26:a:2430:A:H2'  | 2.24                     | 0.47              |
| 26:a:332:A:O2'    | 26:a:334:C:OP2   | 2.23                     | 0.47              |
| 26:a:402:A:H2'    | 26:a:403:U:O4'   | 2.15                     | 0.47              |
| 26:a:1316:U:H2'   | 26:a:1317:G:H8   | 1.79                     | 0.47              |
| 26:a:1366:A:H2'   | 26:a:1367:A:O4'  | 2.14                     | 0.47              |
| 26:a:2106:U:H5'   | 26:a:2107:G:H3'  | 1.97                     | 0.47              |
| 26:a:2638:G:O2'   | 26:a:2778:A:N6   | 2.48                     | 0.47              |
| 26:a:2861:U:H2'   | 26:a:2862:G:C8   | 2.49                     | 0.47              |
| 47:v:25:ARG:HD3   | 47:v:29:GLU:OE1  | 2.14                     | 0.47              |
| 1:A:191:G:H2'     | 1:A:192:A:C8     | 2.49                     | 0.47              |
| 1:A:193:C:H2'     | 1:A:194:C:C6     | 2.50                     | 0.47              |
| 1:A:963:G:C2      | 1:A:964:A:C8     | 3.03                     | 0.47              |
| 1:A:1055:A:O2'    | 3:C:161:GLU:O    | 2.23                     | 0.47              |
| 1:A:1409:C:H2'    | 1:A:1410:A:H8    | 1.80                     | 0.47              |
| 16:P:4:ILE:HG22   | 16:P:71:VAL:HG11 | 1.97                     | 0.47              |
| 22:V:16:C:H1'     | 22:V:60:A:C2     | 2.49                     | 0.47              |
| 26:a:78:U:H2'     | 26:a:79:C:H6     | 1.80                     | 0.47              |
| 26:a:645:C:H2'    | 26:a:647:G:N7    | 2.30                     | 0.47              |
| 26:a:1353:A:OP2   | 26:a:1377:G:N1   | 2.33                     | 0.47              |
| 27:b:78:A:H2'     | 27:b:79:G:O4'    | 2.14                     | 0.47              |
| 32:g:84:THR:HA    | 32:g:133:LEU:O   | 2.15                     | 0.47              |
| 35:j:17:ARG:HD3   | 35:j:17:ARG:HA   | 1.68                     | 0.47              |
| 49:x:19:LEU:HB3   | 49:x:23:ARG:NH1  | 2.29                     | 0.47              |
| 1:A:845:A:H5''    | 1:A:846:G:H8     | 1.80                     | 0.47              |
| 2:B:35:ARG:HH12   | 25:Y:15:GLU:CG   | 2.28                     | 0.47              |
| 9:I:84:THR:O      | 9:I:88:MET:HG2   | 2.15                     | 0.47              |
| 26:a:555:G:O2'    | 26:a:556:A:P     | 2.73                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:645:C:H2'    | 26:a:647:G:C8     | 2.50                     | 0.47              |
| 26:a:784:G:H5'    | 26:a:785:G:OP1    | 2.14                     | 0.47              |
| 26:a:849:A:H2'    | 26:a:850:U:H6     | 1.78                     | 0.47              |
| 26:a:1239:G:H2'   | 26:a:1240:U:O4'   | 2.15                     | 0.47              |
| 26:a:1357:C:H2'   | 26:a:1358:G:O4'   | 2.15                     | 0.47              |
| 26:a:1361:G:H2'   | 26:a:1362:C:C6    | 2.50                     | 0.47              |
| 26:a:1441:G:H2'   | 26:a:1442:U:C6    | 2.50                     | 0.47              |
| 29:d:110:THR:HG23 | 29:d:202:ILE:HB   | 1.96                     | 0.47              |
| 33:h:51:ARG:O     | 33:h:53:GLU:N     | 2.48                     | 0.47              |
| 34:i:3:THR:HG21   | 41:p:57:PHE:CE1   | 2.50                     | 0.47              |
| 1:A:1010:C:H2'    | 1:A:1011:C:H6     | 1.80                     | 0.46              |
| 1:A:1297:G:H21    | 7:G:114:LYS:HB3   | 1.79                     | 0.46              |
| 2:B:42:ASN:C      | 2:B:44:GLU:N      | 2.69                     | 0.46              |
| 26:a:391:A:H1'    | 26:a:411:G:O4'    | 2.15                     | 0.46              |
| 26:a:1996:C:H5    | 35:j:32:TYR:HH    | 1.60                     | 0.46              |
| 26:a:2015:A:C6    | 51:z:3:VAL:HG23   | 2.50                     | 0.46              |
| 27:b:32:U:C2      | 27:b:51:G:N2      | 2.83                     | 0.46              |
| 37:l:42:THR:HG22  | 37:l:148:VAL:HG12 | 1.97                     | 0.46              |
| 41:p:86:ALA:HB2   | 41:p:116:ALA:HB2  | 1.97                     | 0.46              |
| 1:A:754:C:OP1     | 15:O:72:ARG:NH2   | 2.49                     | 0.46              |
| 5:E:85:VAL:HG23   | 5:E:96:MET:HE3    | 1.98                     | 0.46              |
| 6:F:102:MET:CE    | 18:R:26:ILE:HG23  | 2.45                     | 0.46              |
| 8:H:46:ILE:HD13   | 8:H:61:LEU:HD23   | 1.95                     | 0.46              |
| 11:K:27:PHE:HE1   | 21:U:33:ARG:HH22  | 1.49                     | 0.46              |
| 13:M:85:CYS:HB3   | 19:S:74:PHE:CE1   | 2.50                     | 0.46              |
| 18:R:13:PHE:HE2   | 18:R:55:LEU:HD13  | 1.80                     | 0.46              |
| 26:a:641:U:O2'    | 26:a:2350:C:OP1   | 2.31                     | 0.46              |
| 26:a:723:C:H2'    | 26:a:724:U:O4'    | 2.16                     | 0.46              |
| 26:a:893:C:H2'    | 26:a:894:U:C6     | 2.51                     | 0.46              |
| 26:a:2834:G:H2'   | 26:a:2879:A:N6    | 2.31                     | 0.46              |
| 26:a:2881:U:O2'   | 38:m:95:THR:O     | 2.33                     | 0.46              |
| 33:h:50:ARG:HD2   | 33:h:51:ARG:N     | 2.30                     | 0.46              |
| 1:A:219:U:H2'     | 1:A:220:G:H8      | 1.81                     | 0.46              |
| 1:A:236:A:H2'     | 1:A:237:G:C8      | 2.50                     | 0.46              |
| 1:A:626:G:O3'     | 16:P:51:ARG:NH2   | 2.48                     | 0.46              |
| 1:A:925:G:C2      | 1:A:927:G:C8      | 3.03                     | 0.46              |
| 1:A:950:U:H2'     | 1:A:951:G:C8      | 2.50                     | 0.46              |
| 3:C:53:SER:HB2    | 3:C:112:ASP:OD2   | 2.15                     | 0.46              |
| 14:N:14:VAL:HA    | 14:N:60:GLN:NE2   | 2.29                     | 0.46              |
| 18:R:63:ARG:HB3   | 18:R:70:TYR:CE1   | 2.51                     | 0.46              |
| 21:U:54:LYS:O     | 21:U:56:HIS:N     | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:V:32:G:H2'     | 22:V:33:C:H6      | 1.80                     | 0.46              |
| 25:Y:171:ARG:HB2  | 25:Y:173:VAL:HG22 | 1.98                     | 0.46              |
| 26:a:580:U:H2'    | 26:a:581:C:C6     | 2.51                     | 0.46              |
| 26:a:627:A:H5''   | 36:k:78:ARG:NH2   | 2.30                     | 0.46              |
| 26:a:1870:C:H3'   | 26:a:1871:A:C8    | 2.50                     | 0.46              |
| 26:a:2287:A:N7    | 26:a:2289:G:C8    | 2.83                     | 0.46              |
| 26:a:2635:A:H2'   | 26:a:2636:C:O4'   | 2.15                     | 0.46              |
| 31:f:94:GLU:HG3   | 31:f:98:GLU:OE2   | 2.16                     | 0.46              |
| 32:g:89:LEU:HD11  | 32:g:96:ALA:HB2   | 1.97                     | 0.46              |
| 33:h:90:LEU:HB3   | 33:h:123:ARG:O    | 2.15                     | 0.46              |
| 44:s:2:ILE:HB     | 44:s:7:LEU:HD11   | 1.97                     | 0.46              |
| 1:A:3:A:N1        | 1:A:628:G:O2'     | 2.44                     | 0.46              |
| 1:A:1033:G:H2'    | 1:A:1034:G:H8     | 1.75                     | 0.46              |
| 1:A:1305:G:O2'    | 1:A:1306:A:H8     | 1.95                     | 0.46              |
| 2:B:15:HIS:CE1    | 2:B:16:PHE:CE1    | 3.04                     | 0.46              |
| 26:a:1474:U:H3'   | 26:a:1475:G:C8    | 2.50                     | 0.46              |
| 26:a:2228:G:H2'   | 26:a:2229:U:C6    | 2.51                     | 0.46              |
| 26:a:2696:U:H2'   | 26:a:2697:G:H8    | 1.80                     | 0.46              |
| 26:a:2813:A:H2'   | 26:a:2814:A:H8    | 1.80                     | 0.46              |
| 27:b:16:G:N2      | 27:b:69:G:H1'     | 2.30                     | 0.46              |
| 32:g:117:LEU:HD11 | 32:g:123:ALA:HB2  | 1.97                     | 0.46              |
| 39:n:115:LEU:HD23 | 39:n:115:LEU:HA   | 1.79                     | 0.46              |
| 48:w:68:LEU:HD23  | 48:w:78:TYR:CZ    | 2.50                     | 0.46              |
| 1:A:1062:U:H2'    | 1:A:1063:C:C6     | 2.51                     | 0.46              |
| 1:A:1216:A:H5''   | 14:N:5:SER:HB3    | 1.96                     | 0.46              |
| 19:S:11:ILE:HG21  | 19:S:16:LEU:HD12  | 1.98                     | 0.46              |
| 22:V:51:U:H2'     | 22:V:52:C:H6      | 1.75                     | 0.46              |
| 26:a:18:U:OP1     | 41:p:30:ARG:NH1   | 2.36                     | 0.46              |
| 26:a:150:U:H2'    | 26:a:151:C:C6     | 2.51                     | 0.46              |
| 26:a:162:U:O2'    | 26:a:163:C:O5'    | 2.25                     | 0.46              |
| 26:a:884:U:H5'    | 26:a:885:C:O5'    | 2.15                     | 0.46              |
| 26:a:2689:U:OP1   | 26:a:2719:G:N1    | 2.33                     | 0.46              |
| 33:h:47:PHE:O     | 33:h:52:ALA:N     | 2.45                     | 0.46              |
| 44:s:92:ASN:OD1   | 44:s:93:LEU:N     | 2.48                     | 0.46              |
| 51:z:38:HIS:HB3   | 51:z:44:THR:HG22  | 1.97                     | 0.46              |
| 54:2:26:HIS:NE2   | 54:2:48:ALA:HB2   | 2.31                     | 0.46              |
| 1:A:1500:A:H5''   | 1:A:1508:A:H5'    | 1.97                     | 0.46              |
| 22:V:20:G:O6      | 31:f:80:ARG:NH2   | 2.48                     | 0.46              |
| 26:a:1370:C:H2'   | 26:a:1371:G:O4'   | 2.15                     | 0.46              |
| 26:a:1394:U:H4'   | 26:a:1603:A:H4'   | 1.97                     | 0.46              |
| 26:a:1667:G:O2'   | 26:a:1991:U:O4    | 2.31                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:2247:A:H2'  | 26:a:2248:C:C6    | 2.49                     | 0.46              |
| 26:a:2469:A:H2'  | 26:a:2470:G:O4'   | 2.14                     | 0.46              |
| 26:a:2743:U:H2'  | 26:a:2744:G:O4'   | 2.16                     | 0.46              |
| 30:e:127:GLU:C   | 30:e:156:ASN:HD21 | 2.24                     | 0.46              |
| 1:A:399:G:H2'    | 1:A:400:C:C6      | 2.51                     | 0.46              |
| 2:B:59:LYS:O     | 2:B:62:SER:OG     | 2.27                     | 0.46              |
| 4:D:105:MET:SD   | 4:D:180:GLY:HA3   | 2.55                     | 0.46              |
| 7:G:51:ALA:HB2   | 7:G:58:GLU:HG3    | 1.98                     | 0.46              |
| 10:J:50:THR:HG22 | 10:J:62:ARG:HH11  | 1.81                     | 0.46              |
| 26:a:782:A:C2    | 28:c:225:MET:HG2  | 2.50                     | 0.46              |
| 26:a:879:G:H2'   | 26:a:880:G:O4'    | 2.15                     | 0.46              |
| 26:a:2529:G:H5'' | 32:g:175:LYS:HG2  | 1.97                     | 0.46              |
| 38:m:103:ARG:HD3 | 38:m:110:MET:HE2  | 1.97                     | 0.46              |
| 50:y:48:ILE:HG21 | 50:y:57:VAL:HG21  | 1.98                     | 0.46              |
| 56:4:17:SER:C    | 56:4:19:GLY:H     | 2.24                     | 0.46              |
| 1:A:911:U:H2'    | 1:A:912:C:C6      | 2.51                     | 0.46              |
| 2:B:114:LEU:HB3  | 2:B:144:LEU:HD13  | 1.98                     | 0.46              |
| 4:D:124:MET:HG3  | 4:D:146:ARG:HG2   | 1.97                     | 0.46              |
| 17:Q:49:GLU:O    | 17:Q:50:ASN:HB3   | 2.14                     | 0.46              |
| 22:V:16:C:O2'    | 22:V:61:U:H1'     | 2.16                     | 0.46              |
| 26:a:287:G:H2'   | 26:a:288:U:H6     | 1.81                     | 0.46              |
| 26:a:1153:C:OP1  | 41:p:92:ARG:NH2   | 2.38                     | 0.46              |
| 26:a:1315:C:H2'  | 26:a:1316:U:C6    | 2.51                     | 0.46              |
| 26:a:1416:G:O2'  | 26:a:1417:C:O5'   | 2.33                     | 0.46              |
| 26:a:1709:U:H2'  | 26:a:1710:G:C8    | 2.51                     | 0.46              |
| 26:a:1753:G:H5'' | 40:o:93:ARG:HD3   | 1.98                     | 0.46              |
| 26:a:2364:C:OP1  | 47:v:55:ARG:NH1   | 2.44                     | 0.46              |
| 30:e:46:GLN:HB3  | 30:e:83:VAL:HG21  | 1.98                     | 0.46              |
| 47:v:42:GLY:O    | 47:v:44:LYS:N     | 2.46                     | 0.46              |
| 1:A:958:A:OP1    | 19:S:55:ARG:NH1   | 2.41                     | 0.46              |
| 1:A:1034:G:C2'   | 1:A:1035:A:H5'    | 2.46                     | 0.46              |
| 1:A:1348:U:H2'   | 1:A:1349:A:H8     | 1.81                     | 0.46              |
| 2:B:23:TRP:CD1   | 2:B:39:HIS:HE2    | 2.33                     | 0.46              |
| 4:D:188:ARG:NE   | 4:D:197:GLU:OE1   | 2.42                     | 0.46              |
| 6:F:4:TYR:CD2    | 6:F:71:ILE:HG13   | 2.51                     | 0.46              |
| 26:a:57:C:H2'    | 26:a:58:G:O4'     | 2.16                     | 0.46              |
| 26:a:322:A:OP2   | 30:e:163:ASN:HB2  | 2.16                     | 0.46              |
| 26:a:577:G:O2'   | 26:a:1254:A:OP1   | 2.34                     | 0.46              |
| 26:a:686:U:H2'   | 26:a:788:A:N1     | 2.30                     | 0.46              |
| 26:a:884:U:C4    | 26:a:893:C:N3     | 2.84                     | 0.46              |
| 26:a:1087:G:H1   | 26:a:1102:C:N4    | 2.14                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:a:1105:U:H2'   | 26:a:1106:G:C8    | 2.51                     | 0.46              |
| 26:a:1151:A:H4'   | 41:p:81:ASN:ND2   | 2.31                     | 0.46              |
| 26:a:1468:U:H2'   | 26:a:1522:A:N6    | 2.31                     | 0.46              |
| 26:a:1672:A:C2    | 26:a:2582:G:H5'   | 2.50                     | 0.46              |
| 26:a:2292:U:H2'   | 26:a:2293:G:C8    | 2.50                     | 0.46              |
| 26:a:2567:G:H2'   | 26:a:2568:U:C6    | 2.51                     | 0.46              |
| 48:w:5:CYS:SG     | 48:w:8:THR:OG1    | 2.61                     | 0.46              |
| 50:y:7:ILE:HG22   | 50:y:29:LEU:HD11  | 1.98                     | 0.46              |
| 1:A:160:A:H2'     | 1:A:161:A:O4'     | 2.15                     | 0.46              |
| 1:A:204:G:H3'     | 1:A:205:A:C8      | 2.48                     | 0.46              |
| 1:A:625:U:H2'     | 1:A:626:G:C8      | 2.51                     | 0.46              |
| 3:C:134:MET:HE1   | 3:C:167:TRP:HA    | 1.98                     | 0.46              |
| 6:F:41:ASP:OD1    | 6:F:60:VAL:HG22   | 2.16                     | 0.46              |
| 21:U:63:GLU:H     | 21:U:65:ALA:H     | 1.62                     | 0.46              |
| 23:W:70:C:H2'     | 23:W:71:G:C8      | 2.51                     | 0.46              |
| 26:a:594:U:H2'    | 26:a:595:C:H6     | 1.81                     | 0.46              |
| 26:a:2037:A:H2'   | 26:a:2038:G:C8    | 2.51                     | 0.46              |
| 52:0:27:LYS:HB2   | 52:0:28:ARG:NH1   | 2.31                     | 0.46              |
| 1:A:404:G:N7      | 4:D:2:ALA:HB3     | 2.31                     | 0.45              |
| 1:A:625:U:H2'     | 1:A:626:G:H8      | 1.81                     | 0.45              |
| 3:C:73:PRO:HG3    | 3:C:105:GLU:OE1   | 2.16                     | 0.45              |
| 5:E:72:ILE:HD12   | 5:E:145:GLU:HB3   | 1.98                     | 0.45              |
| 5:E:112:ARG:O     | 5:E:116:GLU:HG3   | 2.16                     | 0.45              |
| 8:H:54:ASP:OD1    | 8:H:54:ASP:N      | 2.45                     | 0.45              |
| 12:L:76:GLU:N     | 12:L:76:GLU:OE1   | 2.49                     | 0.45              |
| 23:W:77:A:H5''    | 48:w:22:LEU:HD22  | 1.98                     | 0.45              |
| 25:Y:111:VAL:HG22 | 25:Y:123:GLU:HA   | 1.97                     | 0.45              |
| 25:Y:138:VAL:HA   | 25:Y:157:ILE:HG12 | 1.97                     | 0.45              |
| 26:a:659:G:N2     | 30:e:30:GLN:OE1   | 2.41                     | 0.45              |
| 26:a:764:A:H5''   | 28:c:209:GLY:HA2  | 1.97                     | 0.45              |
| 26:a:955:PSU:H5'  | 37:l:141:LYS:HE2  | 1.98                     | 0.45              |
| 26:a:1168:G:H2'   | 26:a:1169:A:C8    | 2.52                     | 0.45              |
| 26:a:1871:A:H2'   | 26:a:1872:A:C8    | 2.52                     | 0.45              |
| 26:a:2696:U:H2'   | 26:a:2697:G:C8    | 2.51                     | 0.45              |
| 26:a:2808:G:H2'   | 26:a:2890:G:C6    | 2.52                     | 0.45              |
| 29:d:9:VAL:CG2    | 29:d:28:GLU:HB2   | 2.46                     | 0.45              |
| 32:g:33:LEU:HD13  | 32:g:75:MET:HG2   | 1.98                     | 0.45              |
| 1:A:56:U:H2'      | 1:A:57:G:H8       | 1.78                     | 0.45              |
| 1:A:79:G:H22      | 1:A:90:C:N4       | 2.15                     | 0.45              |
| 1:A:227:G:O2'     | 16:P:63:GLN:OE1   | 2.33                     | 0.45              |
| 1:A:333:U:OP1     | 20:T:2:ALA:N      | 2.49                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:530:G:H2'    | 1:A:530:G:N3     | 2.30                     | 0.45              |
| 1:A:855:U:OP2    | 1:A:871:U:N3     | 2.37                     | 0.45              |
| 8:H:18:GLN:HE21  | 8:H:63:LEU:HD22  | 1.80                     | 0.45              |
| 13:M:92:ARG:HD3  | 26:a:888:C:C5    | 2.51                     | 0.45              |
| 14:N:79:LEU:HB2  | 14:N:84:VAL:HG23 | 1.98                     | 0.45              |
| 26:a:95:A:H2'    | 26:a:96:C:O4'    | 2.16                     | 0.45              |
| 26:a:127:A:H5''  | 26:a:128:C:O4'   | 2.16                     | 0.45              |
| 26:a:1171:G:N2   | 26:a:1180:U:C4   | 2.84                     | 0.45              |
| 38:m:57:THR:HG23 | 38:m:62:ASN:HD21 | 1.82                     | 0.45              |
| 46:u:48:MET:HE3  | 46:u:51:GLN:NE2  | 2.31                     | 0.45              |
| 56:4:41:HIS:HB3  | 56:4:44:PHE:CD1  | 2.51                     | 0.45              |
| 1:A:123:U:OP1    | 1:A:311:C:O2'    | 2.34                     | 0.45              |
| 1:A:246:A:C2     | 1:A:282:A:C5     | 3.04                     | 0.45              |
| 1:A:593:U:H2'    | 1:A:594:U:C6     | 2.51                     | 0.45              |
| 5:E:159:LYS:HE3  | 8:H:43:GLU:HA    | 1.97                     | 0.45              |
| 11:K:36:ASP:OD1  | 11:K:36:ASP:N    | 2.47                     | 0.45              |
| 26:a:245:G:O2'   | 26:a:384:A:N1    | 2.41                     | 0.45              |
| 26:a:1773:A:N7   | 26:a:1829:A:H1'  | 2.31                     | 0.45              |
| 26:a:1794:A:H2'  | 26:a:1795:C:H6   | 1.82                     | 0.45              |
| 38:m:57:THR:HG23 | 38:m:62:ASN:ND2  | 2.31                     | 0.45              |
| 52:0:38:LYS:HB2  | 52:0:49:TYR:CD1  | 2.51                     | 0.45              |
| 55:3:2:LYS:NZ    | 55:3:32:LYS:O    | 2.45                     | 0.45              |
| 1:A:215:C:H2'    | 1:A:216:U:H6     | 1.78                     | 0.45              |
| 1:A:1162:C:H2'   | 1:A:1163:A:H8    | 1.81                     | 0.45              |
| 2:B:186:ILE:HG13 | 2:B:200:ILE:O    | 2.16                     | 0.45              |
| 7:G:107:ALA:O    | 7:G:111:ARG:HG3  | 2.17                     | 0.45              |
| 22:V:6:G:H2'     | 22:V:7:G:H8      | 1.82                     | 0.45              |
| 26:a:30:G:H2'    | 26:a:31:C:H6     | 1.82                     | 0.45              |
| 26:a:298:G:N1    | 26:a:339:U:OP2   | 2.29                     | 0.45              |
| 26:a:2513:A:H2'  | 26:a:2514:U:C6   | 2.52                     | 0.45              |
| 1:A:957:U:H4'    | 19:S:79:THR:HB   | 1.99                     | 0.45              |
| 1:A:1144:G:O6    | 1:A:1145:A:N6    | 2.50                     | 0.45              |
| 1:A:1236:A:H4'   | 1:A:1304:G:H4'   | 1.98                     | 0.45              |
| 8:H:22:LYS:O     | 8:H:65:TYR:OH    | 2.35                     | 0.45              |
| 13:M:81:MET:CE   | 13:M:91:HIS:HB3  | 2.46                     | 0.45              |
| 17:Q:21:ILE:HG13 | 17:Q:46:VAL:HB   | 1.97                     | 0.45              |
| 18:R:18:VAL:O    | 18:R:20:GLU:N    | 2.50                     | 0.45              |
| 26:a:24:G:H2'    | 26:a:25:U:C6     | 2.51                     | 0.45              |
| 26:a:139:U:H2'   | 26:a:140:C:C5    | 2.51                     | 0.45              |
| 26:a:242:G:H5''  | 54:2:64:TYR:CE2  | 2.50                     | 0.45              |
| 26:a:1051:G:H2'  | 26:a:1052:C:C6   | 2.52                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:1110:G:H2'  | 26:a:1111:A:C8    | 2.52                     | 0.45              |
| 26:a:1405:U:H2'  | 26:a:1406:U:C6    | 2.52                     | 0.45              |
| 26:a:1779:U:O2   | 26:a:1783:A:N6    | 2.50                     | 0.45              |
| 26:a:2333:A:H4'  | 26:a:2334:U:O5'   | 2.16                     | 0.45              |
| 27:b:28:C:H2'    | 27:b:29:A:C8      | 2.52                     | 0.45              |
| 28:c:243:HIS:O   | 28:c:245:VAL:HG13 | 2.17                     | 0.45              |
| 29:d:25:THR:OG1  | 29:d:191:GLY:O    | 2.30                     | 0.45              |
| 33:h:57:LYS:HE2  | 33:h:57:LYS:HA    | 1.99                     | 0.45              |
| 56:4:8:LYS:HZ1   | 56:4:29:GLY:N     | 2.15                     | 0.45              |
| 1:A:17:U:H2'     | 1:A:18:C:C6       | 2.51                     | 0.45              |
| 1:A:1118:U:H1'   | 1:A:1179:A:C5     | 2.52                     | 0.45              |
| 6:F:36:ILE:HG22  | 6:F:64:VAL:HG12   | 1.99                     | 0.45              |
| 25:Y:112:ILE:CG2 | 25:Y:145:LEU:HD13 | 2.46                     | 0.45              |
| 26:a:693:A:O2'   | 26:a:1353:A:N3    | 2.41                     | 0.45              |
| 26:a:998:C:OP1   | 41:p:84:LYS:NZ    | 2.27                     | 0.45              |
| 26:a:1197:G:H2'  | 26:a:1198:U:H6    | 1.81                     | 0.45              |
| 31:f:16:LEU:HD12 | 31:f:28:VAL:HG13  | 1.99                     | 0.45              |
| 53:1:34:ARG:NE   | 53:1:42:LEU:O     | 2.49                     | 0.45              |
| 1:A:745:G:H2'    | 1:A:746:A:C8      | 2.51                     | 0.45              |
| 1:A:1052:U:O2'   | 1:A:1055:A:OP2    | 2.20                     | 0.45              |
| 1:A:1226:C:O2'   | 13:M:110:LYS:NZ   | 2.50                     | 0.45              |
| 1:A:1347:G:O2'   | 1:A:1373:G:N1     | 2.36                     | 0.45              |
| 25:Y:63:GLN:O    | 25:Y:64:VAL:C     | 2.59                     | 0.45              |
| 26:a:257:C:H2'   | 26:a:258:G:O4'    | 2.16                     | 0.45              |
| 26:a:488:G:H1'   | 26:a:492:A:N6     | 2.31                     | 0.45              |
| 26:a:593:U:H2'   | 26:a:594:U:C6     | 2.52                     | 0.45              |
| 26:a:671:C:H2'   | 26:a:672:C:H6     | 1.82                     | 0.45              |
| 26:a:1771:C:H2'  | 26:a:1772:A:C8    | 2.50                     | 0.45              |
| 26:a:1771:C:H2'  | 26:a:1772:A:H8    | 1.81                     | 0.45              |
| 26:a:1873:G:H2'  | 26:a:1874:C:H6    | 1.80                     | 0.45              |
| 26:a:1927:A:H8   | 26:a:1927:A:O5'   | 2.00                     | 0.45              |
| 26:a:2133:G:C4   | 26:a:2157:G:H1'   | 2.51                     | 0.45              |
| 33:h:14:SER:OG   | 33:h:17:ASP:HB2   | 2.16                     | 0.45              |
| 33:h:47:PHE:CD1  | 33:h:51:ARG:HD2   | 2.52                     | 0.45              |
| 43:r:4:ILE:HD12  | 43:r:6:LYS:HE3    | 1.98                     | 0.45              |
| 44:s:38:ALA:O    | 44:s:81:LYS:NZ    | 2.39                     | 0.45              |
| 1:A:592:G:H2'    | 1:A:593:U:H6      | 1.82                     | 0.45              |
| 2:B:17:GLY:O     | 2:B:18:HIS:O      | 2.34                     | 0.45              |
| 14:N:73:PHE:CZ   | 14:N:78:GLY:HA2   | 2.51                     | 0.45              |
| 17:Q:17:MET:HB3  | 17:Q:20:SER:HB3   | 1.98                     | 0.45              |
| 17:Q:28:PHE:CE2  | 17:Q:37:PHE:HB3   | 2.51                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:R:9:LYS:HG2   | 18:R:10:PHE:N     | 2.32                     | 0.45              |
| 23:W:20:G:C2     | 23:W:58:A:H1'     | 2.51                     | 0.45              |
| 26:a:277:G:O5'   | 26:a:278:A:N6     | 2.50                     | 0.45              |
| 26:a:580:U:O3'   | 41:p:31:VAL:HG13  | 2.17                     | 0.45              |
| 26:a:893:C:H2'   | 26:a:894:U:N1     | 2.32                     | 0.45              |
| 26:a:1484:U:H2'  | 26:a:1485:U:H6    | 1.81                     | 0.45              |
| 26:a:2756:U:OP2  | 55:3:19:ARG:NE    | 2.40                     | 0.45              |
| 26:a:2780:G:OP2  | 34:i:120:ARG:HD3  | 2.17                     | 0.45              |
| 26:a:2812:G:H2'  | 26:a:2813:A:C8    | 2.52                     | 0.45              |
| 35:j:76:VAL:HG22 | 40:o:73:VAL:HB    | 1.98                     | 0.45              |
| 37:l:53:MET:HG2  | 37:l:160:MET:HE1  | 1.99                     | 0.45              |
| 41:p:78:LYS:HE3  | 41:p:117:LEU:HD13 | 1.99                     | 0.45              |
| 1:A:121:U:H5''   | 1:A:122:G:OP2     | 2.17                     | 0.45              |
| 1:A:739:C:OP1    | 6:F:2:ARG:NH2     | 2.48                     | 0.45              |
| 1:A:1007:U:H2'   | 1:A:1008:U:C6     | 2.52                     | 0.45              |
| 8:H:43:GLU:OE1   | 8:H:112:THR:HG21  | 2.17                     | 0.45              |
| 23:W:72:C:H2'    | 23:W:73:A:C8      | 2.52                     | 0.45              |
| 25:Y:155:LYS:HE3 | 25:Y:155:LYS:HB3  | 1.61                     | 0.45              |
| 26:a:351:C:H2'   | 26:a:352:A:H8     | 1.78                     | 0.45              |
| 26:a:1593:A:H2'  | 26:a:1594:U:C6    | 2.52                     | 0.45              |
| 26:a:2461:A:H2'  | 26:a:2462:C:C6    | 2.51                     | 0.45              |
| 26:a:2784:U:H4'  | 29:d:43:ASP:OD1   | 2.17                     | 0.45              |
| 29:d:152:PRO:HG3 | 29:d:156:PHE:CZ   | 2.52                     | 0.45              |
| 30:e:6:LYS:HG3   | 30:e:7:ASP:N      | 2.32                     | 0.45              |
| 31:f:50:LEU:HD21 | 31:f:67:ILE:HD12  | 1.99                     | 0.45              |
| 33:h:16:GLY:HA3  | 33:h:47:PHE:HE2   | 1.82                     | 0.45              |
| 33:h:62:LEU:O    | 33:h:65:ALA:N     | 2.49                     | 0.45              |
| 35:j:88:ASN:OD1  | 35:j:89:ASN:N     | 2.50                     | 0.45              |
| 1:A:413:G:H1'    | 1:A:428:G:H21     | 1.81                     | 0.45              |
| 1:A:1055:A:C6    | 1:A:1206:G:C5     | 3.05                     | 0.45              |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6     | 2.52                     | 0.45              |
| 4:D:196:ASN:OD1  | 4:D:198:HIS:NE2   | 2.50                     | 0.45              |
| 9:I:26:GLY:N     | 9:I:62:ASP:OD1    | 2.50                     | 0.45              |
| 22:V:26:C:H2'    | 22:V:27:G:O4'     | 2.17                     | 0.45              |
| 26:a:1077:A:OP1  | 26:a:1077:A:H8    | 2.00                     | 0.45              |
| 26:a:1111:A:H2'  | 26:a:1111:A:N3    | 2.32                     | 0.45              |
| 26:a:1173:U:H2'  | 26:a:1174:U:H4'   | 1.97                     | 0.45              |
| 26:a:1710:G:H2'  | 26:a:1711:A:H8    | 1.81                     | 0.45              |
| 26:a:1954:G:O2'  | 26:a:1956:U:O4    | 2.33                     | 0.45              |
| 33:h:136:SER:O   | 33:h:137:GLU:OE2  | 2.30                     | 0.45              |
| 35:j:92:GLU:OE1  | 35:j:111:LYS:NZ   | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 44:s:30:ILE:HG21 | 44:s:93:LEU:HD23 | 1.98                     | 0.45              |
| 46:u:30:ILE:HD11 | 46:u:40:ILE:HD13 | 1.99                     | 0.45              |
| 1:A:268:U:C2     | 1:A:269:C:C5     | 3.06                     | 0.44              |
| 1:A:639:G:O6     | 1:A:640:A:N6     | 2.51                     | 0.44              |
| 1:A:1071:C:H2'   | 1:A:1072:G:C8    | 2.51                     | 0.44              |
| 1:A:1513:A:H2'   | 1:A:1514:G:C8    | 2.52                     | 0.44              |
| 1:A:1517:G:H3'   | 1:A:1518:MA6:H8  | 1.97                     | 0.44              |
| 5:E:104:GLY:O    | 5:E:122:ASN:HA   | 2.17                     | 0.44              |
| 25:Y:27:VAL:H    | 25:Y:40:ALA:CB   | 2.30                     | 0.44              |
| 26:a:169:G:H2'   | 26:a:170:U:C6    | 2.52                     | 0.44              |
| 26:a:169:G:H2'   | 26:a:170:U:H6    | 1.82                     | 0.44              |
| 26:a:1004:U:H1'  | 26:a:1010:A:H2'  | 1.99                     | 0.44              |
| 26:a:1505:A:H2'  | 26:a:1506:U:C6   | 2.52                     | 0.44              |
| 31:f:5:HIS:HB2   | 31:f:97:TRP:CD1  | 2.52                     | 0.44              |
| 31:f:139:PRO:HG2 | 56:4:32:LEU:HD21 | 1.99                     | 0.44              |
| 34:i:110:PRO:O   | 34:i:115:GLY:HA3 | 2.17                     | 0.44              |
| 37:l:41:LEU:HD23 | 37:l:41:LEU:HA   | 1.84                     | 0.44              |
| 1:A:768:A:H4'    | 1:A:1523:G:N2    | 2.32                     | 0.44              |
| 1:A:818:G:O2'    | 1:A:819:A:OP1    | 2.33                     | 0.44              |
| 1:A:920:U:H2'    | 1:A:921:U:C6     | 2.51                     | 0.44              |
| 1:A:1266:G:N2    | 1:A:1269:A:OP2   | 2.39                     | 0.44              |
| 1:A:1464:U:H2'   | 1:A:1465:A:C8    | 2.49                     | 0.44              |
| 5:E:85:VAL:HG11  | 5:E:147:MET:HB2  | 1.99                     | 0.44              |
| 26:a:764:A:H5''  | 28:c:209:GLY:HA3 | 1.99                     | 0.44              |
| 26:a:1683:U:H2'  | 26:a:1684:G:C8   | 2.52                     | 0.44              |
| 26:a:2320:U:O2'  | 26:a:2322:A:N7   | 2.44                     | 0.44              |
| 26:a:2430:A:H5'  | 26:a:2431:U:OP2  | 2.17                     | 0.44              |
| 26:a:2542:A:H5'' | 26:a:2766:A:O2'  | 2.18                     | 0.44              |
| 32:g:69:ARG:NH1  | 32:g:73:ASN:HB2  | 2.33                     | 0.44              |
| 33:h:2:GLN:O     | 33:h:39:ALA:HB3  | 2.17                     | 0.44              |
| 37:l:26:VAL:HG13 | 37:l:159:GLU:HG2 | 2.00                     | 0.44              |
| 37:l:65:ILE:HG12 | 37:l:158:TYR:CE1 | 2.52                     | 0.44              |
| 45:t:47:LYS:HG3  | 45:t:48:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:33:A:H2'     | 1:A:34:C:C6      | 2.52                     | 0.44              |
| 1:A:911:U:OP2    | 12:L:94:ARG:NH2  | 2.50                     | 0.44              |
| 1:A:1309:G:OP1   | 13:M:87:ARG:NH1  | 2.50                     | 0.44              |
| 4:D:117:LEU:HG   | 4:D:154:ARG:HH21 | 1.82                     | 0.44              |
| 8:H:102:ALA:O    | 8:H:104:VAL:HG23 | 2.18                     | 0.44              |
| 10:J:53:ILE:HG12 | 10:J:61:ALA:O    | 2.17                     | 0.44              |
| 26:a:1072:C:H3'  | 26:a:1094:U:O4   | 2.17                     | 0.44              |
| 26:a:1360:G:N7   | 26:a:1361:G:C8   | 2.85                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:a:1509:A:H2'  | 26:a:1510:G:H8    | 1.81                     | 0.44              |
| 26:a:2122:U:H5'  | 26:a:2123:G:H5''  | 1.98                     | 0.44              |
| 26:a:2648:G:H2'  | 26:a:2649:C:C6    | 2.52                     | 0.44              |
| 27:b:32:U:H2'    | 27:b:33:G:H8      | 1.83                     | 0.44              |
| 33:h:40:THR:O    | 33:h:43:ASN:N     | 2.50                     | 0.44              |
| 39:n:52:SER:O    | 39:n:55:GLU:HG2   | 2.17                     | 0.44              |
| 43:r:65:ASP:OD1  | 43:r:66:ILE:N     | 2.51                     | 0.44              |
| 1:A:1478:U:H2'   | 1:A:1479:C:C6     | 2.52                     | 0.44              |
| 21:U:35:ARG:HG2  | 21:U:35:ARG:HH11  | 1.83                     | 0.44              |
| 26:a:534:U:O2'   | 41:p:49:ASP:OD2   | 2.26                     | 0.44              |
| 26:a:1049:C:C2   | 26:a:1050:A:C8    | 3.05                     | 0.44              |
| 26:a:1528:A:N6   | 26:a:1543:G:O2'   | 2.51                     | 0.44              |
| 26:a:1594:U:H2'  | 26:a:1595:C:H6    | 1.82                     | 0.44              |
| 33:h:8:LYS:HZ1   | 33:h:14:SER:C     | 2.26                     | 0.44              |
| 40:o:14:LYS:HD2  | 40:o:77:HIS:HA    | 1.98                     | 0.44              |
| 43:r:4:ILE:HG22  | 43:r:106:VAL:HG22 | 1.98                     | 0.44              |
| 1:A:181:A:H61    | 1:A:194:C:H2'     | 1.83                     | 0.44              |
| 1:A:672:U:H2'    | 1:A:673:A:C8      | 2.53                     | 0.44              |
| 1:A:845:A:H1'    | 18:R:9:LYS:HZ2    | 1.82                     | 0.44              |
| 1:A:868:C:H2'    | 1:A:869:G:O4'     | 2.18                     | 0.44              |
| 1:A:890:G:O2'    | 1:A:891:U:P       | 2.76                     | 0.44              |
| 1:A:1095:U:H2'   | 1:A:1096:C:H6     | 1.82                     | 0.44              |
| 1:A:1230:C:H2'   | 1:A:1231:G:H8     | 1.83                     | 0.44              |
| 2:B:41:ILE:HG21  | 2:B:202:GLY:HA2   | 1.99                     | 0.44              |
| 3:C:22:TRP:NE1   | 3:C:36:ASP:OD2    | 2.50                     | 0.44              |
| 21:U:40:LYS:HB2  | 21:U:40:LYS:HE3   | 1.74                     | 0.44              |
| 25:Y:14:LYS:HE3  | 25:Y:14:LYS:HB3   | 1.45                     | 0.44              |
| 26:a:373:U:H2'   | 26:a:374:A:C8     | 2.50                     | 0.44              |
| 26:a:602:A:O2'   | 26:a:604:G:O2'    | 2.29                     | 0.44              |
| 26:a:813:U:H2'   | 26:a:814:C:C6     | 2.51                     | 0.44              |
| 26:a:1565:C:O2'  | 26:a:1566:A:H8    | 2.01                     | 0.44              |
| 26:a:1914:C:OP2  | 26:a:1915:3TD:H10 | 2.16                     | 0.44              |
| 26:a:2040:G:H2'  | 26:a:2041:U:O4'   | 2.18                     | 0.44              |
| 31:f:38:MET:SD   | 31:f:53:ALA:HB1   | 2.57                     | 0.44              |
| 32:g:115:HIS:HB2 | 32:g:151:TYR:HE2  | 1.82                     | 0.44              |
| 38:m:47:VAL:O    | 38:m:51:LEU:HD23  | 2.17                     | 0.44              |
| 1:A:579:A:O2'    | 15:O:54:ARG:NH1   | 2.50                     | 0.44              |
| 1:A:579:A:H2'    | 1:A:580:C:C6      | 2.52                     | 0.44              |
| 1:A:632:U:H3'    | 1:A:633:G:H5'     | 1.98                     | 0.44              |
| 4:D:28:ILE:HD11  | 4:D:34:ILE:HD12   | 2.00                     | 0.44              |
| 9:I:5:GLN:HG2    | 9:I:22:LYS:CE     | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:Y:13:LEU:HD23  | 25:Y:13:LEU:HA    | 1.86                     | 0.44              |
| 25:Y:70:VAL:CG1   | 25:Y:88:LYS:HG3   | 2.48                     | 0.44              |
| 26:a:492:A:H2'    | 26:a:493:G:O4'    | 2.18                     | 0.44              |
| 26:a:801:G:C8     | 30:e:50:ALA:HB2   | 2.53                     | 0.44              |
| 26:a:941:A:H2'    | 26:a:942:G:O4'    | 2.17                     | 0.44              |
| 26:a:2017:U:H4'   | 51:z:5:GLN:O      | 2.17                     | 0.44              |
| 26:a:2562:U:OP1   | 35:j:40:LYS:NZ    | 2.42                     | 0.44              |
| 28:c:132:MET:HE1  | 28:c:144:VAL:HG13 | 1.99                     | 0.44              |
| 38:m:24:MET:HE3   | 38:m:36:THR:HG21  | 1.99                     | 0.44              |
| 38:m:38:LEU:HB3   | 38:m:39:PRO:HD3   | 2.00                     | 0.44              |
| 56:4:35:ASP:OD1   | 56:4:36:VAL:N     | 2.51                     | 0.44              |
| 1:A:581:G:N2      | 1:A:759:A:OP2     | 2.46                     | 0.44              |
| 1:A:599:C:H2'     | 1:A:600:A:H8      | 1.82                     | 0.44              |
| 1:A:1008:U:H2'    | 1:A:1009:U:H6     | 1.83                     | 0.44              |
| 1:A:1179:A:H2'    | 1:A:1180:A:O4'    | 2.18                     | 0.44              |
| 1:A:1412:C:H2'    | 1:A:1413:A:C8     | 2.53                     | 0.44              |
| 21:U:62:ARG:O     | 21:U:62:ARG:CG    | 2.65                     | 0.44              |
| 22:V:64:G:H5''    | 47:v:11:ARG:NH1   | 2.32                     | 0.44              |
| 23:W:63:C:H2'     | 23:W:64:G:C8      | 2.53                     | 0.44              |
| 25:Y:112:ILE:HD11 | 25:Y:170:ARG:HG3  | 2.00                     | 0.44              |
| 25:Y:135:LEU:HB2  | 25:Y:139:ARG:HH22 | 1.82                     | 0.44              |
| 26:a:1073:A:N6    | 26:a:1074:G:N3    | 2.66                     | 0.44              |
| 26:a:1827:U:H2'   | 26:a:1828:G:O4'   | 2.18                     | 0.44              |
| 26:a:2305:U:C2    | 31:f:151:GLY:HA3  | 2.53                     | 0.44              |
| 26:a:2392:A:C2    | 36:k:55:MET:HE3   | 2.53                     | 0.44              |
| 26:a:2474:U:OP2   | 26:a:2475:C:N4    | 2.35                     | 0.44              |
| 26:a:2547:A:H2'   | 26:a:2548:U:C6    | 2.53                     | 0.44              |
| 37:l:33:LEU:HD13  | 37:l:172:PHE:HB3  | 2.00                     | 0.44              |
| 43:r:10:ALA:O     | 43:r:12:SER:N     | 2.49                     | 0.44              |
| 1:A:838:G:C6      | 1:A:849:G:C6      | 3.06                     | 0.44              |
| 1:A:1074:G:O2'    | 2:B:102:THR:OG1   | 2.29                     | 0.44              |
| 1:A:1095:U:P      | 1:A:1108:G:H1     | 2.41                     | 0.44              |
| 1:A:1220:G:O2'    | 19:S:52:HIS:ND1   | 2.40                     | 0.44              |
| 6:F:70:VAL:HA     | 6:F:73:GLU:OE1    | 2.17                     | 0.44              |
| 11:K:27:PHE:HE1   | 21:U:33:ARG:NH2   | 2.05                     | 0.44              |
| 12:L:16:VAL:HG23  | 12:L:17:ALA:H     | 1.83                     | 0.44              |
| 25:Y:5:PHE:C      | 25:Y:7:GLN:H      | 2.24                     | 0.44              |
| 25:Y:12:SER:O     | 25:Y:15:GLU:HB3   | 2.18                     | 0.44              |
| 25:Y:83:LEU:HB3   | 25:Y:84:LEU:H     | 1.58                     | 0.44              |
| 26:a:2692:G:H1'   | 26:a:2847:U:H1'   | 1.99                     | 0.44              |
| 29:d:25:THR:HG21  | 29:d:193:VAL:HG22 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:h:57:LYS:C     | 33:h:61:VAL:HG22  | 2.43                     | 0.44              |
| 33:h:69:ALA:HB3   | 33:h:134:VAL:HG21 | 2.00                     | 0.44              |
| 1:A:45:G:H2'      | 1:A:46:G:H8       | 1.83                     | 0.44              |
| 1:A:1371:G:O3'    | 9:I:71:GLY:HA3    | 2.18                     | 0.44              |
| 1:A:1402:4OC:HM23 | 1:A:1402:4OC:H1'  | 1.77                     | 0.44              |
| 1:A:1539:C:H42    | 24:X:2:G:H1       | 1.65                     | 0.44              |
| 3:C:114:LYS:HB2   | 3:C:185:ASN:ND2   | 2.32                     | 0.44              |
| 8:H:11:LEU:HD12   | 8:H:77:ARG:HB2    | 2.00                     | 0.44              |
| 9:I:87:LEU:HA     | 9:I:90:TYR:HB3    | 2.00                     | 0.44              |
| 11:K:63:ALA:HB1   | 11:K:96:THR:OG1   | 2.18                     | 0.44              |
| 11:K:64:GLN:HG3   | 11:K:99:ALA:HB2   | 1.99                     | 0.44              |
| 22:V:48:U:H5''    | 22:V:49:C:H5'     | 2.00                     | 0.44              |
| 25:Y:128:ARG:HE   | 25:Y:128:ARG:HB3  | 1.64                     | 0.44              |
| 25:Y:158:LYS:HB3  | 25:Y:158:LYS:HE3  | 1.30                     | 0.44              |
| 26:a:138:U:O2'    | 26:a:140:C:OP1    | 2.30                     | 0.44              |
| 26:a:910:A:H2'    | 26:a:911:A:C8     | 2.53                     | 0.44              |
| 26:a:1056:G:H5''  | 26:a:1057:A:OP1   | 2.18                     | 0.44              |
| 26:a:1064:C:H42   | 26:a:1074:G:H1    | 1.66                     | 0.44              |
| 26:a:1299:G:N1    | 26:a:1640:A:OP2   | 2.25                     | 0.44              |
| 26:a:1581:G:H2'   | 26:a:1582:C:O4'   | 2.16                     | 0.44              |
| 26:a:2837:A:H2'   | 26:a:2838:G:H8    | 1.82                     | 0.44              |
| 26:a:2850:A:H2'   | 26:a:2851:A:C8    | 2.53                     | 0.44              |
| 31:f:50:LEU:HD21  | 31:f:67:ILE:HG23  | 1.99                     | 0.44              |
| 31:f:117:LEU:HD12 | 31:f:176:PRO:HG2  | 1.98                     | 0.44              |
| 32:g:98:VAL:HG23  | 32:g:125:CYS:SG   | 2.58                     | 0.44              |
| 33:h:4:ILE:HG22   | 33:h:37:VAL:O     | 2.17                     | 0.44              |
| 33:h:57:LYS:O     | 33:h:58:LEU:C     | 2.61                     | 0.44              |
| 33:h:80:ILE:CG2   | 33:h:146:VAL:HG22 | 2.48                     | 0.44              |
| 1:A:31:G:C8       | 1:A:306:A:H1'     | 2.53                     | 0.43              |
| 1:A:875:U:O2'     | 8:H:15:ARG:HD2    | 2.18                     | 0.43              |
| 1:A:1226:C:H4'    | 19:S:80:TYR:CZ    | 2.52                     | 0.43              |
| 6:F:40:GLU:OE1    | 6:F:42:TRP:CD1    | 2.71                     | 0.43              |
| 6:F:69:GLU:O      | 6:F:73:GLU:OE1    | 2.35                     | 0.43              |
| 6:F:90:MET:CE     | 18:R:61:ARG:HH11  | 2.28                     | 0.43              |
| 7:G:26:PHE:CE2    | 7:G:120:LEU:HD21  | 2.53                     | 0.43              |
| 15:O:36:ILE:O     | 15:O:40:GLN:HG2   | 2.18                     | 0.43              |
| 16:P:21:VAL:HG11  | 16:P:60:TRP:NE1   | 2.33                     | 0.43              |
| 26:a:27:G:O2'     | 26:a:28:A:OP2     | 2.28                     | 0.43              |
| 26:a:538:A:H5''   | 34:i:7:LYS:HE3    | 2.00                     | 0.43              |
| 26:a:1099:G:H8    | 26:a:1099:G:OP2   | 2.00                     | 0.43              |
| 26:a:1255:U:C5    | 30:e:68:ALA:HA    | 2.53                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:a:1889:A:H2'    | 26:a:1890:A:H8    | 1.83                     | 0.43              |
| 26:a:2137:U:O2'    | 26:a:2153:C:H2'   | 2.18                     | 0.43              |
| 26:a:2455:G:H2'    | 26:a:2456:C:C6    | 2.53                     | 0.43              |
| 26:a:2801:G:H2'    | 26:a:2802:A:H8    | 1.83                     | 0.43              |
| 26:a:2809:A:H2'    | 26:a:2810:A:C8    | 2.53                     | 0.43              |
| 28:c:205:LEU:HB3   | 28:c:210:ALA:HB3  | 2.00                     | 0.43              |
| 30:e:48:THR:HG23   | 30:e:86:ALA:HB3   | 2.00                     | 0.43              |
| 31:f:100:PHE:CZ    | 31:f:104:ILE:HD11 | 2.52                     | 0.43              |
| 1:A:79:G:H2'       | 1:A:80:A:C8       | 2.53                     | 0.43              |
| 1:A:889:A:H8       | 1:A:889:A:OP1     | 2.01                     | 0.43              |
| 5:E:107:ALA:HB1    | 5:E:111:MET:HB2   | 2.00                     | 0.43              |
| 7:G:54:SER:OG      | 7:G:55:GLY:N      | 2.50                     | 0.43              |
| 10:J:37:ARG:HB2    | 10:J:75:ASP:HB2   | 1.99                     | 0.43              |
| 17:Q:6:ARG:C       | 17:Q:7:THR:CG2    | 2.91                     | 0.43              |
| 17:Q:52:GLU:N      | 17:Q:52:GLU:OE1   | 2.51                     | 0.43              |
| 26:a:8:C:H2'       | 26:a:9:G:O4'      | 2.17                     | 0.43              |
| 26:a:1412:U:H2'    | 26:a:1413:A:H8    | 1.83                     | 0.43              |
| 26:a:2202:U:O2'    | 26:a:2204:G:OP1   | 2.33                     | 0.43              |
| 26:a:2286:G:H5''   | 26:a:2287:A:OP1   | 2.18                     | 0.43              |
| 26:a:2316:G:H2'    | 26:a:2317:A:H8    | 1.83                     | 0.43              |
| 26:a:2513:A:C6     | 26:a:2574:G:C6    | 3.06                     | 0.43              |
| 26:a:2552:OMU:HM23 | 26:a:2552:OMU:H1' | 1.61                     | 0.43              |
| 26:a:2609:U:H5'    | 26:a:2610:C:OP2   | 2.18                     | 0.43              |
| 26:a:2700:A:H2'    | 26:a:2701:U:H6    | 1.83                     | 0.43              |
| 33:h:54:LEU:HB2    | 33:h:55:GLU:OE1   | 2.18                     | 0.43              |
| 37:l:53:MET:HE2    | 37:l:53:MET:HB3   | 1.79                     | 0.43              |
| 1:A:739:C:P        | 6:F:2:ARG:HH22    | 2.40                     | 0.43              |
| 1:A:1008:U:H2'     | 1:A:1009:U:C6     | 2.53                     | 0.43              |
| 1:A:1320:C:O2      | 19:S:36:ARG:NH2   | 2.51                     | 0.43              |
| 2:B:7:ARG:HA       | 2:B:7:ARG:CZ      | 2.48                     | 0.43              |
| 4:D:159:LEU:O      | 4:D:163:GLU:HG2   | 2.18                     | 0.43              |
| 5:E:76:LEU:HD23    | 5:E:76:LEU:HA     | 1.82                     | 0.43              |
| 12:L:90:LEU:HA     | 12:L:91:PRO:HD3   | 1.88                     | 0.43              |
| 22:V:9:G:O2'       | 22:V:10:G:N7      | 2.48                     | 0.43              |
| 26:a:30:G:O2'      | 26:a:1214:A:N3    | 2.40                     | 0.43              |
| 26:a:217:A:H2'     | 26:a:218:A:C8     | 2.53                     | 0.43              |
| 26:a:219:A:H2'     | 26:a:220:G:O4'    | 2.18                     | 0.43              |
| 26:a:846:C:O2'     | 26:a:847:U:O5'    | 2.36                     | 0.43              |
| 26:a:884:U:N3      | 26:a:893:C:C2     | 2.76                     | 0.43              |
| 26:a:1080:A:H1'    | 26:a:1081:U:N3    | 2.33                     | 0.43              |
| 26:a:1587:G:H2'    | 26:a:1588:G:C8    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:a:1751:U:H2'  | 26:a:1752:C:C6   | 2.53                     | 0.43              |
| 26:a:1918:A:O2'  | 26:a:1920:C:N4   | 2.51                     | 0.43              |
| 26:a:2514:U:H2'  | 26:a:2515:C:H6   | 1.80                     | 0.43              |
| 26:a:2700:A:H2'  | 26:a:2701:U:C6   | 2.53                     | 0.43              |
| 26:a:2796:C:O2'  | 26:a:2797:U:O5'  | 2.35                     | 0.43              |
| 29:d:10:GLY:HA3  | 40:o:5:ILE:HD11  | 1.99                     | 0.43              |
| 30:e:22:ASP:OD1  | 30:e:22:ASP:N    | 2.48                     | 0.43              |
| 32:g:176:LYS:HG3 | 32:g:177:LYS:HG3 | 1.99                     | 0.43              |
| 33:h:69:ALA:O    | 33:h:73:ASN:N    | 2.28                     | 0.43              |
| 35:j:93:GLN:HG3  | 35:j:114:LYS:HE3 | 2.00                     | 0.43              |
| 40:o:27:GLU:HG2  | 40:o:87:LYS:HE2  | 2.00                     | 0.43              |
| 43:r:24:ILE:HD13 | 43:r:36:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:137:U:H3     | 1:A:226:G:H1     | 1.66                     | 0.43              |
| 1:A:404:G:O2'    | 1:A:498:A:N1     | 2.45                     | 0.43              |
| 1:A:415:A:C4     | 1:A:416:G:C8     | 3.06                     | 0.43              |
| 1:A:1143:G:H2'   | 1:A:1144:G:C8    | 2.53                     | 0.43              |
| 1:A:1148:U:H2'   | 1:A:1149:C:O4'   | 2.19                     | 0.43              |
| 1:A:1306:A:N6    | 1:A:1331:G:H1'   | 2.33                     | 0.43              |
| 1:A:1458:G:OP1   | 20:T:30:THR:OG1  | 2.21                     | 0.43              |
| 1:A:1522:U:H2'   | 1:A:1523:G:H8    | 1.82                     | 0.43              |
| 4:D:121:LYS:HG2  | 4:D:131:ASN:HB3  | 2.00                     | 0.43              |
| 5:E:55:GLU:HG3   | 5:E:57:PRO:HD2   | 1.99                     | 0.43              |
| 23:W:77:A:H5''   | 48:w:22:LEU:CD2  | 2.49                     | 0.43              |
| 26:a:64:A:H2'    | 26:a:65:U:H6     | 1.83                     | 0.43              |
| 26:a:225:C:H2'   | 26:a:226:A:O4'   | 2.19                     | 0.43              |
| 26:a:356:G:H2'   | 26:a:357:C:H6    | 1.84                     | 0.43              |
| 26:a:851:C:H2'   | 26:a:852:U:C6    | 2.53                     | 0.43              |
| 26:a:852:U:H2'   | 26:a:853:C:H6    | 1.84                     | 0.43              |
| 26:a:1075:C:H5'' | 26:a:1076:C:C5   | 2.53                     | 0.43              |
| 26:a:1604:C:O2'  | 26:a:1610:A:N1   | 2.38                     | 0.43              |
| 26:a:1683:U:H2'  | 26:a:1684:G:H8   | 1.83                     | 0.43              |
| 26:a:1734:C:H2'  | 26:a:1735:G:C8   | 2.52                     | 0.43              |
| 37:l:36:VAL:HG22 | 46:u:82:TYR:HB2  | 1.99                     | 0.43              |
| 38:m:55:ALA:HA   | 38:m:80:PHE:CE1  | 2.54                     | 0.43              |
| 56:4:20:ASN:HD22 | 56:4:39:LYS:HD3  | 1.83                     | 0.43              |
| 1:A:161:A:H2'    | 1:A:162:A:C8     | 2.53                     | 0.43              |
| 1:A:821:G:H2'    | 1:A:822:U:C6     | 2.54                     | 0.43              |
| 1:A:881:G:H2'    | 1:A:882:C:O4'    | 2.18                     | 0.43              |
| 1:A:1150:A:H4'   | 10:J:43:PRO:HG3  | 2.00                     | 0.43              |
| 5:E:77:ASN:ND2   | 5:E:82:GLN:OE1   | 2.47                     | 0.43              |
| 7:G:108:ALA:O    | 7:G:119:ARG:HD2  | 2.17                     | 0.43              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 26:a:659:G:O2'  | 30:e:95:LYS:O     | 2.36                     | 0.43              |
| 26:a:1196:C:C2  | 26:a:1197:G:C8    | 3.07                     | 0.43              |
| 26:a:1932:A:H2' | 26:a:1933:G:O4'   | 2.19                     | 0.43              |
| 26:a:2752:C:H2' | 26:a:2753:A:O4'   | 2.19                     | 0.43              |
| 27:b:14:U:OP2   | 27:b:70:C:O2'     | 2.33                     | 0.43              |
| 27:b:35:C:H2'   | 27:b:36:C:H4'     | 2.00                     | 0.43              |
| 31:f:119:ALA:O  | 31:f:167:ARG:NH1  | 2.49                     | 0.43              |
| 33:h:53:GLU:N   | 33:h:53:GLU:OE2   | 2.52                     | 0.43              |
| 37:l:69:PRO:HA  | 37:l:149:ALA:HB2  | 2.00                     | 0.43              |
| 1:A:428:G:OP2   | 4:D:7:PRO:HG2     | 2.18                     | 0.43              |
| 1:A:490:C:C2    | 1:A:491:G:C8      | 3.07                     | 0.43              |
| 1:A:866:C:C4    | 1:A:867:G:H1'     | 2.54                     | 0.43              |
| 1:A:1441:A:N3   | 40:o:114:LEU:HD11 | 2.33                     | 0.43              |
| 4:D:194:ASP:OD1 | 4:D:194:ASP:N     | 2.51                     | 0.43              |
| 21:U:4:ILE:HD11 | 21:U:18:ARG:CZ    | 2.49                     | 0.43              |
| 23:W:14:A:H3'   | 23:W:15:G:H8      | 1.82                     | 0.43              |
| 26:a:181:A:H1'  | 26:a:435:C:H5'    | 2.01                     | 0.43              |
| 26:a:279:A:H2'  | 26:a:279:A:N3     | 2.33                     | 0.43              |
| 26:a:1364:G:OP2 | 48:w:50:ARG:NH1   | 2.43                     | 0.43              |
| 26:a:2572:A:N6  | 29:d:150:MEQ:HE1  | 2.33                     | 0.43              |
| 33:h:1:MET:O    | 33:h:20:ASN:HA    | 2.18                     | 0.43              |
| 42:q:6:GLN:HB3  | 42:q:37:GLU:CG    | 2.49                     | 0.43              |
| 49:x:10:SER:OG  | 49:x:11:VAL:N     | 2.51                     | 0.43              |
| 52:0:7:GLU:HB2  | 52:0:27:LYS:HZ3   | 1.84                     | 0.43              |
| 1:A:427:U:H3'   | 1:A:428:G:H2'     | 2.00                     | 0.43              |
| 1:A:1314:C:H2'  | 1:A:1315:U:H6     | 1.83                     | 0.43              |
| 1:A:1376:U:H2'  | 1:A:1377:A:C8     | 2.54                     | 0.43              |
| 3:C:72:ARG:HD3  | 3:C:75:ILE:HG13   | 2.01                     | 0.43              |
| 3:C:121:THR:O   | 3:C:125:GLU:HG3   | 2.19                     | 0.43              |
| 4:D:4:TYR:CE2   | 4:D:11:LEU:HD11   | 2.53                     | 0.43              |
| 6:F:35:LYS:O    | 6:F:65:GLU:N      | 2.48                     | 0.43              |
| 9:I:51:PRO:O    | 9:I:55:VAL:HG12   | 2.19                     | 0.43              |
| 26:a:754:U:H2'  | 26:a:755:U:C6     | 2.54                     | 0.43              |
| 26:a:794:A:H2'  | 26:a:795:C:C6     | 2.53                     | 0.43              |
| 26:a:1657:U:H2' | 26:a:1658:C:H6    | 1.83                     | 0.43              |
| 26:a:2107:G:C2  | 26:a:2108:A:H1'   | 2.54                     | 0.43              |
| 26:a:2391:G:H2' | 26:a:2424:C:N4    | 2.31                     | 0.43              |
| 26:a:2459:A:H2  | 37:l:78:LEU:HD11  | 1.83                     | 0.43              |
| 27:b:108:A:O2'  | 27:b:109:A:OP2    | 2.32                     | 0.43              |
| 38:m:2:ARG:NH2  | 38:m:5:LYS:O      | 2.52                     | 0.43              |
| 38:m:24:MET:HE1 | 38:m:40:LYS:HB3   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:u:28:ALA:HB3  | 46:u:40:ILE:HG13 | 2.00                     | 0.43              |
| 54:2:17:THR:OG1  | 54:2:18:GLY:N    | 2.52                     | 0.43              |
| 1:A:91:U:H2'     | 1:A:92:U:C6      | 2.54                     | 0.43              |
| 1:A:140:U:H3     | 1:A:223:A:H62    | 1.66                     | 0.43              |
| 1:A:323:U:H2'    | 1:A:324:G:O4'    | 2.18                     | 0.43              |
| 1:A:939:G:H21    | 1:A:1375:A:H2    | 1.65                     | 0.43              |
| 4:D:170:TRP:CD2  | 4:D:186:PRO:HB3  | 2.54                     | 0.43              |
| 5:E:147:MET:HE2  | 5:E:147:MET:HB3  | 1.79                     | 0.43              |
| 10:J:15:HIS:HA   | 10:J:18:ILE:HG22 | 2.00                     | 0.43              |
| 10:J:35:GLN:HE22 | 10:J:77:VAL:HB   | 1.82                     | 0.43              |
| 10:J:53:ILE:HD11 | 10:J:61:ALA:HB1  | 2.00                     | 0.43              |
| 26:a:499:U:H2'   | 26:a:500:G:O4'   | 2.19                     | 0.43              |
| 26:a:570:G:H2'   | 26:a:2030:6MZ:N7 | 2.34                     | 0.43              |
| 26:a:742:A:H2'   | 26:a:743:A:C8    | 2.54                     | 0.43              |
| 26:a:852:U:H2'   | 26:a:853:C:C6    | 2.53                     | 0.43              |
| 26:a:891:G:N1    | 26:a:892:A:N7    | 2.66                     | 0.43              |
| 26:a:2674:G:H2'  | 26:a:2675:A:C8   | 2.54                     | 0.43              |
| 28:c:96:TYR:HE1  | 28:c:102:ARG:HD2 | 1.83                     | 0.43              |
| 28:c:227:PRO:HG3 | 28:c:234:GLY:HA3 | 2.00                     | 0.43              |
| 30:e:73:ILE:HG13 | 30:e:78:TRP:CZ3  | 2.54                     | 0.43              |
| 41:p:78:LYS:HE3  | 41:p:78:LYS:HB3  | 1.81                     | 0.43              |
| 1:A:140:U:H3     | 1:A:223:A:N6     | 2.17                     | 0.43              |
| 1:A:363:A:C6     | 12:L:28:PRO:HD2  | 2.54                     | 0.43              |
| 1:A:678:U:H2'    | 1:A:679:C:H6     | 1.84                     | 0.43              |
| 1:A:1157:A:C2    | 1:A:1181:G:C4    | 3.06                     | 0.43              |
| 21:U:69:ARG:HA   | 21:U:69:ARG:HD2  | 1.54                     | 0.43              |
| 26:a:532:A:H2'   | 26:a:532:A:N3    | 2.34                     | 0.43              |
| 26:a:1799:G:O2'  | 28:c:180:GLU:OE2 | 2.32                     | 0.43              |
| 32:g:42:GLU:CB   | 32:g:55:ARG:HE   | 2.31                     | 0.43              |
| 38:m:69:ARG:O    | 38:m:71:ARG:N    | 2.50                     | 0.43              |
| 56:4:3:LYS:O     | 56:4:5:ILE:N     | 2.49                     | 0.43              |
| 56:4:41:HIS:HB3  | 56:4:44:PHE:HD1  | 1.84                     | 0.43              |
| 1:A:26:A:N6      | 1:A:558:G:H1'    | 2.34                     | 0.43              |
| 1:A:1120:U:H2'   | 1:A:1121:U:C6    | 2.53                     | 0.43              |
| 1:A:1163:A:H2'   | 1:A:1164:G:C8    | 2.54                     | 0.43              |
| 1:A:1536:C:H2'   | 1:A:1537:U:C6    | 2.53                     | 0.43              |
| 16:P:54:LEU:HD11 | 16:P:75:ILE:HG23 | 2.01                     | 0.43              |
| 20:T:35:VAL:HG12 | 20:T:79:LEU:HD22 | 2.00                     | 0.43              |
| 25:Y:53:PHE:HB3  | 25:Y:62:ILE:HD12 | 2.01                     | 0.43              |
| 26:a:240:C:OP2   | 26:a:241:A:O2'   | 2.34                     | 0.43              |
| 26:a:558:U:H2'   | 26:a:559:G:H8    | 1.83                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:a:1248:G:P     | 30:e:44:ARG:HH22 | 2.38                     | 0.43              |
| 26:a:1532:A:C6    | 26:a:1540:G:C6   | 3.07                     | 0.43              |
| 26:a:2271:G:OP1   | 47:v:18:ALA:HB1  | 2.19                     | 0.43              |
| 26:a:2412:A:H2'   | 26:a:2413:G:O4'  | 2.19                     | 0.43              |
| 26:a:2743:U:OP2   | 26:a:2755:C:N4   | 2.52                     | 0.43              |
| 35:j:58:LEU:HA    | 35:j:89:ASN:ND2  | 2.34                     | 0.43              |
| 37:l:190:VAL:HG13 | 37:l:191:MET:HG3 | 2.00                     | 0.43              |
| 50:y:19:LYS:HB2   | 50:y:19:LYS:HE3  | 1.77                     | 0.43              |
| 1:A:410:G:N1      | 1:A:431:A:OP2    | 2.30                     | 0.42              |
| 1:A:842:U:H2'     | 1:A:844:G:OP2    | 2.19                     | 0.42              |
| 1:A:1034:G:C2     | 1:A:1035:A:C8    | 3.07                     | 0.42              |
| 1:A:1512:U:H2'    | 1:A:1513:A:H8    | 1.83                     | 0.42              |
| 7:G:143:ARG:HH11  | 23:W:43:G:H5'    | 1.83                     | 0.42              |
| 9:I:72:ILE:H      | 9:I:72:ILE:HD12  | 1.83                     | 0.42              |
| 20:T:78:ASN:O     | 20:T:82:GLN:HG2  | 2.19                     | 0.42              |
| 26:a:304:U:H2'    | 26:a:305:C:C6    | 2.54                     | 0.42              |
| 26:a:971:G:OP1    | 26:a:974:G:O2'   | 2.35                     | 0.42              |
| 26:a:1054:A:C2    | 26:a:1106:G:C6   | 3.07                     | 0.42              |
| 26:a:1075:C:H3'   | 26:a:1076:C:C6   | 2.53                     | 0.42              |
| 26:a:1087:G:O6    | 26:a:1090:A:N6   | 2.52                     | 0.42              |
| 26:a:1428:C:C5    | 26:a:1569:A:H5'' | 2.54                     | 0.42              |
| 26:a:1779:U:C5    | 26:a:1784:A:N7   | 2.85                     | 0.42              |
| 26:a:2130:U:H5'   | 26:a:2159:G:H22  | 1.83                     | 0.42              |
| 26:a:2163:A:H2'   | 26:a:2164:C:H5'  | 2.00                     | 0.42              |
| 26:a:2184:A:H8    | 26:a:2185:U:C5   | 2.35                     | 0.42              |
| 26:a:2262:U:H2'   | 26:a:2263:C:H6   | 1.84                     | 0.42              |
| 26:a:2516:A:O2'   | 26:a:2517:C:H5'  | 2.19                     | 0.42              |
| 1:A:186:C:H2'     | 1:A:187:G:C8     | 2.54                     | 0.42              |
| 1:A:401:C:OP2     | 4:D:70:ARG:NH1   | 2.52                     | 0.42              |
| 1:A:438:U:O2'     | 1:A:439:U:P      | 2.76                     | 0.42              |
| 1:A:438:U:HO2'    | 1:A:439:U:P      | 2.42                     | 0.42              |
| 1:A:1004:A:C6     | 1:A:1026:G:H1'   | 2.54                     | 0.42              |
| 1:A:1007:U:H2'    | 1:A:1008:U:H6    | 1.84                     | 0.42              |
| 4:D:35:GLU:H      | 4:D:35:GLU:CD    | 2.26                     | 0.42              |
| 10:J:7:ARG:HD3    | 10:J:7:ARG:HA    | 1.88                     | 0.42              |
| 14:N:34:VAL:HG23  | 14:N:35:ASN:OD1  | 2.19                     | 0.42              |
| 25:Y:81:GLU:H     | 25:Y:81:GLU:HG2  | 1.58                     | 0.42              |
| 25:Y:121:THR:C    | 25:Y:128:ARG:HG2 | 2.44                     | 0.42              |
| 26:a:205:G:O2'    | 26:a:206:U:OP2   | 2.37                     | 0.42              |
| 26:a:246:C:O2'    | 26:a:385:C:H4'   | 2.19                     | 0.42              |
| 26:a:621:A:OP2    | 36:k:99:ASN:ND2  | 2.52                     | 0.42              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 26:a:835:C:C2   | 26:a:836:G:C8     | 3.07                     | 0.42              |
| 26:a:919:U:H2'  | 26:a:920:A:O4'    | 2.19                     | 0.42              |
| 26:a:947:A:H2'  | 26:a:948:C:C6     | 2.54                     | 0.42              |
| 26:a:1104:C:H2' | 26:a:1105:U:C5    | 2.54                     | 0.42              |
| 26:a:1171:G:O6  | 26:a:1178:C:H2'   | 2.18                     | 0.42              |
| 26:a:2144:G:N3  | 26:a:2146:C:H1'   | 2.34                     | 0.42              |
| 27:b:5:U:H2'    | 27:b:6:G:C8       | 2.51                     | 0.42              |
| 32:g:140:VAL:O  | 32:g:144:VAL:HG23 | 2.18                     | 0.42              |
| 47:v:53:CYS:SG  | 47:v:57:HIS:HA    | 2.58                     | 0.42              |
| 1:A:17:U:H2'    | 1:A:18:C:H6       | 1.84                     | 0.42              |
| 1:A:474:G:H2'   | 1:A:475:C:O4'     | 2.18                     | 0.42              |
| 1:A:1397:C:P    | 5:E:29:ARG:HH22   | 2.41                     | 0.42              |
| 5:E:80:THR:OG1  | 5:E:122:ASN:O     | 2.27                     | 0.42              |
| 26:a:150:U:H2'  | 26:a:151:C:H6     | 1.84                     | 0.42              |
| 26:a:160:A:N3   | 26:a:2208:C:O2'   | 2.45                     | 0.42              |
| 26:a:638:G:H2'  | 26:a:639:U:C6     | 2.55                     | 0.42              |
| 26:a:674:G:H5'' | 30:e:71:GLY:N     | 2.34                     | 0.42              |
| 26:a:807:U:O2'  | 26:a:2060:A:N1    | 2.50                     | 0.42              |
| 26:a:818:G:N1   | 26:a:1188:U:OP2   | 2.36                     | 0.42              |
| 26:a:894:U:O2'  | 26:a:895:U:H2'    | 2.19                     | 0.42              |
| 26:a:964:C:O2   | 26:a:2273:A:H2    | 2.02                     | 0.42              |
| 26:a:2187:U:H2' | 26:a:2188:U:C6    | 2.54                     | 0.42              |
| 26:a:2191:A:H2' | 26:a:2192:U:C6    | 2.54                     | 0.42              |
| 26:a:2294:G:OP1 | 39:n:10:ARG:HD2   | 2.19                     | 0.42              |
| 26:a:2591:C:H2' | 26:a:2592:G:H8    | 1.84                     | 0.42              |
| 30:e:6:LYS:HE2  | 30:e:6:LYS:HB2    | 1.88                     | 0.42              |
| 1:A:844:G:H1    | 25:Y:96:ILE:CG2   | 2.32                     | 0.42              |
| 1:A:908:A:H2'   | 1:A:909:A:C8      | 2.54                     | 0.42              |
| 2:B:42:ASN:C    | 2:B:44:GLU:H      | 2.26                     | 0.42              |
| 3:C:88:ARG:HG3  | 3:C:101:ILE:HG12  | 2.01                     | 0.42              |
| 7:G:59:LEU:O    | 7:G:63:GLU:HG2    | 2.19                     | 0.42              |
| 8:H:66:PHE:O    | 8:H:68:GLY:N      | 2.53                     | 0.42              |
| 19:S:36:ARG:NH2 | 19:S:72:GLY:O     | 2.53                     | 0.42              |
| 19:S:44:MET:HB3 | 19:S:62:VAL:HG11  | 2.01                     | 0.42              |
| 26:a:144:A:H2'  | 26:a:145:C:C6     | 2.53                     | 0.42              |
| 26:a:532:A:H4'  | 26:a:533:G:C8     | 2.54                     | 0.42              |
| 26:a:709:U:H2'  | 26:a:710:U:C6     | 2.55                     | 0.42              |
| 26:a:901:C:C4   | 26:a:902:C:C4     | 3.07                     | 0.42              |
| 26:a:934:U:H2'  | 26:a:935:C:C6     | 2.54                     | 0.42              |
| 26:a:1433:A:H2' | 26:a:1434:A:O4'   | 2.18                     | 0.42              |
| 26:a:1440:U:H2' | 26:a:1441:G:C8    | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:a:2808:G:O2'  | 26:a:2809:A:P    | 2.78                     | 0.42              |
| 31:f:4:LEU:HD23  | 31:f:4:LEU:HA    | 1.87                     | 0.42              |
| 33:h:90:LEU:HD21 | 33:h:92:GLY:O    | 2.18                     | 0.42              |
| 41:p:80:ILE:HG22 | 41:p:84:LYS:HE2  | 2.02                     | 0.42              |
| 1:A:171:A:H2'    | 1:A:172:A:C8     | 2.55                     | 0.42              |
| 1:A:1374:A:C6    | 1:A:1375:A:C6    | 3.08                     | 0.42              |
| 2:B:223:GLU:OE1  | 2:B:223:GLU:N    | 2.52                     | 0.42              |
| 19:S:13:LEU:O    | 19:S:17:LYS:HG2  | 2.20                     | 0.42              |
| 19:S:36:ARG:HB3  | 19:S:72:GLY:HA3  | 2.01                     | 0.42              |
| 20:T:28:MET:HG3  | 20:T:58:VAL:HG12 | 2.00                     | 0.42              |
| 26:a:10:A:C6     | 26:a:2800:A:C2   | 3.07                     | 0.42              |
| 26:a:685:A:C8    | 26:a:773:U:C4    | 3.07                     | 0.42              |
| 26:a:1071:G:OP1  | 26:a:1088:A:H2'  | 2.19                     | 0.42              |
| 26:a:1281:G:H2'  | 26:a:1282:U:C6   | 2.54                     | 0.42              |
| 1:A:356:A:N3     | 1:A:368:U:O2'    | 2.43                     | 0.42              |
| 1:A:780:A:H5''   | 11:K:125:LYS:HD3 | 2.00                     | 0.42              |
| 1:A:1258:G:H2'   | 1:A:1259:C:C6    | 2.55                     | 0.42              |
| 25:Y:51:GLU:HA   | 25:Y:56:ALA:HB1  | 2.02                     | 0.42              |
| 26:a:297:G:H2'   | 26:a:298:G:O4'   | 2.20                     | 0.42              |
| 26:a:705:A:C2    | 26:a:727:A:H1'   | 2.54                     | 0.42              |
| 26:a:891:G:N1    | 26:a:892:A:C5    | 2.87                     | 0.42              |
| 26:a:1177:G:H3'  | 26:a:1178:C:H5'' | 2.01                     | 0.42              |
| 26:a:1206:G:O6   | 26:a:1240:U:O2   | 2.38                     | 0.42              |
| 26:a:1841:U:C2   | 26:a:1842:G:C8   | 3.08                     | 0.42              |
| 26:a:2615:U:C2   | 51:z:4:GLN:HA    | 2.54                     | 0.42              |
| 29:d:60:VAL:HG12 | 29:d:65:ALA:HB2  | 2.01                     | 0.42              |
| 32:g:105:LEU:HB2 | 32:g:113:VAL:HB  | 2.02                     | 0.42              |
| 44:s:30:ILE:HD13 | 44:s:93:LEU:HD23 | 2.00                     | 0.42              |
| 49:x:19:LEU:HD23 | 49:x:19:LEU:HA   | 1.85                     | 0.42              |
| 1:A:246:A:N1     | 1:A:278:G:O2'    | 2.47                     | 0.42              |
| 1:A:678:U:H2'    | 1:A:679:C:C6     | 2.54                     | 0.42              |
| 1:A:783:C:H2'    | 1:A:784:A:H8     | 1.85                     | 0.42              |
| 6:F:37:HIS:CD2   | 6:F:65:GLU:HB2   | 2.55                     | 0.42              |
| 7:G:113:ASP:HB3  | 7:G:114:LYS:H    | 1.58                     | 0.42              |
| 8:H:27:MET:HE3   | 8:H:61:LEU:HD13  | 2.02                     | 0.42              |
| 12:L:39:THR:HG22 | 12:L:51:LYS:HG3  | 2.02                     | 0.42              |
| 25:Y:70:VAL:HB   | 25:Y:82:THR:OG1  | 2.20                     | 0.42              |
| 26:a:143:C:H2'   | 26:a:144:A:C8    | 2.55                     | 0.42              |
| 26:a:591:U:C2    | 26:a:592:A:C8    | 3.07                     | 0.42              |
| 26:a:832:U:H2'   | 26:a:833:A:C8    | 2.54                     | 0.42              |
| 26:a:881:G:N1    | 26:a:895:U:N3    | 2.16                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:a:896:A:H2'   | 26:a:897:C:H5'   | 2.02                     | 0.42              |
| 26:a:971:G:O2'   | 26:a:983:A:N3    | 2.47                     | 0.42              |
| 26:a:1283:G:N2   | 26:a:1286:A:H5'  | 2.34                     | 0.42              |
| 26:a:2376:A:H2'  | 26:a:2377:A:O4'  | 2.18                     | 0.42              |
| 26:a:2552:OMU:H5 | 26:a:2556:C:H41  | 1.85                     | 0.42              |
| 26:a:2576:G:H8   | 26:a:2581:G:O6   | 2.02                     | 0.42              |
| 26:a:2576:G:O2'  | 26:a:2579:C:OP2  | 2.34                     | 0.42              |
| 26:a:2895:G:H2'  | 26:a:2896:C:H6   | 1.85                     | 0.42              |
| 31:f:140:GLU:OE1 | 31:f:140:GLU:N   | 2.48                     | 0.42              |
| 1:A:563:A:H2'    | 1:A:567:G:C8     | 2.55                     | 0.42              |
| 1:A:951:G:C6     | 1:A:1231:G:C6    | 3.08                     | 0.42              |
| 1:A:1003:G:N2    | 1:A:1005:A:O5'   | 2.52                     | 0.42              |
| 1:A:1181:G:H1'   | 1:A:1182:G:C4    | 2.55                     | 0.42              |
| 19:S:11:ILE:HB   | 19:S:41:PHE:CE1  | 2.55                     | 0.42              |
| 25:Y:51:GLU:O    | 25:Y:52:GLN:HG3  | 2.19                     | 0.42              |
| 26:a:452:G:N2    | 26:a:457:A:O2'   | 2.53                     | 0.42              |
| 26:a:549:G:H2'   | 26:a:550:C:H6    | 1.83                     | 0.42              |
| 26:a:1038:G:H2'  | 26:a:1039:A:C8   | 2.54                     | 0.42              |
| 26:a:1236:G:O2'  | 26:a:1237:A:H8   | 2.03                     | 0.42              |
| 26:a:1930:G:HO2' | 26:a:1931:U:P    | 2.43                     | 0.42              |
| 26:a:2112:G:O6   | 26:a:2119:A:N7   | 2.53                     | 0.42              |
| 26:a:2144:G:H1'  | 26:a:2147:A:N6   | 2.31                     | 0.42              |
| 26:a:2167:U:H2'  | 26:a:2169:A:OP2  | 2.20                     | 0.42              |
| 26:a:2788:C:H2'  | 26:a:2789:C:C6   | 2.54                     | 0.42              |
| 46:u:75:GLN:HB2  | 46:u:92:VAL:HG23 | 2.01                     | 0.42              |
| 50:y:41:THR:HG22 | 50:y:43:ALA:H    | 1.84                     | 0.42              |
| 1:A:322:C:H2'    | 1:A:323:U:C6     | 2.54                     | 0.42              |
| 1:A:489:C:H2'    | 1:A:490:C:H6     | 1.84                     | 0.42              |
| 1:A:1010:C:H2'   | 1:A:1011:C:C6    | 2.55                     | 0.42              |
| 1:A:1107:C:C4    | 1:A:1108:G:C8    | 3.08                     | 0.42              |
| 1:A:1120:U:C2    | 1:A:1121:U:C5    | 3.08                     | 0.42              |
| 1:A:1147:C:H4'   | 9:I:7:TYR:CE2    | 2.55                     | 0.42              |
| 1:A:1152:A:OP1   | 10:J:70:HIS:ND1  | 2.52                     | 0.42              |
| 1:A:1159:U:C4    | 1:A:1182:G:C4    | 3.08                     | 0.42              |
| 1:A:1176:A:H3'   | 1:A:1177:G:H8    | 1.85                     | 0.42              |
| 1:A:1314:C:H2'   | 1:A:1315:U:C6    | 2.55                     | 0.42              |
| 4:D:19:LEU:HB2   | 4:D:21:LEU:HG    | 2.02                     | 0.42              |
| 6:F:97:THR:HG22  | 6:F:97:THR:O     | 2.20                     | 0.42              |
| 10:J:24:GLU:OE1  | 10:J:90:LEU:HD21 | 2.19                     | 0.42              |
| 10:J:28:THR:HA   | 10:J:31:ARG:HG2  | 2.01                     | 0.42              |
| 18:R:13:PHE:HD1  | 18:R:18:VAL:HG11 | 1.85                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:a:12:U:O2      | 26:a:2626:C:H4'  | 2.20                     | 0.42              |
| 26:a:77:G:H2'     | 26:a:78:U:C6     | 2.55                     | 0.42              |
| 26:a:98:G:H22     | 45:t:7:ARG:NH1   | 2.18                     | 0.42              |
| 26:a:197:A:H2     | 26:a:2434:A:H62  | 1.68                     | 0.42              |
| 26:a:249:C:O2     | 54:2:12:LYS:NZ   | 2.46                     | 0.42              |
| 26:a:708:G:H2'    | 26:a:709:U:C6    | 2.55                     | 0.42              |
| 26:a:878:A:H3'    | 26:a:879:G:C8    | 2.55                     | 0.42              |
| 26:a:882:G:O2'    | 26:a:883:G:O4'   | 2.35                     | 0.42              |
| 26:a:892:A:C8     | 26:a:893:C:C4    | 3.07                     | 0.42              |
| 26:a:1064:C:N4    | 26:a:1074:G:H22  | 2.18                     | 0.42              |
| 26:a:1131:G:N2    | 26:a:1132:U:O4   | 2.47                     | 0.42              |
| 26:a:1408:G:H2'   | 26:a:1409:U:C6   | 2.54                     | 0.42              |
| 26:a:1862:G:H1    | 26:a:1880:U:H3   | 1.66                     | 0.42              |
| 26:a:2101:A:H2'   | 26:a:2102:G:C8   | 2.54                     | 0.42              |
| 26:a:2192:U:H2'   | 26:a:2193:G:H8   | 1.84                     | 0.42              |
| 26:a:2293:G:H2'   | 26:a:2294:G:O4'  | 2.20                     | 0.42              |
| 27:b:39:A:H2'     | 27:b:40:U:C6     | 2.55                     | 0.42              |
| 32:g:60:ASP:OD2   | 32:g:64:GLN:NE2  | 2.48                     | 0.42              |
| 33:h:122:LEU:HB3  | 33:h:128:HIS:CD2 | 2.54                     | 0.42              |
| 34:i:3:THR:HG21   | 41:p:57:PHE:HE1  | 1.85                     | 0.42              |
| 35:j:58:LEU:HA    | 35:j:89:ASN:HD21 | 1.85                     | 0.42              |
| 36:k:121:THR:HG23 | 36:k:121:THR:O   | 2.20                     | 0.42              |
| 47:v:32:LEU:HA    | 47:v:64:ASP:OD1  | 2.20                     | 0.42              |
| 1:A:1539:C:H1'    | 1:A:1540:U:P     | 2.60                     | 0.42              |
| 2:B:142:GLU:HA    | 2:B:142:GLU:OE2  | 2.20                     | 0.42              |
| 5:E:72:ILE:CD1    | 5:E:145:GLU:HB3  | 2.50                     | 0.42              |
| 8:H:102:ALA:HB3   | 8:H:113:ASP:HB3  | 2.00                     | 0.42              |
| 13:M:49:SER:O     | 13:M:53:ILE:HD12 | 2.19                     | 0.42              |
| 25:Y:5:PHE:N      | 25:Y:5:PHE:CD1   | 2.88                     | 0.42              |
| 26:a:274:C:N4     | 26:a:275:C:H41   | 2.18                     | 0.42              |
| 26:a:704:G:H2'    | 26:a:726:G:N2    | 2.35                     | 0.42              |
| 26:a:1056:G:O2'   | 26:a:1086:A:O2'  | 2.38                     | 0.42              |
| 26:a:1230:A:H2'   | 26:a:1231:U:O4'  | 2.20                     | 0.42              |
| 26:a:1453:A:H61   | 38:m:74:GLU:HG2  | 1.85                     | 0.42              |
| 26:a:2219:U:H2'   | 26:a:2220:U:O4'  | 2.19                     | 0.42              |
| 26:a:2780:G:H1    | 34:i:102:GLU:CD  | 2.28                     | 0.42              |
| 28:c:120:VAL:HG23 | 28:c:134:ASN:OD1 | 2.20                     | 0.42              |
| 47:v:72:LYS:HB3   | 47:v:79:PHE:CD1  | 2.55                     | 0.42              |
| 1:A:151:A:C5      | 1:A:152:A:C8     | 3.08                     | 0.41              |
| 1:A:672:U:H2'     | 1:A:673:A:H8     | 1.85                     | 0.41              |
| 1:A:1158:C:C4     | 1:A:1160:G:C8    | 3.08                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1223:C:P     | 19:S:78:ARG:HH21 | 2.42                     | 0.41              |
| 1:A:1279:G:H5''  | 10:J:9:ARG:NH2   | 2.35                     | 0.41              |
| 1:A:1409:C:H2'   | 1:A:1410:A:C8    | 2.55                     | 0.41              |
| 3:C:70:THR:HG21  | 3:C:76:VAL:HG11  | 2.01                     | 0.41              |
| 5:E:96:MET:HE3   | 5:E:96:MET:HB2   | 1.79                     | 0.41              |
| 13:M:51:GLY:O    | 13:M:55:THR:HG23 | 2.20                     | 0.41              |
| 14:N:42:TRP:HZ3  | 19:S:9:PRO:HD2   | 1.85                     | 0.41              |
| 14:N:94:PRO:C    | 14:N:96:LEU:H    | 2.28                     | 0.41              |
| 16:P:56:ARG:HD2  | 16:P:56:ARG:HA   | 1.76                     | 0.41              |
| 26:a:84:A:N7     | 26:a:101:A:H2    | 2.18                     | 0.41              |
| 26:a:471:A:H2'   | 26:a:472:A:O4'   | 2.19                     | 0.41              |
| 26:a:940:G:H2'   | 26:a:941:A:O4'   | 2.20                     | 0.41              |
| 26:a:1040:A:N1   | 26:a:1115:G:N2   | 2.66                     | 0.41              |
| 26:a:1326:U:O2'  | 26:a:2010:G:O2'  | 2.37                     | 0.41              |
| 26:a:1542:U:H2'  | 26:a:1543:G:O4'  | 2.19                     | 0.41              |
| 26:a:2025:C:H2'  | 26:a:2026:U:C6   | 2.55                     | 0.41              |
| 26:a:2725:A:O2'  | 26:a:2726:A:C8   | 2.71                     | 0.41              |
| 26:a:2744:G:C6   | 26:a:2761:A:C6   | 3.08                     | 0.41              |
| 33:h:17:ASP:O    | 33:h:19:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:201:G:H2'    | 1:A:202:G:C8     | 2.55                     | 0.41              |
| 1:A:245:U:H2'    | 1:A:246:A:H5''   | 2.01                     | 0.41              |
| 1:A:1112:C:O2    | 1:A:1112:C:H2'   | 2.20                     | 0.41              |
| 1:A:1119:C:H2'   | 1:A:1120:U:H6    | 1.85                     | 0.41              |
| 1:A:1124:G:N2    | 1:A:1125:U:O4    | 2.46                     | 0.41              |
| 1:A:1172:C:H2'   | 1:A:1173:U:C6    | 2.55                     | 0.41              |
| 1:A:1319:A:C8    | 1:A:1323:G:C5    | 3.07                     | 0.41              |
| 2:B:14:VAL:HG12  | 2:B:43:LEU:HD21  | 2.01                     | 0.41              |
| 2:B:19:GLN:HA    | 2:B:38:VAL:HG22  | 2.01                     | 0.41              |
| 4:D:4:TYR:CD2    | 4:D:11:LEU:HD11  | 2.56                     | 0.41              |
| 9:I:55:VAL:HG21  | 9:I:94:LEU:HD13  | 2.02                     | 0.41              |
| 23:W:11:A:H2'    | 23:W:12:G:C8     | 2.55                     | 0.41              |
| 26:a:414:C:H2'   | 26:a:415:A:H8    | 1.83                     | 0.41              |
| 26:a:500:G:N2    | 26:a:503:A:H5'   | 2.32                     | 0.41              |
| 26:a:639:U:C2    | 26:a:640:C:C5    | 3.08                     | 0.41              |
| 26:a:729:G:O2'   | 26:a:763:G:H4'   | 2.20                     | 0.41              |
| 26:a:1326:U:H2'  | 26:a:1327:A:H8   | 1.85                     | 0.41              |
| 26:a:1614:A:C2   | 43:r:93:ALA:HB2  | 2.55                     | 0.41              |
| 26:a:2220:U:H4'  | 33:h:97:ARG:HH22 | 1.85                     | 0.41              |
| 26:a:2241:A:H2'  | 26:a:2242:G:C8   | 2.55                     | 0.41              |
| 26:a:2405:G:HO2' | 26:a:2406:A:P    | 2.42                     | 0.41              |
| 26:a:2808:G:O2'  | 26:a:2809:A:O5'  | 2.32                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:g:42:GLU:HB2   | 32:g:55:ARG:NE    | 2.33                     | 0.41              |
| 34:i:109:LEU:HD23 | 34:i:109:LEU:HA   | 1.82                     | 0.41              |
| 42:q:1:MET:HE3    | 42:q:101:ILE:HB   | 2.02                     | 0.41              |
| 1:A:284:C:H2'     | 1:A:285:C:C6      | 2.56                     | 0.41              |
| 1:A:355:C:C4      | 1:A:356:A:N7      | 2.88                     | 0.41              |
| 1:A:552:U:H2'     | 1:A:553:A:C8      | 2.48                     | 0.41              |
| 1:A:818:G:N1      | 1:A:820:U:O2'     | 2.50                     | 0.41              |
| 1:A:1118:U:H1'    | 1:A:1179:A:C4     | 2.55                     | 0.41              |
| 1:A:1260:G:OP1    | 1:A:1284:C:H4'    | 2.19                     | 0.41              |
| 1:A:1326:U:H2'    | 1:A:1327:C:H6     | 1.85                     | 0.41              |
| 1:A:1345:U:H5''   | 1:A:1346:A:OP1    | 2.20                     | 0.41              |
| 3:C:15:VAL:HG11   | 3:C:179:ARG:HA    | 2.02                     | 0.41              |
| 19:S:30:PRO:HA    | 19:S:48:THR:O     | 2.20                     | 0.41              |
| 21:U:16:LEU:O     | 21:U:19:PHE:HB3   | 2.21                     | 0.41              |
| 25:Y:76:GLU:C     | 25:Y:78:GLY:H     | 2.28                     | 0.41              |
| 26:a:242:G:H5''   | 54:2:64:TYR:CD2   | 2.55                     | 0.41              |
| 26:a:607:U:O2     | 26:a:608:A:C8     | 2.74                     | 0.41              |
| 26:a:640:C:H2'    | 26:a:641:U:C6     | 2.55                     | 0.41              |
| 26:a:1394:U:H2'   | 26:a:1395:A:O4'   | 2.20                     | 0.41              |
| 26:a:1631:G:N1    | 26:a:1634:A:OP2   | 2.48                     | 0.41              |
| 26:a:1799:G:N7    | 28:c:178:SER:OG   | 2.46                     | 0.41              |
| 26:a:2230:G:H2'   | 26:a:2231:U:H6    | 1.85                     | 0.41              |
| 26:a:2461:A:H2'   | 26:a:2462:C:H6    | 1.85                     | 0.41              |
| 45:t:96:PHE:CE2   | 45:t:103:ILE:HG12 | 2.54                     | 0.41              |
| 52:0:15:ALA:HB2   | 52:0:47:VAL:HG11  | 2.02                     | 0.41              |
| 1:A:264:C:H2'     | 1:A:265:G:O4'     | 2.21                     | 0.41              |
| 1:A:890:G:H2'     | 1:A:906:A:N6      | 2.36                     | 0.41              |
| 6:F:11:HIS:CE1    | 6:F:54:LEU:HD21   | 2.55                     | 0.41              |
| 13:M:11:ASP:HA    | 13:M:45:ILE:HB    | 2.01                     | 0.41              |
| 26:a:593:U:H2'    | 26:a:594:U:H6     | 1.85                     | 0.41              |
| 26:a:1419:A:C8    | 26:a:1579:A:N6    | 2.88                     | 0.41              |
| 26:a:1504:A:H2'   | 26:a:1505:A:C8    | 2.55                     | 0.41              |
| 26:a:1588:G:O2'   | 26:a:1589:U:OP1   | 2.34                     | 0.41              |
| 26:a:1637:A:H4'   | 26:a:2711:A:O2'   | 2.20                     | 0.41              |
| 26:a:2846:G:H2'   | 26:a:2847:U:C6    | 2.56                     | 0.41              |
| 26:a:2900:A:H2'   | 26:a:2901:C:C6    | 2.55                     | 0.41              |
| 34:i:104:ALA:O    | 34:i:108:MET:HG3  | 2.20                     | 0.41              |
| 38:m:114:GLU:HG2  | 38:m:115:LEU:O    | 2.20                     | 0.41              |
| 52:0:37:LYS:HE2   | 52:0:37:LYS:HB3   | 1.94                     | 0.41              |
| 1:A:373:A:C2      | 1:A:374:A:C8      | 3.09                     | 0.41              |
| 1:A:962:C:C2      | 1:A:963:G:C8      | 3.09                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1116:U:O2'   | 9:I:110:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:1273:C:H2'   | 1:A:1274:A:O4'   | 2.21                     | 0.41              |
| 1:A:1432:G:H1'   | 1:A:1468:A:N6    | 2.34                     | 0.41              |
| 2:B:23:TRP:CE3   | 2:B:25:PRO:HA    | 2.55                     | 0.41              |
| 12:L:16:VAL:HG23 | 12:L:17:ALA:N    | 2.35                     | 0.41              |
| 13:M:67:GLY:HA3  | 31:f:113:ASP:CG  | 2.45                     | 0.41              |
| 16:P:12:LYS:C    | 16:P:14:ARG:H    | 2.28                     | 0.41              |
| 22:V:24:C:H2'    | 22:V:25:U:H6     | 1.84                     | 0.41              |
| 26:a:38:A:H2'    | 26:a:39:G:O4'    | 2.21                     | 0.41              |
| 26:a:100:U:H5''  | 26:a:101:A:OP1   | 2.20                     | 0.41              |
| 26:a:831:G:H2'   | 26:a:832:U:O4'   | 2.20                     | 0.41              |
| 26:a:1306:C:H2'  | 26:a:1307:A:H8   | 1.86                     | 0.41              |
| 26:a:2146:C:H4'  | 26:a:2147:A:C5   | 2.55                     | 0.41              |
| 26:a:2370:G:H4'  | 52:0:44:ARG:NH1  | 2.34                     | 0.41              |
| 26:a:2405:G:O2'  | 26:a:2412:A:N6   | 2.53                     | 0.41              |
| 26:a:2568:U:H2'  | 26:a:2569:G:O4'  | 2.20                     | 0.41              |
| 26:a:2813:A:C4   | 26:a:2814:A:C8   | 3.08                     | 0.41              |
| 31:f:145:LYS:HE2 | 31:f:145:LYS:HA  | 2.01                     | 0.41              |
| 33:h:58:LEU:O    | 33:h:62:LEU:HB2  | 2.21                     | 0.41              |
| 54:2:31:HIS:HD2  | 54:2:32:ILE:HD12 | 1.81                     | 0.41              |
| 56:4:42:PRO:HB2  | 56:4:48:GLN:HG3  | 2.01                     | 0.41              |
| 1:A:160:A:H1'    | 1:A:344:A:C5     | 2.56                     | 0.41              |
| 1:A:765:G:N1     | 1:A:812:G:O2'    | 2.38                     | 0.41              |
| 1:A:846:G:H2'    | 1:A:847:G:H8     | 1.81                     | 0.41              |
| 1:A:923:A:OP1    | 5:E:26:LYS:HD3   | 2.21                     | 0.41              |
| 1:A:1240:U:C5    | 7:G:116:MET:HE3  | 2.55                     | 0.41              |
| 2:B:24:ASN:HA    | 2:B:25:PRO:HD3   | 1.96                     | 0.41              |
| 2:B:101:LEU:HB2  | 2:B:175:GLU:HB3  | 2.03                     | 0.41              |
| 13:M:49:SER:O    | 13:M:52:GLN:N    | 2.54                     | 0.41              |
| 16:P:8:ARG:O     | 16:P:29:ASN:ND2  | 2.54                     | 0.41              |
| 21:U:58:LYS:HG3  | 21:U:59:LYS:N    | 2.30                     | 0.41              |
| 25:Y:165:ASN:O   | 25:Y:166:VAL:C   | 2.63                     | 0.41              |
| 26:a:1583:A:H4'  | 26:a:1585:C:C4   | 2.54                     | 0.41              |
| 26:a:1746:A:H2'  | 26:a:1747:U:H6   | 1.84                     | 0.41              |
| 26:a:1873:G:H2'  | 26:a:1874:C:C6   | 2.55                     | 0.41              |
| 26:a:2079:U:H2'  | 26:a:2080:A:O4'  | 2.20                     | 0.41              |
| 26:a:2747:G:O6   | 26:a:2755:C:H5'' | 2.21                     | 0.41              |
| 28:c:171:TYR:HE1 | 28:c:185:GLU:HG2 | 1.86                     | 0.41              |
| 32:g:12:PRO:HG2  | 32:g:80:THR:HG21 | 2.03                     | 0.41              |
| 33:h:104:THR:HA  | 33:h:108:VAL:O   | 2.21                     | 0.41              |
| 34:i:84:ILE:HG23 | 34:i:84:ILE:O    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 45:t:22:ARG:HG3   | 45:t:22:ARG:NH1  | 2.35                     | 0.41              |
| 46:u:80:HIS:CG    | 46:u:83:LYS:HB2  | 2.56                     | 0.41              |
| 56:4:61:ASN:O     | 56:4:65:ASN:HB3  | 2.21                     | 0.41              |
| 1:A:59:A:H5''     | 1:A:387:U:H5''   | 2.02                     | 0.41              |
| 1:A:208:U:O2'     | 1:A:211:G:N2     | 2.53                     | 0.41              |
| 1:A:691:G:O2'     | 1:A:797:C:H4'    | 2.20                     | 0.41              |
| 1:A:999:C:H2'     | 1:A:1000:A:C8    | 2.55                     | 0.41              |
| 1:A:1447:A:H5''   | 1:A:1448:C:C5    | 2.49                     | 0.41              |
| 2:B:50:PHE:O      | 2:B:54:LEU:HD23  | 2.21                     | 0.41              |
| 6:F:14:GLN:OE1    | 6:F:14:GLN:N     | 2.54                     | 0.41              |
| 6:F:49:TYR:CE1    | 18:R:66:SER:HA   | 2.55                     | 0.41              |
| 11:K:83:GLU:HG2   | 11:K:109:ASN:HB2 | 2.02                     | 0.41              |
| 11:K:122:ARG:HE   | 11:K:122:ARG:HB3 | 1.77                     | 0.41              |
| 22:V:17:C:H5''    | 22:V:62:C:OP1    | 2.20                     | 0.41              |
| 26:a:222:A:C2     | 26:a:233:A:H5''  | 2.56                     | 0.41              |
| 26:a:283:G:H2'    | 26:a:284:U:C6    | 2.55                     | 0.41              |
| 26:a:458:G:H2'    | 26:a:469:G:O6    | 2.20                     | 0.41              |
| 26:a:582:A:H2'    | 26:a:583:G:C8    | 2.55                     | 0.41              |
| 26:a:2116:G:H1    | 26:a:2171:A:N6   | 2.18                     | 0.41              |
| 26:a:2287:A:C8    | 26:a:2289:G:C8   | 3.09                     | 0.41              |
| 26:a:2539:C:H4'   | 55:3:3:VAL:HG21  | 2.03                     | 0.41              |
| 26:a:2698:U:H2'   | 26:a:2699:C:H6   | 1.82                     | 0.41              |
| 32:g:175:LYS:HD2  | 32:g:176:LYS:O   | 2.20                     | 0.41              |
| 33:h:68:ARG:O     | 33:h:71:LYS:N    | 2.50                     | 0.41              |
| 34:i:26:GLY:O     | 34:i:30:THR:HG23 | 2.21                     | 0.41              |
| 34:i:36:LEU:O     | 34:i:51:GLY:HA3  | 2.21                     | 0.41              |
| 35:j:21:CYS:HA    | 35:j:41:ILE:HG22 | 2.02                     | 0.41              |
| 36:k:20:GLY:O     | 36:k:21:ARG:HD3  | 2.20                     | 0.41              |
| 36:k:143:GLU:HG3  | 36:k:144:GLU:H   | 1.84                     | 0.41              |
| 1:A:35:G:N3       | 12:L:115:SER:HB2 | 2.36                     | 0.41              |
| 1:A:181:A:C2      | 1:A:195:A:C6     | 3.09                     | 0.41              |
| 1:A:696:A:H2'     | 1:A:697:U:H6     | 1.85                     | 0.41              |
| 1:A:1201:A:H4'    | 1:A:1202:U:H5''  | 2.02                     | 0.41              |
| 7:G:26:PHE:HE2    | 7:G:120:LEU:HD21 | 1.84                     | 0.41              |
| 13:M:14:HIS:ND1   | 13:M:42:ASP:O    | 2.51                     | 0.41              |
| 15:O:5:THR:O      | 15:O:8:THR:OG1   | 2.35                     | 0.41              |
| 20:T:82:GLN:O     | 20:T:85:LYS:HG3  | 2.19                     | 0.41              |
| 25:Y:43:LYS:HG3   | 25:Y:44:SER:H    | 1.86                     | 0.41              |
| 25:Y:124:LEU:HD23 | 25:Y:124:LEU:HA  | 1.85                     | 0.41              |
| 26:a:773:U:O2'    | 28:c:48:ARG:HD3  | 2.21                     | 0.41              |
| 26:a:1068:G:H2'   | 26:a:1068:G:N3   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:a:1798:U:OP2   | 28:c:271:ARG:NH1 | 2.51                     | 0.41              |
| 26:a:1871:A:H2'   | 26:a:1872:A:O4'  | 2.21                     | 0.41              |
| 26:a:2327:A:N7    | 26:a:2388:A:N6   | 2.68                     | 0.41              |
| 26:a:2485:G:O3'   | 37:l:180:PRO:HB3 | 2.21                     | 0.41              |
| 26:a:2684:U:C4    | 26:a:2685:G:N7   | 2.89                     | 0.41              |
| 26:a:2808:G:H2'   | 26:a:2890:G:O6   | 2.21                     | 0.41              |
| 27:b:28:C:H2'     | 27:b:29:A:H8     | 1.85                     | 0.41              |
| 31:f:43:ALA:HB2   | 31:f:50:LEU:HB2  | 2.01                     | 0.41              |
| 35:j:108:ARG:HH21 | 40:o:34:GLU:HB2  | 1.86                     | 0.41              |
| 43:r:70:LYS:O     | 43:r:107:VAL:HA  | 2.20                     | 0.41              |
| 48:w:45:ARG:HG2   | 48:w:46:PHE:N    | 2.35                     | 0.41              |
| 1:A:34:C:H2'      | 1:A:35:G:C8      | 2.56                     | 0.41              |
| 1:A:79:G:H8       | 1:A:79:G:OP2     | 2.04                     | 0.41              |
| 1:A:155:A:H2'     | 1:A:156:C:H6     | 1.85                     | 0.41              |
| 1:A:413:G:H1'     | 1:A:428:G:N2     | 2.36                     | 0.41              |
| 1:A:520:A:OP2     | 12:L:48:ALA:HB1  | 2.20                     | 0.41              |
| 1:A:593:U:C2      | 1:A:594:U:C5     | 3.08                     | 0.41              |
| 1:A:642:A:C5      | 8:H:107:SER:HA   | 2.55                     | 0.41              |
| 1:A:751:U:H2'     | 1:A:752:G:O4'    | 2.20                     | 0.41              |
| 1:A:845:A:N6      | 18:R:11:CYS:SG   | 2.94                     | 0.41              |
| 1:A:954:G:H2'     | 1:A:955:U:H6     | 1.84                     | 0.41              |
| 1:A:1101:A:H5''   | 2:B:171:ILE:HD11 | 2.03                     | 0.41              |
| 1:A:1191:A:OP2    | 1:A:1191:A:C8    | 2.74                     | 0.41              |
| 1:A:1326:U:H2'    | 1:A:1327:C:C6    | 2.55                     | 0.41              |
| 1:A:1352:C:H2'    | 1:A:1353:G:C8    | 2.55                     | 0.41              |
| 6:F:18:VAL:HG21   | 6:F:58:HIS:ND1   | 2.36                     | 0.41              |
| 9:I:33:ARG:HB3    | 9:I:37:GLN:NE2   | 2.36                     | 0.41              |
| 9:I:96:SER:O      | 9:I:100:LYS:HD3  | 2.20                     | 0.41              |
| 11:K:93:ARG:NH2   | 21:U:29:LEU:HD11 | 2.35                     | 0.41              |
| 13:M:80:LEU:HD12  | 13:M:87:ARG:HB2  | 2.02                     | 0.41              |
| 14:N:49:GLN:OE1   | 19:S:13:LEU:N    | 2.52                     | 0.41              |
| 14:N:94:PRO:O     | 14:N:96:LEU:N    | 2.51                     | 0.41              |
| 17:Q:62:ARG:NH1   | 17:Q:76:VAL:HG22 | 2.35                     | 0.41              |
| 20:T:76:LYS:HE3   | 20:T:76:LYS:HB2  | 1.85                     | 0.41              |
| 25:Y:66:ASP:OD1   | 25:Y:66:ASP:C    | 2.64                     | 0.41              |
| 26:a:342:A:H2'    | 26:a:343:C:O4'   | 2.21                     | 0.41              |
| 26:a:588:U:H2'    | 26:a:589:U:H6    | 1.85                     | 0.41              |
| 26:a:607:U:N3     | 26:a:608:A:N7    | 2.69                     | 0.41              |
| 26:a:893:C:H2'    | 26:a:894:U:C2    | 2.55                     | 0.41              |
| 26:a:1013:C:H2'   | 26:a:1014:A:C8   | 2.53                     | 0.41              |
| 26:a:1042:G:H2'   | 26:a:1043:C:C6   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 26:a:1224:U:H4'  | 42:q:88:GLY:O    | 2.21                     | 0.41              |
| 26:a:1231:U:H2'  | 26:a:1232:G:C8   | 2.54                     | 0.41              |
| 26:a:1434:A:H2'  | 26:a:1435:G:C8   | 2.56                     | 0.41              |
| 26:a:1541:C:H2'  | 26:a:1542:U:C6   | 2.56                     | 0.41              |
| 26:a:1778:U:O4   | 26:a:1784:A:H1'  | 2.21                     | 0.41              |
| 26:a:1793:C:O2'  | 26:a:1900:A:N1   | 2.51                     | 0.41              |
| 26:a:1843:C:H2'  | 26:a:1844:C:C6   | 2.54                     | 0.41              |
| 26:a:2131:U:H5'' | 26:a:2132:U:OP1  | 2.21                     | 0.41              |
| 26:a:2196:C:H2'  | 26:a:2197:U:C6   | 2.56                     | 0.41              |
| 26:a:2545:G:H2'  | 26:a:2546:U:O4'  | 2.21                     | 0.41              |
| 28:c:118:SER:OG  | 28:c:189:ARG:NH2 | 2.54                     | 0.41              |
| 37:l:17:ASN:O    | 37:l:38:ARG:HD3  | 2.21                     | 0.41              |
| 41:p:47:TYR:OH   | 41:p:51:ARG:NH2  | 2.54                     | 0.41              |
| 45:t:14:LEU:HD11 | 45:t:71:ALA:HB2  | 2.03                     | 0.41              |
| 45:t:26:LYS:HB3  | 45:t:35:ILE:HG22 | 2.03                     | 0.41              |
| 56:4:59:ARG:O    | 56:4:63:ARG:HG2  | 2.20                     | 0.41              |
| 1:A:689:C:OP1    | 11:K:29:ASN:ND2  | 2.45                     | 0.41              |
| 1:A:1132:C:N4    | 1:A:1133:G:O6    | 2.54                     | 0.41              |
| 1:A:1238:A:N7    | 1:A:1303:C:H1'   | 2.35                     | 0.41              |
| 1:A:1333:A:H2'   | 1:A:1334:G:O4'   | 2.21                     | 0.41              |
| 1:A:1521:C:H2'   | 1:A:1522:U:C6    | 2.56                     | 0.41              |
| 3:C:207:ILE:H    | 3:C:207:ILE:HG13 | 1.70                     | 0.41              |
| 5:E:142:ASP:HA   | 5:E:145:GLU:HG2  | 2.03                     | 0.41              |
| 11:K:60:PRO:O    | 11:K:95:SER:OG   | 2.29                     | 0.41              |
| 15:O:17:ARG:NH1  | 15:O:24:SER:OG   | 2.54                     | 0.41              |
| 22:V:67:C:H2'    | 22:V:68:C:C6     | 2.56                     | 0.41              |
| 26:a:679:C:H2'   | 26:a:680:C:C6    | 2.56                     | 0.41              |
| 26:a:1831:G:H2'  | 26:a:1832:C:C6   | 2.56                     | 0.41              |
| 26:a:2241:A:H2'  | 26:a:2242:G:H8   | 1.86                     | 0.41              |
| 32:g:78:GLY:HA2  | 32:g:82:GLY:HA2  | 2.02                     | 0.41              |
| 38:m:35:LYS:HB2  | 38:m:112:TYR:CE1 | 2.56                     | 0.41              |
| 51:z:33:THR:HG23 | 51:z:34:SER:N    | 2.36                     | 0.41              |
| 1:A:501:C:O2     | 1:A:549:C:O2'    | 2.37                     | 0.40              |
| 1:A:544:G:C6     | 1:A:545:C:C4     | 3.09                     | 0.40              |
| 1:A:685:G:N2     | 1:A:704:A:OP2    | 2.49                     | 0.40              |
| 1:A:891:U:H2'    | 1:A:892:A:H8     | 1.86                     | 0.40              |
| 1:A:1009:U:H2'   | 1:A:1010:C:C6    | 2.56                     | 0.40              |
| 1:A:1241:G:C2    | 1:A:1242:G:C5    | 3.09                     | 0.40              |
| 6:F:51:ILE:HD11  | 18:R:66:SER:OG   | 2.21                     | 0.40              |
| 19:S:17:LYS:O    | 19:S:20:GLU:HG3  | 2.21                     | 0.40              |
| 25:Y:83:LEU:HD13 | 25:Y:83:LEU:HA   | 1.77                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:a:228:C:H5'    | 26:a:229:C:OP1   | 2.21                     | 0.40              |
| 26:a:635:C:O2'    | 26:a:639:U:H5''  | 2.21                     | 0.40              |
| 26:a:679:C:H2'    | 26:a:680:C:H6    | 1.85                     | 0.40              |
| 26:a:1048:A:H2'   | 26:a:1048:A:N3   | 2.35                     | 0.40              |
| 26:a:1857:G:O2'   | 26:a:1858:A:H8   | 2.03                     | 0.40              |
| 26:a:2209:G:H3'   | 26:a:2210:U:H2'  | 2.03                     | 0.40              |
| 26:a:2389:G:H5''  | 26:a:2390:U:O4'  | 2.20                     | 0.40              |
| 26:a:2395:C:H2'   | 26:a:2396:G:O4'  | 2.20                     | 0.40              |
| 26:a:2647:U:H2'   | 26:a:2648:G:C8   | 2.56                     | 0.40              |
| 26:a:2848:G:C8    | 40:o:95:ALA:HB2  | 2.56                     | 0.40              |
| 33:h:143:ILE:HG23 | 33:h:143:ILE:O   | 2.20                     | 0.40              |
| 35:j:108:ARG:NH2  | 40:o:34:GLU:HB2  | 2.36                     | 0.40              |
| 1:A:78:A:C2       | 1:A:79:G:H1'     | 2.56                     | 0.40              |
| 1:A:600:A:C6      | 1:A:639:G:C6     | 3.10                     | 0.40              |
| 1:A:704:A:C4      | 1:A:705:G:C8     | 3.09                     | 0.40              |
| 1:A:720:C:H5''    | 18:R:41:PRO:HA   | 2.03                     | 0.40              |
| 1:A:838:G:H2'     | 1:A:839:C:H6     | 1.86                     | 0.40              |
| 1:A:1537:U:H3'    | 1:A:1538:C:C5'   | 2.51                     | 0.40              |
| 1:A:1539:C:H4'    | 1:A:1540:U:OP1   | 2.21                     | 0.40              |
| 2:B:181:ILE:H     | 2:B:181:ILE:HG13 | 1.68                     | 0.40              |
| 9:I:94:LEU:HA     | 9:I:97:GLU:OE1   | 2.21                     | 0.40              |
| 12:L:107:VAL:HG23 | 12:L:117:TYR:HB3 | 2.02                     | 0.40              |
| 25:Y:94:ALA:O     | 25:Y:95:TRP:HB2  | 2.21                     | 0.40              |
| 26:a:3:U:H2'      | 26:a:4:U:C6      | 2.57                     | 0.40              |
| 26:a:166:U:H2'    | 26:a:167:A:C8    | 2.57                     | 0.40              |
| 26:a:372:G:O2'    | 48:w:54:LYS:HE2  | 2.21                     | 0.40              |
| 26:a:396:G:C6     | 26:a:397:U:C4    | 3.10                     | 0.40              |
| 26:a:1053:C:N4    | 26:a:1054:A:H62  | 2.15                     | 0.40              |
| 26:a:1684:G:H2'   | 26:a:1685:C:C6   | 2.56                     | 0.40              |
| 26:a:1914:C:H3'   | 26:a:1915:3TD:O4 | 2.21                     | 0.40              |
| 26:a:1940:U:H6    | 26:a:1940:U:H2'  | 1.74                     | 0.40              |
| 28:c:121:ASP:HA   | 33:h:91:PHE:HE1  | 1.70                     | 0.40              |
| 30:e:7:ASP:N      | 30:e:7:ASP:OD1   | 2.54                     | 0.40              |
| 33:h:46:PHE:HZ    | 33:h:50:ARG:HH21 | 1.66                     | 0.40              |
| 37:l:81:4D4:NH2   | 47:v:4:LYS:HE2   | 2.36                     | 0.40              |
| 42:q:3:ALA:HB3    | 42:q:59:ILE:HD11 | 2.03                     | 0.40              |
| 45:t:81:ASP:OD2   | 45:t:98:SER:OG   | 2.32                     | 0.40              |
| 48:w:59:ILE:HD13  | 48:w:67:VAL:HG21 | 2.04                     | 0.40              |
| 55:3:33:HIS:O     | 55:3:35:GLN:HG3  | 2.22                     | 0.40              |
| 56:4:35:ASP:OD1   | 56:4:36:VAL:HG12 | 2.21                     | 0.40              |
| 1:A:19:A:H2'      | 1:A:20:U:C6      | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:211:G:H5'    | 1:A:212:G:O4'    | 2.21                     | 0.40              |
| 1:A:371:A:H2'    | 1:A:372:C:O4'    | 2.22                     | 0.40              |
| 1:A:414:A:H2'    | 1:A:415:A:C8     | 2.56                     | 0.40              |
| 1:A:602:A:H2'    | 1:A:603:U:C6     | 2.57                     | 0.40              |
| 1:A:1315:U:O2    | 1:A:1360:A:H2    | 2.04                     | 0.40              |
| 1:A:1539:C:C1'   | 1:A:1540:U:P     | 3.09                     | 0.40              |
| 2:B:192:ASP:OD1  | 2:B:192:ASP:N    | 2.53                     | 0.40              |
| 3:C:33:LEU:HD23  | 3:C:33:LEU:HA    | 1.79                     | 0.40              |
| 3:C:79:LYS:O     | 3:C:81:GLY:N     | 2.55                     | 0.40              |
| 10:J:65:TYR:HB3  | 14:N:96:LEU:HD21 | 2.02                     | 0.40              |
| 15:O:78:TYR:O    | 15:O:82:ILE:HG23 | 2.22                     | 0.40              |
| 26:a:81:G:H2'    | 26:a:82:U:O4'    | 2.21                     | 0.40              |
| 26:a:1364:G:P    | 48:w:50:ARG:HH12 | 2.43                     | 0.40              |
| 26:a:1637:A:H5'  | 26:a:1760:C:O2'  | 2.21                     | 0.40              |
| 26:a:2305:U:H2'  | 26:a:2306:C:C6   | 2.56                     | 0.40              |
| 27:b:32:U:C2     | 27:b:33:G:C8     | 3.10                     | 0.40              |
| 34:i:32:LEU:HD22 | 34:i:54:ILE:HG21 | 2.03                     | 0.40              |
| 45:t:49:VAL:O    | 45:t:54:GLN:HB3  | 2.21                     | 0.40              |
| 1:A:165:G:H2'    | 1:A:166:U:C6     | 2.56                     | 0.40              |
| 1:A:376:G:H4'    | 16:P:5:ARG:HD2   | 2.04                     | 0.40              |
| 1:A:946:A:H2'    | 1:A:947:G:H8     | 1.79                     | 0.40              |
| 1:A:950:U:OP2    | 13:M:101:ARG:HD2 | 2.22                     | 0.40              |
| 1:A:1111:A:H2'   | 1:A:1112:C:H6    | 1.86                     | 0.40              |
| 1:A:1238:A:H2    | 1:A:1241:G:N3    | 2.19                     | 0.40              |
| 1:A:1271:A:H2'   | 1:A:1272:G:H8    | 1.87                     | 0.40              |
| 2:B:97:LEU:HD12  | 2:B:97:LEU:HA    | 1.94                     | 0.40              |
| 2:B:205:ASP:HB3  | 25:Y:79:PHE:HD2  | 1.86                     | 0.40              |
| 2:B:205:ASP:HB3  | 25:Y:79:PHE:CD2  | 2.55                     | 0.40              |
| 4:D:132:ILE:HG22 | 4:D:135:TYR:N    | 2.36                     | 0.40              |
| 15:O:67:LEU:HD23 | 15:O:67:LEU:HA   | 1.86                     | 0.40              |
| 22:V:76:C:H5''   | 22:V:77:A:OP2    | 2.22                     | 0.40              |
| 25:Y:24:VAL:HG12 | 25:Y:25:ARG:H    | 1.86                     | 0.40              |
| 25:Y:30:ALA:HB3  | 25:Y:37:LEU:HB3  | 2.03                     | 0.40              |
| 25:Y:63:GLN:H    | 25:Y:63:GLN:HG2  | 1.70                     | 0.40              |
| 26:a:49:A:N3     | 26:a:49:A:H2'    | 2.36                     | 0.40              |
| 26:a:447:A:OP1   | 41:p:5:LYS:NZ    | 2.54                     | 0.40              |
| 26:a:692:C:H2'   | 26:a:693:A:H8    | 1.85                     | 0.40              |
| 26:a:894:U:H1'   | 26:a:895:U:O5'   | 2.20                     | 0.40              |
| 26:a:1041:G:C2   | 26:a:1042:G:C8   | 3.10                     | 0.40              |
| 26:a:1110:G:H2'  | 26:a:1111:A:H8   | 1.86                     | 0.40              |
| 26:a:1378:A:O2'  | 26:a:1380:G:N7   | 2.55                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:a:2251:OMG:H1' | 26:a:2251:OMG:HM23 | 1.63                     | 0.40              |
| 26:a:2364:C:H2'   | 26:a:2365:G:O4'    | 2.21                     | 0.40              |
| 27:b:39:A:N1      | 27:b:44:G:C6       | 2.89                     | 0.40              |
| 27:b:44:G:N2      | 27:b:48:U:C2       | 2.89                     | 0.40              |
| 28:c:181:MET:HE2  | 28:c:181:MET:HB2   | 1.86                     | 0.40              |
| 30:e:165:HIS:CG   | 30:e:166:LYS:N     | 2.89                     | 0.40              |
| 34:i:101:ILE:HB   | 34:i:124:VAL:HG11  | 2.03                     | 0.40              |
| 38:m:31:HIS:C     | 38:m:33:ILE:H      | 2.29                     | 0.40              |
| 42:q:32:THR:HA    | 42:q:61:ALA:O      | 2.21                     | 0.40              |
| 49:x:21:LEU:HD23  | 49:x:21:LEU:HA     | 1.91                     | 0.40              |
| 53:l:30:VAL:HG22  | 53:l:33:ARG:NH2    | 2.36                     | 0.40              |
| 1:A:181:A:N6      | 1:A:194:C:H2'      | 2.36                     | 0.40              |
| 1:A:562:U:H1'     | 12:L:12:ARG:HD2    | 2.03                     | 0.40              |
| 1:A:1072:G:H2'    | 1:A:1073:U:C6      | 2.56                     | 0.40              |
| 1:A:1211:U:H4'    | 1:A:1213:A:H1'     | 2.03                     | 0.40              |
| 1:A:1399:C:H4'    | 1:A:1400:C:O5'     | 2.21                     | 0.40              |
| 5:E:115:LEU:HD13  | 5:E:123:VAL:HG11   | 2.03                     | 0.40              |
| 6:F:21:MET:HA     | 6:F:24:ARG:HH11    | 1.87                     | 0.40              |
| 8:H:87:LYS:HB2    | 8:H:125:ILE:HD11   | 2.04                     | 0.40              |
| 8:H:103:VAL:HB    | 8:H:127:CYS:SG     | 2.62                     | 0.40              |
| 9:I:5:GLN:HG2     | 9:I:22:LYS:HE3     | 2.04                     | 0.40              |
| 12:L:90:LEU:HA    | 12:L:90:LEU:HD23   | 1.88                     | 0.40              |
| 13:M:83:LEU:HD21  | 19:S:65:GLU:CD     | 2.46                     | 0.40              |
| 14:N:56:SER:HB3   | 14:N:59:ARG:HG2    | 2.03                     | 0.40              |
| 17:Q:44:LEU:HD22  | 17:Q:73:TRP:CD1    | 2.57                     | 0.40              |
| 23:W:51:U:H3      | 23:W:65:G:H1       | 1.70                     | 0.40              |
| 26:a:479:A:H4'    | 26:a:480:A:OP1     | 2.22                     | 0.40              |
| 26:a:629:G:OP1    | 26:a:650:C:O2'     | 2.30                     | 0.40              |
| 26:a:1024:G:C6    | 26:a:1025:G:C6     | 3.09                     | 0.40              |
| 26:a:1055:G:C8    | 26:a:1056:G:C6     | 3.09                     | 0.40              |
| 26:a:1383:A:H1'   | 26:a:1405:U:O2'    | 2.21                     | 0.40              |
| 26:a:1475:G:O2'   | 26:a:1476:U:O5'    | 2.38                     | 0.40              |
| 26:a:2081:U:H2'   | 26:a:2082:A:H8     | 1.86                     | 0.40              |
| 26:a:2215:C:H2'   | 26:a:2216:G:C8     | 2.57                     | 0.40              |
| 27:b:76:G:O3'     | 46:u:21:ARG:NH2    | 2.40                     | 0.40              |
| 29:d:109:VAL:HG11 | 29:d:193:VAL:HB    | 2.04                     | 0.40              |
| 30:e:149:ILE:HG22 | 30:e:192:ALA:HB1   | 2.03                     | 0.40              |
| 32:g:89:LEU:HD22  | 32:g:162:VAL:HG22  | 2.02                     | 0.40              |
| 33:h:4:ILE:HG22   | 33:h:37:VAL:HB     | 2.04                     | 0.40              |
| 33:h:50:ARG:NH1   | 33:h:55:GLU:OE1    | 2.54                     | 0.40              |
| 35:j:38:ILE:HD11  | 35:j:112:PHE:HZ    | 1.87                     | 0.40              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 41:p:35:ALA:O  | 41:p:39:VAL:HG23 | 2.22                     | 0.40              |
| 44:s:64:LYS:HA | 44:s:79:ASP:OD1  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | B     | 222/224 (99%) | 192 (86%) | 27 (12%) | 3 (1%)   | 9           | 31  |
| 3   | C     | 204/206 (99%) | 191 (94%) | 11 (5%)  | 2 (1%)   | 12          | 39  |
| 4   | D     | 203/206 (98%) | 194 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 5   | E     | 154/167 (92%) | 147 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 6   | F     | 101/135 (75%) | 96 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 7   | G     | 151/179 (84%) | 142 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 8   | H     | 127/130 (98%) | 116 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 9   | I     | 125/130 (96%) | 121 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 10  | J     | 96/103 (93%)  | 89 (93%)  | 6 (6%)   | 1 (1%)   | 12          | 39  |
| 11  | K     | 115/129 (89%) | 107 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 12  | L     | 120/124 (97%) | 108 (90%) | 11 (9%)  | 1 (1%)   | 16          | 44  |
| 13  | M     | 113/118 (96%) | 107 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 14  | N     | 98/101 (97%)  | 97 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 15  | O     | 86/89 (97%)   | 83 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 16  | P     | 79/82 (96%)   | 71 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 17  | Q     | 77/84 (92%)   | 73 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 18  | R     | 64/75 (85%)   | 48 (75%)  | 13 (20%) | 3 (5%)   | 2           | 12  |
| 19  | S     | 82/92 (89%)   | 77 (94%)  | 5 (6%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 20  | T     | 84/87 (97%)   | 83 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 21  | U     | 66/71 (93%)   | 51 (77%)  | 8 (12%)  | 7 (11%)  | 0           | 3   |
| 25  | Y     | 170/557 (30%) | 88 (52%)  | 68 (40%) | 14 (8%)  | 0           | 4   |
| 28  | c     | 269/273 (98%) | 258 (96%) | 11 (4%)  | 0        | 100         | 100 |
| 29  | d     | 206/209 (99%) | 196 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 30  | e     | 199/201 (99%) | 190 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 31  | f     | 175/179 (98%) | 158 (90%) | 17 (10%) | 0        | 100         | 100 |
| 32  | g     | 174/177 (98%) | 158 (91%) | 14 (8%)  | 2 (1%)   | 11          | 37  |
| 33  | h     | 147/149 (99%) | 110 (75%) | 35 (24%) | 2 (1%)   | 9           | 31  |
| 34  | i     | 140/142 (99%) | 136 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 35  | j     | 121/123 (98%) | 115 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 36  | k     | 142/144 (99%) | 132 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 37  | l     | 132/136 (97%) | 126 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 38  | m     | 116/127 (91%) | 111 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 39  | n     | 114/117 (97%) | 109 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | o     | 112/115 (97%) | 108 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 41  | p     | 115/118 (98%) | 111 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 42  | q     | 101/103 (98%) | 95 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 43  | r     | 108/110 (98%) | 103 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 44  | s     | 91/100 (91%)  | 83 (91%)  | 7 (8%)   | 1 (1%)   | 11          | 37  |
| 45  | t     | 100/104 (96%) | 83 (83%)  | 17 (17%) | 0        | 100         | 100 |
| 46  | u     | 92/94 (98%)   | 88 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 47  | v     | 82/85 (96%)   | 73 (89%)  | 9 (11%)  | 0        | 100         | 100 |
| 48  | w     | 75/78 (96%)   | 72 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 49  | x     | 60/63 (95%)   | 58 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 50  | y     | 56/59 (95%)   | 55 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 51  | z     | 54/57 (95%)   | 53 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 52  | 0     | 49/55 (89%)   | 49 (100%) | 0        | 0        | 100         | 100 |
| 53  | 1     | 44/46 (96%)   | 43 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 54  | 2     | 62/65 (95%)   | 59 (95%)  | 2 (3%)   | 1 (2%)   | 7           | 29  |
| 55  | 3     | 36/38 (95%)   | 35 (97%)  | 1 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 56  | 4     | 64/70 (91%)     | 56 (88%)   | 8 (12%)  | 0        | 100         | 100 |
| All | All   | 5773/6426 (90%) | 5304 (92%) | 432 (8%) | 37 (1%)  | 23          | 49  |

All (37) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 18  | HIS  |
| 12  | L     | 16  | VAL  |
| 21  | U     | 57  | ALA  |
| 21  | U     | 62  | ARG  |
| 21  | U     | 65  | ALA  |
| 21  | U     | 66  | ARG  |
| 21  | U     | 67  | ARG  |
| 25  | Y     | 17  | GLU  |
| 32  | g     | 47  | ASP  |
| 32  | g     | 61  | GLY  |
| 33  | h     | 137 | GLU  |
| 10  | J     | 57  | VAL  |
| 18  | R     | 13  | PHE  |
| 21  | U     | 55  | ARG  |
| 21  | U     | 63  | GLU  |
| 25  | Y     | 64  | VAL  |
| 25  | Y     | 95  | TRP  |
| 25  | Y     | 98  | LEU  |
| 25  | Y     | 101 | ALA  |
| 25  | Y     | 166 | VAL  |
| 25  | Y     | 173 | VAL  |
| 2   | B     | 5   | SER  |
| 25  | Y     | 81  | GLU  |
| 18  | R     | 11  | CYS  |
| 18  | R     | 14  | THR  |
| 25  | Y     | 19  | ARG  |
| 25  | Y     | 44  | SER  |
| 44  | s     | 89  | GLU  |
| 3   | C     | 80  | LYS  |
| 25  | Y     | 16  | ILE  |
| 25  | Y     | 96  | ILE  |
| 25  | Y     | 122 | VAL  |
| 54  | 2     | 32  | ILE  |
| 33  | h     | 126 | GLY  |
| 2   | B     | 207 | ILE  |
| 3   | C     | 81  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | Y     | 49  | 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | B     | 186/186 (100%) | 174 (94%)  | 12 (6%)  | 15          | 41  |
| 3   | C     | 170/170 (100%) | 170 (100%) | 0        | 100         | 100 |
| 4   | D     | 172/173 (99%)  | 170 (99%)  | 2 (1%)   | 63          | 72  |
| 5   | E     | 119/126 (94%)  | 119 (100%) | 0        | 100         | 100 |
| 6   | F     | 90/116 (78%)   | 90 (100%)  | 0        | 100         | 100 |
| 7   | G     | 126/147 (86%)  | 126 (100%) | 0        | 100         | 100 |
| 8   | H     | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 9   | I     | 105/107 (98%)  | 105 (100%) | 0        | 100         | 100 |
| 10  | J     | 86/90 (96%)    | 86 (100%)  | 0        | 100         | 100 |
| 11  | K     | 90/99 (91%)    | 88 (98%)   | 2 (2%)   | 45          | 63  |
| 12  | L     | 102/103 (99%)  | 102 (100%) | 0        | 100         | 100 |
| 13  | M     | 93/96 (97%)    | 93 (100%)  | 0        | 100         | 100 |
| 14  | N     | 83/84 (99%)    | 83 (100%)  | 0        | 100         | 100 |
| 15  | O     | 76/77 (99%)    | 76 (100%)  | 0        | 100         | 100 |
| 16  | P     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 17  | Q     | 73/78 (94%)    | 73 (100%)  | 0        | 100         | 100 |
| 18  | R     | 57/65 (88%)    | 53 (93%)   | 4 (7%)   | 14          | 39  |
| 19  | S     | 72/79 (91%)    | 72 (100%)  | 0        | 100         | 100 |
| 20  | T     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 21  | U     | 58/61 (95%)    | 44 (76%)   | 14 (24%) | 1           | 2   |
| 25  | Y     | 144/461 (31%)  | 77 (54%)   | 67 (46%) | 0           | 0   |
| 28  | c     | 216/218 (99%)  | 216 (100%) | 0        | 100         | 100 |
| 29  | d     | 163/163 (100%) | 163 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 30  | e     | 165/165 (100%)  | 164 (99%)  | 1 (1%)   | 78          | 80  |
| 31  | f     | 148/150 (99%)   | 148 (100%) | 0        | 100         | 100 |
| 32  | g     | 137/138 (99%)   | 137 (100%) | 0        | 100         | 100 |
| 33  | h     | 114/114 (100%)  | 114 (100%) | 0        | 100         | 100 |
| 34  | i     | 116/116 (100%)  | 116 (100%) | 0        | 100         | 100 |
| 35  | j     | 104/104 (100%)  | 104 (100%) | 0        | 100         | 100 |
| 36  | k     | 103/103 (100%)  | 103 (100%) | 0        | 100         | 100 |
| 37  | l     | 107/107 (100%)  | 107 (100%) | 0        | 100         | 100 |
| 38  | m     | 98/103 (95%)    | 98 (100%)  | 0        | 100         | 100 |
| 39  | n     | 86/87 (99%)     | 86 (100%)  | 0        | 100         | 100 |
| 40  | o     | 99/100 (99%)    | 99 (100%)  | 0        | 100         | 100 |
| 41  | p     | 89/90 (99%)     | 89 (100%)  | 0        | 100         | 100 |
| 42  | q     | 84/84 (100%)    | 84 (100%)  | 0        | 100         | 100 |
| 43  | r     | 93/93 (100%)    | 93 (100%)  | 0        | 100         | 100 |
| 44  | s     | 80/84 (95%)     | 80 (100%)  | 0        | 100         | 100 |
| 45  | t     | 83/85 (98%)     | 83 (100%)  | 0        | 100         | 100 |
| 46  | u     | 78/78 (100%)    | 78 (100%)  | 0        | 100         | 100 |
| 47  | v     | 62/63 (98%)     | 62 (100%)  | 0        | 100         | 100 |
| 48  | w     | 67/68 (98%)     | 67 (100%)  | 0        | 100         | 100 |
| 49  | x     | 54/55 (98%)     | 54 (100%)  | 0        | 100         | 100 |
| 50  | y     | 48/49 (98%)     | 48 (100%)  | 0        | 100         | 100 |
| 51  | z     | 47/48 (98%)     | 47 (100%)  | 0        | 100         | 100 |
| 52  | 0     | 46/49 (94%)     | 46 (100%)  | 0        | 100         | 100 |
| 53  | 1     | 38/38 (100%)    | 38 (100%)  | 0        | 100         | 100 |
| 54  | 2     | 51/52 (98%)     | 51 (100%)  | 0        | 100         | 100 |
| 55  | 3     | 34/34 (100%)    | 34 (100%)  | 0        | 100         | 100 |
| 56  | 4     | 59/62 (95%)     | 59 (100%)  | 0        | 100         | 100 |
| All | All   | 4805/5254 (92%) | 4703 (98%) | 102 (2%) | 46          | 64  |

All (102) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 4   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 6   | MET  |
| 2   | B     | 7   | ARG  |
| 2   | B     | 10  | LEU  |
| 2   | B     | 15  | HIS  |
| 2   | B     | 31  | ILE  |
| 2   | B     | 35  | ARG  |
| 2   | B     | 45  | LYS  |
| 2   | B     | 63  | ARG  |
| 2   | B     | 74  | ARG  |
| 2   | B     | 204 | ASP  |
| 2   | B     | 207 | ILE  |
| 4   | D     | 55  | LEU  |
| 4   | D     | 58  | LYS  |
| 11  | K     | 119 | ASN  |
| 11  | K     | 122 | ARG  |
| 18  | R     | 9   | LYS  |
| 18  | R     | 10  | PHE  |
| 18  | R     | 11  | CYS  |
| 18  | R     | 16  | GLU  |
| 21  | U     | 17  | ARG  |
| 21  | U     | 24  | GLU  |
| 21  | U     | 25  | LYS  |
| 21  | U     | 33  | ARG  |
| 21  | U     | 35  | ARG  |
| 21  | U     | 44  | GLU  |
| 21  | U     | 47  | ARG  |
| 21  | U     | 54  | LYS  |
| 21  | U     | 58  | LYS  |
| 21  | U     | 63  | GLU  |
| 21  | U     | 66  | ARG  |
| 21  | U     | 67  | ARG  |
| 21  | U     | 68  | THR  |
| 21  | U     | 69  | ARG  |
| 25  | Y     | 5   | PHE  |
| 25  | Y     | 8   | LEU  |
| 25  | Y     | 14  | LYS  |
| 25  | Y     | 15  | GLU  |
| 25  | Y     | 19  | ARG  |
| 25  | Y     | 25  | ARG  |
| 25  | Y     | 29  | VAL  |
| 25  | Y     | 31  | ILE  |
| 25  | Y     | 33  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | Y     | 35  | VAL  |
| 25  | Y     | 36  | VAL  |
| 25  | Y     | 37  | LEU  |
| 25  | Y     | 38  | VAL  |
| 25  | Y     | 39  | ASP  |
| 25  | Y     | 42  | LEU  |
| 25  | Y     | 44  | SER  |
| 25  | Y     | 45  | GLU  |
| 25  | Y     | 60  | LEU  |
| 25  | Y     | 61  | GLU  |
| 25  | Y     | 62  | ILE  |
| 25  | Y     | 64  | VAL  |
| 25  | Y     | 68  | VAL  |
| 25  | Y     | 75  | VAL  |
| 25  | Y     | 79  | PHE  |
| 25  | Y     | 81  | GLU  |
| 25  | Y     | 83  | LEU  |
| 25  | Y     | 84  | LEU  |
| 25  | Y     | 85  | SER  |
| 25  | Y     | 86  | ARG  |
| 25  | Y     | 96  | ILE  |
| 25  | Y     | 97  | THR  |
| 25  | Y     | 98  | LEU  |
| 25  | Y     | 102 | TYR  |
| 25  | Y     | 103 | GLU  |
| 25  | Y     | 107 | THR  |
| 25  | Y     | 108 | VAL  |
| 25  | Y     | 109 | THR  |
| 25  | Y     | 111 | VAL  |
| 25  | Y     | 113 | ASN  |
| 25  | Y     | 115 | LYS  |
| 25  | Y     | 116 | VAL  |
| 25  | Y     | 117 | LYS  |
| 25  | Y     | 120 | PHE  |
| 25  | Y     | 122 | VAL  |
| 25  | Y     | 123 | GLU  |
| 25  | Y     | 125 | ASN  |
| 25  | Y     | 127 | ILE  |
| 25  | Y     | 130 | PHE  |
| 25  | Y     | 144 | THR  |
| 25  | Y     | 145 | LEU  |
| 25  | Y     | 146 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | Y     | 150 | LYS  |
| 25  | Y     | 153 | GLU  |
| 25  | Y     | 154 | PHE  |
| 25  | Y     | 155 | LYS  |
| 25  | Y     | 156 | VAL  |
| 25  | Y     | 157 | ILE  |
| 25  | Y     | 158 | LYS  |
| 25  | Y     | 159 | LEU  |
| 25  | Y     | 160 | ASP  |
| 25  | Y     | 162 | LYS  |
| 25  | Y     | 163 | ARG  |
| 25  | Y     | 166 | VAL  |
| 25  | Y     | 167 | VAL  |
| 25  | Y     | 168 | VAL  |
| 25  | Y     | 170 | ARG  |
| 25  | Y     | 173 | VAL  |
| 30  | e     | 176 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 15  | HIS  |
| 2   | B     | 94  | HIS  |
| 3   | C     | 176 | HIS  |
| 4   | D     | 152 | GLN  |
| 5   | E     | 132 | ASN  |
| 6   | F     | 17  | GLN  |
| 6   | F     | 81  | ASN  |
| 9   | I     | 5   | GLN  |
| 9   | I     | 37  | GLN  |
| 10  | J     | 35  | GLN  |
| 10  | J     | 58  | ASN  |
| 14  | N     | 4   | GLN  |
| 14  | N     | 43  | ASN  |
| 14  | N     | 60  | GLN  |
| 18  | R     | 52  | GLN  |
| 20  | T     | 48  | GLN  |
| 20  | T     | 61  | GLN  |
| 25  | Y     | 7   | GLN  |
| 25  | Y     | 92  | HIS  |
| 29  | d     | 36  | GLN  |
| 29  | d     | 49  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | e     | 62  | GLN  |
| 30  | e     | 136 | GLN  |
| 32  | g     | 38  | ASN  |
| 33  | h     | 18  | GLN  |
| 33  | h     | 128 | HIS  |
| 39  | n     | 116 | GLN  |
| 42  | q     | 6   | GLN  |
| 44  | s     | 70  | HIS  |
| 49  | x     | 27  | ASN  |
| 49  | x     | 39  | GLN  |
| 53  | 1     | 26  | ASN  |
| 54  | 2     | 31  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1538/1539 (99%) | 280 (18%)         | 21 (1%)         |
| 22  | V     | 76/77 (98%)     | 13 (17%)          | 1 (1%)          |
| 23  | W     | 76/77 (98%)     | 43 (56%)          | 3 (3%)          |
| 24  | X     | 5/38 (13%)      | 4 (80%)           | 0               |
| 26  | a     | 2902/2903 (99%) | 581 (20%)         | 0               |
| 27  | b     | 119/120 (99%)   | 18 (15%)          | 0               |
| All | All   | 4716/4754 (99%) | 939 (19%)         | 25 (0%)         |

All (939) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | U    |
| 1   | A     | 7   | A    |
| 1   | A     | 9   | G    |
| 1   | A     | 22  | G    |
| 1   | A     | 31  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 39  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 54  | C    |
| 1   | A     | 66  | A    |
| 1   | A     | 71  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | G    |
| 1   | A     | 77  | A    |
| 1   | A     | 79  | G    |
| 1   | A     | 80  | A    |
| 1   | A     | 82  | G    |
| 1   | A     | 83  | C    |
| 1   | A     | 84  | U    |
| 1   | A     | 85  | U    |
| 1   | A     | 86  | G    |
| 1   | A     | 88  | U    |
| 1   | A     | 94  | G    |
| 1   | A     | 121 | U    |
| 1   | A     | 130 | A    |
| 1   | A     | 132 | C    |
| 1   | A     | 141 | G    |
| 1   | A     | 146 | G    |
| 1   | A     | 149 | A    |
| 1   | A     | 150 | U    |
| 1   | A     | 173 | U    |
| 1   | A     | 177 | G    |
| 1   | A     | 181 | A    |
| 1   | A     | 183 | C    |
| 1   | A     | 184 | G    |
| 1   | A     | 188 | C    |
| 1   | A     | 197 | A    |
| 1   | A     | 204 | G    |
| 1   | A     | 209 | U    |
| 1   | A     | 210 | C    |
| 1   | A     | 211 | G    |
| 1   | A     | 212 | G    |
| 1   | A     | 223 | A    |
| 1   | A     | 240 | G    |
| 1   | A     | 243 | A    |
| 1   | A     | 245 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 279 | A    |
| 1   | A     | 281 | G    |
| 1   | A     | 283 | U    |
| 1   | A     | 289 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 298 | A    |
| 1   | A     | 301 | G    |
| 1   | A     | 306 | A    |
| 1   | A     | 319 | G    |
| 1   | A     | 328 | C    |
| 1   | A     | 330 | C    |
| 1   | A     | 347 | G    |
| 1   | A     | 351 | G    |
| 1   | A     | 352 | C    |
| 1   | A     | 353 | A    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 372 | C    |
| 1   | A     | 383 | A    |
| 1   | A     | 388 | G    |
| 1   | A     | 392 | C    |
| 1   | A     | 406 | G    |
| 1   | A     | 411 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 421 | U    |
| 1   | A     | 422 | C    |
| 1   | A     | 429 | U    |
| 1   | A     | 439 | U    |
| 1   | A     | 448 | A    |
| 1   | A     | 462 | G    |
| 1   | A     | 463 | U    |
| 1   | A     | 465 | A    |
| 1   | A     | 467 | U    |
| 1   | A     | 468 | A    |
| 1   | A     | 469 | C    |
| 1   | A     | 470 | C    |
| 1   | A     | 472 | U    |
| 1   | A     | 476 | U    |
| 1   | A     | 482 | A    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | U    |
| 1   | A     | 486 | U    |
| 1   | A     | 493 | A    |
| 1   | A     | 497 | G    |
| 1   | A     | 509 | A    |
| 1   | A     | 511 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 513 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 521 | G    |
| 1   | A     | 527 | G7M  |
| 1   | A     | 531 | U    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 562 | U    |
| 1   | A     | 564 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | C    |
| 1   | A     | 577 | G    |
| 1   | A     | 596 | A    |
| 1   | A     | 633 | G    |
| 1   | A     | 642 | A    |
| 1   | A     | 650 | G    |
| 1   | A     | 653 | U    |
| 1   | A     | 654 | G    |
| 1   | A     | 661 | G    |
| 1   | A     | 665 | A    |
| 1   | A     | 686 | U    |
| 1   | A     | 694 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |
| 1   | A     | 731 | G    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 781 | A    |
| 1   | A     | 815 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 829 | G    |
| 1   | A     | 841 | C    |
| 1   | A     | 843 | U    |
| 1   | A     | 844 | G    |
| 1   | A     | 845 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 846  | G    |
| 1   | A     | 851  | G    |
| 1   | A     | 872  | A    |
| 1   | A     | 874  | G    |
| 1   | A     | 885  | G    |
| 1   | A     | 889  | A    |
| 1   | A     | 890  | G    |
| 1   | A     | 891  | U    |
| 1   | A     | 900  | A    |
| 1   | A     | 902  | G    |
| 1   | A     | 914  | A    |
| 1   | A     | 926  | G    |
| 1   | A     | 931  | C    |
| 1   | A     | 934  | C    |
| 1   | A     | 935  | A    |
| 1   | A     | 955  | U    |
| 1   | A     | 960  | U    |
| 1   | A     | 961  | U    |
| 1   | A     | 965  | U    |
| 1   | A     | 966  | 2MG  |
| 1   | A     | 967  | 5MC  |
| 1   | A     | 969  | A    |
| 1   | A     | 971  | G    |
| 1   | A     | 975  | A    |
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 982  | U    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 996  | A    |
| 1   | A     | 999  | C    |
| 1   | A     | 1004 | A    |
| 1   | A     | 1016 | A    |
| 1   | A     | 1017 | U    |
| 1   | A     | 1020 | A    |
| 1   | A     | 1023 | G    |
| 1   | A     | 1026 | G    |
| 1   | A     | 1028 | C    |
| 1   | A     | 1030 | U    |
| 1   | A     | 1031 | C    |
| 1   | A     | 1032 | G    |
| 1   | A     | 1033 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1035 | A    |
| 1   | A     | 1036 | A    |
| 1   | A     | 1042 | A    |
| 1   | A     | 1043 | G    |
| 1   | A     | 1055 | A    |
| 1   | A     | 1064 | G    |
| 1   | A     | 1085 | U    |
| 1   | A     | 1089 | G    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1108 | G    |
| 1   | A     | 1121 | U    |
| 1   | A     | 1122 | U    |
| 1   | A     | 1124 | G    |
| 1   | A     | 1136 | C    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1143 | G    |
| 1   | A     | 1157 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1160 | G    |
| 1   | A     | 1168 | U    |
| 1   | A     | 1174 | G    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1191 | A    |
| 1   | A     | 1193 | G    |
| 1   | A     | 1196 | A    |
| 1   | A     | 1197 | A    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1214 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1250 | A    |
| 1   | A     | 1251 | A    |
| 1   | A     | 1255 | G    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | A    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1260 | G    |
| 1   | A     | 1261 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1262 | C    |
| 1   | A     | 1270 | G    |
| 1   | A     | 1275 | A    |
| 1   | A     | 1279 | G    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1286 | U    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1290 | G    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1331 | G    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1348 | U    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1368 | A    |
| 1   | A     | 1370 | G    |
| 1   | A     | 1379 | G    |
| 1   | A     | 1381 | U    |
| 1   | A     | 1394 | A    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1399 | C    |
| 1   | A     | 1400 | C    |
| 1   | A     | 1419 | G    |
| 1   | A     | 1421 | G    |
| 1   | A     | 1422 | G    |
| 1   | A     | 1432 | G    |
| 1   | A     | 1433 | A    |
| 1   | A     | 1434 | A    |
| 1   | A     | 1441 | A    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1448 | C    |
| 1   | A     | 1451 | U    |
| 1   | A     | 1452 | C    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1493 | A    |
| 1   | A     | 1494 | G    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1502 | A    |
| 1   | A     | 1503 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1506 | U    |
| 1   | A     | 1507 | A    |
| 1   | A     | 1508 | A    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1519 | MA6  |
| 1   | A     | 1520 | C    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1533 | C    |
| 1   | A     | 1534 | A    |
| 1   | A     | 1535 | C    |
| 1   | A     | 1538 | C    |
| 1   | A     | 1539 | C    |
| 1   | A     | 1540 | U    |
| 22  | V     | 2    | G    |
| 22  | V     | 5    | G    |
| 22  | V     | 9    | G    |
| 22  | V     | 14   | A    |
| 22  | V     | 17   | C    |
| 22  | V     | 18   | U    |
| 22  | V     | 19   | G    |
| 22  | V     | 21   | H2U  |
| 22  | V     | 22   | A    |
| 22  | V     | 23   | G    |
| 22  | V     | 59   | A    |
| 22  | V     | 65   | G    |
| 22  | V     | 77   | A    |
| 23  | W     | 2    | G    |
| 23  | W     | 4    | G    |
| 23  | W     | 7    | G    |
| 23  | W     | 9    | G    |
| 23  | W     | 10   | G    |
| 23  | W     | 11   | A    |
| 23  | W     | 14   | A    |
| 23  | W     | 15   | G    |
| 23  | W     | 16   | C    |
| 23  | W     | 17   | C    |
| 23  | W     | 18   | U    |
| 23  | W     | 19   | G    |
| 23  | W     | 20   | G    |
| 23  | W     | 21   | U    |
| 23  | W     | 25   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | W     | 27  | G    |
| 23  | W     | 31  | G    |
| 23  | W     | 32  | G    |
| 23  | W     | 33  | C    |
| 23  | W     | 34  | U    |
| 23  | W     | 35  | C    |
| 23  | W     | 36  | A    |
| 23  | W     | 37  | U    |
| 23  | W     | 40  | C    |
| 23  | W     | 41  | C    |
| 23  | W     | 43  | G    |
| 23  | W     | 46  | G    |
| 23  | W     | 47  | G    |
| 23  | W     | 48  | U    |
| 23  | W     | 49  | C    |
| 23  | W     | 50  | G    |
| 23  | W     | 53  | G    |
| 23  | W     | 56  | U    |
| 23  | W     | 60  | A    |
| 23  | W     | 62  | C    |
| 23  | W     | 64  | G    |
| 23  | W     | 67  | C    |
| 23  | W     | 70  | C    |
| 23  | W     | 71  | G    |
| 23  | W     | 73  | A    |
| 23  | W     | 75  | C    |
| 23  | W     | 76  | C    |
| 23  | W     | 77  | A    |
| 24  | X     | 2   | G    |
| 24  | X     | 3   | G    |
| 24  | X     | 5   | G    |
| 24  | X     | 6   | G    |
| 26  | a     | 10  | A    |
| 26  | a     | 14  | A    |
| 26  | a     | 15  | G    |
| 26  | a     | 34  | U    |
| 26  | a     | 35  | G    |
| 26  | a     | 42  | A    |
| 26  | a     | 45  | G    |
| 26  | a     | 46  | G    |
| 26  | a     | 50  | U    |
| 26  | a     | 51  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | a     | 58  | G    |
| 26  | a     | 60  | G    |
| 26  | a     | 61  | C    |
| 26  | a     | 62  | U    |
| 26  | a     | 63  | A    |
| 26  | a     | 71  | A    |
| 26  | a     | 74  | A    |
| 26  | a     | 75  | G    |
| 26  | a     | 96  | C    |
| 26  | a     | 101 | A    |
| 26  | a     | 102 | U    |
| 26  | a     | 103 | A    |
| 26  | a     | 118 | A    |
| 26  | a     | 119 | A    |
| 26  | a     | 120 | U    |
| 26  | a     | 138 | U    |
| 26  | a     | 139 | U    |
| 26  | a     | 140 | C    |
| 26  | a     | 160 | A    |
| 26  | a     | 162 | U    |
| 26  | a     | 196 | A    |
| 26  | a     | 199 | A    |
| 26  | a     | 215 | G    |
| 26  | a     | 216 | A    |
| 26  | a     | 222 | A    |
| 26  | a     | 229 | C    |
| 26  | a     | 233 | A    |
| 26  | a     | 239 | C    |
| 26  | a     | 242 | G    |
| 26  | a     | 243 | U    |
| 26  | a     | 248 | G    |
| 26  | a     | 250 | G    |
| 26  | a     | 255 | A    |
| 26  | a     | 265 | A    |
| 26  | a     | 275 | C    |
| 26  | a     | 276 | U    |
| 26  | a     | 277 | G    |
| 26  | a     | 278 | A    |
| 26  | a     | 279 | A    |
| 26  | a     | 280 | U    |
| 26  | a     | 285 | G    |
| 26  | a     | 286 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | a     | 301 | G    |
| 26  | a     | 311 | A    |
| 26  | a     | 323 | C    |
| 26  | a     | 329 | G    |
| 26  | a     | 330 | A    |
| 26  | a     | 346 | A    |
| 26  | a     | 358 | U    |
| 26  | a     | 361 | G    |
| 26  | a     | 362 | A    |
| 26  | a     | 372 | G    |
| 26  | a     | 373 | U    |
| 26  | a     | 386 | G    |
| 26  | a     | 395 | U    |
| 26  | a     | 396 | G    |
| 26  | a     | 403 | U    |
| 26  | a     | 404 | A    |
| 26  | a     | 405 | U    |
| 26  | a     | 411 | G    |
| 26  | a     | 412 | A    |
| 26  | a     | 417 | C    |
| 26  | a     | 422 | A    |
| 26  | a     | 424 | G    |
| 26  | a     | 436 | C    |
| 26  | a     | 448 | U    |
| 26  | a     | 455 | C    |
| 26  | a     | 457 | A    |
| 26  | a     | 458 | G    |
| 26  | a     | 459 | U    |
| 26  | a     | 481 | G    |
| 26  | a     | 482 | A    |
| 26  | a     | 490 | C    |
| 26  | a     | 491 | G    |
| 26  | a     | 501 | A    |
| 26  | a     | 503 | A    |
| 26  | a     | 505 | A    |
| 26  | a     | 506 | G    |
| 26  | a     | 509 | C    |
| 26  | a     | 510 | C    |
| 26  | a     | 513 | A    |
| 26  | a     | 518 | G    |
| 26  | a     | 528 | A    |
| 26  | a     | 529 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | a     | 530 | G    |
| 26  | a     | 531 | C    |
| 26  | a     | 532 | A    |
| 26  | a     | 546 | U    |
| 26  | a     | 547 | A    |
| 26  | a     | 549 | G    |
| 26  | a     | 556 | A    |
| 26  | a     | 563 | A    |
| 26  | a     | 573 | U    |
| 26  | a     | 575 | A    |
| 26  | a     | 603 | A    |
| 26  | a     | 609 | A    |
| 26  | a     | 613 | A    |
| 26  | a     | 614 | A    |
| 26  | a     | 627 | A    |
| 26  | a     | 637 | A    |
| 26  | a     | 645 | C    |
| 26  | a     | 646 | U    |
| 26  | a     | 647 | G    |
| 26  | a     | 655 | A    |
| 26  | a     | 669 | G    |
| 26  | a     | 678 | C    |
| 26  | a     | 685 | A    |
| 26  | a     | 686 | U    |
| 26  | a     | 711 | G    |
| 26  | a     | 717 | C    |
| 26  | a     | 726 | G    |
| 26  | a     | 729 | G    |
| 26  | a     | 730 | A    |
| 26  | a     | 738 | G    |
| 26  | a     | 746 | PSU  |
| 26  | a     | 747 | 5MU  |
| 26  | a     | 753 | A    |
| 26  | a     | 764 | A    |
| 26  | a     | 765 | C    |
| 26  | a     | 775 | G    |
| 26  | a     | 782 | A    |
| 26  | a     | 783 | A    |
| 26  | a     | 784 | G    |
| 26  | a     | 785 | G    |
| 26  | a     | 789 | A    |
| 26  | a     | 792 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 805  | G    |
| 26  | a     | 812  | C    |
| 26  | a     | 819  | A    |
| 26  | a     | 827  | U    |
| 26  | a     | 828  | U    |
| 26  | a     | 846  | C    |
| 26  | a     | 847  | U    |
| 26  | a     | 858  | G    |
| 26  | a     | 869  | G    |
| 26  | a     | 877  | A    |
| 26  | a     | 878  | A    |
| 26  | a     | 884  | U    |
| 26  | a     | 885  | C    |
| 26  | a     | 886  | A    |
| 26  | a     | 888  | C    |
| 26  | a     | 891  | G    |
| 26  | a     | 892  | A    |
| 26  | a     | 893  | C    |
| 26  | a     | 894  | U    |
| 26  | a     | 895  | U    |
| 26  | a     | 896  | A    |
| 26  | a     | 906  | U    |
| 26  | a     | 907  | G    |
| 26  | a     | 910  | A    |
| 26  | a     | 927  | A    |
| 26  | a     | 941  | A    |
| 26  | a     | 946  | C    |
| 26  | a     | 953  | G    |
| 26  | a     | 958  | U    |
| 26  | a     | 961  | C    |
| 26  | a     | 973  | A    |
| 26  | a     | 974  | G    |
| 26  | a     | 983  | A    |
| 26  | a     | 989  | G    |
| 26  | a     | 995  | C    |
| 26  | a     | 996  | A    |
| 26  | a     | 1005 | C    |
| 26  | a     | 1012 | U    |
| 26  | a     | 1013 | C    |
| 26  | a     | 1023 | U    |
| 26  | a     | 1026 | G    |
| 26  | a     | 1033 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 1045 | C    |
| 26  | a     | 1046 | A    |
| 26  | a     | 1047 | G    |
| 26  | a     | 1053 | C    |
| 26  | a     | 1055 | G    |
| 26  | a     | 1057 | A    |
| 26  | a     | 1059 | G    |
| 26  | a     | 1060 | U    |
| 26  | a     | 1061 | U    |
| 26  | a     | 1062 | G    |
| 26  | a     | 1063 | G    |
| 26  | a     | 1064 | C    |
| 26  | a     | 1065 | U    |
| 26  | a     | 1067 | A    |
| 26  | a     | 1068 | G    |
| 26  | a     | 1069 | A    |
| 26  | a     | 1070 | A    |
| 26  | a     | 1072 | C    |
| 26  | a     | 1073 | A    |
| 26  | a     | 1074 | G    |
| 26  | a     | 1076 | C    |
| 26  | a     | 1077 | A    |
| 26  | a     | 1078 | U    |
| 26  | a     | 1079 | C    |
| 26  | a     | 1080 | A    |
| 26  | a     | 1081 | U    |
| 26  | a     | 1083 | U    |
| 26  | a     | 1084 | A    |
| 26  | a     | 1085 | A    |
| 26  | a     | 1087 | G    |
| 26  | a     | 1088 | A    |
| 26  | a     | 1089 | A    |
| 26  | a     | 1090 | A    |
| 26  | a     | 1091 | G    |
| 26  | a     | 1092 | C    |
| 26  | a     | 1093 | G    |
| 26  | a     | 1094 | U    |
| 26  | a     | 1096 | A    |
| 26  | a     | 1099 | G    |
| 26  | a     | 1101 | U    |
| 26  | a     | 1102 | C    |
| 26  | a     | 1103 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 1104 | C    |
| 26  | a     | 1105 | U    |
| 26  | a     | 1106 | G    |
| 26  | a     | 1111 | A    |
| 26  | a     | 1112 | G    |
| 26  | a     | 1132 | U    |
| 26  | a     | 1133 | A    |
| 26  | a     | 1135 | C    |
| 26  | a     | 1139 | G    |
| 26  | a     | 1142 | A    |
| 26  | a     | 1149 | G    |
| 26  | a     | 1171 | G    |
| 26  | a     | 1172 | C    |
| 26  | a     | 1174 | U    |
| 26  | a     | 1176 | U    |
| 26  | a     | 1177 | G    |
| 26  | a     | 1178 | C    |
| 26  | a     | 1179 | G    |
| 26  | a     | 1180 | U    |
| 26  | a     | 1212 | G    |
| 26  | a     | 1225 | G    |
| 26  | a     | 1237 | A    |
| 26  | a     | 1250 | G    |
| 26  | a     | 1253 | A    |
| 26  | a     | 1256 | G    |
| 26  | a     | 1262 | A    |
| 26  | a     | 1271 | G    |
| 26  | a     | 1272 | A    |
| 26  | a     | 1273 | U    |
| 26  | a     | 1275 | A    |
| 26  | a     | 1286 | A    |
| 26  | a     | 1289 | C    |
| 26  | a     | 1300 | G    |
| 26  | a     | 1301 | A    |
| 26  | a     | 1302 | A    |
| 26  | a     | 1306 | C    |
| 26  | a     | 1314 | C    |
| 26  | a     | 1321 | A    |
| 26  | a     | 1332 | G    |
| 26  | a     | 1345 | C    |
| 26  | a     | 1352 | U    |
| 26  | a     | 1365 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 1368 | G    |
| 26  | a     | 1378 | A    |
| 26  | a     | 1379 | U    |
| 26  | a     | 1383 | A    |
| 26  | a     | 1389 | G    |
| 26  | a     | 1395 | A    |
| 26  | a     | 1403 | A    |
| 26  | a     | 1404 | C    |
| 26  | a     | 1414 | C    |
| 26  | a     | 1416 | G    |
| 26  | a     | 1428 | C    |
| 26  | a     | 1451 | C    |
| 26  | a     | 1453 | A    |
| 26  | a     | 1455 | G    |
| 26  | a     | 1458 | U    |
| 26  | a     | 1459 | G    |
| 26  | a     | 1461 | C    |
| 26  | a     | 1471 | G    |
| 26  | a     | 1475 | G    |
| 26  | a     | 1476 | U    |
| 26  | a     | 1482 | G    |
| 26  | a     | 1487 | U    |
| 26  | a     | 1490 | A    |
| 26  | a     | 1491 | G    |
| 26  | a     | 1493 | C    |
| 26  | a     | 1494 | A    |
| 26  | a     | 1497 | U    |
| 26  | a     | 1508 | A    |
| 26  | a     | 1509 | A    |
| 26  | a     | 1515 | A    |
| 26  | a     | 1522 | A    |
| 26  | a     | 1524 | G    |
| 26  | a     | 1531 | C    |
| 26  | a     | 1535 | A    |
| 26  | a     | 1538 | G    |
| 26  | a     | 1547 | C    |
| 26  | a     | 1554 | U    |
| 26  | a     | 1558 | C    |
| 26  | a     | 1559 | U    |
| 26  | a     | 1560 | G    |
| 26  | a     | 1569 | A    |
| 26  | a     | 1578 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 1583 | A    |
| 26  | a     | 1585 | C    |
| 26  | a     | 1589 | U    |
| 26  | a     | 1608 | A    |
| 26  | a     | 1610 | A    |
| 26  | a     | 1618 | 6MZ  |
| 26  | a     | 1619 | G    |
| 26  | a     | 1634 | A    |
| 26  | a     | 1639 | C    |
| 26  | a     | 1647 | U    |
| 26  | a     | 1648 | U    |
| 26  | a     | 1649 | G    |
| 26  | a     | 1674 | G    |
| 26  | a     | 1675 | C    |
| 26  | a     | 1698 | A    |
| 26  | a     | 1713 | A    |
| 26  | a     | 1715 | G    |
| 26  | a     | 1716 | U    |
| 26  | a     | 1729 | U    |
| 26  | a     | 1730 | U    |
| 26  | a     | 1731 | G    |
| 26  | a     | 1736 | U    |
| 26  | a     | 1738 | G    |
| 26  | a     | 1744 | A    |
| 26  | a     | 1756 | G    |
| 26  | a     | 1758 | U    |
| 26  | a     | 1759 | A    |
| 26  | a     | 1764 | C    |
| 26  | a     | 1773 | A    |
| 26  | a     | 1786 | A    |
| 26  | a     | 1800 | C    |
| 26  | a     | 1801 | A    |
| 26  | a     | 1802 | A    |
| 26  | a     | 1808 | A    |
| 26  | a     | 1811 | G    |
| 26  | a     | 1816 | C    |
| 26  | a     | 1817 | G    |
| 26  | a     | 1819 | A    |
| 26  | a     | 1828 | G    |
| 26  | a     | 1829 | A    |
| 26  | a     | 1858 | A    |
| 26  | a     | 1870 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 1884 | G    |
| 26  | a     | 1901 | A    |
| 26  | a     | 1903 | G    |
| 26  | a     | 1906 | G    |
| 26  | a     | 1913 | A    |
| 26  | a     | 1914 | C    |
| 26  | a     | 1915 | 3TD  |
| 26  | a     | 1919 | A    |
| 26  | a     | 1924 | C    |
| 26  | a     | 1926 | U    |
| 26  | a     | 1929 | G    |
| 26  | a     | 1930 | G    |
| 26  | a     | 1931 | U    |
| 26  | a     | 1937 | A    |
| 26  | a     | 1938 | A    |
| 26  | a     | 1939 | 5MU  |
| 26  | a     | 1940 | U    |
| 26  | a     | 1941 | C    |
| 26  | a     | 1943 | U    |
| 26  | a     | 1954 | G    |
| 26  | a     | 1955 | U    |
| 26  | a     | 1966 | A    |
| 26  | a     | 1967 | C    |
| 26  | a     | 1970 | A    |
| 26  | a     | 1971 | U    |
| 26  | a     | 1972 | G    |
| 26  | a     | 1975 | G    |
| 26  | a     | 1991 | U    |
| 26  | a     | 1993 | U    |
| 26  | a     | 1996 | C    |
| 26  | a     | 1997 | C    |
| 26  | a     | 2020 | A    |
| 26  | a     | 2022 | U    |
| 26  | a     | 2023 | C    |
| 26  | a     | 2027 | G    |
| 26  | a     | 2030 | 6MZ  |
| 26  | a     | 2031 | A    |
| 26  | a     | 2033 | A    |
| 26  | a     | 2043 | C    |
| 26  | a     | 2049 | G    |
| 26  | a     | 2052 | A    |
| 26  | a     | 2055 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 2056 | G    |
| 26  | a     | 2060 | A    |
| 26  | a     | 2061 | G    |
| 26  | a     | 2062 | A    |
| 26  | a     | 2069 | G7M  |
| 26  | a     | 2072 | C    |
| 26  | a     | 2080 | A    |
| 26  | a     | 2093 | G    |
| 26  | a     | 2100 | G    |
| 26  | a     | 2104 | C    |
| 26  | a     | 2105 | U    |
| 26  | a     | 2106 | U    |
| 26  | a     | 2107 | G    |
| 26  | a     | 2108 | A    |
| 26  | a     | 2111 | U    |
| 26  | a     | 2112 | G    |
| 26  | a     | 2113 | U    |
| 26  | a     | 2116 | G    |
| 26  | a     | 2117 | A    |
| 26  | a     | 2118 | U    |
| 26  | a     | 2119 | A    |
| 26  | a     | 2122 | U    |
| 26  | a     | 2123 | G    |
| 26  | a     | 2124 | G    |
| 26  | a     | 2125 | G    |
| 26  | a     | 2126 | A    |
| 26  | a     | 2127 | G    |
| 26  | a     | 2131 | U    |
| 26  | a     | 2132 | U    |
| 26  | a     | 2133 | G    |
| 26  | a     | 2135 | A    |
| 26  | a     | 2136 | G    |
| 26  | a     | 2137 | U    |
| 26  | a     | 2138 | G    |
| 26  | a     | 2139 | U    |
| 26  | a     | 2140 | G    |
| 26  | a     | 2141 | G    |
| 26  | a     | 2144 | G    |
| 26  | a     | 2145 | C    |
| 26  | a     | 2146 | C    |
| 26  | a     | 2147 | A    |
| 26  | a     | 2150 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 2152 | G    |
| 26  | a     | 2153 | C    |
| 26  | a     | 2155 | U    |
| 26  | a     | 2157 | G    |
| 26  | a     | 2158 | A    |
| 26  | a     | 2161 | C    |
| 26  | a     | 2164 | C    |
| 26  | a     | 2165 | C    |
| 26  | a     | 2168 | G    |
| 26  | a     | 2170 | A    |
| 26  | a     | 2172 | U    |
| 26  | a     | 2173 | A    |
| 26  | a     | 2174 | C    |
| 26  | a     | 2176 | A    |
| 26  | a     | 2178 | C    |
| 26  | a     | 2179 | C    |
| 26  | a     | 2180 | U    |
| 26  | a     | 2181 | U    |
| 26  | a     | 2184 | A    |
| 26  | a     | 2185 | U    |
| 26  | a     | 2186 | G    |
| 26  | a     | 2187 | U    |
| 26  | a     | 2189 | U    |
| 26  | a     | 2198 | A    |
| 26  | a     | 2203 | U    |
| 26  | a     | 2204 | G    |
| 26  | a     | 2211 | A    |
| 26  | a     | 2212 | A    |
| 26  | a     | 2214 | C    |
| 26  | a     | 2225 | A    |
| 26  | a     | 2238 | G    |
| 26  | a     | 2239 | G    |
| 26  | a     | 2243 | U    |
| 26  | a     | 2250 | G    |
| 26  | a     | 2266 | A    |
| 26  | a     | 2268 | A    |
| 26  | a     | 2279 | G    |
| 26  | a     | 2283 | C    |
| 26  | a     | 2287 | A    |
| 26  | a     | 2305 | U    |
| 26  | a     | 2308 | G    |
| 26  | a     | 2309 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 2312 | U    |
| 26  | a     | 2320 | U    |
| 26  | a     | 2322 | A    |
| 26  | a     | 2325 | G    |
| 26  | a     | 2334 | U    |
| 26  | a     | 2335 | A    |
| 26  | a     | 2345 | G    |
| 26  | a     | 2347 | C    |
| 26  | a     | 2350 | C    |
| 26  | a     | 2354 | C    |
| 26  | a     | 2361 | G    |
| 26  | a     | 2379 | G    |
| 26  | a     | 2382 | G    |
| 26  | a     | 2383 | G    |
| 26  | a     | 2385 | C    |
| 26  | a     | 2391 | G    |
| 26  | a     | 2392 | A    |
| 26  | a     | 2396 | G    |
| 26  | a     | 2402 | U    |
| 26  | a     | 2403 | C    |
| 26  | a     | 2406 | A    |
| 26  | a     | 2425 | A    |
| 26  | a     | 2427 | C    |
| 26  | a     | 2429 | G    |
| 26  | a     | 2430 | A    |
| 26  | a     | 2432 | A    |
| 26  | a     | 2435 | A    |
| 26  | a     | 2441 | U    |
| 26  | a     | 2445 | 2MG  |
| 26  | a     | 2448 | A    |
| 26  | a     | 2452 | C    |
| 26  | a     | 2453 | A    |
| 26  | a     | 2459 | A    |
| 26  | a     | 2473 | U    |
| 26  | a     | 2474 | U    |
| 26  | a     | 2475 | C    |
| 26  | a     | 2476 | A    |
| 26  | a     | 2478 | A    |
| 26  | a     | 2484 | G    |
| 26  | a     | 2492 | U    |
| 26  | a     | 2494 | G    |
| 26  | a     | 2498 | OMC  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 2502 | G    |
| 26  | a     | 2503 | 2MA  |
| 26  | a     | 2504 | PSU  |
| 26  | a     | 2505 | G    |
| 26  | a     | 2518 | A    |
| 26  | a     | 2529 | G    |
| 26  | a     | 2535 | G    |
| 26  | a     | 2547 | A    |
| 26  | a     | 2554 | U    |
| 26  | a     | 2555 | U    |
| 26  | a     | 2566 | A    |
| 26  | a     | 2567 | G    |
| 26  | a     | 2572 | A    |
| 26  | a     | 2573 | C    |
| 26  | a     | 2585 | U    |
| 26  | a     | 2586 | U    |
| 26  | a     | 2602 | A    |
| 26  | a     | 2604 | PSU  |
| 26  | a     | 2609 | U    |
| 26  | a     | 2613 | U    |
| 26  | a     | 2615 | U    |
| 26  | a     | 2623 | G    |
| 26  | a     | 2629 | U    |
| 26  | a     | 2630 | G    |
| 26  | a     | 2636 | C    |
| 26  | a     | 2646 | C    |
| 26  | a     | 2654 | A    |
| 26  | a     | 2655 | G    |
| 26  | a     | 2656 | U    |
| 26  | a     | 2673 | G    |
| 26  | a     | 2682 | A    |
| 26  | a     | 2685 | G    |
| 26  | a     | 2689 | U    |
| 26  | a     | 2690 | U    |
| 26  | a     | 2702 | G    |
| 26  | a     | 2714 | G    |
| 26  | a     | 2716 | C    |
| 26  | a     | 2718 | G    |
| 26  | a     | 2720 | U    |
| 26  | a     | 2726 | A    |
| 26  | a     | 2727 | A    |
| 26  | a     | 2733 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | a     | 2744 | G    |
| 26  | a     | 2748 | A    |
| 26  | a     | 2765 | A    |
| 26  | a     | 2776 | A    |
| 26  | a     | 2777 | G    |
| 26  | a     | 2778 | A    |
| 26  | a     | 2779 | U    |
| 26  | a     | 2786 | U    |
| 26  | a     | 2791 | G    |
| 26  | a     | 2797 | U    |
| 26  | a     | 2798 | U    |
| 26  | a     | 2800 | A    |
| 26  | a     | 2809 | A    |
| 26  | a     | 2818 | U    |
| 26  | a     | 2820 | A    |
| 26  | a     | 2833 | U    |
| 26  | a     | 2835 | A    |
| 26  | a     | 2849 | U    |
| 26  | a     | 2867 | G    |
| 26  | a     | 2868 | A    |
| 26  | a     | 2872 | A    |
| 26  | a     | 2873 | A    |
| 26  | a     | 2880 | C    |
| 26  | a     | 2884 | U    |
| 26  | a     | 2891 | U    |
| 27  | b     | 4    | C    |
| 27  | b     | 9    | G    |
| 27  | b     | 24   | G    |
| 27  | b     | 32   | U    |
| 27  | b     | 36   | C    |
| 27  | b     | 37   | C    |
| 27  | b     | 41   | G    |
| 27  | b     | 45   | A    |
| 27  | b     | 51   | G    |
| 27  | b     | 52   | A    |
| 27  | b     | 56   | G    |
| 27  | b     | 57   | A    |
| 27  | b     | 67   | G    |
| 27  | b     | 87   | U    |
| 27  | b     | 88   | C    |
| 27  | b     | 89   | U    |
| 27  | b     | 109  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | b     | 120 | U    |

All (25) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 242  | G    |
| 1   | A     | 361  | G    |
| 1   | A     | 413  | G    |
| 1   | A     | 428  | G    |
| 1   | A     | 438  | U    |
| 1   | A     | 481  | G    |
| 1   | A     | 490  | C    |
| 1   | A     | 561  | U    |
| 1   | A     | 652  | U    |
| 1   | A     | 774  | G    |
| 1   | A     | 818  | G    |
| 1   | A     | 890  | G    |
| 1   | A     | 1111 | A    |
| 1   | A     | 1190 | G    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1399 | C    |
| 1   | A     | 1432 | G    |
| 1   | A     | 1475 | G    |
| 1   | A     | 1539 | C    |
| 22  | V     | 20   | G    |
| 23  | W     | 9    | G    |
| 23  | W     | 17   | C    |
| 23  | W     | 76   | C    |

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

43 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 |
| 26  | PSU  | a     | 1911 | 26    | 18,21,22     | 1.09 | 2 (11%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 26  | PSU  | a     | 2605 | 26    | 18,21,22     | 1.45 | 3 (16%)  | 22,30,33    | 1.87 | 4 (18%)  |
| 1   | 5MC  | A     | 1407 | 1     | 18,22,23     | 3.52 | 7 (38%)  | 26,32,35    | 1.00 | 1 (3%)   |
| 12  | D2T  | L     | 89   | 12    | 7,9,10       | 1.37 | 1 (14%)  | 6,11,13     | 2.60 | 4 (66%)  |
| 26  | G7M  | a     | 2069 | 26    | 23,26,27     | 1.51 | 4 (17%)  | 35,39,42    | 1.87 | 6 (17%)  |
| 26  | H2U  | a     | 2449 | 26    | 18,21,22     | 2.70 | 5 (27%)  | 21,30,33    | 2.11 | 5 (23%)  |
| 26  | 1MG  | a     | 745  | 26    | 22,26,27     | 1.11 | 2 (9%)   | 33,39,42    | 1.91 | 8 (24%)  |
| 26  | 6MZ  | a     | 2030 | 26    | 22,25,26     | 2.69 | 5 (22%)  | 30,36,39    | 2.49 | 12 (40%) |
| 26  | PSU  | a     | 2580 | 26    | 18,21,22     | 1.44 | 2 (11%)  | 22,30,33    | 2.05 | 4 (18%)  |
| 1   | 5MC  | A     | 967  | 1     | 18,22,23     | 3.59 | 7 (38%)  | 26,32,35    | 1.05 | 1 (3%)   |
| 22  | 4SU  | V     | 8    | 22    | 18,21,22     | 3.71 | 7 (38%)  | 26,30,33    | 2.35 | 6 (23%)  |
| 26  | OMC  | a     | 2498 | 26,57 | 19,22,23     | 3.12 | 8 (42%)  | 26,31,34    | 0.71 | 0        |
| 26  | 2MA  | a     | 2503 | 26,57 | 22,25,26     | 1.49 | 4 (18%)  | 33,37,40    | 2.33 | 10 (30%) |
| 26  | OMU  | a     | 2552 | 26,57 | 19,22,23     | 2.81 | 8 (42%)  | 26,31,34    | 1.82 | 4 (15%)  |
| 1   | 2MG  | A     | 1516 | 1     | 23,26,27     | 1.33 | 4 (17%)  | 32,38,41    | 2.35 | 9 (28%)  |
| 1   | MA6  | A     | 1519 | 1     | 23,26,27     | 1.62 | 5 (21%)  | 34,38,41    | 2.37 | 13 (38%) |
| 26  | PSU  | a     | 746  | 26    | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.98 | 4 (18%)  |
| 1   | 2MG  | A     | 966  | 1     | 23,26,27     | 1.30 | 4 (17%)  | 32,38,41    | 2.35 | 8 (25%)  |
| 22  | PSU  | V     | 56   | 22    | 18,21,22     | 1.46 | 3 (16%)  | 22,30,33    | 1.79 | 3 (13%)  |
| 26  | 5MU  | a     | 747  | 26    | 19,22,23     | 1.49 | 5 (26%)  | 28,32,35    | 2.13 | 10 (35%) |
| 26  | 5MC  | a     | 1962 | 26    | 18,22,23     | 3.53 | 7 (38%)  | 26,32,35    | 1.12 | 1 (3%)   |
| 26  | PSU  | a     | 955  | 26    | 18,21,22     | 1.11 | 2 (11%)  | 22,30,33    | 1.87 | 4 (18%)  |
| 26  | PSU  | a     | 2457 | 26    | 18,21,22     | 1.57 | 3 (16%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 1   | UR3  | A     | 1498 | 1     | 19,22,23     | 2.77 | 7 (36%)  | 26,32,35    | 1.40 | 2 (7%)   |
| 1   | 2MG  | A     | 1207 | 1     | 23,26,27     | 1.32 | 4 (17%)  | 32,38,41    | 2.27 | 7 (21%)  |
| 26  | OMG  | a     | 2251 | 22,26 | 23,26,27     | 1.26 | 3 (13%)  | 33,38,41    | 1.99 | 6 (18%)  |
| 26  | PSU  | a     | 2504 | 26    | 18,21,22     | 1.55 | 2 (11%)  | 22,30,33    | 2.02 | 5 (22%)  |
| 1   | MA6  | A     | 1518 | 1     | 23,26,27     | 1.49 | 3 (13%)  | 34,38,41    | 2.61 | 16 (47%) |
| 37  | 4D4  | l     | 81   | 37    | 9,11,12      | 1.90 | 2 (22%)  | 8,13,15     | 1.85 | 2 (25%)  |
| 1   | PSU  | A     | 516  | 1,57  | 18,21,22     | 1.49 | 2 (11%)  | 22,30,33    | 1.97 | 3 (13%)  |
| 26  | 2MG  | a     | 1835 | 26    | 23,26,27     | 1.31 | 4 (17%)  | 32,38,41    | 2.26 | 6 (18%)  |
| 26  | 2MG  | a     | 2445 | 26    | 23,26,27     | 1.36 | 3 (13%)  | 32,38,41    | 2.21 | 8 (25%)  |
| 22  | H2U  | V     | 21   | 22    | 18,21,22     | 2.91 | 5 (27%)  | 21,30,33    | 1.98 | 5 (23%)  |
| 26  | 6MZ  | a     | 1618 | 26    | 22,25,26     | 2.63 | 5 (22%)  | 30,36,39    | 2.47 | 12 (40%) |
| 1   | G7M  | A     | 527  | 1     | 23,26,27     | 1.51 | 3 (13%)  | 35,39,42    | 1.91 | 6 (17%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | PSU  | a     | 2604 | 26   | 18,21,22     | 1.46 | 2 (11%)  | 22,30,33    | 2.00 | 4 (18%)  |
| 1   | 4OC  | A     | 1402 | 1    | 20,23,24     | 3.03 | 8 (40%)  | 26,32,35    | 0.92 | 2 (7%)   |
| 37  | MS6  | l     | 137  | 37   | 5,7,8        | 0.70 | 0        | 2,7,9       | 1.50 | 0        |
| 26  | 3TD  | a     | 1915 | 26   | 18,22,23     | 4.32 | 7 (38%)  | 22,32,35    | 1.73 | 4 (18%)  |
| 26  | PSU  | a     | 1917 | 26   | 18,21,22     | 1.53 | 3 (16%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 29  | MEQ  | d     | 150  | 29   | 8,9,10       | 0.95 | 0        | 5,10,12     | 1.13 | 1 (20%)  |
| 22  | 5MU  | V     | 55   | 22   | 19,22,23     | 1.45 | 6 (31%)  | 28,32,35    | 1.74 | 8 (28%)  |
| 26  | 5MU  | a     | 1939 | 26   | 19,22,23     | 1.51 | 6 (31%)  | 28,32,35    | 2.16 | 8 (28%)  |

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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 26  | PSU  | a     | 1911 | 26    | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | PSU  | a     | 2605 | 26    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 1407 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 12  | D2T  | L     | 89   | 12    | -       | 3/7/12/14  | -       |
| 26  | G7M  | a     | 2069 | 26    | -       | 2/7/25/26  | 0/3/3/3 |
| 26  | H2U  | a     | 2449 | 26    | -       | 0/7/38/39  | 0/2/2/2 |
| 26  | 1MG  | a     | 745  | 26    | -       | 0/7/25/26  | 0/3/3/3 |
| 26  | 6MZ  | a     | 2030 | 26    | -       | 2/9/27/28  | 0/3/3/3 |
| 26  | PSU  | a     | 2580 | 26    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 967  | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 22  | 4SU  | V     | 8    | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | OMC  | a     | 2498 | 26,57 | -       | 2/9/27/28  | 0/2/2/2 |
| 26  | 2MA  | a     | 2503 | 26,57 | -       | 3/7/25/26  | 0/3/3/3 |
| 26  | OMU  | a     | 2552 | 26,57 | -       | 3/9/27/28  | 0/2/2/2 |
| 1   | 2MG  | A     | 1516 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | MA6  | A     | 1519 | 1     | -       | 5/11/29/30 | 0/3/3/3 |
| 26  | PSU  | a     | 746  | 26    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | A     | 966  | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 22  | PSU  | V     | 56   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | 5MU  | a     | 747  | 26    | -       | 1/7/25/26  | 0/2/2/2 |
| 26  | 5MC  | a     | 1962 | 26    | -       | 2/7/25/26  | 0/2/2/2 |
| 26  | PSU  | a     | 955  | 26    | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | PSU  | a     | 2457 | 26    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | UR3  | A     | 1498 | 1     | -       | 2/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | 2MG  | A     | 1207 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 26  | OMG  | a     | 2251 | 22,26 | -       | 1/9/27/28  | 0/3/3/3 |
| 26  | PSU  | a     | 2504 | 26    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | MA6  | A     | 1518 | 1     | -       | 2/11/29/30 | 0/3/3/3 |
| 37  | 4D4  | l     | 81   | 37    | -       | 2/11/12/14 | -       |
| 1   | PSU  | A     | 516  | 1,57  | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | 2MG  | a     | 1835 | 26    | -       | 2/9/27/28  | 0/3/3/3 |
| 26  | 2MG  | a     | 2445 | 26    | -       | 2/9/27/28  | 0/3/3/3 |
| 22  | H2U  | V     | 21   | 22    | -       | 7/7/38/39  | 0/2/2/2 |
| 26  | 6MZ  | a     | 1618 | 26    | -       | 4/9/27/28  | 0/3/3/3 |
| 1   | G7M  | A     | 527  | 1     | -       | 1/7/25/26  | 0/3/3/3 |
| 26  | PSU  | a     | 2604 | 26    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | A     | 1402 | 1     | -       | 1/9/29/30  | 0/2/2/2 |
| 37  | MS6  | l     | 137  | 37    | -       | 2/4/6/8    | -       |
| 26  | 3TD  | a     | 1915 | 26    | -       | 6/7/25/26  | 0/2/2/2 |
| 26  | PSU  | a     | 1917 | 26    | -       | 0/7/25/26  | 0/2/2/2 |
| 29  | MEQ  | d     | 150  | 29    | -       | 2/8/9/11   | -       |
| 22  | 5MU  | V     | 55   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | 5MU  | a     | 1939 | 26    | -       | 2/7/25/26  | 0/2/2/2 |

All (175) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 26  | a     | 1915 | 3TD  | C6-C5 | 12.35 | 1.49        | 1.35     |
| 26  | a     | 2030 | 6MZ  | C6-N6 | 11.00 | 1.46        | 1.34     |
| 26  | a     | 1618 | 6MZ  | C6-N6 | 10.77 | 1.45        | 1.34     |
| 1   | A     | 1407 | 5MC  | C6-C5 | 9.35  | 1.50        | 1.34     |
| 1   | A     | 967  | 5MC  | C6-C5 | 9.26  | 1.49        | 1.34     |
| 22  | V     | 21   | H2U  | C2-N1 | 9.23  | 1.48        | 1.35     |
| 26  | a     | 1915 | 3TD  | C2-N1 | 9.13  | 1.49        | 1.37     |
| 26  | a     | 1962 | 5MC  | C6-C5 | 8.98  | 1.49        | 1.34     |
| 22  | V     | 8    | 4SU  | C4-N3 | 8.33  | 1.46        | 1.37     |
| 26  | a     | 2449 | H2U  | C2-N1 | 8.07  | 1.47        | 1.35     |
| 22  | V     | 8    | 4SU  | C2-N3 | 7.13  | 1.50        | 1.38     |
| 1   | A     | 1402 | 4OC  | C4-N3 | 6.74  | 1.44        | 1.32     |
| 1   | A     | 1498 | UR3  | C2-N1 | 6.53  | 1.47        | 1.38     |
| 22  | V     | 8    | 4SU  | C2-N1 | 6.49  | 1.48        | 1.38     |
| 26  | a     | 1962 | 5MC  | C4-N3 | 6.41  | 1.45        | 1.34     |
| 1   | A     | 967  | 5MC  | C4-N3 | 6.35  | 1.44        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 26  | a     | 2498 | OMC  | C6-C5   | 6.26  | 1.49        | 1.35     |
| 1   | A     | 967  | 5MC  | C2-N3   | 6.25  | 1.49        | 1.36     |
| 26  | a     | 1962 | 5MC  | C2-N3   | 6.22  | 1.49        | 1.36     |
| 26  | a     | 2498 | OMC  | C2-N3   | 6.19  | 1.48        | 1.36     |
| 1   | A     | 1402 | 4OC  | C6-C5   | 6.16  | 1.49        | 1.35     |
| 26  | a     | 2498 | OMC  | C4-N4   | 6.10  | 1.48        | 1.33     |
| 1   | A     | 1407 | 5MC  | C2-N3   | 6.04  | 1.48        | 1.36     |
| 22  | V     | 21   | H2U  | C2-N3   | 5.92  | 1.48        | 1.38     |
| 1   | A     | 1407 | 5MC  | C4-N3   | 5.88  | 1.44        | 1.34     |
| 1   | A     | 1498 | UR3  | C6-C5   | 5.88  | 1.48        | 1.35     |
| 26  | a     | 2552 | OMU  | C2-N1   | 5.84  | 1.47        | 1.38     |
| 22  | V     | 8    | 4SU  | C6-C5   | 5.74  | 1.48        | 1.35     |
| 26  | a     | 2552 | OMU  | C2-N3   | 5.69  | 1.48        | 1.38     |
| 26  | a     | 1915 | 3TD  | C6-N1   | 5.66  | 1.45        | 1.36     |
| 1   | A     | 1402 | 4OC  | C2-N3   | 5.65  | 1.47        | 1.36     |
| 26  | a     | 2449 | H2U  | C2-N3   | 5.55  | 1.47        | 1.38     |
| 26  | a     | 1915 | 3TD  | C5'-C4' | -5.21 | 1.35        | 1.51     |
| 1   | A     | 1498 | UR3  | C2-N3   | 5.13  | 1.48        | 1.39     |
| 26  | a     | 2498 | OMC  | C4-N3   | 5.02  | 1.44        | 1.34     |
| 26  | a     | 2552 | OMU  | O2-C2   | -4.77 | 1.14        | 1.23     |
| 1   | A     | 527  | G7M  | C5-N7   | -4.75 | 1.33        | 1.39     |
| 37  | l     | 81   | 4D4  | CZ-NE   | 4.74  | 1.42        | 1.33     |
| 26  | a     | 2069 | G7M  | C5-N7   | -4.67 | 1.33        | 1.39     |
| 1   | A     | 1519 | MA6  | C5-C4   | 4.60  | 1.47        | 1.39     |
| 26  | a     | 2552 | OMU  | C6-C5   | 4.57  | 1.45        | 1.35     |
| 1   | A     | 967  | 5MC  | C6-N1   | 4.54  | 1.45        | 1.38     |
| 22  | V     | 21   | H2U  | C4-N3   | 4.50  | 1.45        | 1.37     |
| 1   | A     | 1407 | 5MC  | C6-N1   | 4.47  | 1.45        | 1.38     |
| 26  | a     | 1915 | 3TD  | C2-N3   | 4.47  | 1.48        | 1.38     |
| 26  | a     | 2503 | 2MA  | C5-C4   | 4.47  | 1.47        | 1.39     |
| 1   | A     | 1518 | MA6  | C5-C4   | 4.45  | 1.47        | 1.39     |
| 1   | A     | 1407 | 5MC  | C4-N4   | 4.41  | 1.45        | 1.34     |
| 1   | A     | 967  | 5MC  | C4-N4   | 4.40  | 1.45        | 1.34     |
| 26  | a     | 1962 | 5MC  | C6-N1   | 4.38  | 1.45        | 1.38     |
| 26  | a     | 1962 | 5MC  | C4-N4   | 4.37  | 1.45        | 1.34     |
| 1   | A     | 1402 | 4OC  | C4-N4   | 4.35  | 1.44        | 1.35     |
| 22  | V     | 8    | 4SU  | C5-C4   | 4.35  | 1.48        | 1.42     |
| 22  | V     | 8    | 4SU  | C4-S4   | -4.34 | 1.60        | 1.68     |
| 26  | a     | 2498 | OMC  | C2-N1   | 4.25  | 1.49        | 1.40     |
| 26  | a     | 2504 | PSU  | C6-C5   | 4.09  | 1.40        | 1.35     |
| 26  | a     | 2449 | H2U  | C4-N3   | 4.06  | 1.44        | 1.37     |
| 26  | a     | 1962 | 5MC  | C2-N1   | 3.88  | 1.48        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 967  | 5MC  | C2-N1 | 3.87  | 1.48        | 1.40     |
| 1   | A     | 1402 | 4OC  | C5-C4 | 3.79  | 1.48        | 1.40     |
| 1   | A     | 1402 | 4OC  | C2-N1 | 3.78  | 1.48        | 1.40     |
| 26  | a     | 2605 | PSU  | C6-C5 | 3.78  | 1.39        | 1.35     |
| 26  | a     | 2552 | OMU  | O4-C4 | -3.73 | 1.17        | 1.24     |
| 22  | V     | 56   | PSU  | C6-C5 | 3.71  | 1.39        | 1.35     |
| 1   | A     | 1407 | 5MC  | C2-N1 | 3.63  | 1.47        | 1.40     |
| 26  | a     | 2457 | PSU  | C6-C5 | 3.61  | 1.39        | 1.35     |
| 1   | A     | 1498 | UR3  | C6-N1 | 3.56  | 1.46        | 1.38     |
| 26  | a     | 2604 | PSU  | C6-C5 | 3.54  | 1.39        | 1.35     |
| 1   | A     | 516  | PSU  | C6-C5 | 3.45  | 1.39        | 1.35     |
| 26  | a     | 1917 | PSU  | C6-C5 | 3.44  | 1.39        | 1.35     |
| 1   | A     | 527  | G7M  | C5-C4 | 3.44  | 1.47        | 1.38     |
| 26  | a     | 2069 | G7M  | C5-C4 | 3.38  | 1.46        | 1.38     |
| 26  | a     | 2580 | PSU  | C6-C5 | 3.35  | 1.39        | 1.35     |
| 26  | a     | 2457 | PSU  | C4-N3 | -3.32 | 1.32        | 1.38     |
| 26  | a     | 2030 | 6MZ  | C5-C4 | -3.26 | 1.32        | 1.39     |
| 26  | a     | 2498 | OMC  | O2-C2 | -3.20 | 1.17        | 1.23     |
| 26  | a     | 746  | PSU  | C6-C5 | 3.17  | 1.39        | 1.35     |
| 26  | a     | 2498 | OMC  | C6-N1 | 3.16  | 1.45        | 1.38     |
| 1   | A     | 1402 | 4OC  | O2-C2 | -3.14 | 1.17        | 1.23     |
| 26  | a     | 1911 | PSU  | C6-C5 | 3.14  | 1.39        | 1.35     |
| 26  | a     | 2251 | OMG  | C5-C4 | 3.13  | 1.47        | 1.38     |
| 26  | a     | 2552 | OMU  | C4-N3 | 3.12  | 1.44        | 1.38     |
| 1   | A     | 516  | PSU  | C4-N3 | -3.08 | 1.33        | 1.38     |
| 26  | a     | 1618 | 6MZ  | C5-C4 | -3.05 | 1.33        | 1.39     |
| 1   | A     | 1207 | 2MG  | C5-C4 | 3.05  | 1.47        | 1.38     |
| 26  | a     | 745  | 1MG  | C5-C4 | 3.04  | 1.47        | 1.38     |
| 1   | A     | 1498 | UR3  | O2-C2 | -3.04 | 1.17        | 1.22     |
| 22  | V     | 55   | 5MU  | C4-N3 | -3.03 | 1.33        | 1.38     |
| 1   | A     | 966  | 2MG  | C5-C4 | 3.03  | 1.47        | 1.38     |
| 26  | a     | 1835 | 2MG  | C5-C4 | 3.02  | 1.47        | 1.38     |
| 1   | A     | 1519 | MA6  | C5-C6 | 3.01  | 1.49        | 1.41     |
| 1   | A     | 1516 | 2MG  | C5-C4 | 2.99  | 1.47        | 1.38     |
| 26  | a     | 2445 | 2MG  | C5-C4 | 2.97  | 1.47        | 1.38     |
| 1   | A     | 1407 | 5MC  | O2-C2 | -2.96 | 1.18        | 1.23     |
| 26  | a     | 1962 | 5MC  | O2-C2 | -2.95 | 1.18        | 1.23     |
| 1   | A     | 967  | 5MC  | O2-C2 | -2.94 | 1.18        | 1.23     |
| 22  | V     | 8    | 4SU  | C6-N1 | 2.94  | 1.45        | 1.38     |
| 1   | A     | 1402 | 4OC  | C6-N1 | 2.89  | 1.45        | 1.38     |
| 26  | a     | 955  | PSU  | C6-C5 | 2.88  | 1.38        | 1.35     |
| 22  | V     | 56   | PSU  | C4-N3 | -2.84 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 26  | a     | 2605 | PSU  | C4-N3   | -2.82 | 1.33        | 1.38     |
| 26  | a     | 2604 | PSU  | C4-N3   | -2.80 | 1.33        | 1.38     |
| 26  | a     | 2580 | PSU  | C4-N3   | -2.78 | 1.33        | 1.38     |
| 26  | a     | 747  | 5MU  | C2-N1   | 2.78  | 1.42        | 1.38     |
| 26  | a     | 1917 | PSU  | C4-N3   | -2.76 | 1.33        | 1.38     |
| 26  | a     | 747  | 5MU  | C4-N3   | -2.75 | 1.33        | 1.38     |
| 26  | a     | 2030 | 6MZ  | C5-N7   | -2.68 | 1.33        | 1.39     |
| 26  | a     | 1939 | 5MU  | C4-N3   | -2.68 | 1.33        | 1.38     |
| 1   | A     | 1498 | UR3  | O4-C4   | -2.67 | 1.17        | 1.23     |
| 26  | a     | 2503 | 2MA  | C5-C6   | 2.66  | 1.48        | 1.41     |
| 1   | A     | 1207 | 2MG  | C6-N1   | -2.66 | 1.33        | 1.38     |
| 26  | a     | 2449 | H2U  | O2-C2   | -2.66 | 1.18        | 1.23     |
| 26  | a     | 2445 | 2MG  | C6-N1   | -2.66 | 1.33        | 1.38     |
| 26  | a     | 1939 | 5MU  | C6-C5   | 2.65  | 1.39        | 1.34     |
| 26  | a     | 2251 | OMG  | C6-N1   | -2.63 | 1.34        | 1.38     |
| 26  | a     | 2504 | PSU  | C4-N3   | -2.61 | 1.34        | 1.38     |
| 22  | V     | 55   | 5MU  | C6-C5   | 2.60  | 1.38        | 1.34     |
| 1   | A     | 527  | G7M  | C6-N1   | -2.60 | 1.34        | 1.38     |
| 26  | a     | 1915 | 3TD  | O4-C4   | -2.60 | 1.17        | 1.23     |
| 26  | a     | 2552 | OMU  | C6-N1   | 2.59  | 1.44        | 1.38     |
| 26  | a     | 2449 | H2U  | O4-C4   | -2.59 | 1.18        | 1.23     |
| 26  | a     | 747  | 5MU  | C6-C5   | 2.59  | 1.38        | 1.34     |
| 26  | a     | 746  | PSU  | C4-N3   | -2.57 | 1.34        | 1.38     |
| 26  | a     | 1618 | 6MZ  | C5-N7   | -2.57 | 1.34        | 1.39     |
| 26  | a     | 2069 | G7M  | C6-N1   | -2.56 | 1.34        | 1.38     |
| 26  | a     | 1835 | 2MG  | C6-N1   | -2.56 | 1.34        | 1.38     |
| 1   | A     | 1519 | MA6  | C8-N7   | 2.56  | 1.36        | 1.31     |
| 1   | A     | 1498 | UR3  | C5-C4   | 2.55  | 1.50        | 1.43     |
| 1   | A     | 966  | 2MG  | C6-N1   | -2.55 | 1.34        | 1.38     |
| 1   | A     | 1516 | 2MG  | C6-N1   | -2.52 | 1.34        | 1.38     |
| 1   | A     | 1518 | MA6  | C5-C6   | 2.52  | 1.48        | 1.41     |
| 26  | a     | 1915 | 3TD  | C4-N3   | 2.49  | 1.45        | 1.40     |
| 26  | a     | 2030 | 6MZ  | C8-N9   | -2.47 | 1.33        | 1.37     |
| 26  | a     | 1917 | PSU  | C2'-C1' | -2.45 | 1.50        | 1.53     |
| 22  | V     | 55   | 5MU  | C2-N3   | -2.38 | 1.33        | 1.38     |
| 1   | A     | 1516 | 2MG  | C5-N7   | -2.38 | 1.34        | 1.39     |
| 26  | a     | 1939 | 5MU  | C4-C5   | 2.38  | 1.48        | 1.44     |
| 26  | a     | 2251 | OMG  | C5-N7   | -2.37 | 1.34        | 1.39     |
| 26  | a     | 747  | 5MU  | C4-C5   | 2.37  | 1.48        | 1.44     |
| 26  | a     | 2503 | 2MA  | C8-N7   | 2.37  | 1.36        | 1.31     |
| 26  | a     | 2445 | 2MG  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 22  | V     | 21   | H2U  | O2-C2   | -2.33 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 26  | a     | 1618 | 6MZ  | C6-N1   | -2.32 | 1.31        | 1.35     |
| 26  | a     | 2457 | PSU  | C2-N3   | -2.29 | 1.33        | 1.37     |
| 1   | A     | 1518 | MA6  | C5-N7   | -2.29 | 1.34        | 1.39     |
| 26  | a     | 1618 | 6MZ  | C8-N9   | -2.28 | 1.33        | 1.37     |
| 26  | a     | 2030 | 6MZ  | C6-N1   | -2.28 | 1.31        | 1.35     |
| 26  | a     | 1835 | 2MG  | C5-N7   | -2.25 | 1.34        | 1.39     |
| 26  | a     | 2503 | 2MA  | C5-N7   | -2.25 | 1.34        | 1.39     |
| 26  | a     | 1939 | 5MU  | C2-N3   | -2.25 | 1.34        | 1.38     |
| 1   | A     | 966  | 2MG  | C5-N7   | -2.24 | 1.34        | 1.39     |
| 1   | A     | 1519 | MA6  | O3'-C3' | 2.24  | 1.48        | 1.43     |
| 26  | a     | 1939 | 5MU  | C2-N1   | 2.24  | 1.42        | 1.38     |
| 1   | A     | 1519 | MA6  | C5-N7   | -2.22 | 1.34        | 1.39     |
| 22  | V     | 55   | 5MU  | C2-N1   | 2.22  | 1.42        | 1.38     |
| 1   | A     | 1207 | 2MG  | C5-N7   | -2.22 | 1.34        | 1.39     |
| 26  | a     | 1835 | 2MG  | C2-N3   | 2.21  | 1.36        | 1.31     |
| 26  | a     | 745  | 1MG  | C5-N7   | -2.19 | 1.34        | 1.39     |
| 1   | A     | 1207 | 2MG  | C2-N3   | 2.16  | 1.36        | 1.31     |
| 26  | a     | 955  | PSU  | C4-C5   | -2.16 | 1.38        | 1.44     |
| 1   | A     | 966  | 2MG  | C2-N3   | 2.16  | 1.36        | 1.31     |
| 37  | l     | 81   | 4D4  | CZ-NH1  | 2.16  | 1.43        | 1.34     |
| 22  | V     | 21   | H2U  | O4-C4   | -2.13 | 1.18        | 1.23     |
| 26  | a     | 1939 | 5MU  | C6-N1   | -2.13 | 1.34        | 1.38     |
| 26  | a     | 2498 | OMC  | C5-C4   | 2.13  | 1.47        | 1.42     |
| 1   | A     | 1516 | 2MG  | C2-N3   | 2.08  | 1.35        | 1.31     |
| 22  | V     | 56   | PSU  | C2-N3   | -2.08 | 1.34        | 1.37     |
| 26  | a     | 2069 | G7M  | C5-C6   | 2.07  | 1.49        | 1.43     |
| 26  | a     | 1911 | PSU  | C4-C5   | -2.06 | 1.38        | 1.44     |
| 26  | a     | 2552 | OMU  | C5-C4   | 2.04  | 1.48        | 1.43     |
| 22  | V     | 55   | 5MU  | C4-C5   | 2.02  | 1.48        | 1.44     |
| 22  | V     | 55   | 5MU  | C6-N1   | -2.02 | 1.34        | 1.38     |
| 26  | a     | 2605 | PSU  | C2-N3   | -2.01 | 1.34        | 1.37     |
| 12  | L     | 89   | D2T  | CB1-SB  | -2.01 | 1.75        | 1.79     |
| 26  | a     | 747  | 5MU  | C2-N3   | -2.01 | 1.34        | 1.38     |

All (237) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 26  | a     | 2503 | 2MA  | C5-C4-N3 | -8.16 | 118.02      | 127.19   |
| 22  | V     | 8    | 4SU  | C4-N3-C2 | -7.94 | 119.62      | 127.34   |
| 26  | a     | 1835 | 2MG  | C2-N3-C4 | 7.71  | 121.60      | 112.04   |
| 1   | A     | 966  | 2MG  | C2-N3-C4 | 7.70  | 121.58      | 112.04   |
| 1   | A     | 1516 | 2MG  | C2-N3-C4 | 7.51  | 121.35      | 112.04   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 1207 | 2MG  | C2-N3-C4 | 7.40  | 121.21      | 112.04   |
| 26  | a     | 2445 | 2MG  | C2-N3-C4 | 7.18  | 120.94      | 112.04   |
| 26  | a     | 2449 | H2U  | C4-N3-C2 | -6.98 | 120.00      | 125.79   |
| 22  | V     | 21   | H2U  | C4-N3-C2 | -6.55 | 120.36      | 125.79   |
| 1   | A     | 1518 | MA6  | N1-C6-N6 | 6.43  | 124.11      | 117.08   |
| 26  | a     | 2251 | OMG  | C5-C4-N3 | -6.40 | 118.07      | 128.46   |
| 26  | a     | 2457 | PSU  | N1-C2-N3 | 6.37  | 122.35      | 115.13   |
| 1   | A     | 1516 | 2MG  | C5-C4-N3 | -6.37 | 118.12      | 128.46   |
| 1   | A     | 966  | 2MG  | C5-C4-N3 | -6.35 | 118.15      | 128.46   |
| 26  | a     | 1835 | 2MG  | C5-C4-N3 | -6.26 | 118.30      | 128.46   |
| 1   | A     | 516  | PSU  | N1-C2-N3 | 6.23  | 122.18      | 115.13   |
| 26  | a     | 2503 | 2MA  | N3-C4-N9 | 6.18  | 135.56      | 126.99   |
| 1   | A     | 1207 | 2MG  | C5-C4-N3 | -6.14 | 118.49      | 128.46   |
| 26  | a     | 2445 | 2MG  | C5-C4-N3 | -6.07 | 118.62      | 128.46   |
| 1   | A     | 1519 | MA6  | C5-C4-N3 | -6.06 | 118.84      | 126.75   |
| 26  | a     | 746  | PSU  | N1-C2-N3 | 6.06  | 121.99      | 115.13   |
| 26  | a     | 2504 | PSU  | N1-C2-N3 | 6.05  | 121.98      | 115.13   |
| 26  | a     | 2604 | PSU  | N1-C2-N3 | 6.01  | 121.94      | 115.13   |
| 26  | a     | 1917 | PSU  | N1-C2-N3 | 5.93  | 121.85      | 115.13   |
| 1   | A     | 1518 | MA6  | C5-C4-N3 | -5.92 | 119.02      | 126.75   |
| 22  | V     | 56   | PSU  | N1-C2-N3 | 5.80  | 121.70      | 115.13   |
| 26  | a     | 2605 | PSU  | N1-C2-N3 | 5.80  | 121.70      | 115.13   |
| 26  | a     | 2580 | PSU  | N1-C2-N3 | 5.75  | 121.64      | 115.13   |
| 1   | A     | 527  | G7M  | N9-C4-N3 | 5.74  | 137.46      | 125.94   |
| 26  | a     | 2069 | G7M  | C5-C4-N3 | -5.69 | 117.24      | 128.15   |
| 26  | a     | 2552 | OMU  | C4-N3-C2 | -5.67 | 119.11      | 126.58   |
| 1   | A     | 527  | G7M  | C5-C4-N3 | -5.65 | 117.32      | 128.15   |
| 22  | V     | 8    | 4SU  | C5-C4-N3 | 5.57  | 119.86      | 114.69   |
| 26  | a     | 747  | 5MU  | N3-C2-N1 | 5.47  | 122.16      | 114.89   |
| 26  | a     | 1618 | 6MZ  | N1-C2-N3 | -5.42 | 120.12      | 128.60   |
| 26  | a     | 2069 | G7M  | N9-C4-N3 | 5.42  | 136.81      | 125.94   |
| 26  | a     | 1618 | 6MZ  | C5-C4-N3 | -5.41 | 119.70      | 126.75   |
| 26  | a     | 2030 | 6MZ  | C5-C4-N3 | -5.40 | 119.71      | 126.75   |
| 26  | a     | 2030 | 6MZ  | C9-N6-C6 | -5.25 | 118.35      | 122.87   |
| 26  | a     | 1939 | 5MU  | C4-N3-C2 | -5.22 | 120.59      | 127.35   |
| 26  | a     | 2030 | 6MZ  | N1-C2-N3 | -5.21 | 120.45      | 128.60   |
| 26  | a     | 2069 | G7M  | C2-N3-C4 | 5.18  | 121.54      | 112.30   |
| 26  | a     | 1939 | 5MU  | N3-C2-N1 | 5.07  | 121.62      | 114.89   |
| 1   | A     | 1518 | MA6  | N3-C4-N9 | 4.96  | 135.26      | 127.08   |
| 26  | a     | 2251 | OMG  | C2-N3-C4 | 4.93  | 121.08      | 112.30   |
| 26  | a     | 1915 | 3TD  | N1-C2-N3 | 4.92  | 120.02      | 116.14   |
| 26  | a     | 1618 | 6MZ  | C9-N6-C6 | -4.91 | 118.64      | 122.87   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26  | a     | 745  | 1MG  | C5-C4-N3  | -4.91 | 120.50      | 128.46   |
| 26  | a     | 2251 | OMG  | N9-C4-N3  | 4.87  | 135.73      | 125.94   |
| 26  | a     | 1911 | PSU  | C4-N3-C2  | -4.85 | 119.36      | 126.34   |
| 26  | a     | 747  | 5MU  | C4-N3-C2  | -4.83 | 121.09      | 127.35   |
| 1   | A     | 966  | 2MG  | N9-C4-N3  | 4.79  | 135.56      | 125.94   |
| 26  | a     | 1911 | PSU  | N1-C2-N3  | 4.78  | 120.55      | 115.13   |
| 1   | A     | 1498 | UR3  | C4-N3-C2  | -4.73 | 120.11      | 124.56   |
| 26  | a     | 955  | PSU  | N1-C2-N3  | 4.73  | 120.49      | 115.13   |
| 1   | A     | 527  | G7M  | C2-N3-C4  | 4.72  | 120.71      | 112.30   |
| 26  | a     | 2030 | 6MZ  | N9-C8-N7  | -4.72 | 107.46      | 113.91   |
| 26  | a     | 955  | PSU  | C4-N3-C2  | -4.70 | 119.57      | 126.34   |
| 26  | a     | 1939 | 5MU  | C5-C4-N3  | 4.58  | 119.22      | 115.31   |
| 26  | a     | 1618 | 6MZ  | N9-C8-N7  | -4.57 | 107.66      | 113.91   |
| 26  | a     | 1835 | 2MG  | N9-C4-N3  | 4.52  | 135.03      | 125.94   |
| 1   | A     | 1519 | MA6  | C2-N1-C6  | 4.47  | 122.30      | 111.75   |
| 1   | A     | 1207 | 2MG  | N9-C4-N3  | 4.47  | 134.91      | 125.94   |
| 22  | V     | 8    | 4SU  | C5-C4-S4  | -4.42 | 118.77      | 124.47   |
| 22  | V     | 55   | 5MU  | N3-C2-N1  | 4.41  | 120.75      | 114.89   |
| 1   | A     | 1518 | MA6  | C2-N1-C6  | 4.40  | 122.14      | 111.75   |
| 26  | a     | 745  | 1MG  | C2-N3-C4  | 4.38  | 121.82      | 111.98   |
| 1   | A     | 1519 | MA6  | C9-N6-C6  | -4.23 | 109.42      | 120.40   |
| 1   | A     | 1516 | 2MG  | N9-C4-N3  | 4.22  | 134.41      | 125.94   |
| 26  | a     | 2445 | 2MG  | N9-C4-N3  | 4.21  | 134.39      | 125.94   |
| 12  | L     | 89   | D2T  | OD2-CG-CB | 4.13  | 122.07      | 113.15   |
| 26  | a     | 2552 | OMU  | N3-C2-N1  | 4.09  | 120.32      | 114.89   |
| 1   | A     | 1519 | MA6  | C4-C5-N7  | -3.98 | 105.77      | 110.62   |
| 26  | a     | 2030 | 6MZ  | C4-C5-C6  | 3.94  | 119.86      | 116.81   |
| 1   | A     | 1519 | MA6  | N3-C4-N9  | 3.86  | 133.44      | 127.08   |
| 26  | a     | 745  | 1MG  | N9-C4-N3  | 3.83  | 133.63      | 125.94   |
| 1   | A     | 1519 | MA6  | C2-N3-C4  | 3.80  | 120.72      | 111.75   |
| 26  | a     | 2605 | PSU  | C4-N3-C2  | -3.73 | 120.97      | 126.34   |
| 1   | A     | 1518 | MA6  | C5-C6-N6  | -3.72 | 118.82      | 125.30   |
| 1   | A     | 1518 | MA6  | C2-N3-C4  | 3.71  | 120.52      | 111.75   |
| 26  | a     | 1939 | 5MU  | C5-C6-N1  | -3.68 | 119.56      | 123.34   |
| 26  | a     | 2504 | PSU  | C4-N3-C2  | -3.65 | 121.08      | 126.34   |
| 22  | V     | 8    | 4SU  | N3-C2-N1  | 3.63  | 119.71      | 114.89   |
| 26  | a     | 1618 | 6MZ  | C2-N3-C4  | 3.63  | 120.32      | 111.75   |
| 26  | a     | 1618 | 6MZ  | C4-C5-C6  | 3.63  | 119.62      | 116.81   |
| 1   | A     | 1407 | 5MC  | C5-C6-N1  | -3.63 | 119.61      | 123.34   |
| 22  | V     | 55   | 5MU  | C4-N3-C2  | -3.61 | 122.67      | 127.35   |
| 26  | a     | 747  | 5MU  | C5-C4-N3  | 3.61  | 118.39      | 115.31   |
| 26  | a     | 2552 | OMU  | C5-C4-N3  | 3.61  | 120.24      | 114.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | V     | 21   | H2U  | N3-C2-N1    | 3.60  | 120.46      | 116.65   |
| 26  | a     | 2030 | 6MZ  | C2-N3-C4    | 3.60  | 120.25      | 111.75   |
| 26  | a     | 746  | PSU  | C4-N3-C2    | -3.60 | 121.16      | 126.34   |
| 26  | a     | 2449 | H2U  | N3-C2-N1    | 3.59  | 120.44      | 116.65   |
| 1   | A     | 1518 | MA6  | C10-N6-C6   | -3.57 | 111.13      | 120.40   |
| 1   | A     | 527  | G7M  | CN7-N7-C5   | 3.57  | 131.21      | 126.77   |
| 26  | a     | 1915 | 3TD  | C4-N3-C2    | -3.57 | 120.73      | 124.61   |
| 26  | a     | 1939 | 5MU  | O4-C4-C5    | -3.56 | 120.78      | 124.90   |
| 1   | A     | 516  | PSU  | C4-N3-C2    | -3.56 | 121.22      | 126.34   |
| 1   | A     | 1519 | MA6  | C10-N6-C6   | -3.49 | 111.34      | 120.40   |
| 26  | a     | 746  | PSU  | O2-C2-N1    | -3.47 | 118.97      | 122.79   |
| 26  | a     | 2604 | PSU  | C4-N3-C2    | -3.45 | 121.37      | 126.34   |
| 1   | A     | 1518 | MA6  | C9-N6-C6    | -3.45 | 111.46      | 120.40   |
| 1   | A     | 967  | 5MC  | C5-C6-N1    | -3.40 | 119.84      | 123.34   |
| 37  | l     | 81   | 4D4  | O-C-CA      | -3.39 | 115.90      | 124.78   |
| 26  | a     | 2457 | PSU  | C4-N3-C2    | -3.37 | 121.48      | 126.34   |
| 26  | a     | 2580 | PSU  | C4-N3-C2    | -3.37 | 121.48      | 126.34   |
| 26  | a     | 745  | 1MG  | C2'-C1'-N9  | -3.36 | 103.68      | 113.22   |
| 26  | a     | 2030 | 6MZ  | N3-C4-N9    | 3.34  | 132.58      | 127.08   |
| 26  | a     | 2580 | PSU  | O2-C2-N1    | -3.33 | 119.12      | 122.79   |
| 26  | a     | 2030 | 6MZ  | C5-N7-C8    | 3.33  | 108.25      | 103.51   |
| 22  | V     | 55   | 5MU  | C5-C4-N3    | 3.33  | 118.15      | 115.31   |
| 26  | a     | 1618 | 6MZ  | C5-N7-C8    | 3.33  | 108.23      | 103.51   |
| 26  | a     | 2504 | PSU  | C6-C5-C4    | -3.32 | 115.88      | 118.20   |
| 26  | a     | 2504 | PSU  | O2-C2-N1    | -3.31 | 119.14      | 122.79   |
| 26  | a     | 1917 | PSU  | C4-N3-C2    | -3.31 | 121.57      | 126.34   |
| 22  | V     | 56   | PSU  | C4-N3-C2    | -3.29 | 121.60      | 126.34   |
| 26  | a     | 2604 | PSU  | C3'-C2'-C1' | 3.28  | 105.45      | 101.64   |
| 26  | a     | 1962 | 5MC  | C5-C6-N1    | -3.27 | 119.97      | 123.34   |
| 26  | a     | 1618 | 6MZ  | N3-C4-N9    | 3.25  | 132.43      | 127.08   |
| 1   | A     | 516  | PSU  | O2-C2-N1    | -3.24 | 119.22      | 122.79   |
| 26  | a     | 747  | 5MU  | O4-C4-C5    | -3.21 | 121.18      | 124.90   |
| 26  | a     | 2503 | 2MA  | C4-C5-N7    | -3.21 | 106.71      | 110.62   |
| 26  | a     | 1917 | PSU  | O2-C2-N1    | -3.20 | 119.27      | 122.79   |
| 1   | A     | 1207 | 2MG  | C6-C5-N7    | 3.20  | 136.20      | 130.25   |
| 1   | A     | 1518 | MA6  | N1-C2-N3    | -3.18 | 123.62      | 128.60   |
| 26  | a     | 2604 | PSU  | O2-C2-N1    | -3.18 | 119.29      | 122.79   |
| 1   | A     | 1516 | 2MG  | C6-C5-N7    | 3.15  | 136.10      | 130.25   |
| 26  | a     | 1835 | 2MG  | C6-C5-N7    | 3.15  | 136.10      | 130.25   |
| 26  | a     | 2580 | PSU  | C3'-C2'-C1' | 3.14  | 105.29      | 101.64   |
| 26  | a     | 2449 | H2U  | C5-C4-N3    | 3.11  | 120.14      | 116.65   |
| 26  | a     | 2445 | 2MG  | C6-C5-N7    | 3.09  | 136.00      | 130.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 966  | 2MG  | C6-C5-N7    | 3.07  | 135.96      | 130.25   |
| 26  | a     | 746  | PSU  | C3'-C2'-C1' | 3.06  | 105.20      | 101.64   |
| 26  | a     | 2605 | PSU  | O2-C2-N1    | -2.97 | 119.52      | 122.79   |
| 26  | a     | 955  | PSU  | O2-C2-N1    | -2.91 | 119.58      | 122.79   |
| 1   | A     | 1516 | 2MG  | O4'-C1'-N9  | 2.91  | 115.02      | 108.36   |
| 22  | V     | 55   | 5MU  | O4-C4-C5    | -2.91 | 121.53      | 124.90   |
| 1   | A     | 1518 | MA6  | C4-C5-N7    | -2.90 | 107.08      | 110.62   |
| 26  | a     | 2449 | H2U  | O2-C2-N1    | -2.90 | 119.47      | 123.11   |
| 26  | a     | 2552 | OMU  | O4-C4-C5    | -2.89 | 120.07      | 125.16   |
| 26  | a     | 2503 | 2MA  | N6-C6-N1    | 2.84  | 121.05      | 117.03   |
| 26  | a     | 2251 | OMG  | C6-C5-N7    | 2.83  | 135.51      | 130.25   |
| 1   | A     | 1519 | MA6  | C10-N6-C9   | -2.81 | 107.07      | 116.12   |
| 12  | L     | 89   | D2T  | OD1-CG-CB   | -2.81 | 116.56      | 122.44   |
| 26  | a     | 955  | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 1   | A     | 1519 | MA6  | C5-N7-C8    | 2.78  | 107.46      | 103.51   |
| 1   | A     | 1519 | MA6  | N1-C2-N3    | -2.78 | 124.26      | 128.60   |
| 26  | a     | 747  | 5MU  | C5-C6-N1    | -2.75 | 120.51      | 123.34   |
| 22  | V     | 21   | H2U  | C5-C4-N3    | 2.74  | 119.73      | 116.65   |
| 37  | l     | 81   | 4D4  | NE-CZ-NH2   | 2.73  | 125.50      | 120.70   |
| 26  | a     | 1915 | 3TD  | O4'-C4'-C5' | -2.73 | 100.39      | 109.37   |
| 26  | a     | 745  | 1MG  | C6-C5-N7    | 2.71  | 135.48      | 129.35   |
| 26  | a     | 2457 | PSU  | O2-C2-N1    | -2.71 | 119.81      | 122.79   |
| 1   | A     | 1498 | UR3  | C1'-N1-C2   | 2.69  | 121.53      | 116.99   |
| 1   | A     | 1516 | 2MG  | C4-C5-N7    | -2.68 | 106.47      | 110.72   |
| 26  | a     | 2030 | 6MZ  | C4-N9-C8    | 2.67  | 108.62      | 105.73   |
| 26  | a     | 2503 | 2MA  | C2-N1-C6    | 2.66  | 122.23      | 118.08   |
| 26  | a     | 745  | 1MG  | O4'-C1'-N9  | 2.65  | 114.42      | 108.36   |
| 26  | a     | 2503 | 2MA  | C5-N7-C8    | 2.61  | 107.22      | 103.51   |
| 22  | V     | 56   | PSU  | O2-C2-N1    | -2.61 | 119.92      | 122.79   |
| 26  | a     | 2449 | H2U  | C5-C6-N1    | 2.60  | 120.17      | 111.61   |
| 22  | V     | 21   | H2U  | C5-C6-N1    | 2.57  | 120.09      | 111.61   |
| 26  | a     | 747  | 5MU  | O2-C2-N3    | -2.57 | 116.72      | 121.50   |
| 1   | A     | 1518 | MA6  | C4-N9-C8    | 2.54  | 108.48      | 105.73   |
| 26  | a     | 2605 | PSU  | C6-C5-C4    | -2.53 | 116.43      | 118.20   |
| 26  | a     | 745  | 1MG  | C4-C5-N7    | -2.53 | 106.72      | 110.72   |
| 26  | a     | 1835 | 2MG  | C4-C5-N7    | -2.51 | 106.74      | 110.72   |
| 1   | A     | 1207 | 2MG  | C4-C5-N7    | -2.51 | 106.76      | 110.72   |
| 26  | a     | 1917 | PSU  | C3'-C2'-C1' | 2.50  | 104.55      | 101.64   |
| 1   | A     | 1516 | 2MG  | C2-N1-C6    | -2.49 | 121.61      | 124.48   |
| 26  | a     | 2445 | 2MG  | C4-C5-N7    | -2.49 | 106.78      | 110.72   |
| 1   | A     | 966  | 2MG  | C3'-C2'-C1' | 2.48  | 106.15      | 101.43   |
| 26  | a     | 1911 | PSU  | O2-C2-N1    | -2.47 | 120.08      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | a     | 2069 | G7M  | C2'-C3'-C4' | -2.46 | 97.87       | 102.64   |
| 12  | L     | 89   | D2T  | CB-CA-N     | 2.45  | 114.32      | 109.10   |
| 1   | A     | 966  | 2MG  | C4-C5-N7    | -2.43 | 106.88      | 110.72   |
| 26  | a     | 1915 | 3TD  | C5'-C4'-C3' | 2.40  | 124.19      | 115.18   |
| 22  | V     | 21   | H2U  | O2-C2-N1    | -2.39 | 120.10      | 123.11   |
| 26  | a     | 1618 | 6MZ  | C4-N9-C8    | 2.39  | 108.32      | 105.73   |
| 1   | A     | 1519 | MA6  | C6-C5-N7    | 2.37  | 137.25      | 133.28   |
| 26  | a     | 747  | 5MU  | C6-N1-C2    | -2.36 | 118.91      | 121.30   |
| 26  | a     | 1618 | 6MZ  | C5-C6-N1    | 2.36  | 120.71      | 118.20   |
| 1   | A     | 1518 | MA6  | C5-N7-C8    | 2.36  | 106.86      | 103.51   |
| 26  | a     | 2251 | OMG  | C4-C5-N7    | -2.35 | 107.00      | 110.72   |
| 1   | A     | 1402 | 4OC  | CM4-N4-C4   | -2.34 | 117.89      | 122.45   |
| 29  | d     | 150  | MEQ  | CB-CG-CD    | -2.33 | 107.84      | 113.04   |
| 1   | A     | 527  | G7M  | C5-C6-N1    | 2.30  | 116.60      | 111.79   |
| 26  | a     | 2030 | 6MZ  | C5-C6-N1    | 2.29  | 120.65      | 118.20   |
| 22  | V     | 55   | 5MU  | C3'-C2'-C1' | 2.29  | 105.77      | 101.43   |
| 22  | V     | 8    | 4SU  | C1'-N1-C2   | 2.28  | 121.69      | 117.57   |
| 26  | a     | 1917 | PSU  | C6-C5-C4    | -2.28 | 116.61      | 118.20   |
| 26  | a     | 1911 | PSU  | C6-N1-C2    | -2.27 | 120.36      | 122.68   |
| 26  | a     | 747  | 5MU  | O4'-C1'-N1  | 2.27  | 113.55      | 108.36   |
| 1   | A     | 527  | G7M  | O6-C6-C5    | -2.27 | 122.95      | 128.06   |
| 26  | a     | 1939 | 5MU  | O2-C2-N1    | -2.26 | 119.78      | 122.79   |
| 26  | a     | 2503 | 2MA  | O4'-C1'-N9  | 2.26  | 112.50      | 108.06   |
| 26  | a     | 1939 | 5MU  | O5'-C5'-C4' | 2.24  | 116.61      | 108.99   |
| 26  | a     | 2504 | PSU  | O3'-C3'-C4' | 2.24  | 117.51      | 111.05   |
| 26  | a     | 1618 | 6MZ  | C4-C5-N7    | -2.22 | 107.91      | 110.62   |
| 26  | a     | 2503 | 2MA  | C4-N9-C8    | 2.22  | 108.13      | 105.73   |
| 22  | V     | 8    | 4SU  | O2-C2-N1    | -2.22 | 119.84      | 122.79   |
| 1   | A     | 1516 | 2MG  | C2'-C1'-N9  | -2.22 | 106.94      | 113.22   |
| 26  | a     | 2069 | G7M  | C5-C6-N1    | 2.21  | 116.41      | 111.79   |
| 26  | a     | 2251 | OMG  | O6-C6-C5    | -2.20 | 120.75      | 126.60   |
| 1   | A     | 1518 | MA6  | O4'-C1'-N9  | 2.20  | 112.40      | 108.06   |
| 26  | a     | 747  | 5MU  | C5M-C5-C6   | -2.19 | 119.92      | 122.85   |
| 1   | A     | 1518 | MA6  | C2'-C1'-N9  | -2.19 | 107.75      | 113.30   |
| 26  | a     | 1618 | 6MZ  | C4-N9-C1'   | -2.19 | 121.38      | 126.59   |
| 26  | a     | 2069 | G7M  | CN7-N7-C5   | 2.18  | 129.47      | 126.77   |
| 22  | V     | 55   | 5MU  | C5-C6-N1    | -2.18 | 121.10      | 123.34   |
| 26  | a     | 2030 | 6MZ  | C4-C5-N7    | -2.18 | 107.97      | 110.62   |
| 26  | a     | 2445 | 2MG  | O5'-C5'-C4' | -2.17 | 101.61      | 108.99   |
| 26  | a     | 1835 | 2MG  | O6-C6-C5    | -2.16 | 120.87      | 126.60   |
| 26  | a     | 2503 | 2MA  | C6-C5-N7    | 2.16  | 136.04      | 132.02   |
| 26  | a     | 747  | 5MU  | C5M-C5-C4   | 2.15  | 121.14      | 118.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1516 | 2MG  | O6-C6-C5    | -2.15 | 120.91      | 126.60   |
| 1   | A     | 1207 | 2MG  | O6-C6-C5    | -2.13 | 120.95      | 126.60   |
| 1   | A     | 1402 | 4OC  | C6-C5-C4    | 2.12  | 119.56      | 116.96   |
| 26  | a     | 2457 | PSU  | O2-C2-N3    | -2.12 | 117.82      | 121.82   |
| 22  | V     | 55   | 5MU  | O2-C2-N3    | -2.10 | 117.58      | 121.50   |
| 26  | a     | 1911 | PSU  | C6-C5-C4    | 2.10  | 119.67      | 118.20   |
| 26  | a     | 2445 | 2MG  | O6-C6-C5    | -2.09 | 121.04      | 126.60   |
| 1   | A     | 1519 | MA6  | O3'-C3'-C2' | 2.09  | 118.60      | 111.82   |
| 1   | A     | 966  | 2MG  | O6-C6-C5    | -2.09 | 121.06      | 126.60   |
| 26  | a     | 1939 | 5MU  | C2'-C3'-C4' | 2.07  | 106.67      | 102.64   |
| 12  | L     | 89   | D2T  | O-C-CA      | -2.06 | 119.39      | 124.78   |
| 1   | A     | 1519 | MA6  | N1-C6-N6    | 2.05  | 119.33      | 117.08   |
| 1   | A     | 1518 | MA6  | C10-N6-C9   | -2.05 | 109.51      | 116.12   |
| 1   | A     | 966  | 2MG  | C5-C6-N1    | 2.05  | 118.40      | 113.19   |
| 26  | a     | 745  | 1MG  | C3'-C2'-C1' | 2.05  | 105.31      | 101.43   |
| 1   | A     | 1518 | MA6  | C3'-C2'-C1' | 2.04  | 105.30      | 101.43   |
| 26  | a     | 2445 | 2MG  | C2-N1-C6    | -2.03 | 122.15      | 124.48   |
| 26  | a     | 2503 | 2MA  | C2-N3-C4    | 2.02  | 121.97      | 116.99   |
| 26  | a     | 2030 | 6MZ  | C4-N9-C1'   | -2.02 | 121.78      | 126.59   |
| 1   | A     | 1207 | 2MG  | O4'-C1'-N9  | 2.02  | 112.97      | 108.36   |
| 22  | V     | 55   | 5MU  | O4'-C1'-N1  | 2.01  | 112.97      | 108.36   |
| 26  | a     | 2457 | PSU  | C3'-C2'-C1' | 2.00  | 103.97      | 101.64   |

There are no chirality outliers.

All (70) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A     | 1207 | 2MG  | N1-C2-N2-CM2    |
| 1   | A     | 1207 | 2MG  | N3-C2-N2-CM2    |
| 1   | A     | 1498 | UR3  | O4'-C1'-N1-C6   |
| 1   | A     | 1498 | UR3  | O4'-C1'-N1-C2   |
| 1   | A     | 1518 | MA6  | C5-C6-N6-C9     |
| 1   | A     | 1519 | MA6  | C5-C6-N6-C9     |
| 1   | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 1   | A     | 1519 | MA6  | N1-C6-N6-C9     |
| 12  | L     | 89   | D2T  | CA-CB-SB-CB1    |
| 12  | L     | 89   | D2T  | SB-CB-CG-OD2    |
| 22  | V     | 21   | H2U  | O4'-C4'-C5'-O5' |
| 22  | V     | 21   | H2U  | C3'-C4'-C5'-O5' |
| 22  | V     | 21   | H2U  | O4'-C1'-N1-C6   |
| 22  | V     | 21   | H2U  | C2'-C1'-N1-C2   |
| 22  | V     | 21   | H2U  | C2'-C1'-N1-C6   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | a     | 746  | PSU  | O4'-C1'-C5-C4   |
| 26  | a     | 746  | PSU  | O4'-C1'-C5-C6   |
| 26  | a     | 1618 | 6MZ  | C5-C6-N6-C9     |
| 26  | a     | 1618 | 6MZ  | N1-C6-N6-C9     |
| 26  | a     | 1618 | 6MZ  | O4'-C4'-C5'-O5' |
| 26  | a     | 1915 | 3TD  | C2'-C1'-C5-C4   |
| 26  | a     | 1915 | 3TD  | O4'-C1'-C5-C4   |
| 26  | a     | 1915 | 3TD  | O4'-C1'-C5-C6   |
| 26  | a     | 1915 | 3TD  | C3'-C4'-C5'-O5' |
| 26  | a     | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 26  | a     | 1939 | 5MU  | C3'-C4'-C5'-O5' |
| 26  | a     | 1939 | 5MU  | O4'-C4'-C5'-O5' |
| 26  | a     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 26  | a     | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 26  | a     | 2069 | G7M  | C3'-C4'-C5'-O5' |
| 26  | a     | 2251 | OMG  | C1'-C2'-O2'-CM2 |
| 26  | a     | 2445 | 2MG  | C3'-C4'-C5'-O5' |
| 26  | a     | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 26  | a     | 2552 | OMU  | O4'-C1'-N1-C2   |
| 26  | a     | 2552 | OMU  | O4'-C1'-N1-C6   |
| 26  | a     | 2552 | OMU  | C1'-C2'-O2'-CM2 |
| 26  | a     | 2604 | PSU  | C3'-C4'-C5'-O5' |
| 26  | a     | 2604 | PSU  | O4'-C4'-C5'-O5' |
| 26  | a     | 1618 | 6MZ  | C3'-C4'-C5'-O5' |
| 26  | a     | 2498 | OMC  | C3'-C4'-C5'-O5' |
| 26  | a     | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 1   | A     | 967  | 5MC  | O4'-C4'-C5'-O5' |
| 26  | a     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 26  | a     | 2498 | OMC  | O4'-C4'-C5'-O5' |
| 37  | l     | 137  | MS6  | CB-CG-SD-CE     |
| 26  | a     | 1835 | 2MG  | O4'-C4'-C5'-O5' |
| 26  | a     | 2445 | 2MG  | O4'-C4'-C5'-O5' |
| 29  | d     | 150  | MEQ  | OE1-CD-CG-CB    |
| 29  | d     | 150  | MEQ  | NE2-CD-CG-CB    |
| 26  | a     | 1835 | 2MG  | C3'-C4'-C5'-O5' |
| 22  | V     | 21   | H2U  | O4'-C1'-N1-C2   |
| 37  | l     | 137  | MS6  | CA-CB-CG-SD     |
| 1   | A     | 1519 | MA6  | C4'-C5'-O5'-P   |
| 1   | A     | 1518 | MA6  | N1-C6-N6-C9     |
| 1   | A     | 527  | G7M  | C4'-C5'-O5'-P   |
| 26  | a     | 2503 | 2MA  | O4'-C1'-N9-C4   |
| 26  | a     | 1915 | 3TD  | C4'-C5'-O5'-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 26  | a     | 2503 | 2MA  | O4'-C1'-N9-C8   |
| 26  | a     | 747  | 5MU  | C4'-C5'-O5'-P   |
| 1   | A     | 967  | 5MC  | C3'-C4'-C5'-O5' |
| 26  | a     | 1962 | 5MC  | C2'-C1'-N1-C6   |
| 26  | a     | 1962 | 5MC  | O4'-C1'-N1-C6   |
| 26  | a     | 2580 | PSU  | O4'-C4'-C5'-O5' |
| 37  | l     | 81   | 4D4  | NE-CD-CG-CB     |
| 1   | A     | 1519 | MA6  | N1-C6-N6-C10    |
| 12  | L     | 89   | D2T  | CG-CB-SB-CB1    |
| 22  | V     | 21   | H2U  | C4'-C5'-O5'-P   |
| 26  | a     | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 37  | l     | 81   | 4D4  | O-C-CA-CB       |

There are no ring outliers.

12 monomers are involved in 16 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 12  | L     | 89   | D2T  | 2       | 0            |
| 26  | a     | 2030 | 6MZ  | 1       | 0            |
| 26  | a     | 2498 | OMC  | 1       | 0            |
| 26  | a     | 2552 | OMU  | 2       | 0            |
| 1   | A     | 1516 | 2MG  | 1       | 0            |
| 26  | a     | 955  | PSU  | 1       | 0            |
| 26  | a     | 2251 | OMG  | 1       | 0            |
| 1   | A     | 1518 | MA6  | 1       | 0            |
| 37  | l     | 81   | 4D4  | 1       | 0            |
| 1   | A     | 1402 | 4OC  | 1       | 0            |
| 26  | a     | 1915 | 3TD  | 2       | 0            |
| 29  | d     | 150  | MEQ  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 315 ligands modelled in this entry, 315 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

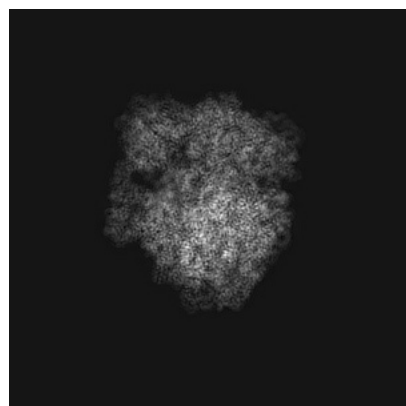
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15116. These allow visual inspection of the internal detail of the map and identification of artifacts.

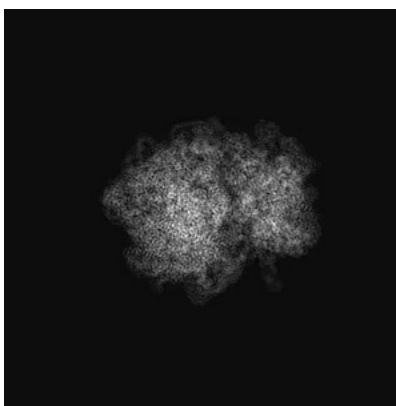
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

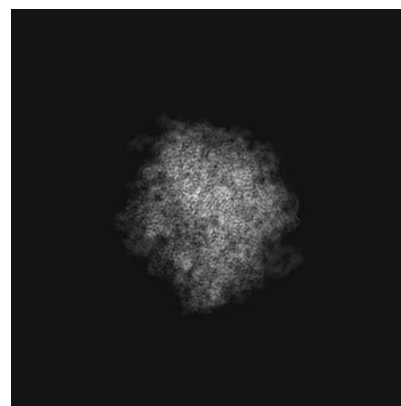
#### 6.1.1 Primary map



X

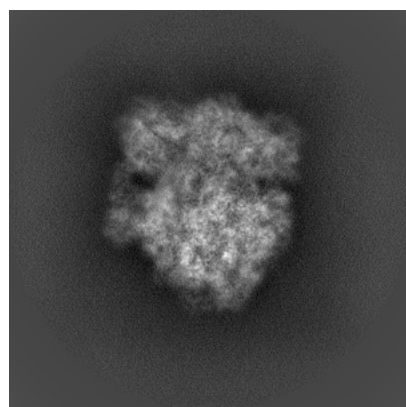


Y

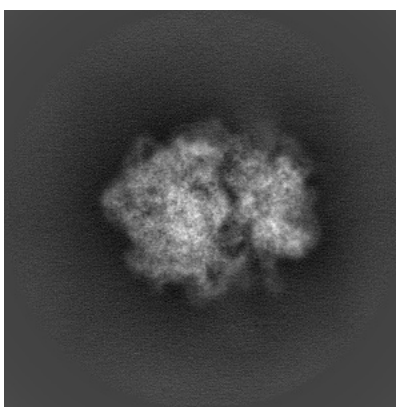


Z

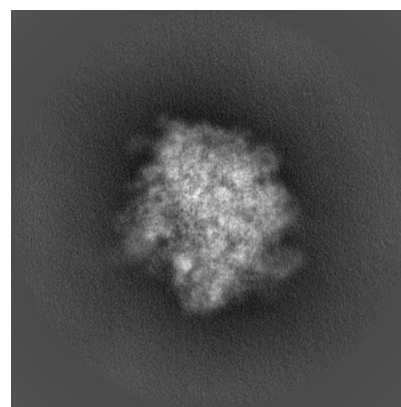
#### 6.1.2 Raw map



X



Y



Z

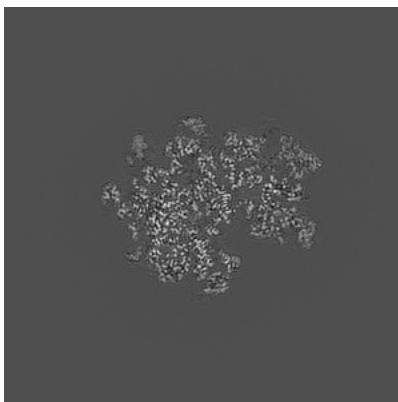
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

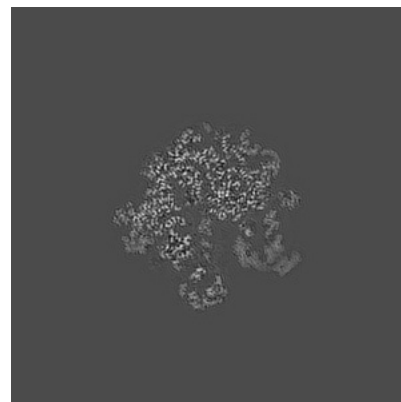
### 6.2.1 Primary map



X Index: 256

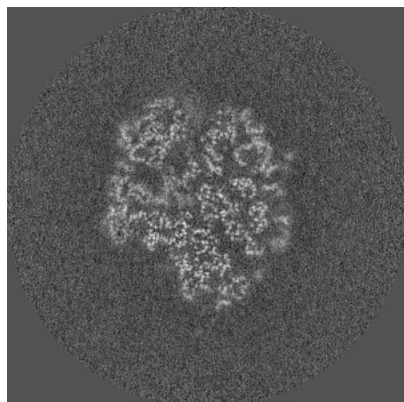


Y Index: 256

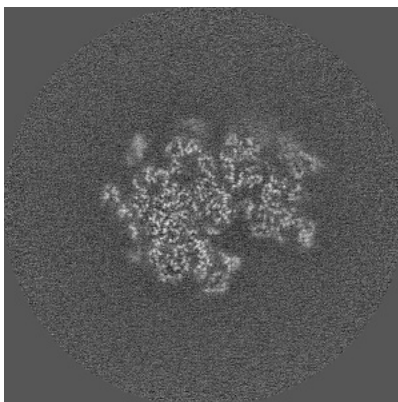


Z Index: 256

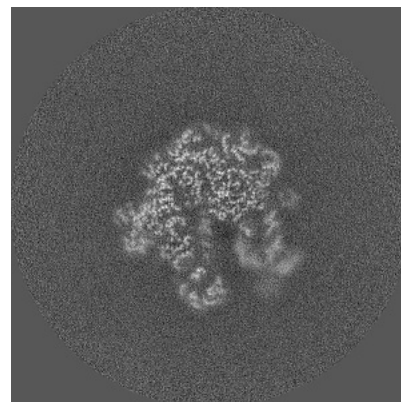
### 6.2.2 Raw map



X Index: 256



Y Index: 256

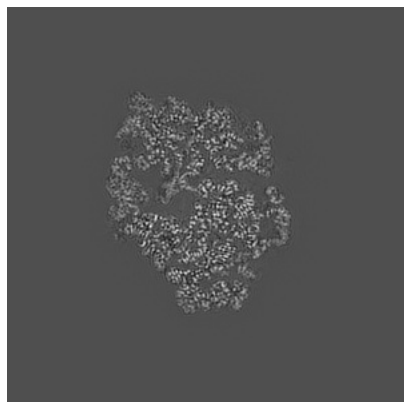


Z Index: 256

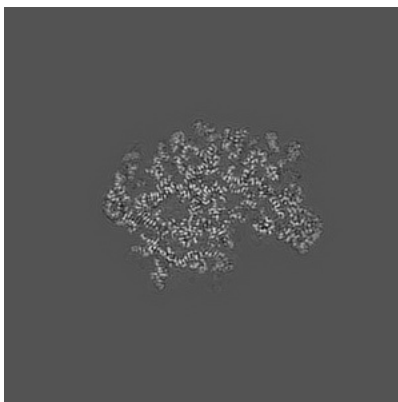
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 267

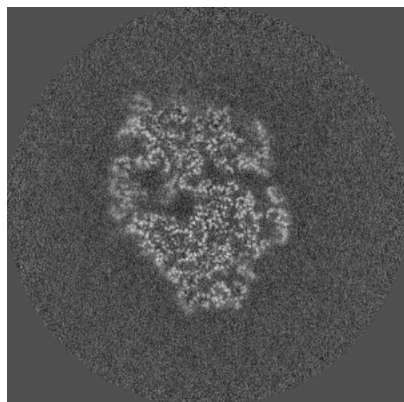


Y Index: 275

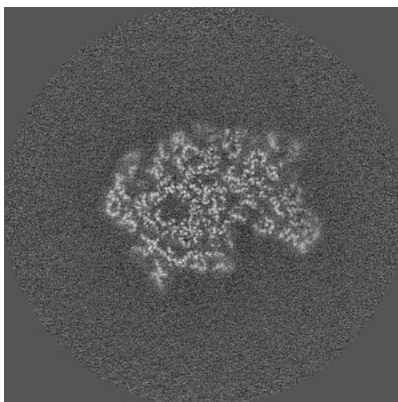


Z Index: 230

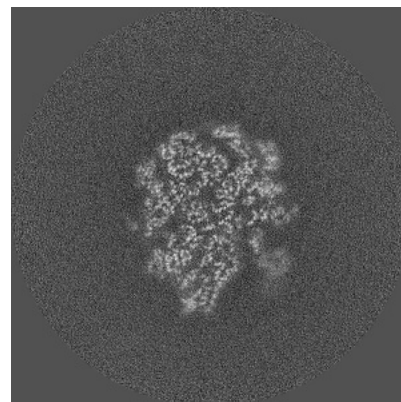
### 6.3.2 Raw map



X Index: 268



Y Index: 275

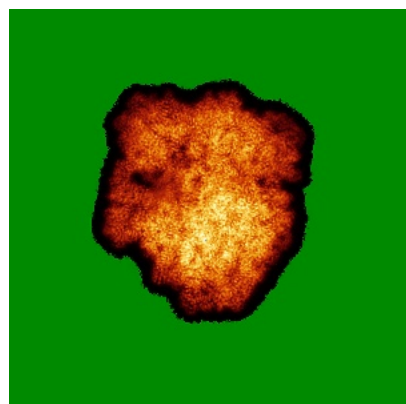


Z Index: 230

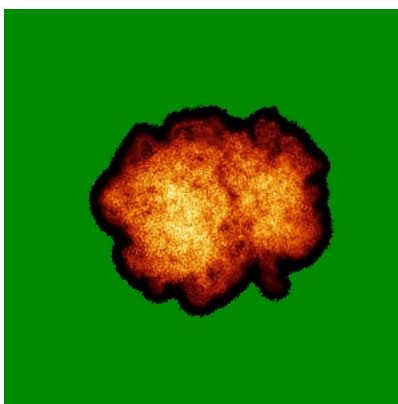
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

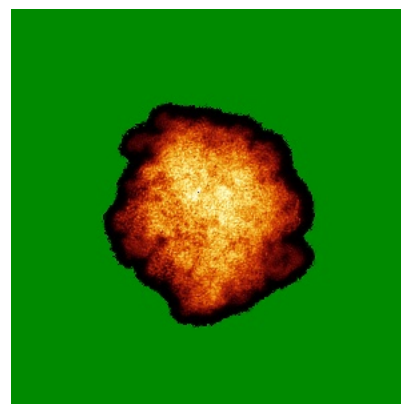
### 6.4.1 Primary map



X

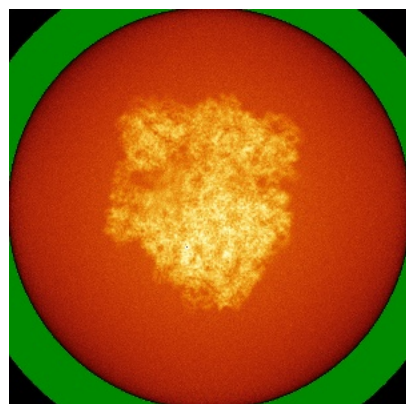


Y

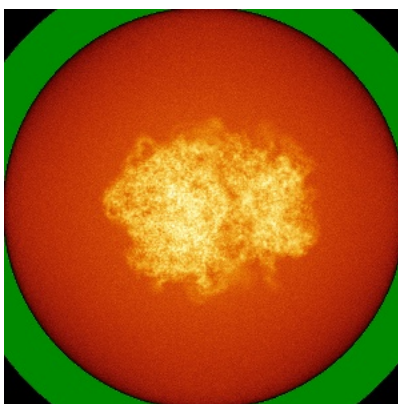


Z

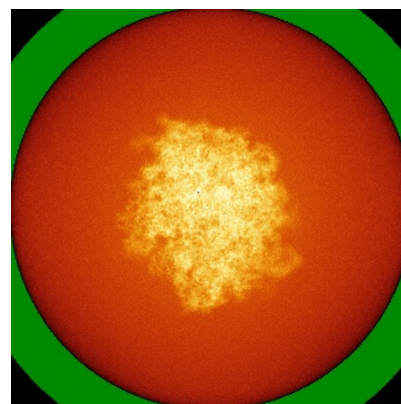
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



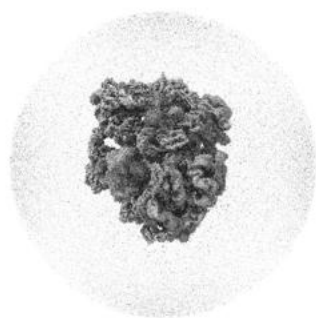
Y



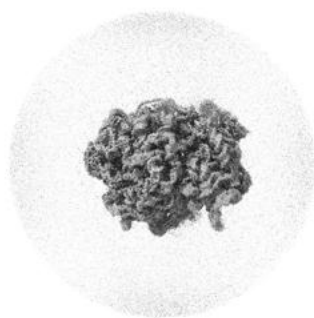
Z

The images above show the 3D surface view of the map at the recommended contour level 4.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

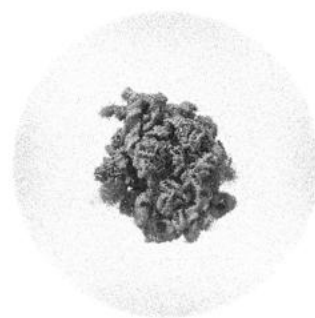
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

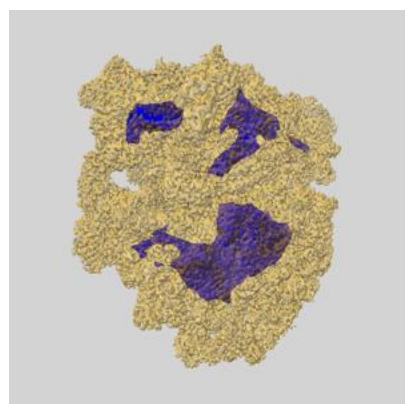
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

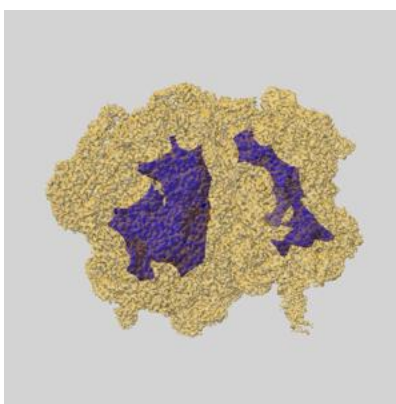
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

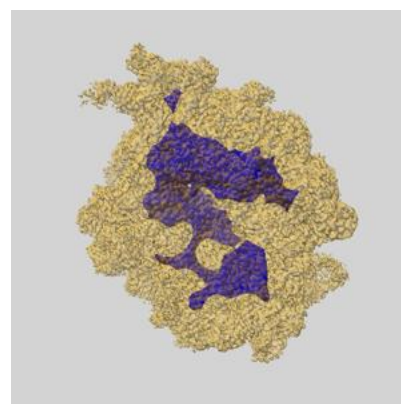
### 6.6.1 emd\_15116\_msk\_1.map [i](#)



X



Y

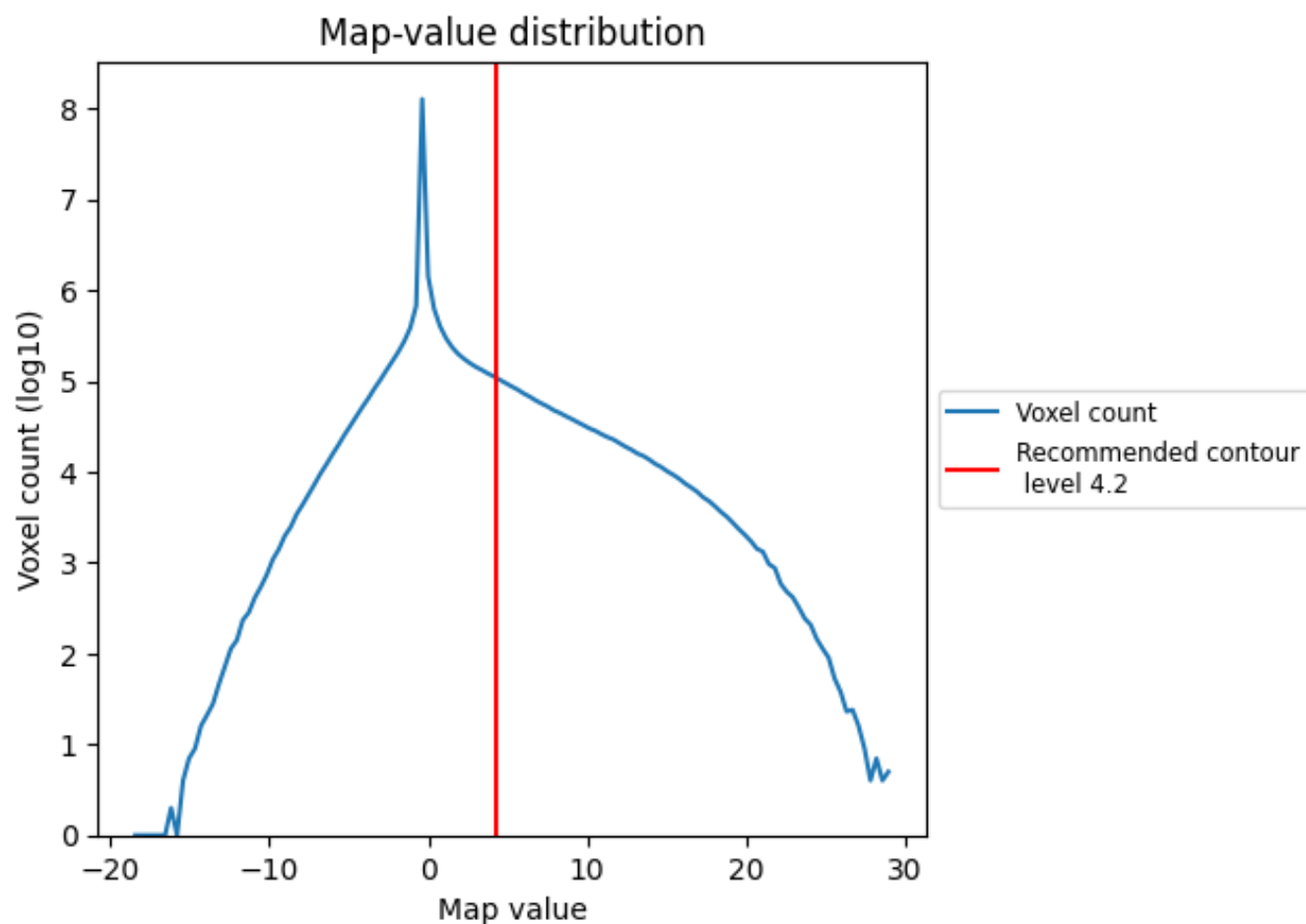


Z

## 7 Map analysis [i](#)

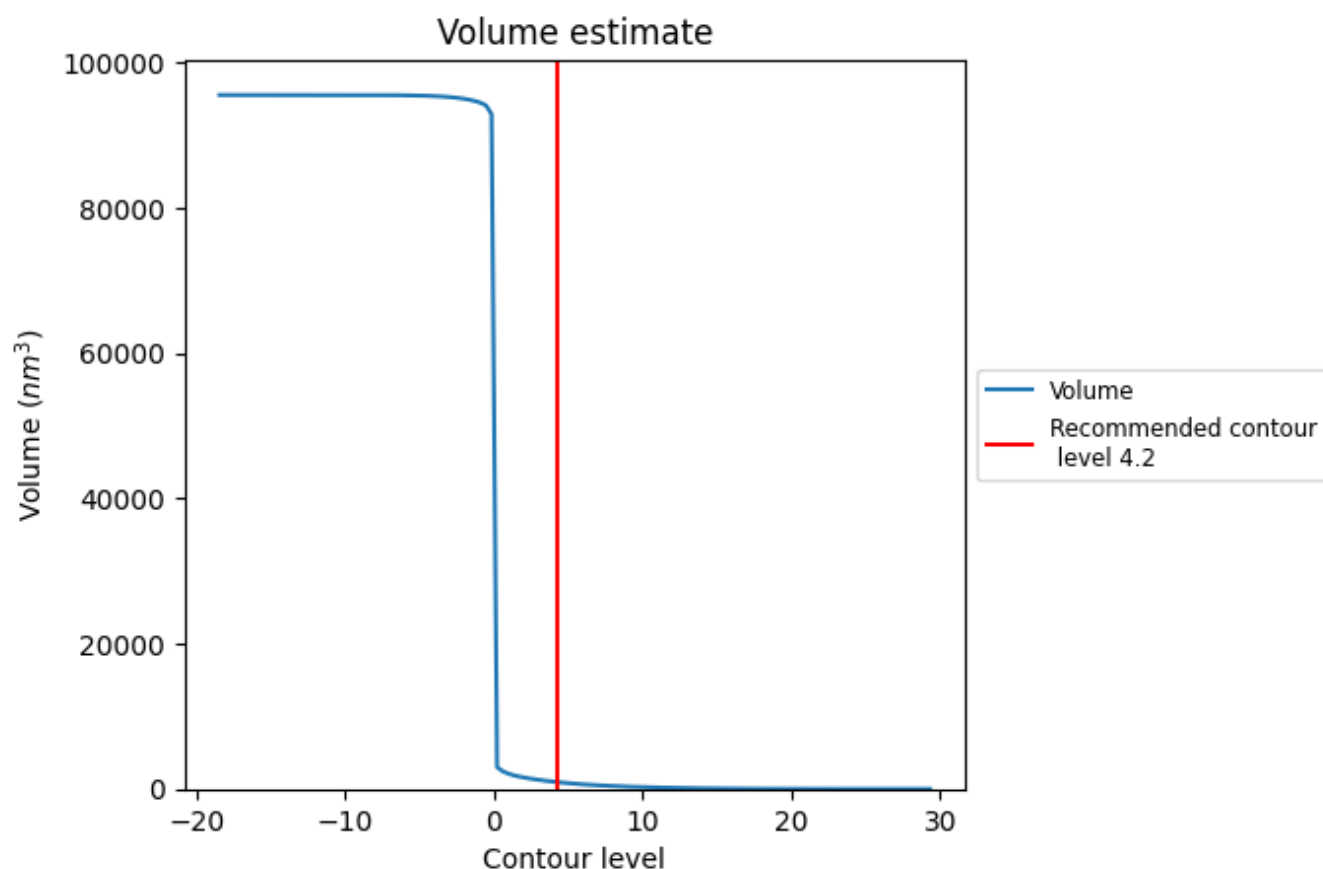
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

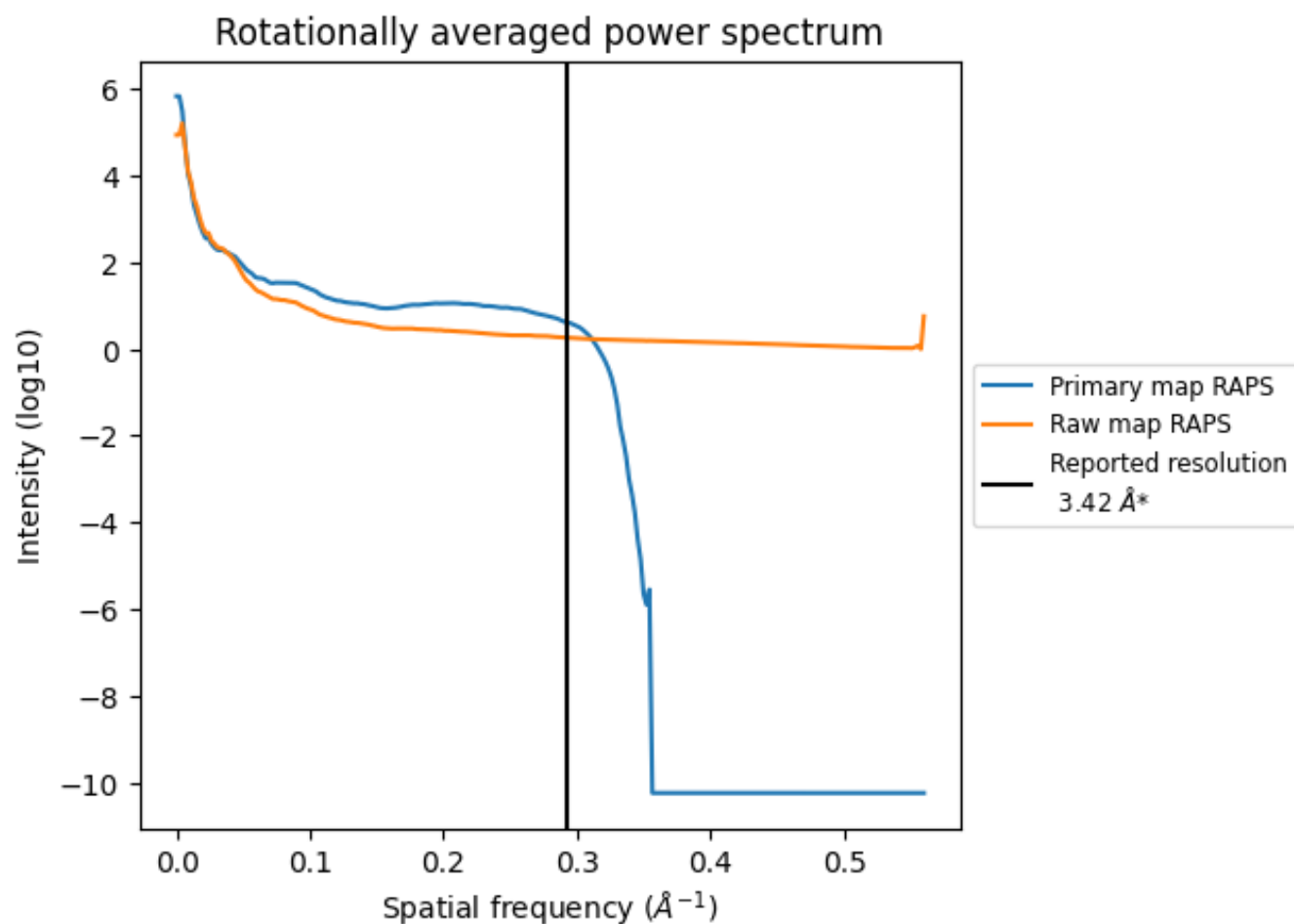
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 957 nm<sup>3</sup>; this corresponds to an approximate mass of 865 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

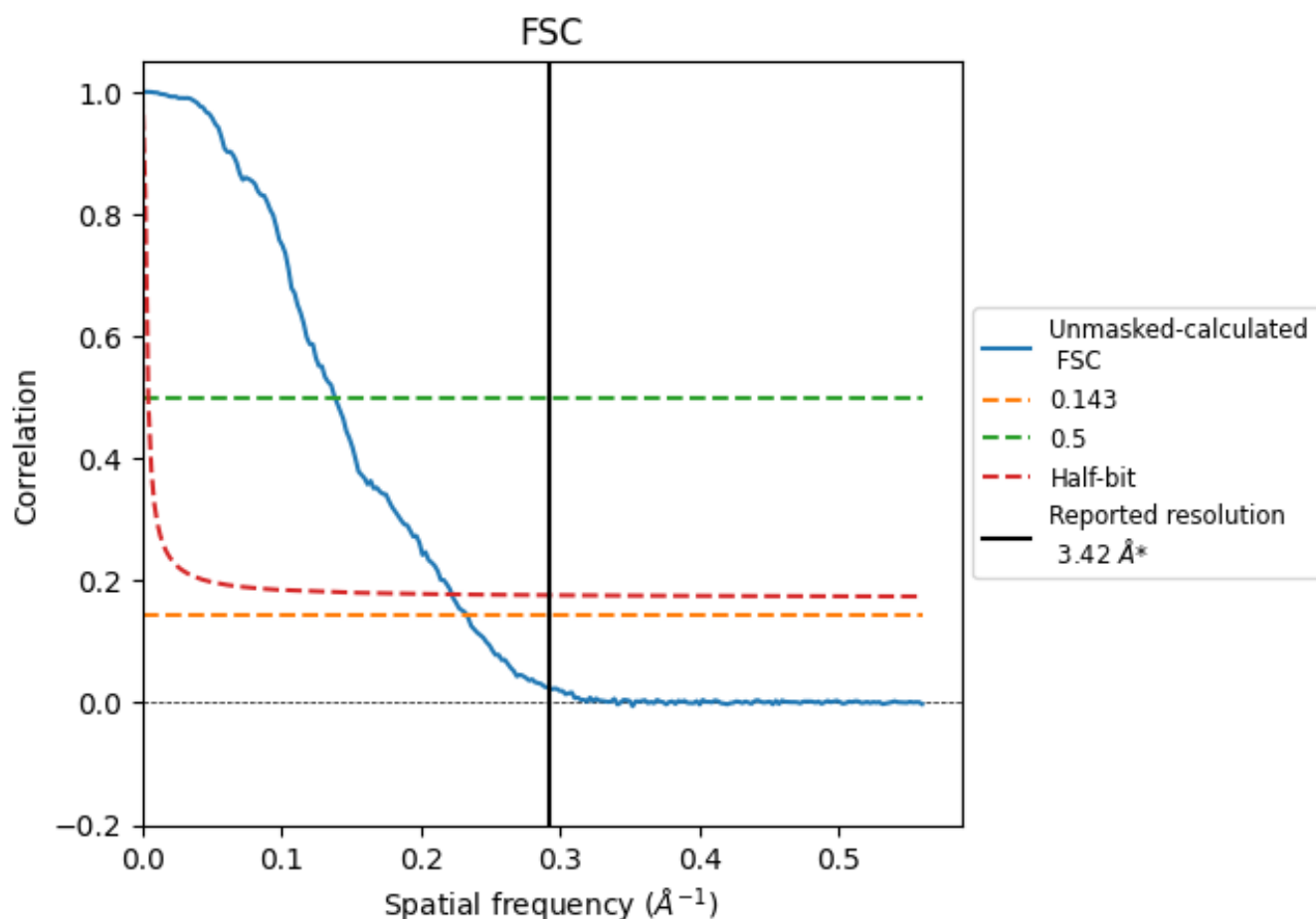


\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.292  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

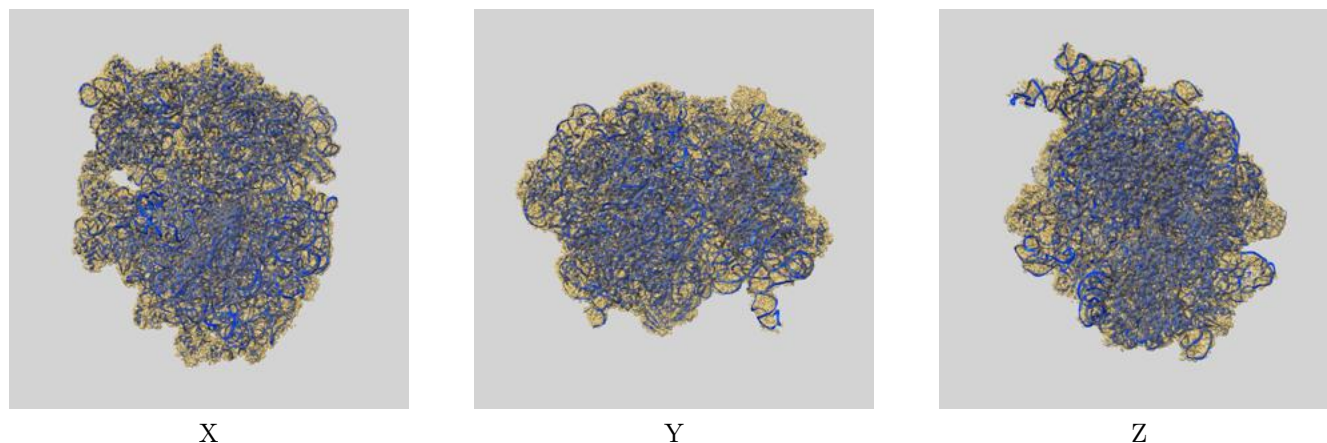
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.42                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.29                               | 7.23 | 4.50     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.29 differs from the reported value 3.42 by more than 10 %

## 9 Map-model fit [i](#)

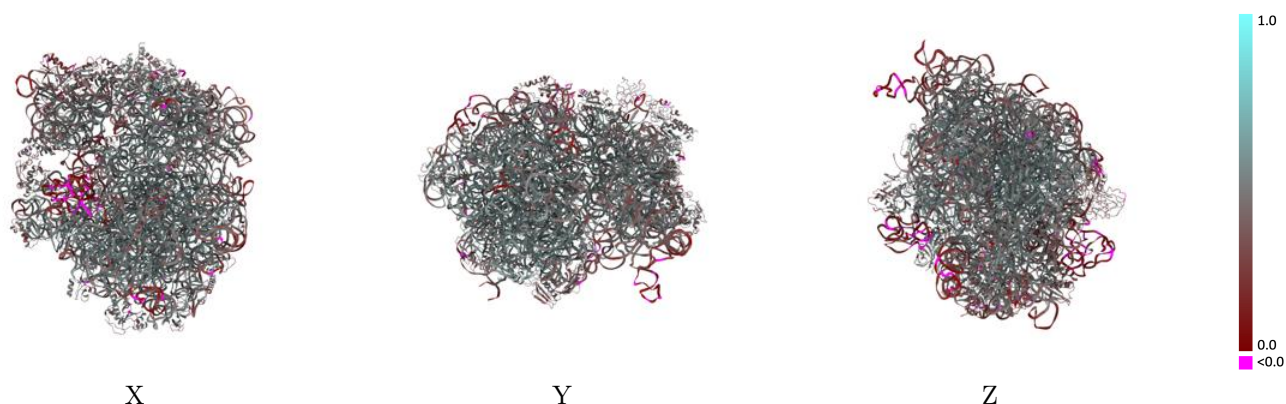
This section contains information regarding the fit between EMDB map EMD-15116 and PDB model 8A3L. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

### 9.1 Map-model overlay [i](#)



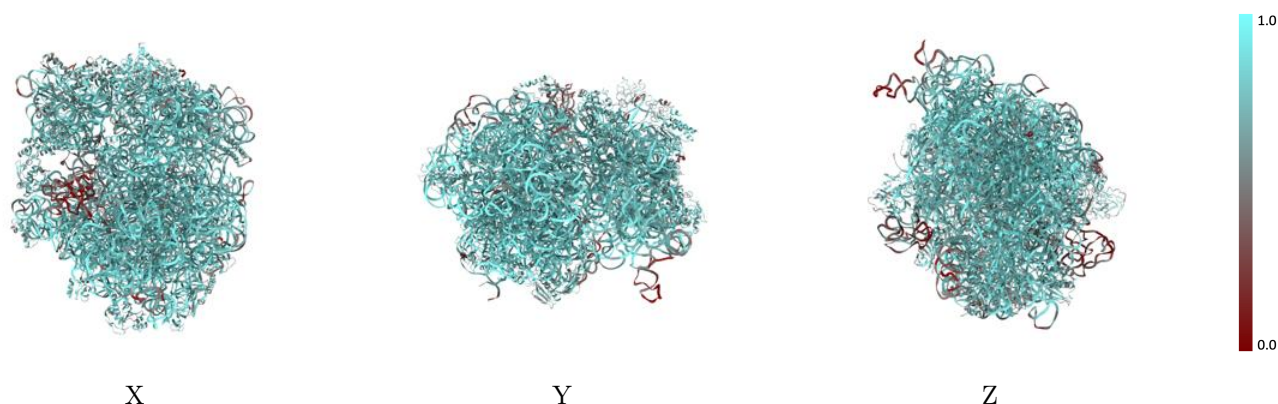
The images above show the 3D surface view of the map at the recommended contour level 4.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



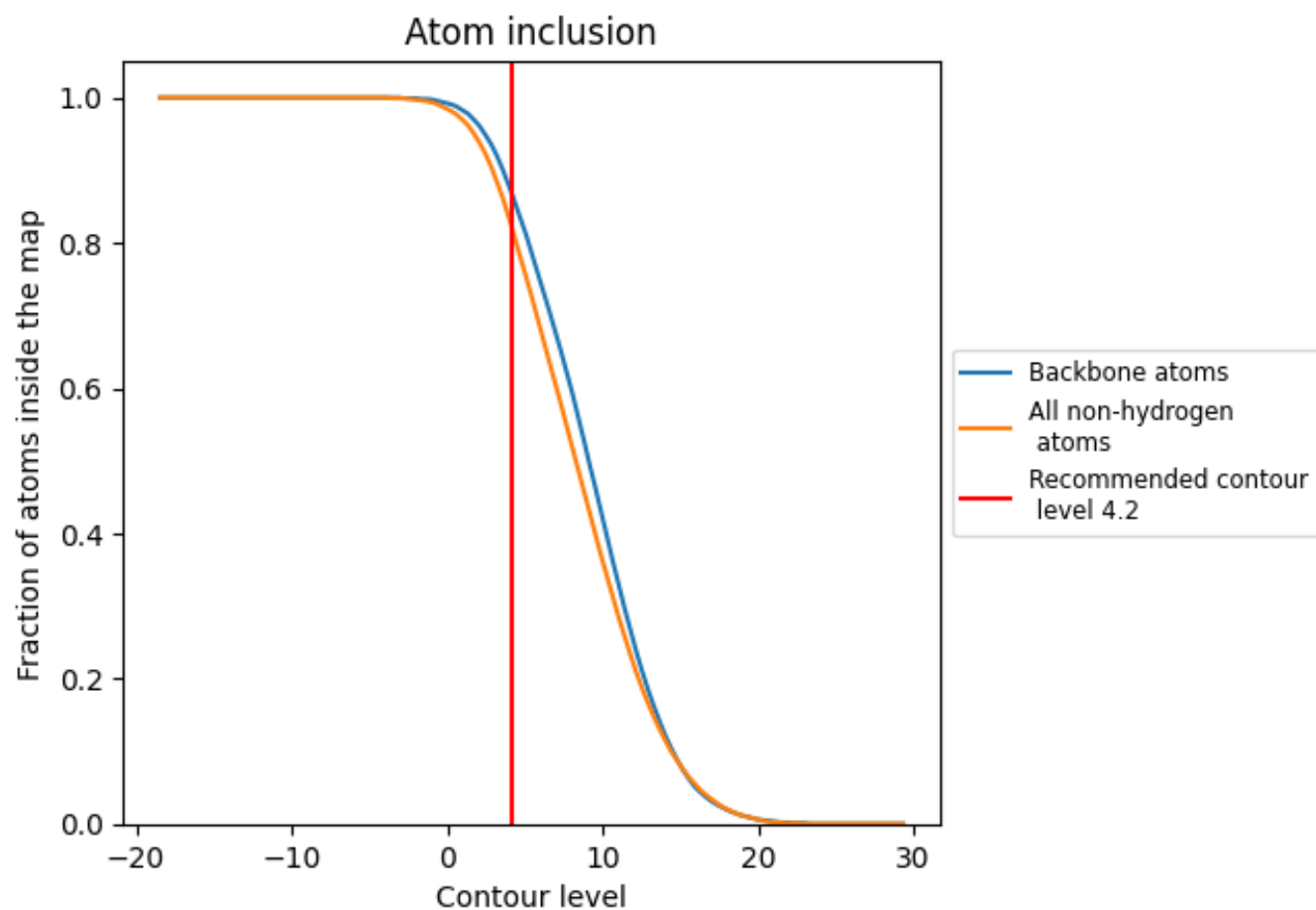
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8190   |  0.4600   |
| 0     |  0.7600   |  0.4700   |
| 1     |  0.8650   |  0.5370   |
| 2     |  0.8640   |  0.5460   |
| 3     |  0.7880   |  0.5050   |
| 4     |  0.6130   |  0.3120   |
| A     |  0.8320   |  0.4470   |
| B     |  0.7850   |  0.4650   |
| C     |  0.7720   |  0.4420   |
| D     |  0.7420   |  0.4260   |
| E     |  0.7900   |  0.4720   |
| F     |  0.7570   |  0.4200   |
| G     |  0.6960   |  0.4000   |
| H     |  0.7650   |  0.4760   |
| I     |  0.7210  |  0.4240  |
| J     |  0.6730 |  0.3670 |
| K     |  0.7940 |  0.4690 |
| L     |  0.7980 |  0.4880 |
| M     |  0.7390 |  0.4400 |
| N     |  0.7470 |  0.4410 |
| O     |  0.7460 |  0.4530 |
| P     |  0.7760 |  0.4630 |
| Q     |  0.7310 |  0.4460 |
| R     |  0.8240 |  0.5000 |
| S     |  0.6930 |  0.4090 |
| T     |  0.7390 |  0.4650 |
| U     |  0.7280 |  0.4750 |
| V     |  0.7430 |  0.3830 |
| W     |  0.4510 |  0.2430 |
| X     |  0.5000 |  0.2320 |
| Y     |  0.6050 |  0.3250 |
| a     |  0.8580 |  0.4760 |
| b     |  0.8280 |  0.4380 |
| c     |  0.8660 |  0.5370 |
| d     |  0.8490 |  0.5220 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| e     |  0.8000   |  0.4840   |
| f     |  0.7340   |  0.4210   |
| g     |  0.6880   |  0.3780   |
| h     |  0.6750   |  0.3770   |
| i     |  0.8280   |  0.5110   |
| j     |  0.8200   |  0.4980   |
| k     |  0.8310   |  0.5050   |
| l     |  0.8180   |  0.5070   |
| m     |  0.8730   |  0.5310   |
| n     |  0.7500   |  0.4610   |
| o     |  0.8160   |  0.4910   |
| p     |  0.8520   |  0.5320   |
| q     |  0.8100   |  0.5030   |
| r     |  0.8160   |  0.5010   |
| s     |  0.7560   |  0.4610   |
| t     |  0.7380   |  0.4380   |
| u     |  0.7630   |  0.4530   |
| v     |  0.7510   |  0.4760   |
| w     |  0.8020   |  0.5000   |
| x     |  0.7080  |  0.4120  |
| y     |  0.7640 |  0.4750 |
| z     |  0.8020 |  0.4910 |