



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 07:04 AM EDT

PDB ID : 8FZF / pdb\_00008fzf  
EMDB ID : EMD-29624  
Title : Cryo-EM structure of an E. coli rotated ribosome complex bound with RF3-ppGpp and p/E-tRNAPhe (Composite state I-C)  
Authors : Rybak, M.Y.; Li, L.; Lin, J.; Gagnon, M.G.  
Deposited on : 2023-01-28  
Resolution : 3.20 Å(reported)  
Based on initial model : 7K00

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:

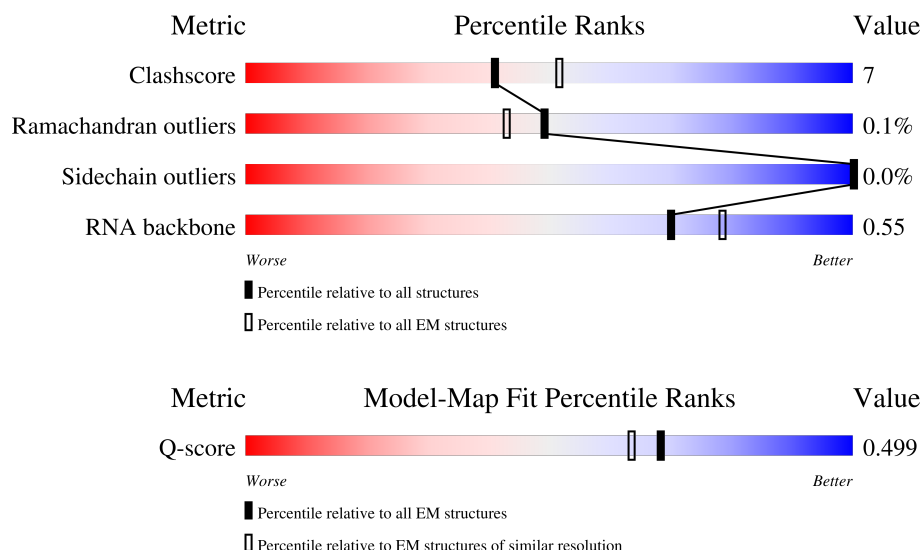
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.20 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.



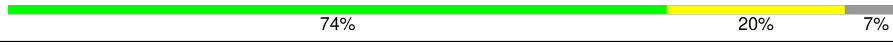
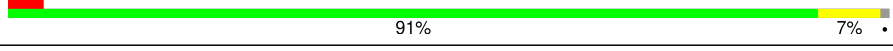
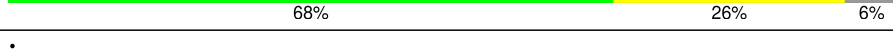
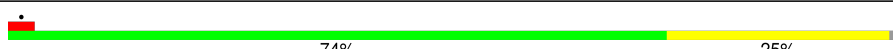
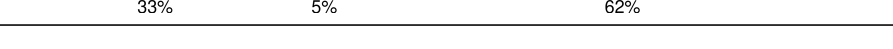
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 15020 ( 2.70 - 3.70 )                                    |

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     | 1542   |                  |
| 2   | b     | 241    |                  |
| 3   | c     | 233    |                  |

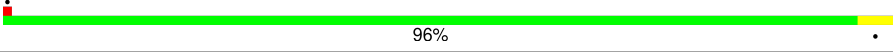
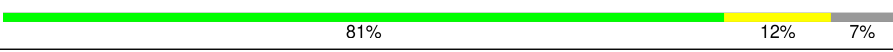
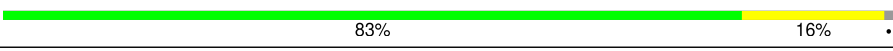
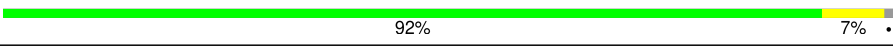
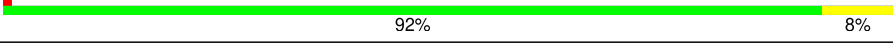
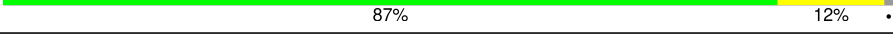
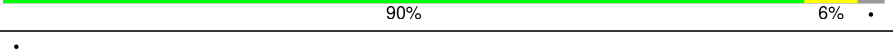
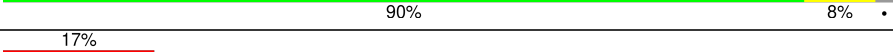
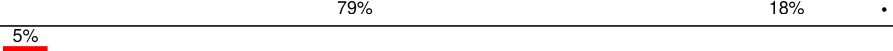
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | d     | 206    |    |
| 5   | e     | 167    |    |
| 6   | f     | 131    |    |
| 7   | g     | 156    |    |
| 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  | x     | 76     |  |
| 23  | z     | 21     |  |
| 24  | v     | 529    |  |
| 25  | A     | 2904   |  |
| 26  | B     | 120    |  |
| 27  | C     | 273    |  |
| 28  | D     | 209    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | E     | 201    |    |
| 30  | F     | 179    |    |
| 31  | G     | 177    |    |
| 32  | I     | 165    |    |
| 33  | J     | 142    |    |
| 34  | L     | 142    |    |
| 35  | M     | 123    |    |
| 36  | N     | 144    |    |
| 37  | O     | 136    |    |
| 38  | P     | 127    |    |
| 39  | Q     | 117    |    |
| 40  | R     | 115    |   |
| 41  | S     | 118    |  |
| 42  | T     | 103    |  |
| 43  | U     | 110    |  |
| 44  | V     | 100    |  |
| 45  | W     | 104    |  |
| 46  | X     | 94     |  |
| 47  | Y     | 85     |  |
| 48  | Z     | 78     |  |
| 49  | 1     | 63     |  |
| 50  | 2     | 59     |  |
| 51  | 3     | 70     |  |
| 52  | 4     | 57     |  |
| 53  | 5     | 55     |  |

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| Mol | Chain | Length | Quality of chain                                    |
|-----|-------|--------|-----------------------------------------------------|
| 54  | 6     | 46     | <div><div></div><div>96%</div><div>.</div></div>    |
| 55  | 7     | 65     | <div><div></div><div>82%</div><div>15%.</div></div> |
| 56  | 8     | 38     | <div><div></div><div>82%</div><div>18%</div></div>  |

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 148897 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     | 1528     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32803 | 14637 | 6019 | 10619 | 1528 |         |       |

- 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     |
|     |       |          | 1754  | 1110 | 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     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1191  | 741 | 230 | 216 | 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 Small ribosomal subunit protein uS9.

| 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 | 173 | 161 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| k     | 119     | IAS      | ASN    | conflict | UNP A0A0H3PWX2 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | l     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 582 | 193 | 162 | 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 Small ribosomal subunit protein uS14.

| 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 Small ribosomal subunit protein uS15.

| 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 Small ribosomal subunit protein uS17.

| 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     | 54       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 446   | 283 | 85 | 78 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | s     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 424 | 126 | 111 | 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     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 460   | 287 | 95 | 77 | 1 |         |       |

- Molecule 22 is a RNA chain called p/E phenylalanyl-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 22  | x     | 74       | Total | C   | N   | O   | P  | S       | 0     | 0 |
|     |       |          | 1588  | 713 | 285 | 515 | 73 | 2       |       |   |

- Molecule 23 is a RNA chain called F-UAA mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 23  | z     | 8        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 168   | 76 | 29 | 55 | 8 |         |       |

- Molecule 24 is a protein called Peptide chain release factor RF3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | v     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3897  | 2471 | 671 | 735 | 20 |         |       |

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 25  | A     | 2899     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62252 | 27778 | 11456 | 20119 | 2899 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 26  | B     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2572  | 1145 | 470 | 837 | 120 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | C     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | D     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 980 | 288 | 294 | 4 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | E     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | F     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | G     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | I     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 988   | 625 | 175 | 183 | 5 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | J     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | L     | 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  | M     | 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  | N     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 653 | 207 | 190 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | O     | 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  |
|-------|---------|----------|--------|----------|------------|
| O     | 82      | MS6      | MET    | conflict | UNP E6BI61 |

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | P     | 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  | Q     | 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  | R     | 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  | S     | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |       |

- Molecule 42 is a protein called Ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | T     | 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  | U     | 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  | V     | 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  | W     | 102      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | X     | 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  | Y     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 582   | 360 | 117 | 104 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Z     | 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  | 1     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 495   | 305 | 97 | 92 | 1 |         |       |

- Molecule 50 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 51 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | 3     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 373   | 232 | 66 | 69 | 6 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52  | 4     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 434   | 263 | 92 | 78 | 1 |         |       |

- Molecule 53 is a protein called Large ribosomal subunit protein bL33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 53  | 5     | 51       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 417   | 269 | 76 | 72 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | 6     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 55  | 7     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

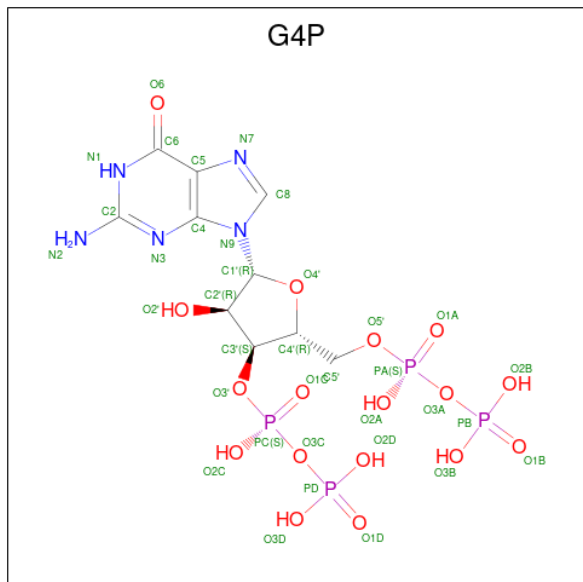
- Molecule 56 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 56  | 8     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 57  | a     | 51       | Total | Mg  | 0       |
|     |       |          | 51    | 51  |         |
| 57  | x     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | A     | 315      | Total | Mg  | 0       |
|     |       |          | 315   | 315 |         |
| 57  | B     | 9        | Total | Mg  | 0       |
|     |       |          | 9     | 9   |         |
| 57  | C     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | D     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | E     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | P     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | S     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | 4     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | 6     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | 7     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 58 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula:  $C_{10}H_{17}N_5O_{17}P_4$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 58  | v     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 36    | 10 | 5 | 17 | 4 |         |

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 59  | 3     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 59  | 8     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 60 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 60  | a     | 6        | Total | O  | 0       |
|     |       |          | 6     | 6  |         |
| 60  | k     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 60  | x     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 60  | A     | 85       | Total | O  | 0       |
|     |       |          | 85    | 85 |         |
| 60  | B     | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |

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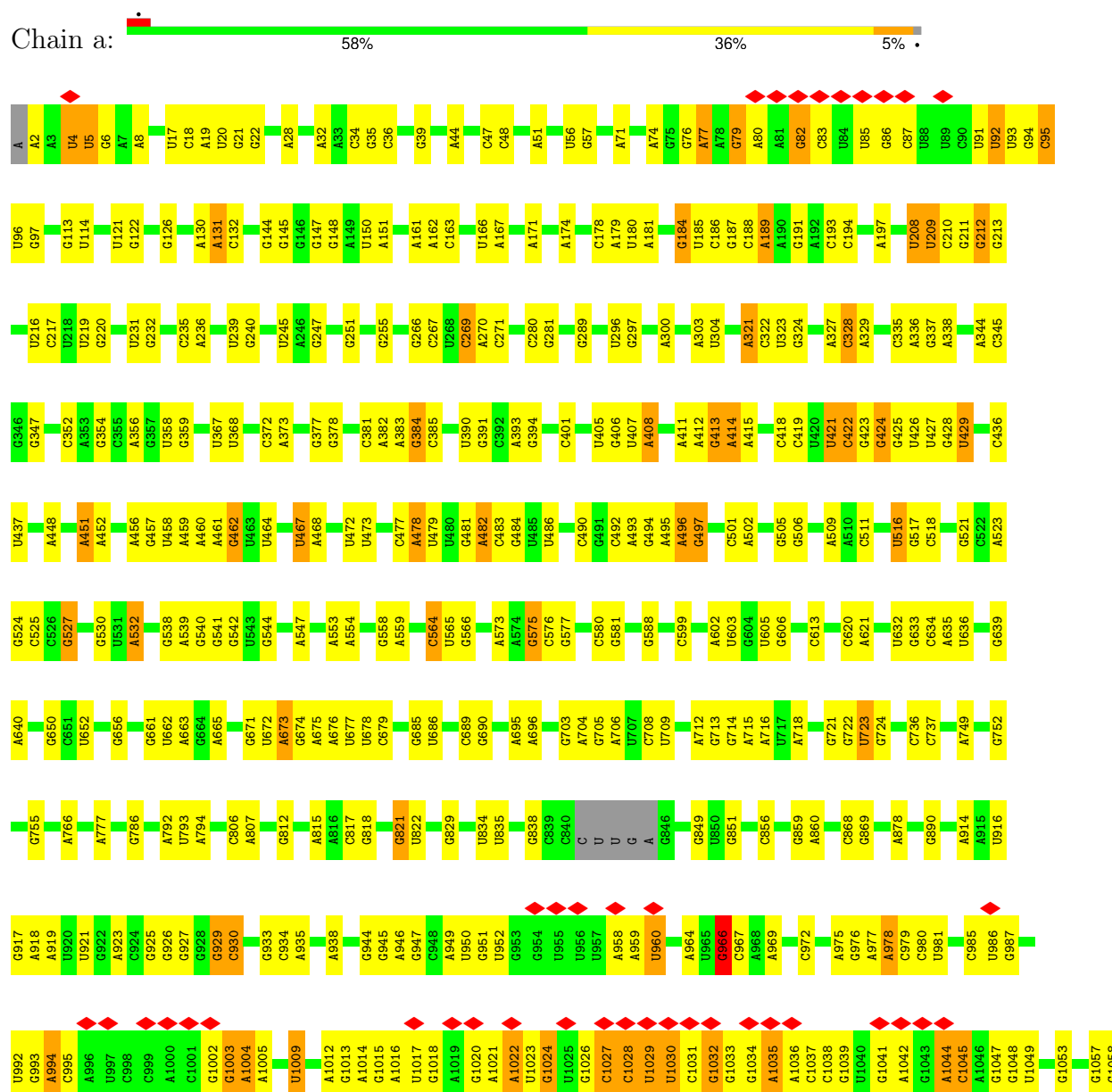
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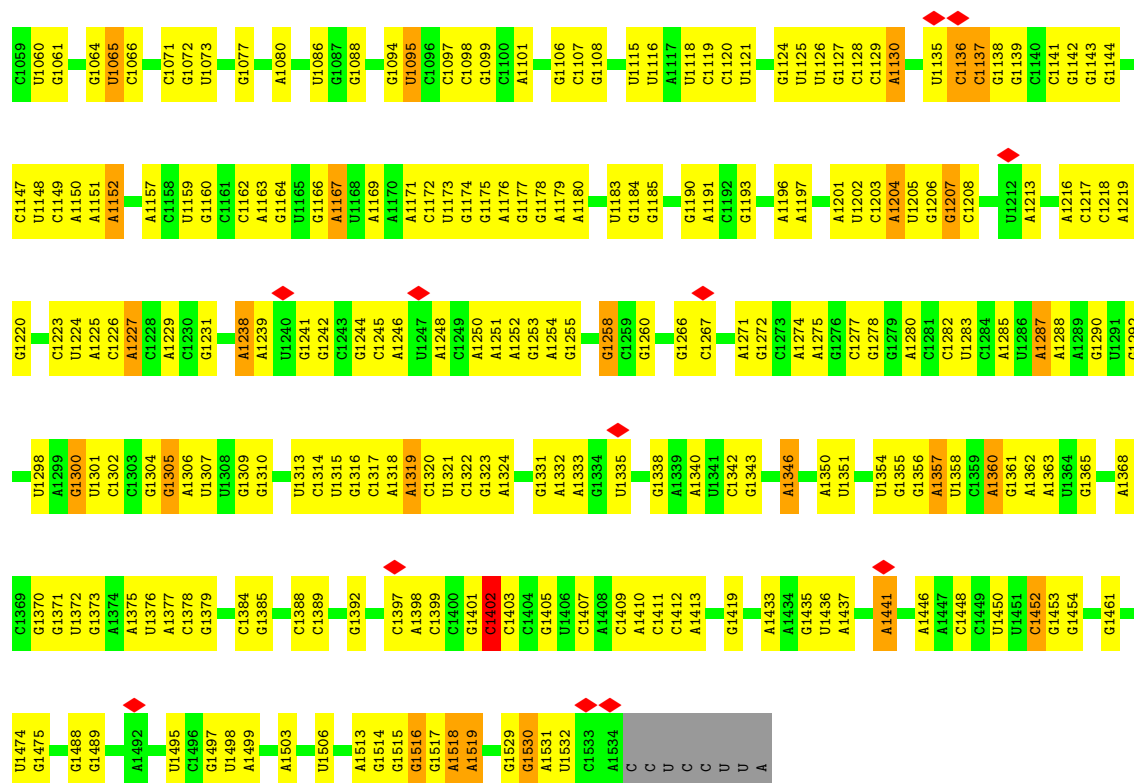
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 60  | C     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

### 3 Residue-property plots

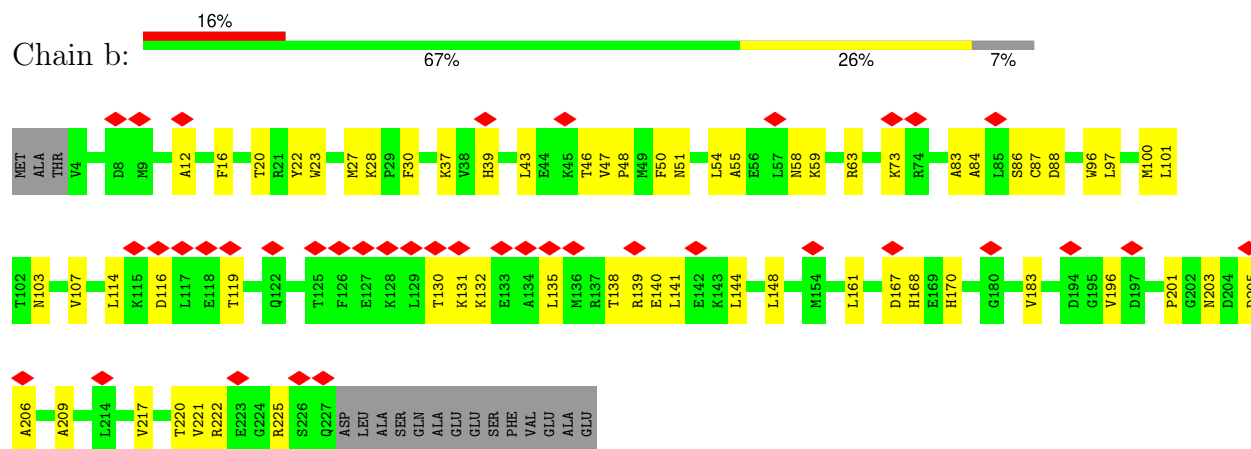
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

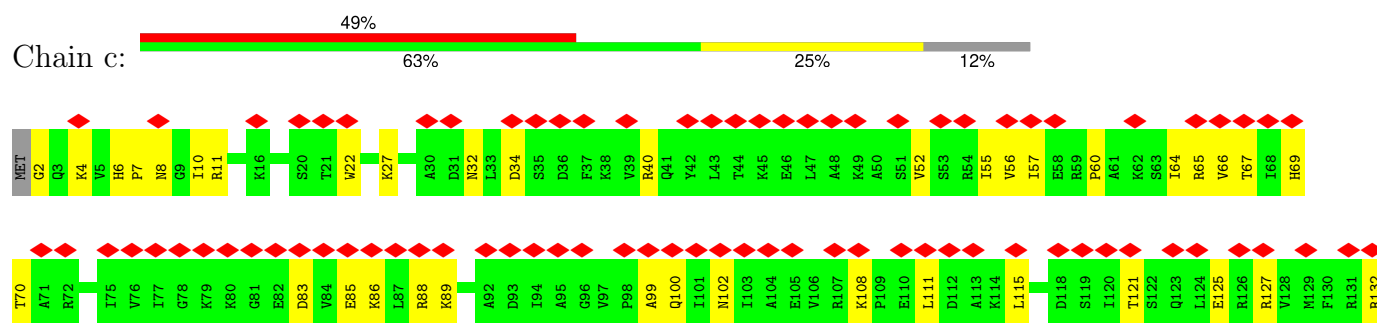


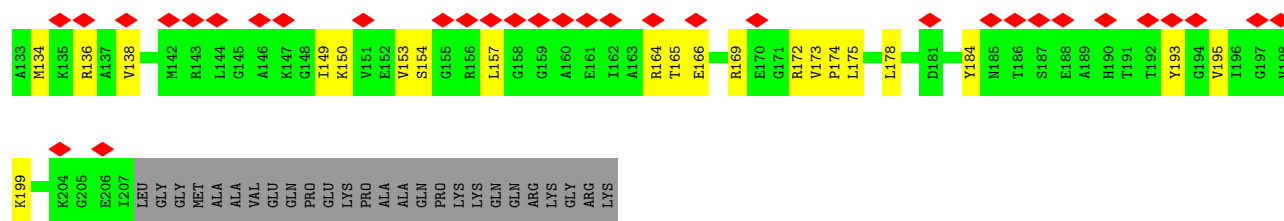


• Molecule 2: 30S ribosomal protein S2

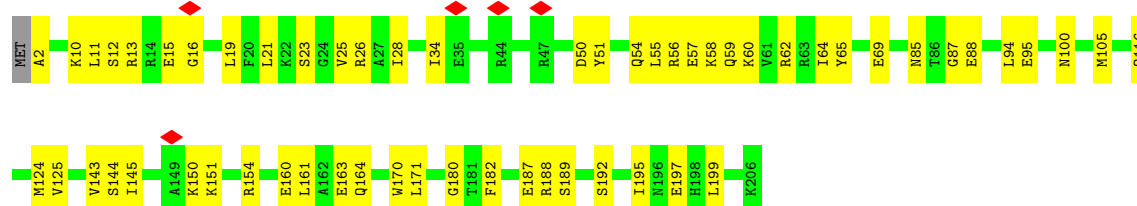


• Molecule 3: 30S ribosomal protein S3





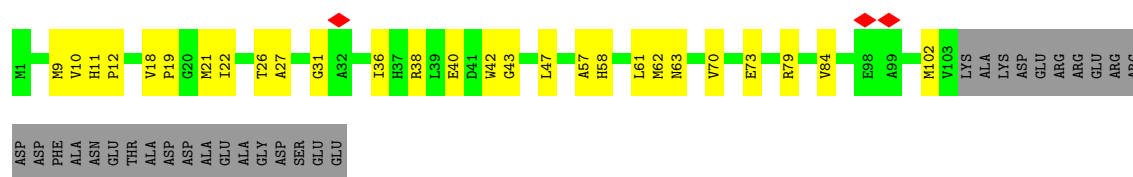
• Molecule 4: 30S ribosomal protein S4



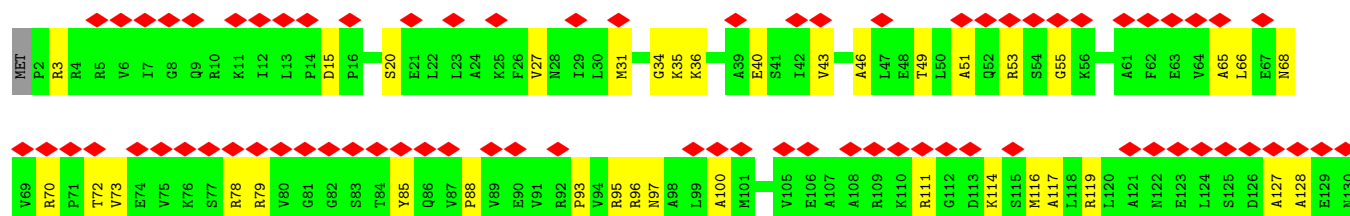
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

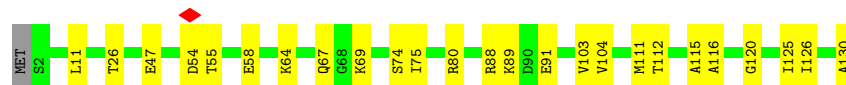
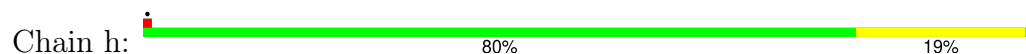


• Molecule 7: 30S ribosomal protein S7

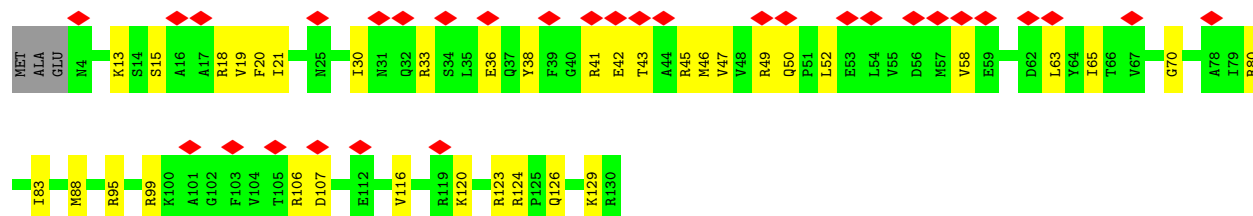




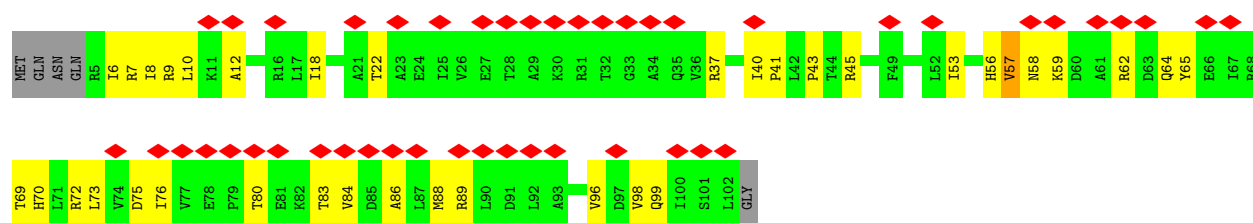
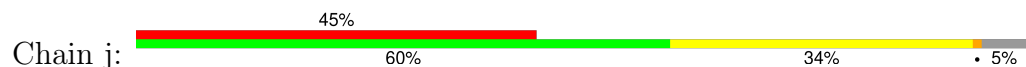
- Molecule 8: 30S ribosomal protein S8



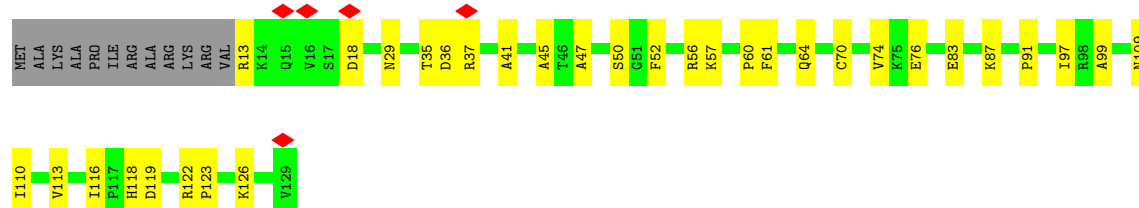
- Molecule 9: Small ribosomal subunit protein uS9



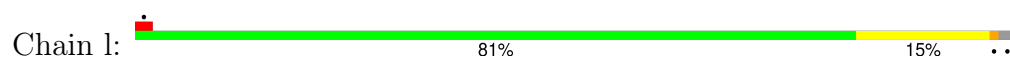
- Molecule 10: 30S ribosomal protein S10

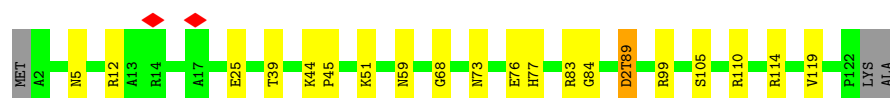


- Molecule 11: 30S ribosomal protein S11

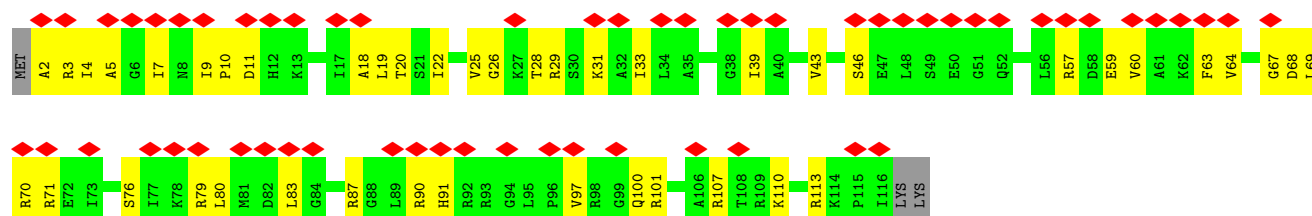


- Molecule 12: 30S ribosomal protein S12

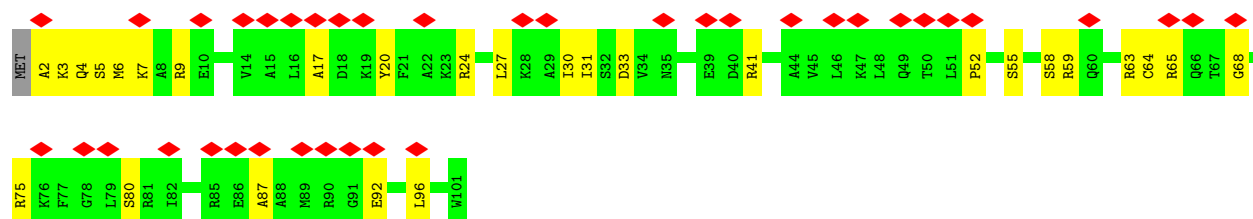




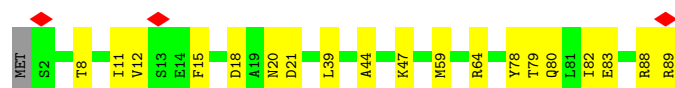
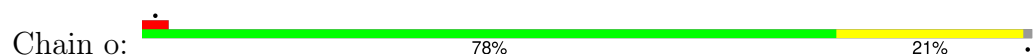
- Molecule 13: 30S ribosomal protein S13



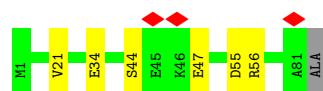
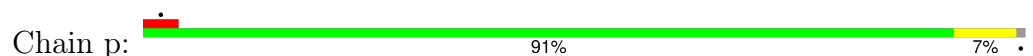
- Molecule 14: Small ribosomal subunit protein uS14



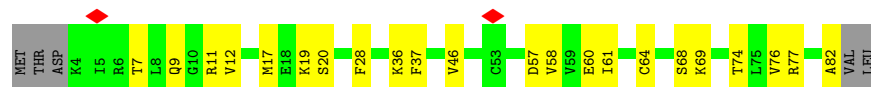
- Molecule 15: Small ribosomal subunit protein uS15



- Molecule 16: 30S ribosomal protein S16



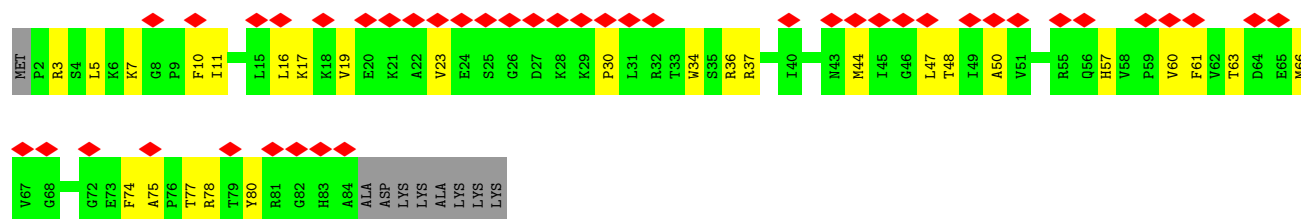
- Molecule 17: Small ribosomal subunit protein uS17



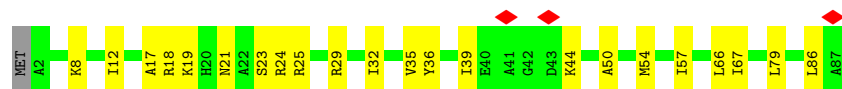
- Molecule 18: 30S ribosomal protein S18



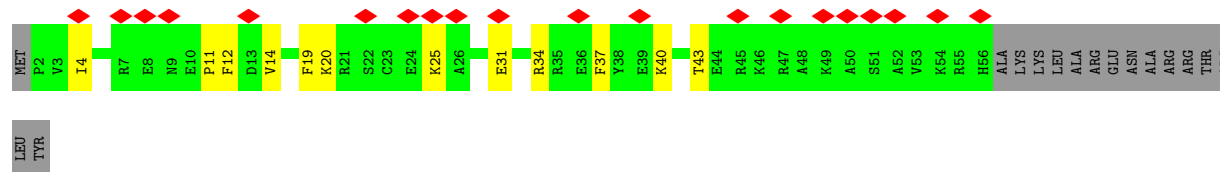
• Molecule 19: 30S ribosomal protein S19



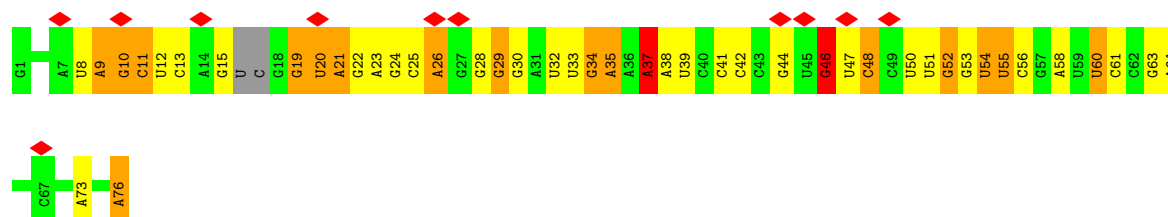
• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein S21

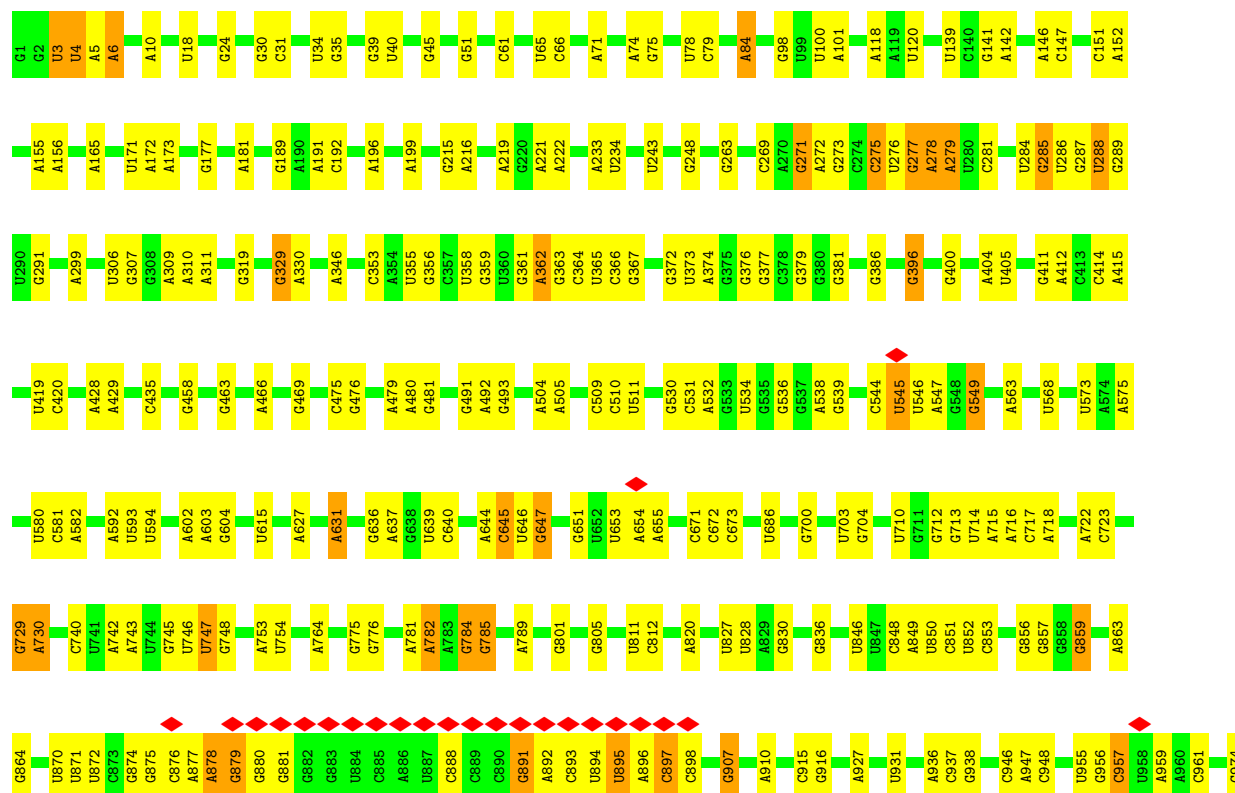


• Molecule 22: p/E phenylalanyl-tRNA

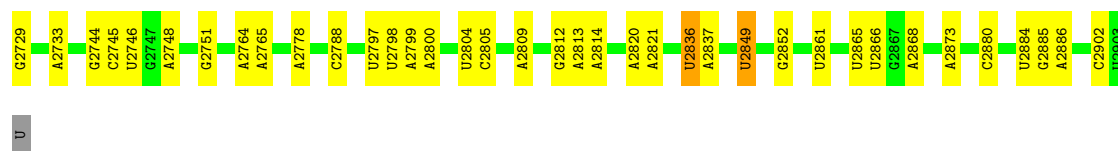


• Molecule 23: F-UAA mRNA

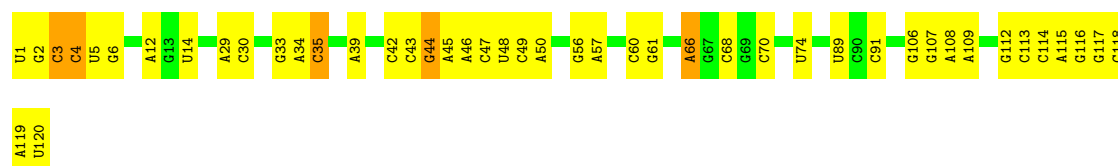




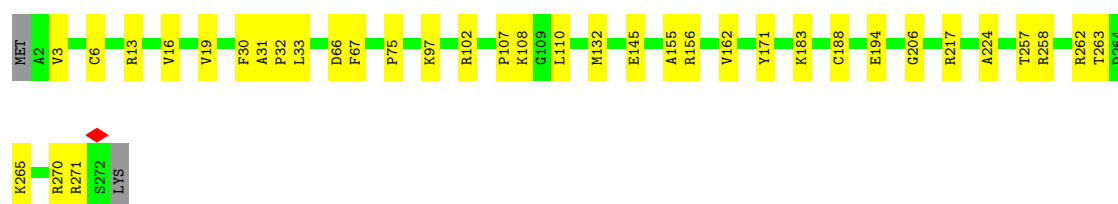
|       |       |       |       |       |       |       |         |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|---------|-------|-------|-------|-------|-------|
| G2595 | A2478 | G2360 | A2241 | U2155 | U2074 | A1928 | C1795   | A1496 | G1338 | U1198 | A1085 | A975  |
| A2598 | G2479 | G2361 | G2242 | G2156 | U2075 | G1929 | U1796   | U1497 | A1353 | U1199 | A1086 | G976  |
| A2602 | G2480 | G2362 | U2243 | G2157 | G2093 | G1930 | U1797   | A1505 | A1354 | U1203 | A1088 | A981  |
| G2603 | G2481 | C2364 | U2245 | A2158 | C2096 | A1937 | U1798   | U1506 | U1361 | G1212 | A1089 | C982  |
| U2604 | G2482 | A2377 | G2246 | G2161 | A2097 | A1938 | U1799   | C1507 | G1362 | A1213 | A1090 | A983  |
| U2605 | G2483 | A2381 | U2247 | A2162 | U2098 | U1939 | C1800   | A1508 | G1361 | G1212 | G1091 | A990  |
| U2609 | G2484 | G2382 | G2248 | A2163 | G2099 | U1955 | A1801   | A1509 | C1362 | A1214 | C1092 | G993  |
| U2613 | G2492 | G2383 | G2250 | A2164 | G2100 | U1962 | A1802   | G1510 | G1363 | G1223 | U1094 | A996  |
| G2614 | G2496 | U2384 | G2251 | U2165 | A2101 | C1962 | A1515   | A1515 | A1364 | U1224 | A1095 |       |
| U2615 | G2497 | C2385 | G2252 | U2166 | G2102 | U1963 | G1524   | G1524 | A1365 | G1235 | U1096 | C1005 |
| C2616 | G2498 | G2386 | A2266 | U2167 | C2103 | G1964 | A1808   |       | C1370 |       | A1097 |       |
| C2617 | G2499 | G2387 | G2271 | U2168 | C2104 | C1965 | A1809   |       |       |       | A1098 |       |
| C2618 | G2502 | G2388 | G2272 | A2169 | U2105 | A1966 | C1816   |       |       |       |       |       |
| C2619 | A2503 | G2389 | G2273 | A2170 | U2106 | A1967 | A1829   |       |       |       | C1102 | A1009 |
| U2629 | U2504 | G2400 | G2274 | A2171 | G2107 | A1970 | G1835   |       |       |       | A1103 | U1012 |
| G2630 | G2505 | U2401 | A2280 | U2172 | A2108 | U1971 | C1836   |       |       |       | C1104 | C1013 |
| C2636 | G2512 | U2402 | G2281 | A2173 | U2109 | G1972 | C1837   |       |       |       | U1105 |       |
| G2655 | C2512 | G2405 | G2282 | C2174 | G2110 | U1991 | U1848   |       |       |       | G1106 | G1022 |
| G2656 | A2513 | A2406 | A2283 | C2175 | U2111 | G1992 | G1849   |       |       |       | U1107 | G1026 |
| G2657 | C2515 | A2411 | G2284 | A2176 | U2112 | U1993 | U1850   |       |       |       | C1108 |       |
| G2661 | U2514 | A2412 | G2285 | G2177 | U2113 | G1996 | U1851   |       |       |       | A1111 | G1031 |
| G2662 | A2518 | G2418 | G2286 | C2178 | A2114 | C2012 | U1852   |       |       |       | A1112 | A1032 |
| G2663 | U2519 | U2419 | G2287 | C2179 | G2115 | U2020 | A1853   |       |       |       | U1113 | U1033 |
| G2664 | G2520 | G2420 | A2288 | U2180 | U2116 | A1958 | A1857   |       |       |       | C1114 | G1038 |
| G2669 | G2523 | G2421 | G2289 | U2181 | A2117 | G2022 | A1866   |       |       |       | U1132 | A1039 |
| U2687 | U2528 | C2424 | U2305 | U2182 | A2118 | U2023 | A1872   |       |       |       | C1135 | C1045 |
| U2688 | G2529 | A2425 | G2308 | U2183 | A2119 | C2023 | A1873   |       |       |       | A1046 | G1047 |
| U2690 | A2547 | G2429 | A2309 | U2184 | A2120 | A2030 | A1878   |       |       |       | G1138 |       |
| C2681 | U2548 | U2441 | G2310 | U2185 | G2123 | A2031 | A1879   |       |       |       | U1141 | G1059 |
| C2682 | U2552 | G2445 | G2311 | U2186 | G2124 | G2032 | C1879   |       |       |       | A1142 | U1060 |
| U2684 | G2553 | G2446 | U2312 | U2187 | U2128 | A2033 | U1882   |       |       |       | U1061 | U1061 |
| U2687 | U2554 | G2447 | G2313 | U2188 | C2129 | U2034 | U1883   |       |       |       | G1062 | G1063 |
| U2688 | U2555 | A2448 | A2314 | U2189 | U2130 | G1884 | U1884   |       |       |       | C1064 | U1065 |
| U2689 | A2566 | U2449 | G2322 | U2190 | U2132 | C2044 | G1907   |       |       |       | U1066 | U1066 |
| U2700 | G2567 | G2454 | G2325 | A2198 | G2133 | A2051 | U1911   |       |       |       | A1067 | A1067 |
| U2701 | A2576 | G2455 | A2328 | G2204 | U2136 | A2052 | A1912   |       |       |       | G1068 | A1069 |
| A2705 | G2577 | C2456 | U2329 | A2211 | G2137 | C2055 | C1914   |       |       |       | A1070 | A1070 |
| G2714 | G2578 | U2457 | A2333 | G2216 | U2140 | G2056 | 3TD1915 |       |       |       | G1071 | G1071 |
| G2715 | C2579 | A2461 | U2334 | G2217 | G2141 | A2060 | A1916   |       |       |       | U1072 | U1072 |
| G2716 | U2580 | C2462 | A2335 | G2218 | A2142 | G2061 | A1917   |       |       |       | A1073 | G1074 |
| G2717 | G2582 | A2469 | G2340 | G2219 | C2143 | C2065 | A1918   |       |       |       | C1075 | C1075 |
| G2718 | U2583 | G2470 | A2341 | A2225 | C2144 | C2066 | A1919   |       |       |       | G1177 | G1076 |
| C2723 | G2585 | U2473 | G2345 | G2230 | C2145 | C2067 | G1920   |       |       |       | U1178 | C1079 |
| A2726 | A2589 | U2474 | G2346 | U2231 | C2146 | G2068 | G1922   |       |       |       | G1179 | A1080 |
|       | C2590 | C2475 | C2350 | C2232 | U2148 | A2070 | C1924   |       |       |       | U1180 | U1081 |
|       | C2591 | U2476 | G2359 | U2233 | C2150 | C2071 | C1925   |       |       |       | U1181 | U1082 |
|       | G2592 | U2477 | G2360 | U2234 | U2151 | C2072 | U1926   |       |       |       | U1183 | U1083 |
|       |       |       |       | G2238 | G2152 | C2073 | A1927   |       |       |       |       | A1084 |
|       |       |       |       | G2239 | C2153 |       |         |       |       |       |       |       |
|       |       |       |       | U2240 | A2154 |       |         |       |       |       |       |       |



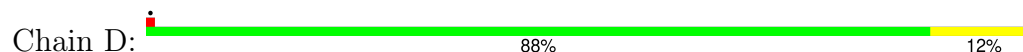
• Molecule 26: 5S Ribosomal RNA



• Molecule 27: 50S ribosomal protein L2



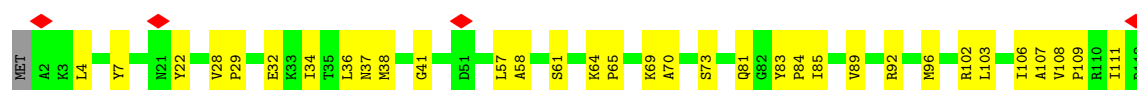
• Molecule 28: 50S ribosomal protein L3

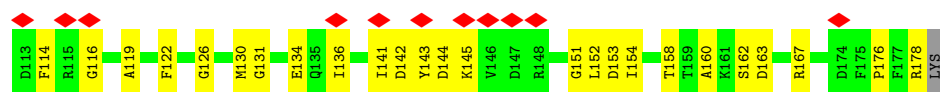


• Molecule 29: 50S ribosomal protein L4

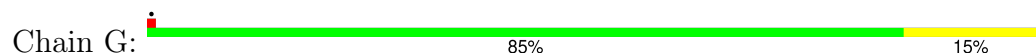


• Molecule 30: 50S ribosomal protein L5

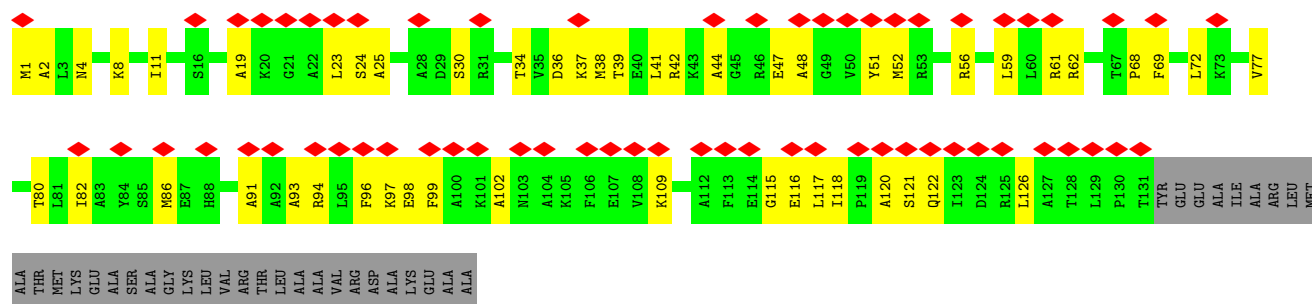




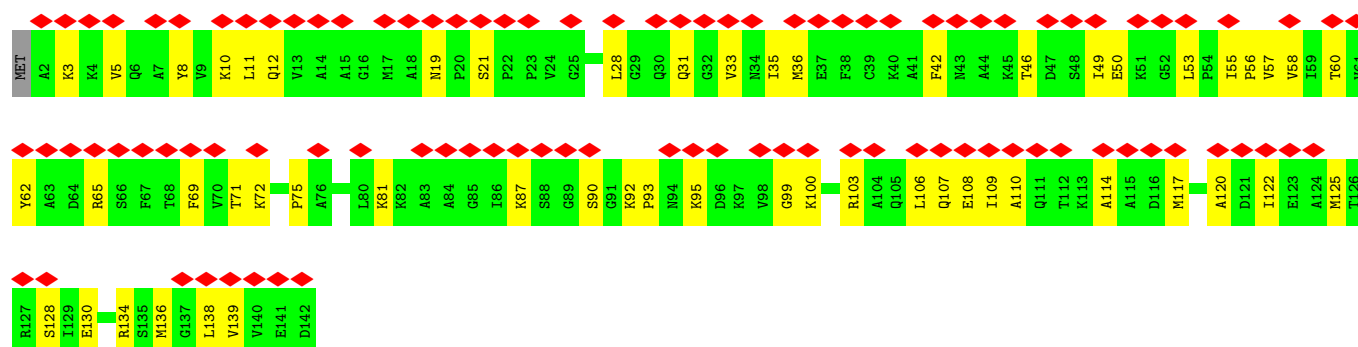
- Molecule 31: 50S ribosomal protein L6



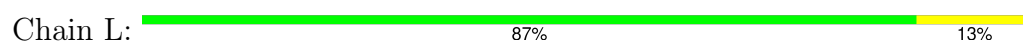
- Molecule 32: 50S ribosomal protein L10



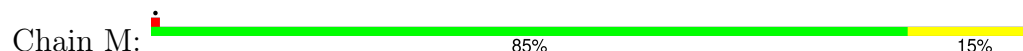
- Molecule 33: 50S ribosomal protein L11

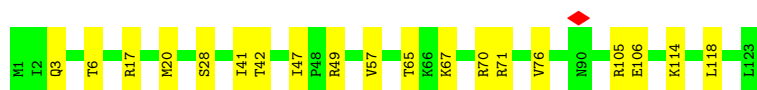


- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14

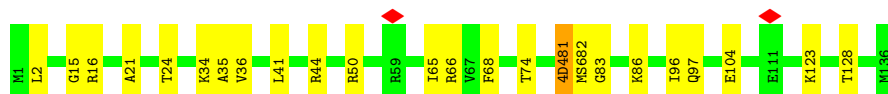
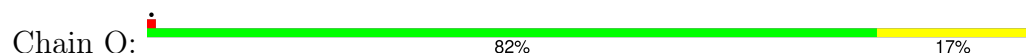




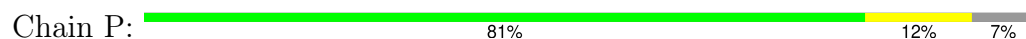
- Molecule 36: 50S ribosomal protein L15



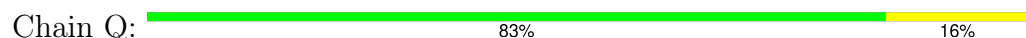
- Molecule 37: 50S ribosomal protein L16



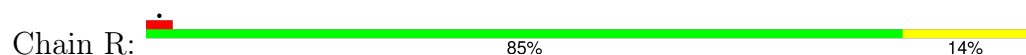
- Molecule 38: Large ribosomal subunit protein bL17



- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19



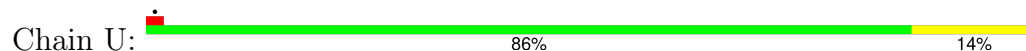
- Molecule 41: 50S ribosomal protein L20



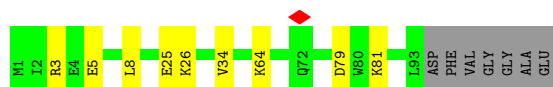
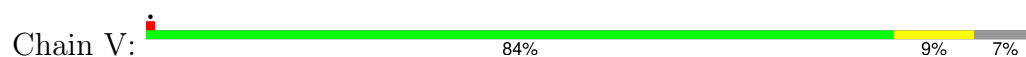
- Molecule 42: Ribosomal protein L21



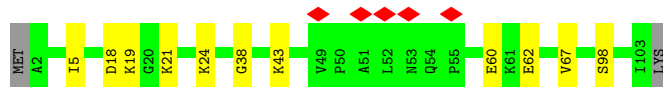
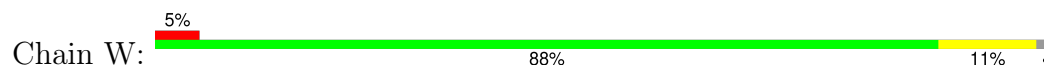
- Molecule 43: 50S ribosomal protein L22



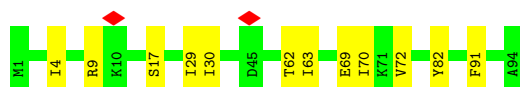
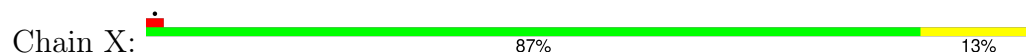
- Molecule 44: 50S ribosomal protein L23



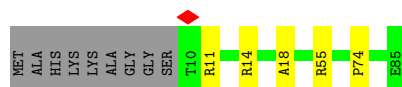
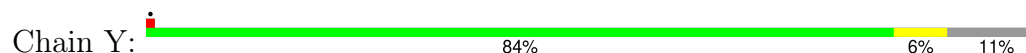
- Molecule 45: 50S ribosomal protein L24



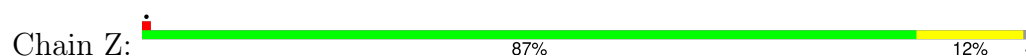
- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29

Chain 1:  90% 6% .



- Molecule 50: Large ribosomal subunit protein uL30

Chain 2:  90% 8% .



- Molecule 51: 50S ribosomal protein L31

Chain 3:  17% 59% 10% 31%



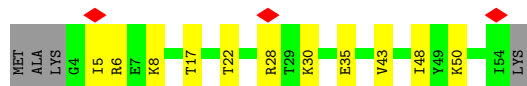
- Molecule 52: 50S ribosomal protein L32

Chain 4:  79% 18% .

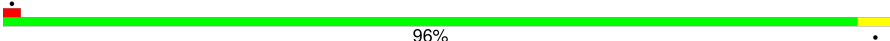


- Molecule 53: Large ribosomal subunit protein bL33

Chain 5:  5% 73% 20% 7%



- Molecule 54: 50S ribosomal protein L34

Chain 6:  96% .

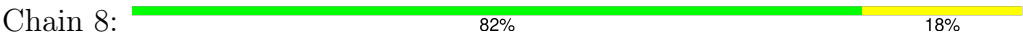


- Molecule 55: 50S ribosomal protein L35

Chain 7:  82% 15% . .



- Molecule 56: 50S ribosomal protein L36



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 33348                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 96000                                   | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 28.006                                  | Depositor |
| Minimum map value                    | -16.348                                 | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 1.015                                   | Depositor |
| Recommended contour level            | 3                                       | Depositor |
| Map size (Å)                         | 435.2, 435.2, 435.2                     | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.85, 0.85, 0.85                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, MIA, H2U, 3TD, 4D4, MA6, 6MZ, 4SU, G4P, MS6, MG, 1MG, 5MU, PSU, 2MG, 5MC, G7M, OMC, 4OC, D2T, MEQ, OMU, OMG, ZN, 2MA, IAS

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     | 0.14         | 0/36450       | 0.26        | 0/56856       |
| 2   | b     | 0.15         | 0/1785        | 0.40        | 0/2404        |
| 3   | c     | 0.12         | 0/1651        | 0.32        | 0/2225        |
| 4   | d     | 0.13         | 0/1665        | 0.26        | 0/2227        |
| 5   | e     | 0.15         | 0/1165        | 0.34        | 0/1568        |
| 6   | f     | 0.15         | 0/858         | 0.39        | 0/1160        |
| 7   | g     | 0.14         | 0/1206        | 0.38        | 0/1617        |
| 8   | h     | 0.14         | 0/989         | 0.32        | 0/1326        |
| 9   | i     | 0.12         | 0/1034        | 0.33        | 0/1375        |
| 10  | j     | 0.13         | 0/796         | 0.39        | 0/1077        |
| 11  | k     | 0.14         | 0/884         | 0.33        | 0/1191        |
| 12  | l     | 0.16         | 0/945         | 0.34        | 0/1268        |
| 13  | m     | 0.12         | 0/900         | 0.32        | 0/1204        |
| 14  | n     | 0.11         | 0/817         | 0.31        | 0/1088        |
| 15  | o     | 0.16         | 0/722         | 0.37        | 0/964         |
| 16  | p     | 0.15         | 0/653         | 0.32        | 0/877         |
| 17  | q     | 0.15         | 0/650         | 0.35        | 0/871         |
| 18  | r     | 0.13         | 0/453         | 0.27        | 0/609         |
| 19  | s     | 0.11         | 0/680         | 0.28        | 0/915         |
| 20  | t     | 0.16         | 0/676         | 0.36        | 0/895         |
| 21  | u     | 0.12         | 0/467         | 0.30        | 0/620         |
| 22  | x     | 0.23         | 2/1602 (0.1%) | 0.31        | 0/2493        |
| 23  | z     | 0.10         | 0/187         | 0.27        | 0/288         |
| 24  | v     | 0.30         | 0/3970        | 0.49        | 1/5367 (0.0%) |
| 25  | A     | 0.20         | 0/69147       | 0.29        | 0/107869      |
| 26  | B     | 0.16         | 0/2876        | 0.28        | 0/4483        |
| 27  | C     | 0.20         | 0/2121        | 0.32        | 0/2852        |
| 28  | D     | 0.21         | 0/1576        | 0.33        | 0/2119        |
| 29  | E     | 0.18         | 0/1571        | 0.27        | 0/2113        |
| 30  | F     | 0.14         | 0/1434        | 0.35        | 0/1926        |
| 31  | G     | 0.16         | 0/1343        | 0.30        | 0/1816        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 32  | I     | 0.14         | 0/1001          | 0.41        | 0/1350          |
| 33  | J     | 0.13         | 0/1046          | 0.43        | 0/1410          |
| 34  | L     | 0.20         | 0/1152          | 0.27        | 0/1551          |
| 35  | M     | 0.19         | 0/955           | 0.30        | 0/1279          |
| 36  | N     | 0.19         | 0/1061          | 0.28        | 0/1412          |
| 37  | O     | 0.16         | 0/1073          | 0.29        | 0/1433          |
| 38  | P     | 0.20         | 0/958           | 0.33        | 0/1281          |
| 39  | Q     | 0.15         | 0/902           | 0.29        | 0/1209          |
| 40  | R     | 0.19         | 0/929           | 0.28        | 0/1242          |
| 41  | S     | 0.22         | 0/960           | 0.26        | 0/1278          |
| 42  | T     | 0.19         | 0/829           | 0.36        | 0/1107          |
| 43  | U     | 0.20         | 0/864           | 0.30        | 0/1156          |
| 44  | V     | 0.18         | 0/744           | 0.28        | 0/994           |
| 45  | W     | 0.19         | 0/787           | 0.42        | 2/1051 (0.2%)   |
| 46  | X     | 0.15         | 0/766           | 0.31        | 0/1025          |
| 47  | Y     | 0.19         | 0/589           | 0.29        | 0/779           |
| 48  | Z     | 0.18         | 0/635           | 0.26        | 0/848           |
| 49  | 1     | 0.15         | 0/496           | 0.25        | 0/660           |
| 50  | 2     | 0.21         | 0/453           | 0.33        | 0/605           |
| 51  | 3     | 0.11         | 0/380           | 0.29        | 0/508           |
| 52  | 4     | 0.20         | 0/440           | 0.31        | 0/588           |
| 53  | 5     | 0.16         | 0/424           | 0.28        | 0/565           |
| 54  | 6     | 0.21         | 0/380           | 0.29        | 0/498           |
| 55  | 7     | 0.19         | 0/513           | 0.33        | 0/676           |
| 56  | 8     | 0.19         | 0/303           | 0.29        | 0/397           |
| All | All   | 0.18         | 2/159913 (0.0%) | 0.30        | 3/238565 (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  | O     | 0                   | 2                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 22  | x     | 46  | G7M  | O3'-P | 5.13 | 1.61        | 1.56     |
| 22  | x     | 8   | 4SU  | O3'-P | 5.03 | 1.61        | 1.56     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | v     | 92  | HIS  | CB-CA-C | -5.77 | 109.94      | 116.63   |
| 45  | W     | 98  | SER  | CA-C-N  | 5.14  | 131.35      | 121.54   |
| 45  | W     | 98  | SER  | C-N-CA  | 5.14  | 131.35      | 121.54   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 37  | O     | 81  | 4D4  | Mainchain |
| 37  | O     | 82  | MS6  | Peptide   |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | a     | 32803 | 0        | 16528    | 427     | 0            |
| 2   | b     | 1754  | 0        | 1782     | 42      | 0            |
| 3   | c     | 1624  | 0        | 1696     | 45      | 0            |
| 4   | d     | 1643  | 0        | 1707     | 37      | 0            |
| 5   | e     | 1152  | 0        | 1196     | 21      | 0            |
| 6   | f     | 839   | 0        | 833      | 17      | 0            |
| 7   | g     | 1191  | 0        | 1245     | 39      | 0            |
| 8   | h     | 979   | 0        | 1031     | 13      | 0            |
| 9   | i     | 1022  | 0        | 1070     | 24      | 0            |
| 10  | j     | 786   | 0        | 828      | 28      | 0            |
| 11  | k     | 877   | 0        | 884      | 23      | 0            |
| 12  | l     | 942   | 0        | 999      | 14      | 0            |
| 13  | m     | 891   | 0        | 952      | 40      | 0            |
| 14  | n     | 805   | 0        | 844      | 27      | 0            |
| 15  | o     | 714   | 0        | 734      | 12      | 0            |
| 16  | p     | 643   | 0        | 661      | 3       | 0            |
| 17  | q     | 641   | 0        | 682      | 14      | 0            |
| 18  | r     | 446   | 0        | 472      | 11      | 0            |
| 19  | s     | 663   | 0        | 688      | 19      | 0            |
| 20  | t     | 670   | 0        | 719      | 14      | 0            |
| 21  | u     | 460   | 0        | 486      | 8       | 0            |
| 22  | x     | 1588  | 0        | 818      | 38      | 0            |
| 23  | z     | 168   | 0        | 86       | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | v     | 3897  | 0        | 3881     | 102     | 0            |
| 25  | A     | 62252 | 0        | 31332    | 454     | 0            |
| 26  | B     | 2572  | 0        | 1301     | 27      | 0            |
| 27  | C     | 2082  | 0        | 2154     | 24      | 0            |
| 28  | D     | 1566  | 0        | 1618     | 20      | 0            |
| 29  | E     | 1552  | 0        | 1619     | 13      | 0            |
| 30  | F     | 1410  | 0        | 1444     | 45      | 0            |
| 31  | G     | 1323  | 0        | 1371     | 15      | 0            |
| 32  | I     | 988   | 0        | 1025     | 37      | 0            |
| 33  | J     | 1032  | 0        | 1085     | 35      | 0            |
| 34  | L     | 1129  | 0        | 1162     | 14      | 0            |
| 35  | M     | 946   | 0        | 1023     | 13      | 0            |
| 36  | N     | 1052  | 0        | 1127     | 6       | 0            |
| 37  | O     | 1075  | 0        | 1145     | 13      | 0            |
| 38  | P     | 945   | 0        | 988      | 11      | 0            |
| 39  | Q     | 892   | 0        | 923      | 12      | 0            |
| 40  | R     | 917   | 0        | 962      | 11      | 0            |
| 41  | S     | 947   | 0        | 1019     | 7       | 0            |
| 42  | T     | 816   | 0        | 839      | 8       | 0            |
| 43  | U     | 857   | 0        | 922      | 9       | 0            |
| 44  | V     | 738   | 0        | 807      | 7       | 0            |
| 45  | W     | 779   | 0        | 831      | 7       | 0            |
| 46  | X     | 753   | 0        | 780      | 8       | 0            |
| 47  | Y     | 582   | 0        | 599      | 4       | 0            |
| 48  | Z     | 625   | 0        | 652      | 5       | 0            |
| 49  | 1     | 495   | 0        | 526      | 4       | 0            |
| 50  | 2     | 449   | 0        | 488      | 3       | 0            |
| 51  | 3     | 373   | 0        | 370      | 6       | 0            |
| 52  | 4     | 434   | 0        | 445      | 9       | 0            |
| 53  | 5     | 417   | 0        | 451      | 8       | 0            |
| 54  | 6     | 377   | 0        | 418      | 2       | 0            |
| 55  | 7     | 504   | 0        | 572      | 8       | 0            |
| 56  | 8     | 302   | 0        | 340      | 5       | 0            |
| 57  | 4     | 1     | 0        | 0        | 0       | 0            |
| 57  | 6     | 1     | 0        | 0        | 0       | 0            |
| 57  | 7     | 1     | 0        | 0        | 0       | 0            |
| 57  | A     | 315   | 0        | 0        | 0       | 0            |
| 57  | B     | 9     | 0        | 0        | 0       | 0            |
| 57  | C     | 1     | 0        | 0        | 0       | 0            |
| 57  | D     | 1     | 0        | 0        | 0       | 0            |
| 57  | E     | 1     | 0        | 0        | 0       | 0            |
| 57  | P     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57  | S     | 1      | 0        | 0        | 0       | 0            |
| 57  | a     | 51     | 0        | 0        | 0       | 0            |
| 57  | x     | 1      | 0        | 0        | 0       | 0            |
| 58  | v     | 36     | 0        | 11       | 8       | 0            |
| 59  | 3     | 1      | 0        | 0        | 0       | 0            |
| 59  | 8     | 1      | 0        | 0        | 0       | 0            |
| 60  | A     | 85     | 0        | 0        | 3       | 0            |
| 60  | B     | 2      | 0        | 0        | 0       | 0            |
| 60  | C     | 1      | 0        | 0        | 0       | 0            |
| 60  | a     | 6      | 0        | 0        | 1       | 0            |
| 60  | k     | 1      | 0        | 0        | 0       | 0            |
| 60  | x     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 148897 | 0        | 101171   | 1679    | 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 7.

All (1679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:x:12:U:C4      | 22:x:23:A:N1      | 2.18                     | 1.11              |
| 58:v:601:G4P:H8   | 58:v:601:G4P:H5'' | 1.33                     | 1.09              |
| 24:v:98:ASP:O     | 24:v:101:ARG:N    | 1.91                     | 1.04              |
| 24:v:98:ASP:O     | 24:v:100:TYR:N    | 1.93                     | 1.01              |
| 1:a:1441:A:H62    | 1:a:1461:G:N2     | 1.57                     | 1.01              |
| 1:a:1357:A:N6     | 1:a:1365:G:H1     | 1.60                     | 0.98              |
| 1:a:150:U:H3      | 1:a:171:A:H62     | 1.09                     | 0.98              |
| 1:a:1441:A:N6     | 1:a:1461:G:H21    | 1.60                     | 0.98              |
| 10:j:57:VAL:HG12  | 10:j:58:ASN:H     | 1.30                     | 0.95              |
| 1:a:1441:A:H62    | 1:a:1461:G:H21    | 1.01                     | 0.93              |
| 1:a:1088:G:H21    | 1:a:1167:A:H61    | 1.22                     | 0.86              |
| 24:v:98:ASP:O     | 24:v:99:THR:C     | 2.18                     | 0.86              |
| 24:v:425:VAL:HG23 | 24:v:440:ALA:HB2  | 1.58                     | 0.85              |
| 33:J:12:GLN:NE2   | 33:J:55:ILE:O     | 2.10                     | 0.84              |
| 1:a:1360:A:H62    | 14:n:58:SER:HB3   | 1.42                     | 0.84              |
| 1:a:1357:A:H61    | 1:a:1365:G:H1     | 0.86                     | 0.83              |
| 1:a:501:C:OP1     | 12:l:114:ARG:NH2  | 2.12                     | 0.82              |
| 25:A:713:G:H21    | 25:A:718:A:H62    | 1.25                     | 0.82              |
| 1:a:1373:G:H4'    | 7:g:31:MET:HE1    | 1.60                     | 0.82              |
| 2:b:87:CYS:O      | 2:b:225:ARG:NH1   | 2.13                     | 0.81              |
| 1:a:1088:G:N2     | 1:a:1167:A:H61    | 1.76                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:g:78:ARG:O      | 7:g:85:TYR:HB2    | 1.81                     | 0.81              |
| 25:A:2123:G:H21   | 25:A:2176:A:H61   | 1.29                     | 0.81              |
| 10:j:9:ARG:HG2    | 10:j:73:LEU:HD13  | 1.64                     | 0.80              |
| 12:l:44:LYS:HD2   | 12:l:45:PRO:HA    | 1.63                     | 0.80              |
| 24:v:92:HIS:NE2   | 58:v:601:G4P:O3B  | 2.15                     | 0.79              |
| 25:A:2144:G:N2    | 25:A:2146:C:O2'   | 2.15                     | 0.79              |
| 25:A:1065:U:O2    | 25:A:1074:G:N1    | 2.13                     | 0.79              |
| 15:o:44:ALA:O     | 15:o:47:LYS:NZ    | 2.14                     | 0.79              |
| 24:v:98:ASP:OD1   | 24:v:99:THR:N     | 2.16                     | 0.79              |
| 26:B:30:C:H1'     | 26:B:57:A:H61     | 1.46                     | 0.79              |
| 32:I:52:MET:HE1   | 32:I:86:MET:H     | 1.48                     | 0.78              |
| 1:a:950:U:H3      | 1:a:1231:G:H1     | 1.31                     | 0.78              |
| 25:A:544:C:N3     | 25:A:549:G:N1     | 2.30                     | 0.78              |
| 32:I:59:LEU:HB3   | 32:I:62:ARG:HB2   | 1.64                     | 0.78              |
| 5:e:45:ARG:HG2    | 5:e:71:MET:HE3    | 1.67                     | 0.77              |
| 24:v:17:ALA:HB2   | 24:v:106:VAL:HG11 | 1.66                     | 0.77              |
| 45:W:18:ASP:HB2   | 45:W:21:LYS:HD2   | 1.64                     | 0.77              |
| 1:a:1086:U:H3     | 1:a:1099:G:H22    | 1.32                     | 0.76              |
| 14:n:33:ASP:O     | 14:n:41:ARG:NH2   | 2.18                     | 0.76              |
| 25:A:1084:A:O2'   | 25:A:1085:A:O5'   | 2.04                     | 0.76              |
| 15:o:18:ASP:HB2   | 15:o:21:ASP:HB2   | 1.66                     | 0.76              |
| 28:D:133:THR:HG22 | 28:D:134:HIS:H    | 1.51                     | 0.76              |
| 22:x:12:U:C5      | 22:x:23:A:N1      | 2.53                     | 0.75              |
| 22:x:15:G:N2      | 22:x:48:C:H42     | 1.82                     | 0.75              |
| 35:M:70:ARG:HG2   | 35:M:76:VAL:HG12  | 1.69                     | 0.75              |
| 25:A:713:G:N2     | 25:A:718:A:H62    | 1.83                     | 0.75              |
| 25:A:2109:U:H2'   | 25:A:2180:U:H3    | 1.52                     | 0.75              |
| 25:A:1925:C:H2'   | 25:A:1926:U:H2'   | 1.67                     | 0.75              |
| 25:A:2313:C:H2'   | 25:A:2314:A:H8    | 1.50                     | 0.75              |
| 1:a:150:U:H3      | 1:a:171:A:N6      | 1.85                     | 0.74              |
| 7:g:70:ARG:HE     | 7:g:96:ARG:HG3    | 1.50                     | 0.74              |
| 25:A:2123:G:N2    | 25:A:2124:G:O6    | 2.21                     | 0.74              |
| 13:m:11:ASP:HB3   | 13:m:46:SER:HB2   | 1.70                     | 0.74              |
| 1:a:181:A:H61     | 1:a:194:C:H3'     | 1.52                     | 0.74              |
| 13:m:4:ILE:HG13   | 13:m:57:ARG:HD2   | 1.70                     | 0.74              |
| 24:v:87:LEU:HD11  | 24:v:364:ILE:HD12 | 1.70                     | 0.74              |
| 1:a:1346:A:N6     | 1:a:1375:A:OP2    | 2.21                     | 0.74              |
| 25:A:1601:G:OP1   | 44:V:64:LYS:NZ    | 2.19                     | 0.74              |
| 1:a:1088:G:H21    | 1:a:1167:A:N6     | 1.86                     | 0.73              |
| 20:t:23:SER:OG    | 20:t:24:ARG:NH1   | 2.22                     | 0.73              |
| 1:a:1009:U:O2     | 1:a:1020:G:N2     | 2.22                     | 0.73              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 25:A:544:C:N4     | 25:A:549:G:O6    | 2.19                     | 0.73              |
| 32:I:30:SER:H     | 32:I:109:LYS:HD2 | 1.55                     | 0.72              |
| 46:X:9:ARG:NH2    | 46:X:17:SER:OG   | 2.22                     | 0.72              |
| 53:5:35:GLU:HG3   | 53:5:50:LYS:HE3  | 1.70                     | 0.72              |
| 3:c:132:ARG:HB3   | 3:c:136:ARG:HH12 | 1.55                     | 0.72              |
| 25:A:713:G:H21    | 25:A:718:A:N6    | 1.87                     | 0.72              |
| 10:j:37:ARG:HB3   | 10:j:75:ASP:HB2  | 1.72                     | 0.72              |
| 1:a:1305:G:N2     | 1:a:1331:G:O2'   | 2.23                     | 0.72              |
| 1:a:1175:G:H2'    | 1:a:1176:A:H8    | 1.55                     | 0.71              |
| 22:x:51:U:H3      | 22:x:63:G:H1     | 1.38                     | 0.71              |
| 25:A:781:A:OP1    | 27:C:217:ARG:NH2 | 2.24                     | 0.71              |
| 58:v:601:G4P:H5'' | 58:v:601:G4P:C8  | 2.18                     | 0.71              |
| 24:v:98:ASP:C     | 24:v:100:TYR:N   | 2.49                     | 0.70              |
| 15:o:88:ARG:NH2   | 25:A:716:A:OP1   | 2.23                     | 0.70              |
| 1:a:1323:G:H2'    | 1:a:1324:A:C8    | 2.27                     | 0.70              |
| 10:j:41:PRO:HB3   | 10:j:72:ARG:HE   | 1.56                     | 0.70              |
| 1:a:1035:A:H1'    | 1:a:1036:A:H2    | 1.57                     | 0.70              |
| 1:a:150:U:H2'     | 1:a:151:A:H8     | 1.56                     | 0.70              |
| 46:X:4:ILE:HB     | 46:X:63:ILE:HG22 | 1.74                     | 0.70              |
| 47:Y:11:ARG:O     | 47:Y:14:ARG:NH1  | 2.25                     | 0.70              |
| 9:i:30:ILE:HG12   | 9:i:65:ILE:HD11  | 1.73                     | 0.70              |
| 22:x:76:A:O2'     | 25:A:2394:C:N3   | 2.25                     | 0.69              |
| 13:m:28:THR:HA    | 13:m:31:LYS:HE2  | 1.72                     | 0.69              |
| 33:J:90:SER:HB2   | 33:J:93:PRO:HG3  | 1.72                     | 0.69              |
| 43:U:11:ARG:NH2   | 43:U:99:ARG:O    | 2.26                     | 0.69              |
| 5:e:55:GLU:HG3    | 5:e:57:PRO:HD2   | 1.75                     | 0.69              |
| 25:A:976:G:HO2'   | 25:A:1155:A:HO2' | 1.38                     | 0.69              |
| 22:x:63:G:H2'     | 22:x:64:A:H8     | 1.56                     | 0.69              |
| 25:A:1798:U:OP2   | 27:C:271:ARG:NH2 | 2.26                     | 0.69              |
| 32:I:117:LEU:HB3  | 32:I:120:ALA:HA  | 1.75                     | 0.69              |
| 1:a:674:G:H2'     | 1:a:675:A:H8     | 1.57                     | 0.69              |
| 1:a:1356:G:H2'    | 1:a:1357:A:C8    | 2.28                     | 0.69              |
| 32:I:44:ALA:HB1   | 32:I:52:MET:HG2  | 1.75                     | 0.69              |
| 7:g:133:THR:O     | 7:g:137:LYS:NZ   | 2.26                     | 0.68              |
| 10:j:86:ALA:HA    | 10:j:89:ARG:HE   | 1.58                     | 0.68              |
| 25:A:1153:C:OP1   | 41:S:92:ARG:NH2  | 2.26                     | 0.68              |
| 25:A:1071:G:H22   | 25:A:1090:A:H62  | 1.41                     | 0.68              |
| 25:A:2483:C:N3    | 37:O:123:LYS:NZ  | 2.39                     | 0.68              |
| 2:b:43:LEU:HA     | 2:b:46:THR:HG22  | 1.75                     | 0.68              |
| 8:h:47:GLU:HG2    | 8:h:64:LYS:HB3   | 1.74                     | 0.68              |
| 25:A:1111:A:O2'   | 25:A:1112:G:OP1  | 2.12                     | 0.68              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 25:A:1918:A:O2'    | 25:A:1920:C:N4   | 2.27                     | 0.68              |
| 1:a:995:C:O2       | 14:n:4:GLN:NE2   | 2.27                     | 0.68              |
| 3:c:11:ARG:NH2     | 3:c:175:LEU:O    | 2.27                     | 0.68              |
| 13:m:33:ILE:HD12   | 13:m:59:GLU:HG3  | 1.75                     | 0.68              |
| 25:A:2498:OMC:HM22 | 25:A:2499:C:H5'  | 1.76                     | 0.68              |
| 22:x:15:G:N2       | 22:x:48:C:N4     | 2.42                     | 0.68              |
| 1:a:673:A:H2'      | 1:a:674:G:C8     | 2.29                     | 0.68              |
| 1:a:1223:C:H5''    | 1:a:1224:U:H5''  | 1.76                     | 0.68              |
| 5:e:36:LEU:HD22    | 5:e:134:ILE:HD13 | 1.76                     | 0.68              |
| 24:v:378:THR:HG21  | 24:v:387:PHE:H   | 1.58                     | 0.68              |
| 25:A:2107:G:O6     | 25:A:2183:A:N6   | 2.26                     | 0.68              |
| 56:8:14:CYS:HA     | 56:8:27:CYS:HB3  | 1.76                     | 0.68              |
| 12:l:25:GLU:OE2    | 12:l:59:ASN:ND2  | 2.27                     | 0.67              |
| 29:E:146:VAL:HG12  | 29:E:185:LYS:HB2 | 1.76                     | 0.67              |
| 9:i:123:ARG:NH1    | 9:i:124:ARG:O    | 2.27                     | 0.67              |
| 22:x:12:U:C4       | 22:x:23:A:C2     | 2.82                     | 0.67              |
| 25:A:1925:C:N4     | 25:A:1928:A:OP2  | 2.27                     | 0.67              |
| 34:L:125:TYR:OH    | 34:L:132:HIS:NE2 | 2.27                     | 0.67              |
| 1:a:544:G:OP1      | 4:d:56:ARG:NH2   | 2.27                     | 0.67              |
| 1:a:401:C:O2'      | 1:a:621:A:N3     | 2.27                     | 0.67              |
| 3:c:10:ILE:HG23    | 3:c:11:ARG:HG3   | 1.76                     | 0.67              |
| 22:x:51:U:O2       | 22:x:63:G:N2     | 2.27                     | 0.67              |
| 22:x:13:C:C2       | 22:x:22:G:N2     | 2.63                     | 0.67              |
| 1:a:1009:U:H3      | 1:a:1020:G:H1    | 1.42                     | 0.67              |
| 22:x:15:G:H22      | 22:x:48:C:N4     | 1.92                     | 0.67              |
| 25:A:2153:C:H2'    | 25:A:2154:A:H8   | 1.59                     | 0.67              |
| 27:C:6:CYS:SG      | 27:C:13:ARG:NH2  | 2.68                     | 0.67              |
| 29:E:1:MET:N       | 29:E:14:VAL:O    | 2.28                     | 0.67              |
| 1:a:1149:C:H2'     | 1:a:1150:A:H8    | 1.60                     | 0.67              |
| 25:A:2405:G:O2'    | 25:A:2411:A:N6   | 2.27                     | 0.67              |
| 25:A:1022:G:O6     | 34:L:68:LYS:NZ   | 2.25                     | 0.66              |
| 25:A:1059:G:OP1    | 33:J:10:LYS:NZ   | 2.25                     | 0.66              |
| 25:A:2512:C:O2'    | 28:D:159:LYS:NZ  | 2.29                     | 0.66              |
| 9:i:46:MET:SD      | 9:i:49:ARG:NH2   | 2.67                     | 0.66              |
| 24:v:78:PRO:HA     | 24:v:83:LEU:HA   | 1.77                     | 0.66              |
| 25:A:61:C:OP2      | 49:1:47:ARG:NH2  | 2.27                     | 0.66              |
| 39:Q:24:THR:HG22   | 39:Q:42:PRO:HD3  | 1.76                     | 0.66              |
| 25:A:2377:A:O2'    | 39:Q:117:PHE:O   | 2.13                     | 0.66              |
| 26:B:1:U:H2'       | 26:B:2:G:C8      | 2.31                     | 0.66              |
| 26:B:14:U:OP2      | 26:B:70:C:O2'    | 2.14                     | 0.66              |
| 1:a:1005:A:OP2     | 1:a:1024:G:N2    | 2.25                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:j:40:ILE:HD11  | 10:j:73:LEU:HD23  | 1.78                     | 0.66              |
| 24:v:450:VAL:HG23 | 24:v:461:ALA:HB3  | 1.78                     | 0.66              |
| 1:a:147:G:H2'     | 1:a:148:G:C8      | 2.30                     | 0.65              |
| 25:A:544:C:O2     | 25:A:549:G:N2     | 2.26                     | 0.65              |
| 37:O:24:THR:O     | 37:O:34:LYS:NZ    | 2.29                     | 0.65              |
| 32:I:38:MET:HA    | 32:I:41:LEU:HB3   | 1.78                     | 0.65              |
| 25:A:476:G:N1     | 25:A:479:A:OP2    | 2.27                     | 0.65              |
| 1:a:713:G:H2'     | 1:a:714:G:C8      | 2.32                     | 0.65              |
| 21:u:4:ILE:HG13   | 21:u:19:PHE:HA    | 1.79                     | 0.65              |
| 1:a:673:A:H2'     | 1:a:674:G:H8      | 1.62                     | 0.65              |
| 33:J:31:GLN:O     | 33:J:65:ARG:NH2   | 2.30                     | 0.65              |
| 1:a:458:U:H2'     | 1:a:459:A:H8      | 1.61                     | 0.65              |
| 24:v:96:SER:HB2   | 24:v:445:GLN:HE21 | 1.61                     | 0.65              |
| 58:v:601:G4P:H8   | 58:v:601:G4P:C5'  | 2.19                     | 0.65              |
| 25:A:1046:A:N6    | 32:I:4:ASN:OD1    | 2.30                     | 0.65              |
| 25:A:2723:C:OP1   | 28:D:114:LYS:NZ   | 2.30                     | 0.65              |
| 40:R:89:ARG:NH1   | 40:R:113:ARG:O    | 2.30                     | 0.65              |
| 44:V:3:ARG:NH1    | 44:V:5:GLU:OE2    | 2.30                     | 0.65              |
| 22:x:21:A:N6      | 22:x:46:G7M:O2'   | 2.30                     | 0.64              |
| 30:F:126:GLY:O    | 30:F:158:THR:OG1  | 2.16                     | 0.64              |
| 1:a:219:U:H2'     | 1:a:220:G:H8      | 1.61                     | 0.64              |
| 1:a:1106:G:O2'    | 3:c:169:ARG:NH2   | 2.30                     | 0.64              |
| 7:g:40:GLU:OE1    | 9:i:41:ARG:NH2    | 2.29                     | 0.64              |
| 31:G:95:ARG:NH2   | 31:G:128:GLN:OE1  | 2.30                     | 0.64              |
| 25:A:177:G:OP2    | 25:A:177:G:N2     | 2.26                     | 0.64              |
| 25:A:1907:G:O6    | 25:A:1923:U:O2    | 2.14                     | 0.64              |
| 24:v:403:LEU:HD13 | 24:v:412:LEU:HB2  | 1.79                     | 0.64              |
| 1:a:1323:G:H2'    | 1:a:1324:A:H8     | 1.63                     | 0.64              |
| 22:x:12:U:O4      | 22:x:23:A:N1      | 2.29                     | 0.64              |
| 24:v:446:PHE:O    | 24:v:449:VAL:HG12 | 1.97                     | 0.64              |
| 43:U:29:VAL:HB    | 43:U:55:ILE:HD11  | 1.79                     | 0.64              |
| 1:a:1143:G:H2'    | 1:a:1144:G:C8     | 2.33                     | 0.64              |
| 25:A:381:G:N7     | 60:A:3411:HOH:O   | 2.30                     | 0.64              |
| 25:A:1799:G:OP1   | 27:C:258:ARG:NH1  | 2.30                     | 0.64              |
| 27:C:270:ARG:HE   | 27:C:271:ARG:H    | 1.46                     | 0.64              |
| 4:d:187:GLU:OE2   | 4:d:189:SER:OG    | 2.15                     | 0.64              |
| 25:A:309:A:N3     | 25:A:329:G:O2'    | 2.31                     | 0.64              |
| 25:A:895:U:N3     | 25:A:897:C:N4     | 2.46                     | 0.64              |
| 1:a:1178:G:N7     | 9:i:99:ARG:NH1    | 2.40                     | 0.64              |
| 24:v:97:GLU:HB2   | 24:v:441:VAL:HG12 | 1.79                     | 0.64              |
| 25:A:2052:A:H4'   | 28:D:148:GLN:O    | 1.97                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:s:11:ILE:HG21  | 19:s:16:LEU:HD22  | 1.80                     | 0.64              |
| 25:A:463:G:N2     | 25:A:466:A:OP2    | 2.29                     | 0.64              |
| 1:a:212:G:H2'     | 1:a:213:G:H8      | 1.63                     | 0.63              |
| 24:v:158:VAL:HG23 | 24:v:162:LEU:HD12 | 1.78                     | 0.63              |
| 25:A:243:U:OP2    | 55:7:8:ARG:NH1    | 2.32                     | 0.63              |
| 38:P:86:ARG:NH1   | 38:P:117:ASP:OD1  | 2.27                     | 0.63              |
| 25:A:1754:A:N1    | 25:A:2716:C:O2'   | 2.31                     | 0.63              |
| 2:b:28:LYS:HA     | 2:b:28:LYS:HE3    | 1.79                     | 0.63              |
| 12:l:110:ARG:HB3  | 12:l:119:VAL:HG11 | 1.79                     | 0.63              |
| 1:a:424:G:H2'     | 1:a:425:G:C8      | 2.33                     | 0.63              |
| 1:a:464:U:N3      | 1:a:467:U:OP2     | 2.24                     | 0.63              |
| 33:J:92:LYS:HB2   | 33:J:95:LYS:HB2   | 1.80                     | 0.63              |
| 25:A:2312:U:O2    | 30:F:37:ASN:ND2   | 2.31                     | 0.63              |
| 1:a:1173:U:H2'    | 1:a:1174:G:H8     | 1.63                     | 0.63              |
| 1:a:1151:A:HO2'   | 1:a:1152:A:H8     | 1.47                     | 0.63              |
| 24:v:147:ASP:OD1  | 25:A:2657:A:H5''  | 1.99                     | 0.62              |
| 12:l:68:GLY:O     | 12:l:99:ARG:NH1   | 2.32                     | 0.62              |
| 25:A:631:A:OP2    | 55:7:23:LYS:NZ    | 2.32                     | 0.62              |
| 33:J:130:GLU:OE1  | 33:J:134:ARG:NH2  | 2.32                     | 0.62              |
| 19:s:10:PHE:HE2   | 19:s:37:ARG:HD2   | 1.63                     | 0.62              |
| 30:F:36:LEU:HB2   | 30:F:89:VAL:HG22  | 1.80                     | 0.62              |
| 1:a:1218:C:H2'    | 1:a:1219:A:C8     | 2.34                     | 0.62              |
| 1:a:1358:U:OP2    | 14:n:75:ARG:NH2   | 2.33                     | 0.62              |
| 24:v:168:PRO:HA   | 24:v:254:VAL:HG22 | 1.81                     | 0.62              |
| 1:a:28:A:O2'      | 1:a:296:U:OP1     | 2.17                     | 0.62              |
| 1:a:1191:A:OP2    | 3:c:2:GLY:N       | 2.33                     | 0.62              |
| 28:D:25:THR:OG1   | 28:D:191:GLY:O    | 2.18                     | 0.62              |
| 21:u:31:GLU:OE2   | 21:u:34:ARG:NH2   | 2.31                     | 0.62              |
| 25:A:2246:G:H2'   | 25:A:2247:A:H8    | 1.64                     | 0.62              |
| 3:c:108:LYS:HB3   | 3:c:111:LEU:HD23  | 1.82                     | 0.62              |
| 24:v:210:LEU:O    | 24:v:228:ARG:NH1  | 2.32                     | 0.62              |
| 25:A:729:G:H5''   | 25:A:730:A:H5''   | 1.81                     | 0.62              |
| 30:F:136:ILE:HG21 | 30:F:143:TYR:HD1  | 1.65                     | 0.62              |
| 5:e:97:GLN:HE21   | 5:e:124:LEU:HD12  | 1.65                     | 0.61              |
| 21:u:20:LYS:HA    | 21:u:20:LYS:HE3   | 1.82                     | 0.61              |
| 25:A:2313:C:O4'   | 30:F:37:ASN:ND2   | 2.33                     | 0.61              |
| 33:J:108:GLU:HG3  | 33:J:109:ILE:HG13 | 1.80                     | 0.61              |
| 31:G:137:ASP:HB3  | 31:G:140:VAL:HG12 | 1.82                     | 0.61              |
| 8:h:67:GLN:HE21   | 8:h:69:LYS:HB2    | 1.64                     | 0.61              |
| 22:x:60:U:OP1     | 22:x:61:C:N4      | 2.22                     | 0.61              |
| 25:A:1084:A:OP1   | 32:I:56:ARG:N     | 2.30                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:m:90:ARG:HB2   | 13:m:97:VAL:HG13  | 1.83                     | 0.61              |
| 1:a:517:G:N2      | 1:a:530:G:OP1     | 2.31                     | 0.61              |
| 1:a:1433:A:N7     | 60:a:3103:HOH:O   | 2.31                     | 0.61              |
| 25:A:276:U:O2'    | 25:A:277:G:O4'    | 2.18                     | 0.61              |
| 27:C:108:LYS:N    | 27:C:194:GLU:O    | 2.34                     | 0.61              |
| 25:A:1203:U:O2'   | 36:N:4:ASN:ND2    | 2.33                     | 0.61              |
| 5:e:111:MET:HE3   | 5:e:127:ALA:HB2   | 1.82                     | 0.61              |
| 14:n:27:LEU:O     | 14:n:31:ILE:HG13  | 2.01                     | 0.61              |
| 24:v:23:ASP:HA    | 58:v:601:G4P:O1B  | 1.99                     | 0.61              |
| 25:A:2116:G:O6    | 25:A:2171:A:N6    | 2.33                     | 0.61              |
| 44:V:25:GLU:HG3   | 44:V:26:LYS:HE2   | 1.82                     | 0.61              |
| 1:a:458:U:H2'     | 1:a:459:A:C8      | 2.35                     | 0.61              |
| 4:d:188:ARG:NH2   | 4:d:195:ILE:O     | 2.34                     | 0.61              |
| 13:m:19:LEU:HD12  | 13:m:22:ILE:HD13  | 1.83                     | 0.61              |
| 25:A:1311:G:OP2   | 25:A:1311:G:N2    | 2.30                     | 0.61              |
| 31:G:86:LYS:HE3   | 31:G:132:VAL:HG22 | 1.82                     | 0.61              |
| 25:A:1250:G:H5''  | 41:S:6:ARG:HD3    | 1.83                     | 0.60              |
| 24:v:32:LYS:NZ    | 24:v:198:GLY:O    | 2.29                     | 0.60              |
| 29:E:58:LYS:NZ    | 29:E:70:SER:O     | 2.34                     | 0.60              |
| 25:A:2115:G:H21   | 25:A:2117:A:H8    | 1.48                     | 0.60              |
| 24:v:360:TYR:HB3  | 24:v:361:PRO:HD2  | 1.82                     | 0.60              |
| 25:A:18:U:OP1     | 41:S:30:ARG:NH2   | 2.35                     | 0.60              |
| 25:A:534:U:O2'    | 41:S:49:ASP:OD2   | 2.14                     | 0.60              |
| 25:A:856:G:H2'    | 25:A:857:G:C8     | 2.35                     | 0.60              |
| 25:A:2286:G:H3'   | 53:5:30:LYS:HE3   | 1.84                     | 0.60              |
| 4:d:125:VAL:HG22  | 4:d:143:VAL:HG22  | 1.84                     | 0.60              |
| 25:A:2157:G:O2'   | 25:A:2158:A:O4'   | 2.20                     | 0.60              |
| 1:a:1035:A:O2'    | 1:a:1037:C:N4     | 2.34                     | 0.60              |
| 22:x:13:C:N3      | 22:x:22:G:N2      | 2.49                     | 0.60              |
| 28:D:10:GLY:HA3   | 40:R:5:ILE:HD11   | 1.82                     | 0.60              |
| 37:O:74:THR:HG21  | 37:O:86:LYS:HE3   | 1.83                     | 0.60              |
| 1:a:1160:G:H1     | 1:a:1176:A:N6     | 2.00                     | 0.59              |
| 24:v:300:VAL:HA   | 24:v:318:MET:HA   | 1.83                     | 0.59              |
| 25:A:848:C:H2'    | 25:A:849:A:H8     | 1.66                     | 0.59              |
| 25:A:2175:C:H2'   | 25:A:2176:A:C8    | 2.37                     | 0.59              |
| 35:M:76:VAL:HG22  | 40:R:73:VAL:HB    | 1.84                     | 0.59              |
| 2:b:86:SER:O      | 2:b:222:ARG:NH2   | 2.35                     | 0.59              |
| 24:v:319:ARG:HH12 | 24:v:362:GLY:HA2  | 1.66                     | 0.59              |
| 30:F:34:ILE:HD13  | 30:F:96:MET:HB2   | 1.84                     | 0.59              |
| 11:k:45:ALA:HB3   | 11:k:70:CYS:HB2   | 1.85                     | 0.59              |
| 25:A:307:G:N1     | 25:A:310:A:OP2    | 2.29                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:F:41:GLY:HA2  | 30:F:85:ILE:HB   | 1.84                     | 0.59              |
| 30:F:109:PRO:HG3 | 51:3:44:PHE:HE2  | 1.67                     | 0.59              |
| 52:4:46:ASP:O    | 52:4:53:LYS:NZ   | 2.35                     | 0.59              |
| 3:c:40:ARG:NH1   | 14:n:92:GLU:HG2  | 2.18                     | 0.59              |
| 17:q:17:MET:SD   | 17:q:20:SER:OG   | 2.60                     | 0.59              |
| 25:A:2139:U:O2   | 25:A:2152:G:O6   | 2.20                     | 0.59              |
| 25:A:2478:A:H5'  | 56:8:32:LYS:HE2  | 1.85                     | 0.59              |
| 30:F:69:LYS:HA   | 30:F:84:PRO:HA   | 1.84                     | 0.59              |
| 1:a:1071:C:H2'   | 1:a:1072:G:H8    | 1.68                     | 0.59              |
| 25:A:2473:U:O2'  | 25:A:2474:U:OP1  | 2.21                     | 0.59              |
| 1:a:1248:A:N7    | 1:a:1290:G:N1    | 2.50                     | 0.59              |
| 12:l:89:D2T:OD1  | 12:l:89:D2T:N    | 2.36                     | 0.59              |
| 25:A:1070:A:H61  | 33:J:11:LEU:HD22 | 1.65                     | 0.59              |
| 25:A:1071:G:H22  | 25:A:1090:A:N6   | 2.00                     | 0.59              |
| 1:a:405:U:O4     | 4:d:2:ALA:N      | 2.36                     | 0.59              |
| 1:a:1224:U:C2    | 1:a:1322:C:H5'   | 2.37                     | 0.59              |
| 24:v:28:THR:HG21 | 58:v:601:G4P:C8  | 2.32                     | 0.59              |
| 25:A:278:A:N6    | 25:A:362:A:N7    | 2.51                     | 0.59              |
| 25:A:2064:C:H2'  | 25:A:2065:C:H6   | 1.68                     | 0.59              |
| 31:G:27:LYS:HD3  | 31:G:32:GLU:HG3  | 1.85                     | 0.59              |
| 32:I:96:PHE:HE2  | 32:I:126:LEU:HB2 | 1.67                     | 0.59              |
| 3:c:154:SER:HB2  | 3:c:165:THR:HG22 | 1.85                     | 0.59              |
| 10:j:7:ARG:NH1   | 10:j:75:ASP:OD2  | 2.36                     | 0.59              |
| 17:q:9:GLN:HE22  | 17:q:58:VAL:HG12 | 1.68                     | 0.59              |
| 24:v:447:ASP:OD1 | 24:v:448:VAL:N   | 2.36                     | 0.59              |
| 1:a:1120:C:H2'   | 1:a:1121:U:H6    | 1.68                     | 0.59              |
| 1:a:1225:A:O4'   | 19:s:78:ARG:NH1  | 2.36                     | 0.59              |
| 10:j:57:VAL:HG12 | 10:j:58:ASN:N    | 2.12                     | 0.58              |
| 25:A:2313:C:H2'  | 25:A:2314:A:C8   | 2.36                     | 0.58              |
| 4:d:65:TYR:HD2   | 4:d:94:LEU:HD22  | 1.68                     | 0.58              |
| 19:s:44:MET:HA   | 19:s:47:LEU:HD12 | 1.84                     | 0.58              |
| 2:b:183:VAL:HG23 | 2:b:196:VAL:HG13 | 1.83                     | 0.58              |
| 25:A:1363:C:O2'  | 25:A:1809:A:N3   | 2.34                     | 0.58              |
| 25:A:2167:U:O2   | 25:A:2169:A:N6   | 2.36                     | 0.58              |
| 26:B:1:U:H2'     | 26:B:2:G:H8      | 1.68                     | 0.58              |
| 32:I:36:ASP:O    | 32:I:39:THR:OG1  | 2.21                     | 0.58              |
| 1:a:1022:A:H2'   | 1:a:1023:U:C6    | 2.39                     | 0.58              |
| 1:a:76:G:O6      | 1:a:77:A:N6      | 2.30                     | 0.58              |
| 1:a:1373:G:H5''  | 7:g:36:LYS:HE3   | 1.85                     | 0.58              |
| 11:k:36:ASP:OD1  | 11:k:37:ARG:N    | 2.33                     | 0.58              |
| 24:v:76:GLN:OE1  | 24:v:85:ASN:ND2  | 2.37                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:D:33:ARG:NH2   | 28:D:53:GLY:O      | 2.32                     | 0.58              |
| 1:a:166:U:H2'     | 1:a:167:A:H8       | 1.67                     | 0.58              |
| 1:a:606:G:N2      | 1:a:632:U:OP1      | 2.34                     | 0.58              |
| 1:a:1253:G:H2'    | 1:a:1254:A:H8      | 1.68                     | 0.58              |
| 3:c:56:VAL:HG23   | 3:c:69:HIS:HE1     | 1.69                     | 0.58              |
| 7:g:150:ALA:HB3   | 11:k:56:ARG:HH12   | 1.68                     | 0.58              |
| 25:A:1032:A:H1'   | 56:8:23:ILE:HD13   | 1.86                     | 0.58              |
| 4:d:50:ASP:OD1    | 4:d:51:TYR:N       | 2.36                     | 0.58              |
| 7:g:150:ALA:HB2   | 11:k:61:PHE:HB2    | 1.86                     | 0.58              |
| 24:v:431:ILE:HG13 | 24:v:494:ALA:HA    | 1.85                     | 0.58              |
| 50:2:10:THR:HG22  | 50:2:56:LYS:HE2    | 1.85                     | 0.58              |
| 24:v:28:THR:HG21  | 58:v:601:G4P:H8    | 1.86                     | 0.58              |
| 33:J:57:VAL:HA    | 33:J:71:THR:HA     | 1.86                     | 0.58              |
| 31:G:175:LYS:HE2  | 31:G:177:LYS:HD2   | 1.86                     | 0.58              |
| 1:a:1405:G:O2'    | 1:a:1518:MA6:O2'   | 2.19                     | 0.57              |
| 13:m:25:VAL:HG23  | 13:m:29:ARG:HB2    | 1.83                     | 0.57              |
| 24:v:392:ASN:OD1  | 24:v:527:ARG:NH2   | 2.37                     | 0.57              |
| 25:A:1837:C:O2'   | 25:A:1927:A:N3     | 2.32                     | 0.57              |
| 1:a:714:G:H2'     | 1:a:715:A:C8       | 2.39                     | 0.57              |
| 1:a:1368:A:OP1    | 10:j:64:GLN:NE2    | 2.34                     | 0.57              |
| 25:A:1107:G:H4'   | 32:I:80:THR:HA     | 1.85                     | 0.57              |
| 25:A:2175:C:N3    | 25:A:2176:A:N6     | 2.51                     | 0.57              |
| 1:a:427:U:O2'     | 1:a:541:G:OP1      | 2.21                     | 0.57              |
| 25:A:1141:U:H4'   | 25:A:1142:A:O4'    | 2.04                     | 0.57              |
| 1:a:166:U:H2'     | 1:a:167:A:C8       | 2.38                     | 0.57              |
| 1:a:921:U:O2      | 5:e:24:THR:OG1     | 2.22                     | 0.57              |
| 4:d:170:TRP:CD1   | 4:d:171:LEU:HG     | 2.39                     | 0.57              |
| 25:A:2292:U:H2'   | 25:A:2293:G:H8     | 1.69                     | 0.57              |
| 30:F:108:VAL:HG11 | 30:F:176:PRO:HG2   | 1.86                     | 0.57              |
| 2:b:167:ASP:O     | 2:b:170:HIS:ND1    | 2.33                     | 0.57              |
| 25:A:2246:G:H2'   | 25:A:2247:A:C8     | 2.40                     | 0.57              |
| 1:a:4:U:H2'       | 1:a:5:U:H5''       | 1.86                     | 0.57              |
| 1:a:269:C:H2'     | 1:a:270:A:H8       | 1.70                     | 0.57              |
| 6:f:19:PRO:O      | 6:f:22:ILE:HG12    | 2.04                     | 0.57              |
| 20:t:66:LEU:HD23  | 20:t:67:ILE:HG13   | 1.86                     | 0.57              |
| 25:A:1715:G:O2'   | 25:A:1743:G:O6     | 2.20                     | 0.57              |
| 25:A:2502:G:H5''  | 25:A:2503:2MA:H5'' | 1.84                     | 0.57              |
| 1:a:878:A:OP1     | 8:h:80:ARG:NH1     | 2.37                     | 0.57              |
| 1:a:1150:A:H4'    | 10:j:43:PRO:HG3    | 1.87                     | 0.57              |
| 14:n:87:ALA:HB1   | 14:n:92:GLU:HB2    | 1.86                     | 0.57              |
| 25:A:372:G:O2'    | 25:A:400:G:O6      | 2.18                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:2:A:N3        | 1:a:613:C:O2'     | 2.38                     | 0.57              |
| 24:v:496:ASP:OD1  | 24:v:500:ASN:N    | 2.37                     | 0.57              |
| 25:A:155:A:H2'    | 25:A:156:A:C8     | 2.40                     | 0.57              |
| 10:j:45:ARG:HB3   | 10:j:69:THR:HB    | 1.87                     | 0.57              |
| 25:A:593:U:H2'    | 25:A:594:U:C6     | 2.39                     | 0.57              |
| 6:f:11:HIS:CD2    | 6:f:12:PRO:HD2    | 2.40                     | 0.56              |
| 9:i:52:LEU:HB3    | 9:i:58:VAL:HG22   | 1.87                     | 0.56              |
| 24:v:287:ARG:HH12 | 24:v:289:VAL:HG22 | 1.70                     | 0.56              |
| 1:a:671:G:O3'     | 6:f:79:ARG:NH2    | 2.36                     | 0.56              |
| 5:e:61:GLN:O      | 5:e:65:GLU:HG2    | 2.05                     | 0.56              |
| 5:e:82:GLN:OE1    | 5:e:150:PRO:HD3   | 2.04                     | 0.56              |
| 8:h:112:THR:HG23  | 8:h:115:ALA:H     | 1.70                     | 0.56              |
| 22:x:10:G:H2'     | 22:x:11:C:C6      | 2.41                     | 0.56              |
| 25:A:1386:C:H2'   | 25:A:1387:A:H8    | 1.71                     | 0.56              |
| 2:b:20:THR:O      | 2:b:23:TRP:HD1    | 1.88                     | 0.56              |
| 25:A:306:U:H3     | 25:A:310:A:H62    | 1.54                     | 0.56              |
| 25:A:1084:A:H2'   | 25:A:1085:A:C8    | 2.41                     | 0.56              |
| 25:A:1250:G:N7    | 36:N:18:ARG:NH2   | 2.53                     | 0.56              |
| 25:A:2064:C:H2'   | 25:A:2065:C:C6    | 2.40                     | 0.56              |
| 30:F:58:ALA:HB1   | 51:3:7:PRO:HG3    | 1.86                     | 0.56              |
| 48:Z:62:LYS:NZ    | 48:Z:70:GLU:OE2   | 2.30                     | 0.56              |
| 1:a:35:G:H2'      | 1:a:36:C:C6       | 2.41                     | 0.56              |
| 3:c:34:ASP:OD2    | 14:n:65:ARG:NH1   | 2.38                     | 0.56              |
| 19:s:3:ARG:HH12   | 19:s:7:LYS:HD2    | 1.70                     | 0.56              |
| 33:J:81:LYS:HD2   | 33:J:87:LYS:HA    | 1.86                     | 0.56              |
| 1:a:1319:A:H8     | 1:a:1323:G:C5     | 2.24                     | 0.56              |
| 1:a:1516:2MG:N2   | 1:a:1519:MA6:OP2  | 2.38                     | 0.56              |
| 2:b:16:PHE:O      | 2:b:203:ASN:ND2   | 2.38                     | 0.56              |
| 4:d:95:GLU:HA     | 4:d:100:ASN:HD22  | 1.71                     | 0.56              |
| 25:A:2578:G:H21   | 28:D:130:GLN:HE21 | 1.53                     | 0.56              |
| 32:I:48:ALA:HB3   | 32:I:51:TYR:HE1   | 1.70                     | 0.56              |
| 1:a:56:U:H2'      | 1:a:57:G:H8       | 1.71                     | 0.56              |
| 3:c:40:ARG:HH12   | 14:n:92:GLU:HG2   | 1.69                     | 0.56              |
| 6:f:9:MET:HE1     | 18:r:65:LEU:HD12  | 1.87                     | 0.56              |
| 24:v:107:ASP:O    | 24:v:135:THR:OG1  | 2.23                     | 0.56              |
| 1:a:216:U:H2'     | 1:a:217:C:H6      | 1.71                     | 0.56              |
| 1:a:712:A:H2'     | 1:a:713:G:C8      | 2.40                     | 0.56              |
| 1:a:1060:U:H5''   | 10:j:53:ILE:HD12  | 1.86                     | 0.56              |
| 4:d:58:LYS:NZ     | 4:d:69:GLU:OE1    | 2.34                     | 0.56              |
| 25:A:981:A:OP2    | 25:A:982:C:N4     | 2.38                     | 0.56              |
| 15:o:78:TYR:OH    | 15:o:89:ARG:OXT   | 2.22                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:A:284:U:H3    | 25:A:356:G:H1     | 1.54                     | 0.56              |
| 25:A:2141:G:H2'  | 25:A:2142:A:C8    | 2.40                     | 0.56              |
| 29:E:46:GLN:O    | 29:E:88:ARG:NH1   | 2.38                     | 0.56              |
| 32:I:23:LEU:HD22 | 32:I:118:ILE:HD12 | 1.87                     | 0.56              |
| 35:M:42:THR:HG22 | 35:M:57:VAL:HG22  | 1.88                     | 0.56              |
| 4:d:59:GLN:OE1   | 4:d:62:ARG:NH2    | 2.39                     | 0.56              |
| 13:m:67:GLY:HA2  | 13:m:70:ARG:HE    | 1.71                     | 0.56              |
| 19:s:36:ARG:HH21 | 19:s:75:ALA:HB3   | 1.70                     | 0.56              |
| 25:A:2183:A:H2'  | 25:A:2184:A:C8    | 2.41                     | 0.56              |
| 1:a:718:A:H2     | 18:r:38:LYS:HG2   | 1.71                     | 0.55              |
| 9:i:106:ARG:NH1  | 9:i:107:ASP:O     | 2.38                     | 0.55              |
| 32:I:77:VAL:HG22 | 32:I:82:ILE:HD13  | 1.88                     | 0.55              |
| 34:L:23:LYS:NZ   | 34:L:142:ILE:OXT  | 2.39                     | 0.55              |
| 1:a:1012:A:OP2   | 19:s:17:LYS:NZ    | 2.37                     | 0.55              |
| 25:A:1266:G:O2'  | 25:A:2012:G:O6    | 2.24                     | 0.55              |
| 25:A:2788:C:O2'  | 25:A:2809:A:N3    | 2.37                     | 0.55              |
| 50:2:11:ARG:HB2  | 50:2:54:MET:HB2   | 1.88                     | 0.55              |
| 1:a:219:U:H2'    | 1:a:220:G:C8      | 2.42                     | 0.55              |
| 1:a:1310:G:OP1   | 13:m:79:ARG:NH2   | 2.40                     | 0.55              |
| 25:A:639:U:H2'   | 25:A:640:C:H6     | 1.71                     | 0.55              |
| 25:A:1263:U:OP1  | 52:4:13:ARG:NH1   | 2.40                     | 0.55              |
| 1:a:131:A:H2'    | 1:a:132:C:C6      | 2.42                     | 0.55              |
| 5:e:56:VAL:O     | 5:e:60:ILE:HG13   | 2.07                     | 0.55              |
| 25:A:2250:G:O2'  | 25:A:2496:C:OP1   | 2.24                     | 0.55              |
| 2:b:58:ASN:HB3   | 2:b:220:THR:OG1   | 2.06                     | 0.55              |
| 14:n:6:MET:HG3   | 14:n:63:ARG:NH1   | 2.22                     | 0.55              |
| 24:v:270:ASP:O   | 24:v:274:GLU:HG2  | 2.06                     | 0.55              |
| 25:A:263:G:O2'   | 25:A:429:A:N3     | 2.38                     | 0.55              |
| 1:a:674:G:H2'    | 1:a:675:A:C8      | 2.39                     | 0.55              |
| 20:t:17:ALA:O    | 20:t:21:ASN:ND2   | 2.39                     | 0.55              |
| 22:x:53:G:H3'    | 22:x:54:5MU:H73   | 1.88                     | 0.55              |
| 25:A:1105:U:H2'  | 25:A:1106:G:H8    | 1.71                     | 0.55              |
| 25:A:2031:A:N3   | 25:A:2455:G:O2'   | 2.35                     | 0.55              |
| 25:A:2149:U:H2'  | 25:A:2150:C:C6    | 2.42                     | 0.55              |
| 1:a:1412:C:H2'   | 1:a:1413:A:C8     | 2.42                     | 0.55              |
| 10:j:57:VAL:CG1  | 10:j:58:ASN:H     | 2.11                     | 0.55              |
| 22:x:13:C:N4     | 22:x:22:G:N1      | 2.55                     | 0.55              |
| 32:I:25:ALA:HA   | 32:I:115:GLY:HA2  | 1.89                     | 0.55              |
| 1:a:421:U:O2     | 3:c:127:ARG:NH2   | 2.40                     | 0.55              |
| 6:f:9:MET:HA     | 6:f:58:HIS:O      | 2.07                     | 0.55              |
| 25:A:645:C:H2'   | 25:A:647:G:C8     | 2.42                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:A:155:A:H2'    | 25:A:156:A:H8     | 1.71                     | 0.55              |
| 25:A:1064:C:N4    | 25:A:1070:A:OP1   | 2.39                     | 0.55              |
| 37:O:36:VAL:HG12  | 46:X:82:TYR:HB2   | 1.88                     | 0.55              |
| 1:a:429:U:OP1     | 4:d:13:ARG:NH1    | 2.40                     | 0.55              |
| 1:a:1125:U:OP1    | 10:j:37:ARG:NE    | 2.40                     | 0.55              |
| 25:A:1918:A:HO2'  | 25:A:1920:C:N4    | 2.05                     | 0.55              |
| 1:a:56:U:H2'      | 1:a:57:G:C8       | 2.42                     | 0.54              |
| 9:i:88:MET:HE1    | 9:i:95:ARG:HA     | 1.88                     | 0.54              |
| 24:v:109:CYS:SG   | 24:v:137:ILE:HG12 | 2.47                     | 0.54              |
| 25:A:1264:A:OP1   | 52:4:16:ARG:NH2   | 2.35                     | 0.54              |
| 26:B:39:A:C2      | 26:B:44:G:C2      | 2.95                     | 0.54              |
| 1:a:1450:U:O2'    | 1:a:1453:G:O6     | 2.21                     | 0.54              |
| 25:A:511:U:H4'    | 25:A:1235:G:H4'   | 1.89                     | 0.54              |
| 25:A:1108:U:H2'   | 25:A:1109:C:C6    | 2.42                     | 0.54              |
| 25:A:1771:C:H2'   | 25:A:1772:A:H8    | 1.72                     | 0.54              |
| 25:A:2155:U:H3'   | 25:A:2156:G:H8    | 1.71                     | 0.54              |
| 43:U:3:THR:HG21   | 43:U:58:ALA:HB2   | 1.90                     | 0.54              |
| 16:p:55:ASP:OD1   | 16:p:56:ARG:N     | 2.40                     | 0.54              |
| 19:s:36:ARG:NH2   | 19:s:75:ALA:O     | 2.41                     | 0.54              |
| 25:A:849:A:H2'    | 25:A:850:U:H6     | 1.73                     | 0.54              |
| 25:A:2291:U:H2'   | 25:A:2292:U:C6    | 2.43                     | 0.54              |
| 2:b:88:ASP:HB2    | 2:b:225:ARG:NH1   | 2.22                     | 0.54              |
| 35:M:71:ARG:NH1   | 35:M:106:GLU:OE2  | 2.41                     | 0.54              |
| 1:a:1163:A:H2'    | 1:a:1164:G:C8     | 2.43                     | 0.54              |
| 2:b:27:MET:HB2    | 2:b:30:PHE:HB2    | 1.89                     | 0.54              |
| 30:F:57:LEU:O     | 30:F:61:SER:OG    | 2.21                     | 0.54              |
| 30:F:102:ARG:HG3  | 30:F:106:ILE:HD11 | 1.89                     | 0.54              |
| 3:c:134:MET:HE2   | 3:c:153:VAL:HB    | 1.88                     | 0.54              |
| 8:h:89:LYS:HD2    | 8:h:120:GLY:HA2   | 1.89                     | 0.54              |
| 33:J:110:ALA:HB1  | 33:J:125:MET:HE2  | 1.90                     | 0.54              |
| 34:L:3:THR:HG21   | 41:S:61:TRP:HE1   | 1.73                     | 0.54              |
| 35:M:114:LYS:HE2  | 35:M:118:LEU:HD11 | 1.90                     | 0.54              |
| 37:O:97:GLN:OE1   | 37:O:97:GLN:N     | 2.41                     | 0.54              |
| 1:a:461:A:H2'     | 1:a:462:G:H8      | 1.73                     | 0.54              |
| 11:k:109:ASN:OD1  | 11:k:110:ILE:N    | 2.41                     | 0.54              |
| 24:v:331:LEU:HD12 | 24:v:379:PHE:HB3  | 1.89                     | 0.54              |
| 24:v:493:LEU:HD21 | 24:v:501:LEU:HD13 | 1.89                     | 0.54              |
| 33:J:19:ASN:O     | 33:J:21:SER:N     | 2.38                     | 0.54              |
| 1:a:929:G:O2'     | 1:a:930:C:OP1     | 2.24                     | 0.54              |
| 1:a:1004:A:H8     | 1:a:1024:G:H21    | 1.55                     | 0.54              |
| 25:A:2359:C:O2'   | 55:7:54:ASP:OD2   | 2.21                     | 0.54              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:a:297:G:N2     | 1:a:300:A:OP2      | 2.37                     | 0.54              |
| 25:A:2071:A:H2'  | 25:A:2072:C:C6     | 2.43                     | 0.54              |
| 25:A:2523:G:HO2' | 25:A:2764:A:HO2'   | 1.56                     | 0.54              |
| 52:4:31:ASP:OD1  | 52:4:32:LYS:N      | 2.39                     | 0.54              |
| 1:a:96:U:H2'     | 1:a:97:G:H8        | 1.73                     | 0.53              |
| 1:a:407:U:H2'    | 1:a:408:A:H8       | 1.74                     | 0.53              |
| 25:A:414:C:H2'   | 25:A:415:A:H8      | 1.73                     | 0.53              |
| 25:A:538:A:H4'   | 34:L:7:LYS:HG2     | 1.90                     | 0.53              |
| 25:A:959:A:HO2'  | 25:A:2457:PSU:HO2' | 1.52                     | 0.53              |
| 1:a:356:A:N3     | 1:a:368:U:O2'      | 2.31                     | 0.53              |
| 1:a:1384:C:H2'   | 1:a:1385:G:H8      | 1.71                     | 0.53              |
| 11:k:87:LYS:HG3  | 11:k:113:VAL:HG23  | 1.89                     | 0.53              |
| 25:A:2189:U:H2'  | 25:A:2190:G:C8     | 2.43                     | 0.53              |
| 25:A:2243:U:H2'  | 25:A:2244:U:C6     | 2.43                     | 0.53              |
| 49:1:38:GLN:H    | 49:1:38:GLN:CD     | 2.16                     | 0.53              |
| 1:a:17:U:H2'     | 1:a:18:C:C6        | 2.43                     | 0.53              |
| 1:a:1282:C:H2'   | 1:a:1283:U:C6      | 2.43                     | 0.53              |
| 24:v:333:GLN:NE2 | 24:v:377:ASP:OD2   | 2.42                     | 0.53              |
| 33:J:99:GLY:HA3  | 33:J:138:LEU:HD23  | 1.91                     | 0.53              |
| 48:Z:32:ASN:OD1  | 48:Z:34:HIS:NE2    | 2.41                     | 0.53              |
| 48:Z:65:ASP:OD1  | 48:Z:66:THR:N      | 2.41                     | 0.53              |
| 3:c:22:TRP:CH2   | 3:c:32:ASN:HB3     | 2.44                     | 0.53              |
| 4:d:144:SER:OG   | 4:d:145:ILE:N      | 2.41                     | 0.53              |
| 25:A:285:G:O6    | 25:A:355:U:O2      | 2.26                     | 0.53              |
| 25:A:1060:U:H3   | 25:A:1080:A:H2     | 1.56                     | 0.53              |
| 34:L:12:LYS:NZ   | 34:L:13:ARG:O      | 2.39                     | 0.53              |
| 1:a:21:G:H2'     | 1:a:22:G:C8        | 2.44                     | 0.53              |
| 1:a:131:A:H2'    | 1:a:132:C:H6       | 1.74                     | 0.53              |
| 1:a:821:G:H2'    | 1:a:822:U:C6       | 2.44                     | 0.53              |
| 1:a:1253:G:H2'   | 1:a:1254:A:C8      | 2.43                     | 0.53              |
| 8:h:74:SER:HB3   | 8:h:130:ALA:HB3    | 1.89                     | 0.53              |
| 22:x:63:G:H2'    | 22:x:64:A:C8       | 2.42                     | 0.53              |
| 24:v:305:ALA:HB1 | 24:v:307:MET:HE3   | 1.91                     | 0.53              |
| 25:A:2103:C:H2'  | 25:A:2104:C:C6     | 2.44                     | 0.53              |
| 31:G:98:VAL:HG12 | 31:G:103:ILE:HG12  | 1.89                     | 0.53              |
| 1:a:178:C:H2'    | 1:a:179:A:H8       | 1.73                     | 0.53              |
| 1:a:539:A:H2'    | 1:a:540:G:C8       | 2.43                     | 0.53              |
| 1:a:1216:A:H5''  | 14:n:5:SER:OG      | 2.08                     | 0.53              |
| 1:a:1219:A:H2'   | 1:a:1220:G:C8      | 2.44                     | 0.53              |
| 22:x:13:C:N3     | 22:x:22:G:C2       | 2.77                     | 0.53              |
| 24:v:79:TYR:CD2  | 24:v:80:HIS:HD2    | 2.27                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:A:1802:A:H2'   | 25:A:1803:A:C8    | 2.43                     | 0.53              |
| 1:a:421:U:OP2     | 1:a:422:C:N4      | 2.42                     | 0.53              |
| 1:a:652:U:O4      | 1:a:752:G:O2'     | 2.21                     | 0.53              |
| 9:i:18:ARG:HH21   | 9:i:20:PHE:HZ     | 1.57                     | 0.53              |
| 25:A:2364:C:OP1   | 47:Y:55:ARG:NH1   | 2.41                     | 0.53              |
| 1:a:1226:C:O2'    | 13:m:110:LYS:NZ   | 2.41                     | 0.53              |
| 1:a:1309:G:OP1    | 13:m:87:ARG:NH2   | 2.42                     | 0.53              |
| 8:h:104:VAL:HG12  | 8:h:125:ILE:HD13  | 1.90                     | 0.53              |
| 10:j:6:ILE:HB     | 10:j:76:ILE:HB    | 1.91                     | 0.53              |
| 26:B:114:C:H2'    | 26:B:115:A:H8     | 1.74                     | 0.53              |
| 33:J:106:LEU:HD22 | 33:J:130:GLU:HG2  | 1.89                     | 0.53              |
| 12:l:76:GLU:HG3   | 12:l:77:HIS:ND1   | 2.24                     | 0.52              |
| 25:A:2179:C:H2'   | 25:A:2180:U:H5''  | 1.90                     | 0.52              |
| 26:B:60:C:H2'     | 26:B:61:G:H8      | 1.74                     | 0.52              |
| 1:a:477:C:H2'     | 1:a:478:A:C8      | 2.45                     | 0.52              |
| 1:a:927:G:H21     | 1:a:1532:U:H5''   | 1.74                     | 0.52              |
| 7:g:141:VAL:HA    | 7:g:144:MET:HE2   | 1.92                     | 0.52              |
| 17:q:46:VAL:HG21  | 17:q:61:ILE:HG21  | 1.90                     | 0.52              |
| 25:A:1386:C:H2'   | 25:A:1387:A:C8    | 2.44                     | 0.52              |
| 1:a:1149:C:H2'    | 1:a:1150:A:C8     | 2.42                     | 0.52              |
| 3:c:138:VAL:HA    | 3:c:149:ILE:HD13  | 1.91                     | 0.52              |
| 31:G:84:THR:HG22  | 31:G:134:LYS:HG2  | 1.91                     | 0.52              |
| 1:a:231:U:H2'     | 1:a:232:G:H8      | 1.73                     | 0.52              |
| 4:d:60:LYS:O      | 4:d:64:ILE:HG12   | 2.09                     | 0.52              |
| 24:v:447:ASP:O    | 24:v:450:VAL:HG12 | 2.08                     | 0.52              |
| 25:A:172:A:H2'    | 25:A:173:A:H8     | 1.74                     | 0.52              |
| 32:I:24:SER:HB3   | 32:I:86:MET:HA    | 1.92                     | 0.52              |
| 1:a:1031:C:H4'    | 1:a:1032:G:C2     | 2.44                     | 0.52              |
| 1:a:1178:G:O6     | 9:i:99:ARG:NH2    | 2.28                     | 0.52              |
| 6:f:38:ARG:HB3    | 6:f:63:ASN:HD22   | 1.75                     | 0.52              |
| 15:o:11:ILE:O     | 15:o:15:PHE:HB3   | 2.08                     | 0.52              |
| 1:a:456:A:H2'     | 1:a:457:G:C8      | 2.45                     | 0.52              |
| 1:a:1241:G:H2'    | 1:a:1242:G:H8     | 1.73                     | 0.52              |
| 1:a:1513:A:H2'    | 1:a:1514:G:C8     | 2.44                     | 0.52              |
| 25:A:2128:G:H1'   | 25:A:2173:A:N3    | 2.24                     | 0.52              |
| 1:a:1513:A:H2'    | 1:a:1514:G:H8     | 1.74                     | 0.52              |
| 2:b:55:ALA:HA     | 2:b:58:ASN:ND2    | 2.25                     | 0.52              |
| 22:x:12:U:O4      | 22:x:23:A:C6      | 2.63                     | 0.52              |
| 24:v:319:ARG:NH1  | 24:v:362:GLY:HA2  | 2.24                     | 0.52              |
| 25:A:639:U:H2'    | 25:A:640:C:C6     | 2.44                     | 0.52              |
| 44:V:5:GLU:HG3    | 49:l:19:LEU:HD11  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:a:1125:U:O2'   | 1:a:1126:U:O5'    | 2.24                     | 0.52              |
| 1:a:1203:C:N3    | 1:a:1204:A:N6     | 2.57                     | 0.52              |
| 24:v:25:GLY:HA3  | 24:v:142:ASN:HD22 | 1.74                     | 0.52              |
| 33:J:58:VAL:O    | 33:J:69:PHE:HB2   | 2.10                     | 0.52              |
| 41:S:50:ARG:O    | 41:S:54:LYS:NZ    | 2.42                     | 0.52              |
| 24:v:139:THR:CG2 | 24:v:254:VAL:HG12 | 2.40                     | 0.52              |
| 25:A:189:G:OP2   | 48:Z:26:LYS:NZ    | 2.43                     | 0.52              |
| 30:F:134:GLU:OE1 | 30:F:136:ILE:HG12 | 2.09                     | 0.52              |
| 5:e:115:LEU:HD13 | 5:e:123:VAL:HG11  | 1.91                     | 0.52              |
| 6:f:43:GLY:HA2   | 6:f:58:HIS:CE1    | 2.45                     | 0.52              |
| 11:k:83:GLU:HG2  | 11:k:109:ASN:HB3  | 1.91                     | 0.52              |
| 18:r:29:LEU:HD13 | 18:r:59:ILE:HD13  | 1.91                     | 0.52              |
| 24:v:414:LYS:O   | 24:v:417:VAL:HG12 | 2.09                     | 0.52              |
| 31:G:164:TYR:HB2 | 31:G:167:GLU:HB2  | 1.92                     | 0.52              |
| 2:b:100:MET:HA   | 2:b:107:VAL:HG21  | 1.91                     | 0.51              |
| 4:d:57:GLU:HG3   | 4:d:199:LEU:HG    | 1.92                     | 0.51              |
| 13:m:39:ILE:HD12 | 13:m:43:VAL:HG11  | 1.92                     | 0.51              |
| 25:A:2595:G:N2   | 25:A:2598:A:OP2   | 2.37                     | 0.51              |
| 45:W:43:LYS:NZ   | 45:W:60:GLU:OE2   | 2.40                     | 0.51              |
| 1:a:994:A:H61    | 1:a:1047:G:H4'    | 1.73                     | 0.51              |
| 1:a:1342:C:H2'   | 1:a:1343:G:H8     | 1.75                     | 0.51              |
| 24:v:290:GLU:N   | 24:v:290:GLU:OE1  | 2.43                     | 0.51              |
| 25:A:2138:G:H2'  | 25:A:2139:U:C6    | 2.45                     | 0.51              |
| 1:a:958:A:N6     | 19:s:77:THR:O     | 2.43                     | 0.51              |
| 1:a:1278:G:N7    | 3:c:27:LYS:NZ     | 2.57                     | 0.51              |
| 3:c:134:MET:HE1  | 3:c:166:GLU:HG3   | 1.91                     | 0.51              |
| 25:A:191:A:H2'   | 25:A:192:C:C6     | 2.44                     | 0.51              |
| 25:A:700:G:O2'   | 25:A:1632:A:N3    | 2.40                     | 0.51              |
| 25:A:870:U:O2    | 25:A:907:G:O6     | 2.27                     | 0.51              |
| 25:A:2183:A:H2'  | 25:A:2184:A:H8    | 1.76                     | 0.51              |
| 25:A:2484:G:OP1  | 37:O:44:ARG:NH1   | 2.43                     | 0.51              |
| 33:J:107:GLN:HA  | 33:J:110:ALA:HB3  | 1.92                     | 0.51              |
| 55:7:31:HIS:ND1  | 55:7:32:ILE:HG13  | 2.25                     | 0.51              |
| 1:a:1356:G:H2'   | 1:a:1357:A:H8     | 1.73                     | 0.51              |
| 1:a:1405:G:HO2'  | 1:a:1518:MA6:HO2' | 1.50                     | 0.51              |
| 13:m:4:ILE:HD11  | 13:m:60:VAL:HB    | 1.93                     | 0.51              |
| 24:v:98:ASP:O    | 24:v:100:TYR:C    | 2.53                     | 0.51              |
| 25:A:2241:A:H2'  | 25:A:2242:G:C8    | 2.46                     | 0.51              |
| 1:a:208:U:H4'    | 1:a:209:U:H5      | 1.75                     | 0.51              |
| 1:a:1515:G:H2'   | 1:a:1516:2MG:C8   | 2.45                     | 0.51              |
| 7:g:49:THR:HG22  | 7:g:53:ARG:CZ     | 2.40                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:l:39:THR:HG22 | 12:l:51:LYS:HG3   | 1.93                     | 0.51              |
| 25:A:2141:G:H2'  | 25:A:2142:A:H8    | 1.74                     | 0.51              |
| 33:J:3:LYS:NZ    | 33:J:62:TYR:OH    | 2.42                     | 0.51              |
| 1:a:1313:U:H2'   | 1:a:1314:C:C6     | 2.46                     | 0.51              |
| 25:A:859:G:O2'   | 25:A:916:G:O6     | 2.26                     | 0.51              |
| 29:E:190:ALA:O   | 29:E:194:LYS:NZ   | 2.43                     | 0.51              |
| 43:U:4:ILE:HG13  | 43:U:106:VAL:HG22 | 1.91                     | 0.51              |
| 1:a:923:A:O2'    | 1:a:1399:C:OP2    | 2.29                     | 0.51              |
| 1:a:949:A:H2'    | 1:a:950:U:C6      | 2.46                     | 0.51              |
| 1:a:1073:U:O2'   | 2:b:103:ASN:OD1   | 2.21                     | 0.51              |
| 1:a:1314:C:H2'   | 1:a:1315:U:C6     | 2.46                     | 0.51              |
| 1:a:1314:C:H2'   | 1:a:1315:U:H6     | 1.76                     | 0.51              |
| 2:b:47:VAL:O     | 2:b:51:ASN:ND2    | 2.43                     | 0.51              |
| 13:m:4:ILE:HG13  | 13:m:57:ARG:HH11  | 1.76                     | 0.51              |
| 5:e:45:ARG:HA    | 5:e:72:ILE:O      | 2.11                     | 0.51              |
| 8:h:54:ASP:OD1   | 8:h:55:THR:N      | 2.41                     | 0.51              |
| 13:m:2:ALA:HA    | 13:m:9:ILE:HB     | 1.93                     | 0.51              |
| 25:A:1727:C:H2'  | 25:A:1728:C:O4'   | 2.11                     | 0.51              |
| 33:J:114:ALA:HB2 | 33:J:125:MET:HG2  | 1.93                     | 0.51              |
| 25:A:1073:A:H2'  | 25:A:1074:G:O4'   | 2.11                     | 0.51              |
| 25:A:1085:A:O2'  | 25:A:1086:A:O4'   | 2.25                     | 0.51              |
| 18:r:55:LEU:O    | 18:r:59:ILE:HG12  | 2.11                     | 0.51              |
| 24:v:409:GLN:O   | 24:v:412:LEU:HB3  | 2.11                     | 0.51              |
| 26:B:49:C:OP1    | 39:Q:102:ARG:HG2  | 2.11                     | 0.51              |
| 51:3:16:CYS:SG   | 51:3:17:SER:N     | 2.84                     | 0.51              |
| 1:a:1136:C:OP2   | 1:a:1137:C:N4     | 2.44                     | 0.50              |
| 1:a:1313:U:H2'   | 1:a:1314:C:H6     | 1.76                     | 0.50              |
| 4:d:188:ARG:NH1  | 4:d:192:SER:O     | 2.43                     | 0.50              |
| 25:A:1794:A:H2'  | 25:A:1795:C:C6    | 2.46                     | 0.50              |
| 25:A:2189:U:O2'  | 25:A:2190:G:OP1   | 2.22                     | 0.50              |
| 25:A:2812:G:H2'  | 25:A:2813:A:C8    | 2.46                     | 0.50              |
| 46:X:72:VAL:HB   | 46:X:91:PHE:HB3   | 1.93                     | 0.50              |
| 1:a:966:2MG:N2   | 22:x:34:G:H5'     | 2.26                     | 0.50              |
| 1:a:1004:A:H2'   | 1:a:1005:A:C4     | 2.46                     | 0.50              |
| 3:c:85:GLU:HA    | 3:c:88:ARG:HG2    | 1.93                     | 0.50              |
| 25:A:1009:A:N3   | 25:A:1153:C:O2'   | 2.44                     | 0.50              |
| 33:J:103:ARG:HA  | 33:J:106:LEU:HD23 | 1.93                     | 0.50              |
| 38:P:38:LEU:HB3  | 38:P:39:PRO:HD3   | 1.93                     | 0.50              |
| 1:a:1183:U:O2'   | 1:a:1185:G:OP2    | 2.29                     | 0.50              |
| 8:h:26:THR:OG1   | 8:h:58:GLU:OE2    | 2.26                     | 0.50              |
| 10:j:12:ALA:HB2  | 10:j:96:VAL:HG13  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:n:64:CYS:HB3  | 14:n:68:GLY:H     | 1.77                     | 0.50              |
| 24:v:287:ARG:NH1 | 24:v:289:VAL:HG22 | 2.26                     | 0.50              |
| 25:A:820:A:H4'   | 25:A:836:G:H22    | 1.76                     | 0.50              |
| 25:A:1138:G:H21  | 34:L:108:MET:HE2  | 1.77                     | 0.50              |
| 37:O:50:ARG:HD3  | 37:O:65:ILE:HD11  | 1.93                     | 0.50              |
| 1:a:408:A:O3'    | 4:d:23:SER:OG     | 2.27                     | 0.50              |
| 1:a:1157:A:N7    | 1:a:1180:A:N6     | 2.59                     | 0.50              |
| 1:a:1163:A:H2'   | 1:a:1164:G:H8     | 1.77                     | 0.50              |
| 7:g:78:ARG:NH1   | 7:g:79:ARG:O      | 2.45                     | 0.50              |
| 8:h:103:VAL:HG23 | 8:h:126:ILE:HB    | 1.94                     | 0.50              |
| 19:s:48:THR:HG22 | 19:s:61:PHE:HD1   | 1.77                     | 0.50              |
| 19:s:63:THR:H    | 19:s:66:MET:HE2   | 1.74                     | 0.50              |
| 24:v:211:ASN:HA  | 24:v:228:ARG:NH1  | 2.26                     | 0.50              |
| 32:I:42:ARG:HA   | 32:I:42:ARG:NE    | 2.26                     | 0.50              |
| 1:a:1065:U:H5''  | 1:a:1190:G:H22    | 1.77                     | 0.50              |
| 3:c:55:ILE:HG22  | 3:c:57:ILE:HD11   | 1.92                     | 0.50              |
| 10:j:18:ILE:HG13 | 10:j:70:HIS:HB2   | 1.94                     | 0.50              |
| 17:q:57:ASP:OD1  | 17:q:82:ALA:N     | 2.45                     | 0.50              |
| 17:q:64:CYS:SG   | 17:q:74:THR:OG1   | 2.59                     | 0.50              |
| 25:A:275:C:O2'   | 25:A:276:U:O4'    | 2.17                     | 0.50              |
| 25:A:361:G:H8    | 25:A:361:G:OP2    | 1.95                     | 0.50              |
| 1:a:1271:A:H2'   | 1:a:1272:G:C8     | 2.46                     | 0.50              |
| 4:d:116:GLN:HE21 | 4:d:154:ARG:HH12  | 1.60                     | 0.50              |
| 9:i:33:ARG:HH21  | 9:i:38:TYR:HA     | 1.75                     | 0.50              |
| 25:A:2153:C:H2'  | 25:A:2154:A:C8    | 2.44                     | 0.50              |
| 25:A:2216:G:H2'  | 25:A:2217:G:H8    | 1.76                     | 0.50              |
| 25:A:2328:A:H2'  | 25:A:2329:U:C6    | 2.47                     | 0.50              |
| 26:B:12:A:O2'    | 47:Y:74:PRO:O     | 2.30                     | 0.50              |
| 26:B:66:A:OP2    | 26:B:108:A:N6     | 2.45                     | 0.50              |
| 40:R:90:GLY:O    | 40:R:113:ARG:NH1  | 2.44                     | 0.50              |
| 43:U:108:SER:OG  | 43:U:110:ARG:OXT  | 2.28                     | 0.50              |
| 52:4:46:ASP:N    | 52:4:46:ASP:OD1   | 2.44                     | 0.50              |
| 1:a:456:A:H2'    | 1:a:457:G:H8      | 1.77                     | 0.50              |
| 1:a:950:U:H2'    | 1:a:951:G:C8      | 2.47                     | 0.50              |
| 1:a:337:G:H2'    | 1:a:338:A:H8      | 1.76                     | 0.50              |
| 1:a:505:G:H2'    | 1:a:506:G:H8      | 1.76                     | 0.50              |
| 9:i:36:GLU:HG3   | 9:i:45:ARG:HE     | 1.77                     | 0.50              |
| 15:o:39:LEU:HD12 | 15:o:59:MET:HE1   | 1.93                     | 0.50              |
| 25:A:414:C:H2'   | 25:A:415:A:C8     | 2.47                     | 0.50              |
| 25:A:1796:U:H2'  | 25:A:1797:G:H8    | 1.75                     | 0.50              |
| 25:A:1927:A:H2'  | 25:A:1928:A:C8    | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:A:2461:A:H2'   | 25:A:2462:C:C6    | 2.47                     | 0.50              |
| 34:L:73:VAL:HG12  | 34:L:88:THR:HG22  | 1.93                     | 0.50              |
| 1:a:685:G:H2'     | 1:a:686:U:C6      | 2.46                     | 0.50              |
| 1:a:1307:U:OP1    | 13:m:100:GLN:NE2  | 2.45                     | 0.50              |
| 2:b:135:LEU:O     | 2:b:139:ARG:HG3   | 2.12                     | 0.50              |
| 11:k:76:GLU:OE1   | 11:k:76:GLU:N     | 2.39                     | 0.50              |
| 25:A:1315:C:O2'   | 25:A:1392:A:N3    | 2.43                     | 0.50              |
| 25:A:1636:U:O2'   | 25:A:1760:C:O2    | 2.26                     | 0.50              |
| 1:a:662:U:H2'     | 1:a:663:A:C8      | 2.47                     | 0.49              |
| 1:a:1012:A:H2'    | 1:a:1013:G:C8     | 2.47                     | 0.49              |
| 25:A:30:G:H2'     | 25:A:31:C:C6      | 2.47                     | 0.49              |
| 28:D:46:ARG:NH1   | 28:D:85:ALA:O     | 2.45                     | 0.49              |
| 30:F:103:LEU:O    | 30:F:108:VAL:HG23 | 2.12                     | 0.49              |
| 1:a:634:C:H2'     | 1:a:635:A:H8      | 1.77                     | 0.49              |
| 1:a:950:U:H3'     | 13:m:101:ARG:HH22 | 1.78                     | 0.49              |
| 1:a:1141:C:H2'    | 1:a:1142:G:H8     | 1.76                     | 0.49              |
| 1:a:1309:G:OP1    | 13:m:91:HIS:NE2   | 2.32                     | 0.49              |
| 6:f:27:ALA:O      | 6:f:31:GLY:N      | 2.42                     | 0.49              |
| 22:x:9:A:H62      | 22:x:23:A:H62     | 1.59                     | 0.49              |
| 25:A:1447:C:O2'   | 25:A:1544:A:N3    | 2.39                     | 0.49              |
| 25:A:1682:G:H2'   | 25:A:1683:U:C6    | 2.47                     | 0.49              |
| 41:S:90:ILE:HA    | 42:T:11:GLN:HE22  | 1.76                     | 0.49              |
| 2:b:20:THR:HG23   | 2:b:39:HIS:HE1    | 1.77                     | 0.49              |
| 18:r:35:GLU:HG3   | 21:u:25:LYS:HE2   | 1.95                     | 0.49              |
| 19:s:60:VAL:HG21  | 19:s:74:PHE:HB3   | 1.92                     | 0.49              |
| 25:A:602:A:O2'    | 25:A:604:G:O2'    | 2.25                     | 0.49              |
| 30:F:119:ALA:O    | 30:F:167:ARG:NH2  | 2.45                     | 0.49              |
| 1:a:216:U:H2'     | 1:a:217:C:C6      | 2.46                     | 0.49              |
| 1:a:676:A:H2'     | 1:a:677:U:C6      | 2.47                     | 0.49              |
| 1:a:966:2MG:HM21  | 9:i:129:LYS:HE2   | 1.94                     | 0.49              |
| 1:a:1319:A:H2'    | 1:a:1323:G:N7     | 2.26                     | 0.49              |
| 25:A:993:G:H1'    | 42:T:91:GLN:HE21  | 1.76                     | 0.49              |
| 25:A:1672:A:C2    | 25:A:2582:G:H5'   | 2.47                     | 0.49              |
| 53:5:5:ILE:HG21   | 53:5:28:ARG:HH12  | 1.77                     | 0.49              |
| 1:a:1021:A:H2'    | 1:a:1022:A:C8     | 2.47                     | 0.49              |
| 15:o:64:ARG:NH2   | 15:o:89:ARG:OXT   | 2.35                     | 0.49              |
| 24:v:303:ILE:HG12 | 24:v:316:ALA:HB2  | 1.94                     | 0.49              |
| 24:v:475:GLU:O    | 24:v:521:VAL:HB   | 2.12                     | 0.49              |
| 25:A:24:G:O2'     | 43:U:78:GLU:O     | 2.29                     | 0.49              |
| 25:A:742:A:H2'    | 25:A:743:A:H8     | 1.76                     | 0.49              |
| 25:A:1992:G:N2    | 25:A:1996:C:O2'   | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:E:119:ILE:HD11 | 29:E:187:VAL:HG22 | 1.95                     | 0.49              |
| 30:F:136:ILE:HA   | 30:F:141:ILE:HG23 | 1.95                     | 0.49              |
| 43:U:73:LYS:HB2   | 43:U:106:VAL:HB   | 1.94                     | 0.49              |
| 1:a:978:A:H61     | 1:a:1316:G:H21    | 1.60                     | 0.49              |
| 1:a:1401:G:H2'    | 1:a:1402:4OC:O4'  | 2.12                     | 0.49              |
| 25:A:742:A:H2'    | 25:A:743:A:C8     | 2.48                     | 0.49              |
| 1:a:382:A:H2'     | 1:a:383:A:C8      | 2.48                     | 0.49              |
| 1:a:736:C:H2'     | 1:a:737:C:C6      | 2.48                     | 0.49              |
| 1:a:1166:G:N1     | 1:a:1169:A:OP2    | 2.46                     | 0.49              |
| 1:a:1238:A:P      | 1:a:1300:G:H22    | 2.36                     | 0.49              |
| 25:A:2281:A:O2'   | 25:A:2282:G:H5'   | 2.13                     | 0.49              |
| 27:C:30:PHE:HD2   | 27:C:33:LEU:HD12  | 1.77                     | 0.49              |
| 1:a:501:C:H2'     | 1:a:502:A:H8      | 1.77                     | 0.49              |
| 1:a:859:G:H2'     | 1:a:860:A:C8      | 2.48                     | 0.49              |
| 10:j:56:HIS:ND1   | 10:j:57:VAL:HG23  | 2.28                     | 0.49              |
| 11:k:64:GLN:HG2   | 11:k:99:ALA:HB2   | 1.94                     | 0.49              |
| 21:u:40:LYS:O     | 21:u:43:THR:OG1   | 2.25                     | 0.49              |
| 22:x:51:U:H2'     | 22:x:52:G:C8      | 2.47                     | 0.49              |
| 25:A:1106:G:C2    | 25:A:1107:G:C8    | 3.01                     | 0.49              |
| 27:C:67:PHE:CE1   | 27:C:156:ARG:HD2  | 2.48                     | 0.49              |
| 32:I:24:SER:HB2   | 32:I:116:GLU:HG2  | 1.95                     | 0.49              |
| 37:O:15:GLY:O     | 37:O:16:ARG:NH1   | 2.36                     | 0.49              |
| 1:a:553:A:H2'     | 1:a:554:A:C8      | 2.48                     | 0.49              |
| 1:a:676:A:H2'     | 1:a:677:U:H6      | 1.78                     | 0.49              |
| 14:n:27:LEU:HD13  | 14:n:30:ILE:HD11  | 1.94                     | 0.49              |
| 25:A:5:A:H2'      | 25:A:6:A:H8       | 1.78                     | 0.49              |
| 25:A:1093:G:N2    | 25:A:1098:A:H62   | 2.10                     | 0.49              |
| 25:A:2175:C:H2'   | 25:A:2176:A:H8    | 1.78                     | 0.49              |
| 30:F:108:VAL:O    | 30:F:111:ILE:HG12 | 2.13                     | 0.49              |
| 1:a:1435:G:H2'    | 1:a:1436:U:C6     | 2.48                     | 0.49              |
| 17:q:28:PHE:HE1   | 17:q:37:PHE:HB3   | 1.77                     | 0.49              |
| 25:A:191:A:H2'    | 25:A:192:C:H6     | 1.78                     | 0.49              |
| 25:A:1907:G:O6    | 25:A:1923:U:C2    | 2.65                     | 0.49              |
| 33:J:117:MET:SD   | 33:J:128:SER:OG   | 2.65                     | 0.49              |
| 39:Q:88:LYS:HG3   | 39:Q:88:LYS:O     | 2.13                     | 0.49              |
| 25:A:1710:G:H2'   | 25:A:1711:A:C8    | 2.49                     | 0.48              |
| 33:J:5:VAL:HA     | 33:J:8:TYR:CZ     | 2.48                     | 0.48              |
| 1:a:413:G:H4'     | 1:a:414:A:H5''    | 1.94                     | 0.48              |
| 2:b:48:PRO:HA     | 2:b:51:ASN:HD22   | 1.78                     | 0.48              |
| 2:b:96:TRP:HZ2    | 2:b:101:LEU:HD23  | 1.77                     | 0.48              |
| 3:c:52:VAL:HB     | 3:c:70:THR:HG22   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:x:33:U:H1'     | 22:x:37:MIA:H151  | 1.95                     | 0.48              |
| 25:A:1045:C:H1'   | 25:A:1047:G:N3    | 2.28                     | 0.48              |
| 38:P:30:ARG:NH2   | 38:P:74:GLU:OE2   | 2.46                     | 0.48              |
| 1:a:950:U:H2'     | 1:a:951:G:H8      | 1.78                     | 0.48              |
| 1:a:1127:G:H22    | 1:a:1147:C:H42    | 1.61                     | 0.48              |
| 3:c:40:ARG:NE     | 3:c:57:ILE:HD13   | 2.28                     | 0.48              |
| 13:m:70:ARG:NH2   | 30:F:144:ASP:HA   | 2.28                     | 0.48              |
| 24:v:189:GLU:OE2  | 24:v:191:TYR:OH   | 2.23                     | 0.48              |
| 25:A:279:A:N6     | 25:A:361:G:O2'    | 2.46                     | 0.48              |
| 25:A:2655:G:O2'   | 25:A:2664:G:O6    | 2.25                     | 0.48              |
| 30:F:142:ASP:OD1  | 30:F:143:TYR:N    | 2.46                     | 0.48              |
| 37:O:35:ALA:HA    | 37:O:128:THR:HG22 | 1.94                     | 0.48              |
| 1:a:718:A:C2      | 18:r:38:LYS:HG2   | 2.49                     | 0.48              |
| 1:a:1118:U:H2'    | 1:a:1119:C:H6     | 1.78                     | 0.48              |
| 2:b:97:LEU:O      | 2:b:100:MET:HG3   | 2.13                     | 0.48              |
| 4:d:11:LEU:O      | 4:d:15:GLU:HG2    | 2.13                     | 0.48              |
| 24:v:126:LEU:O    | 24:v:130:THR:HG23 | 2.14                     | 0.48              |
| 25:A:219:A:N3     | 25:A:234:U:O2'    | 2.31                     | 0.48              |
| 25:A:782:A:O2'    | 27:C:224:ALA:O    | 2.31                     | 0.48              |
| 25:A:2074:U:H2'   | 25:A:2075:U:C6    | 2.48                     | 0.48              |
| 25:A:2099:U:H2'   | 25:A:2100:G:C8    | 2.48                     | 0.48              |
| 25:A:2123:G:N2    | 25:A:2176:A:H61   | 2.07                     | 0.48              |
| 1:a:952:U:H5''    | 1:a:964:A:H61     | 1.78                     | 0.48              |
| 17:q:28:PHE:CE1   | 17:q:37:PHE:HB3   | 2.49                     | 0.48              |
| 25:A:1443:U:H2'   | 25:A:1444:G:H8    | 1.78                     | 0.48              |
| 25:A:2032:G:OP2   | 25:A:2454:G:O2'   | 2.26                     | 0.48              |
| 1:a:393:A:C2      | 1:a:394:G:C8      | 3.01                     | 0.48              |
| 10:j:84:VAL:HG12  | 10:j:88:MET:SD    | 2.53                     | 0.48              |
| 27:C:30:PHE:CE2   | 27:C:32:PRO:HD2   | 2.49                     | 0.48              |
| 43:U:48:LYS:O     | 43:U:52:GLU:HG3   | 2.12                     | 0.48              |
| 1:a:639:G:O6      | 1:a:640:A:N6      | 2.47                     | 0.48              |
| 1:a:972:C:OP2     | 10:j:59:LYS:NZ    | 2.40                     | 0.48              |
| 1:a:1342:C:H2'    | 1:a:1343:G:C8     | 2.48                     | 0.48              |
| 19:s:30:PRO:HA    | 19:s:48:THR:O     | 2.14                     | 0.48              |
| 25:A:1046:A:H4'   | 32:I:61:ARG:HB3   | 1.95                     | 0.48              |
| 25:A:2030:6MZ:N3  | 25:A:2499:C:H5''  | 2.28                     | 0.48              |
| 25:A:2812:G:H2'   | 25:A:2813:A:H8    | 1.78                     | 0.48              |
| 28:D:39:ASP:N     | 28:D:39:ASP:OD1   | 2.46                     | 0.48              |
| 1:a:324:G:N1      | 1:a:327:A:OP2     | 2.46                     | 0.48              |
| 1:a:1402:4OC:HM22 | 1:a:1403:C:H5'    | 1.96                     | 0.48              |
| 2:b:83:ALA:O      | 2:b:87:CYS:HB2    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:A:644:A:H2'    | 25:A:645:C:O4'    | 2.14                     | 0.48              |
| 25:A:849:A:H2'    | 25:A:850:U:C6     | 2.49                     | 0.48              |
| 39:Q:29:HIS:HA    | 39:Q:97:PHE:HE2   | 1.78                     | 0.48              |
| 1:a:126:G:OP1     | 1:a:605:U:O2'     | 2.26                     | 0.48              |
| 1:a:523:A:N6      | 12:l:89:D2T:OD1   | 2.46                     | 0.48              |
| 1:a:1287:A:H2'    | 1:a:1288:A:C8     | 2.48                     | 0.48              |
| 7:g:70:ARG:O      | 7:g:138:ARG:NH2   | 2.47                     | 0.48              |
| 22:x:13:C:C4      | 22:x:22:G:N1      | 2.82                     | 0.48              |
| 24:v:124:ARG:NH1  | 24:v:161:GLU:OE1  | 2.47                     | 0.48              |
| 24:v:138:LEU:HD23 | 24:v:253:PRO:HG2  | 1.95                     | 0.48              |
| 25:A:897:C:H2'    | 25:A:898:C:O4'    | 2.14                     | 0.48              |
| 25:A:1964:G:O2'   | 25:A:1967:C:OP2   | 2.25                     | 0.48              |
| 25:A:2191:A:O2'   | 25:A:2192:U:OP1   | 2.24                     | 0.48              |
| 33:J:49:ILE:HG13  | 33:J:50:GLU:N     | 2.29                     | 0.48              |
| 33:J:50:GLU:OE1   | 33:J:53:LEU:N     | 2.47                     | 0.48              |
| 1:a:185:U:H2'     | 1:a:186:C:H6      | 1.79                     | 0.48              |
| 14:n:7:LYS:HE2    | 14:n:68:GLY:HA3   | 1.96                     | 0.48              |
| 25:A:363:G:H2'    | 25:A:364:C:C6     | 2.48                     | 0.48              |
| 25:A:722:A:H2'    | 25:A:723:C:C6     | 2.49                     | 0.48              |
| 25:A:1138:G:N2    | 34:L:108:MET:HE2  | 2.29                     | 0.48              |
| 25:A:1551:A:H2'   | 25:A:1552:A:O4'   | 2.14                     | 0.48              |
| 25:A:2836:U:H2'   | 25:A:2837:A:C8    | 2.49                     | 0.48              |
| 29:E:164:LEU:HB2  | 29:E:167:VAL:HG22 | 1.95                     | 0.48              |
| 30:F:22:TYR:HD2   | 30:F:28:VAL:HG12  | 1.77                     | 0.48              |
| 1:a:180:U:H2'     | 1:a:181:A:H8      | 1.78                     | 0.47              |
| 1:a:558:G:OP2     | 1:a:559:A:O2'     | 2.31                     | 0.47              |
| 32:I:47:GLU:HG3   | 32:I:48:ALA:H     | 1.79                     | 0.47              |
| 32:I:99:PHE:HA    | 32:I:102:ALA:HB3  | 1.95                     | 0.47              |
| 1:a:542:G:OP1     | 4:d:10:LYS:NZ     | 2.28                     | 0.47              |
| 1:a:1118:U:OP1    | 9:i:106:ARG:NH2   | 2.40                     | 0.47              |
| 7:g:68:ASN:ND2    | 7:g:127:ALA:O     | 2.46                     | 0.47              |
| 24:v:184:HIS:ND1  | 24:v:187:LYS:HG2  | 2.29                     | 0.47              |
| 25:A:480:A:O2'    | 45:W:43:LYS:O     | 2.33                     | 0.47              |
| 25:A:1263:U:O2'   | 52:4:8:PRO:HD2    | 2.14                     | 0.47              |
| 25:A:2101:A:H2'   | 25:A:2102:G:C8    | 2.48                     | 0.47              |
| 1:a:736:C:H2'     | 1:a:737:C:H6      | 1.78                     | 0.47              |
| 1:a:960:U:O2      | 1:a:1225:A:N6     | 2.48                     | 0.47              |
| 1:a:1315:U:H2'    | 1:a:1316:G:O4'    | 2.14                     | 0.47              |
| 5:e:79:GLY:O      | 5:e:121:HIS:N     | 2.40                     | 0.47              |
| 7:g:40:GLU:HA     | 7:g:43:VAL:HG12   | 1.95                     | 0.47              |
| 22:x:47:U:N3      | 22:x:50:U:OP1     | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 25:A:419:U:H2'   | 25:A:420:C:C6    | 2.50                     | 0.47              |
| 25:A:1063:G:N7   | 33:J:90:SER:OG   | 2.34                     | 0.47              |
| 32:I:94:ARG:O    | 32:I:98:GLU:N    | 2.47                     | 0.47              |
| 1:a:113:G:H2'    | 1:a:114:U:C6     | 2.50                     | 0.47              |
| 1:a:255:G:H4'    | 17:q:19:LYS:HD2  | 1.95                     | 0.47              |
| 1:a:599:C:N4     | 1:a:640:A:H61    | 2.13                     | 0.47              |
| 1:a:723:U:H3     | 1:a:856:C:H5'    | 1.78                     | 0.47              |
| 1:a:1246:A:N6    | 1:a:1292:G:O6    | 2.48                     | 0.47              |
| 5:e:97:GLN:NE2   | 5:e:124:LEU:HD12 | 2.29                     | 0.47              |
| 25:A:729:G:OP1   | 27:C:13:ARG:HG2  | 2.15                     | 0.47              |
| 26:B:44:G:N2     | 26:B:48:U:C2     | 2.82                     | 0.47              |
| 44:V:64:LYS:HA   | 44:V:79:ASP:OD1  | 2.14                     | 0.47              |
| 55:7:14:PHE:C    | 55:7:15:LYS:HD3  | 2.40                     | 0.47              |
| 1:a:269:C:H2'    | 1:a:270:A:C8     | 2.48                     | 0.47              |
| 1:a:1244:G:H2'   | 1:a:1245:C:C6    | 2.49                     | 0.47              |
| 3:c:11:ARG:HE    | 3:c:178:LEU:HA   | 1.80                     | 0.47              |
| 3:c:86:LYS:O     | 3:c:89:LYS:HG2   | 2.15                     | 0.47              |
| 25:A:1278:C:OP1  | 38:P:36:THR:HG22 | 2.15                     | 0.47              |
| 1:a:482:A:H2'    | 1:a:483:C:O4'    | 2.15                     | 0.47              |
| 1:a:1515:G:H2'   | 1:a:1516:2MG:H8  | 1.79                     | 0.47              |
| 22:x:15:G:H21    | 22:x:20:U:H3     | 1.62                     | 0.47              |
| 25:A:171:U:H2'   | 25:A:172:A:H8    | 1.80                     | 0.47              |
| 25:A:373:U:H2'   | 25:A:374:A:H8    | 1.79                     | 0.47              |
| 25:A:1353:A:H2'  | 25:A:1354:A:C8   | 2.49                     | 0.47              |
| 25:A:2191:A:HO2' | 25:A:2192:U:P    | 2.37                     | 0.47              |
| 27:C:66:ASP:OD2  | 27:C:102:ARG:NH1 | 2.48                     | 0.47              |
| 30:F:38:MET:HE1  | 30:F:57:LEU:HD11 | 1.96                     | 0.47              |
| 1:a:635:A:H2'    | 1:a:636:U:H6     | 1.80                     | 0.47              |
| 1:a:1027:C:H2'   | 1:a:1028:C:C5    | 2.50                     | 0.47              |
| 1:a:1319:A:C8    | 1:a:1323:G:C8    | 3.03                     | 0.47              |
| 2:b:73:LYS:HZ3   | 2:b:168:HIS:HB2  | 1.80                     | 0.47              |
| 6:f:70:VAL:O     | 6:f:73:GLU:HG3   | 2.14                     | 0.47              |
| 7:g:72:THR:HA    | 7:g:96:ARG:HH12  | 1.79                     | 0.47              |
| 25:A:880:G:H3'   | 25:A:881:G:H8    | 1.80                     | 0.47              |
| 25:A:893:C:H2'   | 25:A:894:U:C6    | 2.50                     | 0.47              |
| 25:A:1771:C:H2'  | 25:A:1772:A:C8   | 2.49                     | 0.47              |
| 25:A:1797:G:O2'  | 27:C:257:THR:OG1 | 2.33                     | 0.47              |
| 25:A:2421:G:OP1  | 53:5:8:LYS:NZ    | 2.47                     | 0.47              |
| 25:A:2636:C:O2'  | 28:D:45:TYR:OH   | 2.29                     | 0.47              |
| 26:B:106:G:H2'   | 26:B:107:G:O4'   | 2.15                     | 0.47              |
| 33:J:42:PHE:O    | 33:J:46:THR:HG23 | 2.13                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 39:Q:94:ARG:HB3  | 39:Q:97:PHE:O     | 2.15                     | 0.47              |
| 1:a:1030:U:H5'   | 1:a:1031:C:C6     | 2.49                     | 0.47              |
| 1:a:1218:C:H2'   | 1:a:1219:A:H8     | 1.78                     | 0.47              |
| 1:a:1488:G:H2'   | 1:a:1489:G:C8     | 2.49                     | 0.47              |
| 10:j:59:LYS:HE2  | 10:j:62:ARG:HH21  | 1.80                     | 0.47              |
| 25:A:1353:A:H2'  | 25:A:1354:A:H8    | 1.79                     | 0.47              |
| 25:A:1668:A:N3   | 25:A:1670:C:N4    | 2.62                     | 0.47              |
| 25:A:2849:U:H4'  | 25:A:2868:A:C2    | 2.50                     | 0.47              |
| 26:B:115:A:H2'   | 26:B:116:G:H8     | 1.80                     | 0.47              |
| 27:C:262:ARG:O   | 27:C:265:LYS:NZ   | 2.48                     | 0.47              |
| 30:F:130:MET:HB2 | 30:F:154:ILE:HB   | 1.96                     | 0.47              |
| 31:G:47:ASP:N    | 31:G:47:ASP:OD1   | 2.47                     | 0.47              |
| 33:J:122:ILE:H   | 33:J:122:ILE:HD12 | 1.80                     | 0.47              |
| 38:P:24:MET:HE3  | 38:P:36:THR:HG21  | 1.95                     | 0.47              |
| 38:P:33:ILE:HD13 | 52:4:55:ILE:HD13  | 1.97                     | 0.47              |
| 38:P:72:ASP:HB3  | 38:P:75:ILE:HB    | 1.97                     | 0.47              |
| 25:A:1198:U:H2'  | 25:A:1199:U:H6    | 1.80                     | 0.47              |
| 25:A:1746:A:H2'  | 25:A:1747:U:C6    | 2.49                     | 0.47              |
| 25:A:2554:U:H2'  | 25:A:2555:U:C6    | 2.50                     | 0.47              |
| 1:a:459:A:H2'    | 1:a:460:A:H8      | 1.79                     | 0.47              |
| 1:a:1250:A:C4    | 1:a:1287:A:N6     | 2.83                     | 0.47              |
| 1:a:1298:U:OP2   | 7:g:114:LYS:NZ    | 2.43                     | 0.47              |
| 2:b:116:ASP:O    | 2:b:119:THR:OG1   | 2.31                     | 0.47              |
| 14:n:31:ILE:O    | 14:n:41:ARG:NH1   | 2.47                     | 0.47              |
| 24:v:25:GLY:HA3  | 24:v:142:ASN:ND2  | 2.30                     | 0.47              |
| 25:A:276:U:H2'   | 25:A:277:G:C8     | 2.50                     | 0.47              |
| 25:A:784:G:H5'   | 25:A:785:G:OP1    | 2.15                     | 0.47              |
| 25:A:2241:A:H2'  | 25:A:2242:G:H8    | 1.80                     | 0.47              |
| 25:A:2547:A:H2'  | 25:A:2548:U:C6    | 2.49                     | 0.47              |
| 25:A:2836:U:H2'  | 25:A:2837:A:H8    | 1.79                     | 0.47              |
| 2:b:87:CYS:SG    | 2:b:221:VAL:HG11  | 2.55                     | 0.46              |
| 20:t:25:ARG:O    | 20:t:29:ARG:HG3   | 2.14                     | 0.46              |
| 24:v:153:GLU:O   | 24:v:157:GLU:HG2  | 2.15                     | 0.46              |
| 25:A:645:C:H2'   | 25:A:647:G:N7     | 2.30                     | 0.46              |
| 25:A:894:U:H2'   | 25:A:895:U:O4'    | 2.14                     | 0.46              |
| 25:A:2145:C:H3'  | 25:A:2146:C:H5'   | 1.96                     | 0.46              |
| 26:B:60:C:H2'    | 26:B:61:G:C8      | 2.50                     | 0.46              |
| 28:D:56:LYS:HB2  | 28:D:59:ARG:HB2   | 1.97                     | 0.46              |
| 35:M:3:GLN:O     | 35:M:6:THR:OG1    | 2.21                     | 0.46              |
| 35:M:65:THR:HG22 | 35:M:67:LYS:H     | 1.79                     | 0.46              |
| 13:m:70:ARG:HH22 | 30:F:144:ASP:HA   | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:v:334:VAL:HG13 | 24:v:334:VAL:O    | 2.14                     | 0.46              |
| 25:A:673:C:OP1    | 29:E:49:ARG:NH1   | 2.41                     | 0.46              |
| 25:A:1584:U:H2'   | 25:A:1585:C:H5'   | 1.98                     | 0.46              |
| 25:A:2185:U:H2'   | 25:A:2186:G:O4'   | 2.16                     | 0.46              |
| 2:b:20:THR:O      | 2:b:22:TYR:N      | 2.49                     | 0.46              |
| 17:q:9:GLN:HE22   | 17:q:58:VAL:CG1   | 2.26                     | 0.46              |
| 24:v:21:HIS:HD2   | 24:v:122:ARG:HB2  | 1.80                     | 0.46              |
| 25:A:1506:U:H2'   | 25:A:1507:C:C6    | 2.50                     | 0.46              |
| 42:T:14:VAL:HG11  | 42:T:20:VAL:HG21  | 1.97                     | 0.46              |
| 46:X:30:ILE:HD13  | 46:X:70:ILE:HD11  | 1.98                     | 0.46              |
| 1:a:122:G:O6      | 1:a:239:U:O2      | 2.32                     | 0.46              |
| 1:a:705:G:C5      | 1:a:706:A:C8      | 3.03                     | 0.46              |
| 5:e:153:VAL:HA    | 5:e:156:LYS:HG2   | 1.97                     | 0.46              |
| 13:m:68:ASP:OD1   | 13:m:69:LEU:N     | 2.48                     | 0.46              |
| 20:t:36:TYR:CE1   | 20:t:79:LEU:HD21  | 2.50                     | 0.46              |
| 25:A:364:C:H2'    | 25:A:365:U:C6     | 2.51                     | 0.46              |
| 25:A:1476:U:H2'   | 25:A:1477:A:H8    | 1.80                     | 0.46              |
| 30:F:136:ILE:HD13 | 30:F:143:TYR:CD1  | 2.50                     | 0.46              |
| 1:a:161:A:H2'     | 1:a:162:A:C8      | 2.51                     | 0.46              |
| 1:a:918:A:H2'     | 1:a:919:A:C8      | 2.50                     | 0.46              |
| 1:a:1360:A:N6     | 14:n:58:SER:HB3   | 2.22                     | 0.46              |
| 3:c:172:ARG:HG2   | 3:c:174:PRO:HD3   | 1.98                     | 0.46              |
| 6:f:26:THR:HG23   | 6:f:36:ILE:HG13   | 1.97                     | 0.46              |
| 24:v:139:THR:HG21 | 24:v:254:VAL:HG12 | 1.97                     | 0.46              |
| 25:A:30:G:O2'     | 25:A:1214:A:N3    | 2.44                     | 0.46              |
| 25:A:1047:G:O2'   | 25:A:1111:A:N6    | 2.49                     | 0.46              |
| 25:A:1093:G:H2'   | 25:A:1098:A:H61   | 1.80                     | 0.46              |
| 25:A:2123:G:H21   | 25:A:2176:A:N6    | 2.05                     | 0.46              |
| 26:B:119:A:H2'    | 26:B:120:U:O4'    | 2.15                     | 0.46              |
| 30:F:37:ASN:OD1   | 30:F:38:MET:N     | 2.47                     | 0.46              |
| 7:g:93:PRO:O      | 7:g:97:ASN:ND2    | 2.49                     | 0.46              |
| 13:m:80:LEU:HD11  | 13:m:87:ARG:HE    | 1.81                     | 0.46              |
| 25:A:891:G:C2     | 25:A:892:A:C5     | 3.04                     | 0.46              |
| 25:A:1038:G:H2'   | 25:A:1039:A:C8    | 2.50                     | 0.46              |
| 25:A:1441:G:H2'   | 25:A:1442:U:C6    | 2.50                     | 0.46              |
| 25:A:2194:U:H2'   | 25:A:2195:U:C6    | 2.51                     | 0.46              |
| 30:F:38:MET:CE    | 30:F:57:LEU:HD11  | 2.45                     | 0.46              |
| 32:I:68:PRO:HA    | 32:I:72:LEU:HD11  | 1.97                     | 0.46              |
| 1:a:575:G:O2'     | 1:a:821:G:OP2     | 2.33                     | 0.46              |
| 1:a:1255:G:H2'    | 1:a:1258:G:H21    | 1.81                     | 0.46              |
| 3:c:88:ARG:HG3    | 3:c:89:LYS:N      | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:o:88:ARG:HH22  | 25:A:716:A:P      | 2.39                     | 0.46              |
| 28:D:11:MET:HG3   | 28:D:24:VAL:O     | 2.16                     | 0.46              |
| 33:J:56:PRO:HD3   | 33:J:75:PRO:HD3   | 1.96                     | 0.46              |
| 44:V:8:LEU:HD13   | 49:1:22:LEU:HB3   | 1.98                     | 0.46              |
| 1:a:144:G:H2'     | 1:a:145:G:H8      | 1.81                     | 0.46              |
| 1:a:188:C:H2'     | 1:a:189:A:N3      | 2.30                     | 0.46              |
| 1:a:459:A:H2'     | 1:a:460:A:C8      | 2.51                     | 0.46              |
| 1:a:635:A:H2'     | 1:a:636:U:C6      | 2.51                     | 0.46              |
| 1:a:1028:C:H3'    | 1:a:1028:C:OP2    | 2.15                     | 0.46              |
| 2:b:46:THR:OG1    | 2:b:201:PRO:HD2   | 2.15                     | 0.46              |
| 13:m:29:ARG:O     | 13:m:33:ILE:HG12  | 2.16                     | 0.46              |
| 22:x:34:G:O2'     | 22:x:35:A:OP1     | 2.29                     | 0.46              |
| 25:A:1570:A:H2'   | 25:A:1571:A:C8    | 2.50                     | 0.46              |
| 25:A:2216:G:H2'   | 25:A:2217:G:C8    | 2.49                     | 0.46              |
| 1:a:1518:MA6:H103 | 1:a:1519:MA6:H102 | 1.98                     | 0.46              |
| 9:i:116:VAL:HG23  | 10:j:62:ARG:HH11  | 1.81                     | 0.46              |
| 20:t:25:ARG:HG3   | 20:t:66:LEU:HD21  | 1.97                     | 0.46              |
| 20:t:44:LYS:HD3   | 20:t:86:LEU:HD12  | 1.97                     | 0.46              |
| 30:F:73:SER:HB2   | 30:F:81:GLN:H     | 1.81                     | 0.46              |
| 1:a:407:U:H2'     | 1:a:408:A:C8      | 2.50                     | 0.46              |
| 1:a:1064:G:H1'    | 1:a:1190:G:N2     | 2.30                     | 0.46              |
| 1:a:1095:U:P      | 1:a:1108:G:H1     | 2.39                     | 0.46              |
| 1:a:1351:U:H3     | 1:a:1371:G:H1     | 1.64                     | 0.46              |
| 11:k:29:ASN:HB2   | 11:k:57:LYS:NZ    | 2.30                     | 0.46              |
| 25:A:544:C:O3'    | 25:A:545:U:H2'    | 2.16                     | 0.46              |
| 25:A:2136:G:H22   | 25:A:2155:U:H3    | 1.64                     | 0.46              |
| 28:D:3:GLY:C      | 28:D:4:LEU:HD12   | 2.40                     | 0.46              |
| 1:a:384:G:H2'     | 1:a:385:C:C6      | 2.51                     | 0.45              |
| 3:c:57:ILE:HG13   | 3:c:66:VAL:HG12   | 1.97                     | 0.45              |
| 3:c:121:THR:O     | 3:c:125:GLU:HG2   | 2.15                     | 0.45              |
| 4:d:150:LYS:HB2   | 4:d:151:LYS:NZ    | 2.31                     | 0.45              |
| 6:f:40:GLU:OE2    | 6:f:61:LEU:HD23   | 2.15                     | 0.45              |
| 7:g:27:VAL:HG22   | 7:g:43:VAL:HG11   | 1.98                     | 0.45              |
| 9:i:42:GLU:O      | 9:i:46:MET:HG2    | 2.15                     | 0.45              |
| 24:v:90:PRO:O     | 24:v:99:THR:OG1   | 2.33                     | 0.45              |
| 24:v:437:ILE:HD11 | 24:v:504:ILE:HD13 | 1.98                     | 0.45              |
| 24:v:495:LEU:HD11 | 24:v:499:ASP:HA   | 1.97                     | 0.45              |
| 36:N:109:LYS:HG2  | 36:N:126:ARG:HB2  | 1.98                     | 0.45              |
| 40:R:14:LYS:HE2   | 40:R:77:HIS:HA    | 1.97                     | 0.45              |
| 1:a:187:G:N1      | 1:a:191:G:O6      | 2.49                     | 0.45              |
| 1:a:358:U:H2'     | 1:a:359:G:H8      | 1.81                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:a:721:G:H4'    | 1:a:722:G:O4'     | 2.16                     | 0.45              |
| 1:a:749:A:O2'    | 15:o:20:ASN:ND2   | 2.50                     | 0.45              |
| 25:A:458:G:O2'   | 25:A:469:G:O6     | 2.29                     | 0.45              |
| 26:B:43:C:O2     | 30:F:92:ARG:NE    | 2.32                     | 0.45              |
| 32:I:1:MET:HE3   | 32:I:2:ALA:H      | 1.82                     | 0.45              |
| 37:O:66:ARG:HD2  | 37:O:104:GLU:OE1  | 2.16                     | 0.45              |
| 38:P:103:ARG:HD2 | 38:P:106:ASP:OD1  | 2.15                     | 0.45              |
| 55:7:62:LEU:HB3  | 55:7:65:ALA:HB3   | 1.99                     | 0.45              |
| 1:a:1044:A:H2'   | 1:a:1045:C:H4'    | 1.99                     | 0.45              |
| 1:a:1319:A:C8    | 1:a:1323:G:C5     | 3.04                     | 0.45              |
| 1:a:1409:C:H2'   | 1:a:1410:A:H8     | 1.80                     | 0.45              |
| 2:b:50:PHE:O     | 2:b:54:LEU:HD23   | 2.17                     | 0.45              |
| 4:d:95:GLU:HA    | 4:d:100:ASN:ND2   | 2.30                     | 0.45              |
| 6:f:47:LEU:HD21  | 6:f:57:ALA:HB3    | 1.97                     | 0.45              |
| 25:A:1720:U:H2'  | 25:A:1721:G:O4'   | 2.15                     | 0.45              |
| 25:A:2345:G:N3   | 25:A:2381:A:H2'   | 2.31                     | 0.45              |
| 25:A:2745:C:H2'  | 25:A:2746:U:C6    | 2.51                     | 0.45              |
| 9:i:19:VAL:HA    | 9:i:65:ILE:HG22   | 1.98                     | 0.45              |
| 9:i:80:ARG:O     | 9:i:83:ILE:HG22   | 2.15                     | 0.45              |
| 14:n:64:CYS:HB3  | 14:n:68:GLY:N     | 2.31                     | 0.45              |
| 24:v:97:GLU:O    | 24:v:97:GLU:HG2   | 2.15                     | 0.45              |
| 24:v:299:PHE:HE1 | 24:v:390:ILE:HG12 | 1.81                     | 0.45              |
| 25:A:1046:A:H61  | 32:I:8:LYS:HE2    | 1.81                     | 0.45              |
| 31:G:24:ILE:HD11 | 31:G:43:VAL:HG21  | 1.98                     | 0.45              |
| 35:M:47:ILE:HG22 | 35:M:49:ARG:H     | 1.81                     | 0.45              |
| 1:a:381:C:H2'    | 1:a:382:A:O4'     | 2.15                     | 0.45              |
| 1:a:418:C:H2'    | 1:a:419:C:C6      | 2.51                     | 0.45              |
| 1:a:639:G:C6     | 1:a:640:A:N6      | 2.85                     | 0.45              |
| 2:b:138:THR:HA   | 2:b:141:LEU:HD23  | 1.98                     | 0.45              |
| 2:b:161:LEU:HB3  | 2:b:183:VAL:HG12  | 1.99                     | 0.45              |
| 4:d:55:LEU:HD11  | 4:d:59:GLN:HE21   | 1.81                     | 0.45              |
| 8:h:111:MET:HE2  | 8:h:116:ALA:HA    | 1.98                     | 0.45              |
| 25:A:30:G:H2'    | 25:A:31:C:H6      | 1.80                     | 0.45              |
| 25:A:1283:G:N2   | 25:A:1285:A:H3'   | 2.31                     | 0.45              |
| 1:a:933:G:O6     | 7:g:3:ARG:NH2     | 2.49                     | 0.45              |
| 1:a:1002:G:C2    | 1:a:1003:G:H1'    | 2.52                     | 0.45              |
| 1:a:1072:G:H2'   | 1:a:1073:U:C6     | 2.51                     | 0.45              |
| 4:d:54:GLN:HA    | 4:d:199:LEU:HD12  | 1.99                     | 0.45              |
| 7:g:111:ARG:O    | 7:g:119:ARG:NH2   | 2.50                     | 0.45              |
| 15:o:79:THR:HA   | 15:o:82:ILE:HG12  | 1.97                     | 0.45              |
| 20:t:32:ILE:HG12 | 20:t:54:MET:HE2   | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:t:35:VAL:HG22  | 20:t:50:ALA:HB1   | 1.96                     | 0.45              |
| 25:A:1079:C:H2'   | 25:A:1080:A:O4'   | 2.17                     | 0.45              |
| 25:A:2115:G:H21   | 25:A:2117:A:H3'   | 1.81                     | 0.45              |
| 25:A:2271:G:OP1   | 47:Y:18:ALA:HB1   | 2.17                     | 0.45              |
| 31:G:28:GLY:HA3   | 31:G:79:VAL:HB    | 1.98                     | 0.45              |
| 1:a:501:C:H2'     | 1:a:502:A:C8      | 2.51                     | 0.45              |
| 1:a:523:A:H61     | 12:l:89:D2T:CG    | 2.29                     | 0.45              |
| 2:b:59:LYS:HB3    | 2:b:63:ARG:HH12   | 1.81                     | 0.45              |
| 16:p:21:VAL:HG12  | 16:p:34:GLU:O     | 2.17                     | 0.45              |
| 24:v:260:LEU:HD21 | 25:A:2655:G:H5'   | 1.98                     | 0.45              |
| 25:A:1198:U:H2'   | 25:A:1199:U:C6    | 2.51                     | 0.45              |
| 25:A:2687:U:H2'   | 25:A:2688:G:O4'   | 2.17                     | 0.45              |
| 38:P:24:MET:CE    | 38:P:36:THR:HG21  | 2.47                     | 0.45              |
| 56:8:16:ILE:HD13  | 56:8:25:VAL:HG22  | 1.98                     | 0.45              |
| 1:a:945:G:H2'     | 1:a:945:G:N3      | 2.31                     | 0.45              |
| 20:t:19:LYS:HA    | 20:t:19:LYS:HD2   | 1.68                     | 0.45              |
| 25:A:753:A:H2'    | 25:A:754:U:H6     | 1.81                     | 0.45              |
| 25:A:1429:G:H2'   | 25:A:1430:G:H8    | 1.81                     | 0.45              |
| 25:A:2155:U:H3'   | 25:A:2156:G:C8    | 2.52                     | 0.45              |
| 25:A:2305:U:H5''  | 30:F:131:GLY:HA3  | 1.99                     | 0.45              |
| 27:C:171:TYR:HD1  | 27:C:183:LYS:HB3  | 1.82                     | 0.45              |
| 28:D:133:THR:HG22 | 28:D:134:HIS:N    | 2.27                     | 0.45              |
| 31:G:27:LYS:HG3   | 31:G:28:GLY:H     | 1.82                     | 0.45              |
| 51:3:18:CYS:SG    | 51:3:20:ASN:HB2   | 2.57                     | 0.45              |
| 1:a:539:A:H2'     | 1:a:540:G:H8      | 1.82                     | 0.45              |
| 1:a:696:A:N3      | 1:a:786:G:O2'     | 2.42                     | 0.45              |
| 1:a:1028:C:O2'    | 1:a:1029:U:O5'    | 2.26                     | 0.45              |
| 1:a:1162:C:H2'    | 1:a:1163:A:H8     | 1.81                     | 0.45              |
| 1:a:1175:G:H2'    | 1:a:1176:A:C8     | 2.43                     | 0.45              |
| 1:a:1271:A:H2'    | 1:a:1272:G:H8     | 1.81                     | 0.45              |
| 1:a:1317:C:OP1    | 14:n:24:ARG:NH2   | 2.50                     | 0.45              |
| 4:d:87:GLY:HA3    | 4:d:197:GLU:HG3   | 1.99                     | 0.45              |
| 5:e:153:VAL:HG23  | 5:e:156:LYS:HE3   | 1.99                     | 0.45              |
| 17:q:68:SER:OG    | 17:q:69:LYS:N     | 2.48                     | 0.45              |
| 24:v:324:LYS:HE3  | 24:v:360:TYR:HE1  | 1.82                     | 0.45              |
| 25:A:1224:U:H4'   | 42:T:88:GLY:O     | 2.16                     | 0.45              |
| 31:G:123:ALA:HB2  | 31:G:133:LEU:HD23 | 1.99                     | 0.45              |
| 39:Q:27:VAL:HA    | 39:Q:93:ASP:HB3   | 1.98                     | 0.45              |
| 1:a:868:C:H2'     | 1:a:869:G:O4'     | 2.17                     | 0.45              |
| 1:a:925:G:C2      | 1:a:927:G:C8      | 3.05                     | 0.45              |
| 1:a:1350:A:N7     | 9:i:120:LYS:NZ    | 2.66                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:1371:G:H2'    | 1:a:1372:U:C6     | 2.52                     | 0.45              |
| 3:c:60:PRO:HG3    | 3:c:65:ARG:CZ     | 2.47                     | 0.45              |
| 25:A:1179:G:H2'   | 25:A:1180:U:C6    | 2.52                     | 0.45              |
| 53:5:17:THR:HG21  | 53:5:43:VAL:HG13  | 1.99                     | 0.45              |
| 1:a:492:C:H2'     | 1:a:493:A:C8      | 2.52                     | 0.44              |
| 11:k:97:ILE:HG22  | 21:u:12:PHE:HZ    | 1.81                     | 0.44              |
| 25:A:1796:U:H2'   | 25:A:1797:G:C8    | 2.52                     | 0.44              |
| 54:6:22:MET:HE3   | 54:6:22:MET:HB3   | 1.86                     | 0.44              |
| 1:a:337:G:H2'     | 1:a:338:A:C8      | 2.52                     | 0.44              |
| 1:a:494:G:O2'     | 1:a:496:A:H1'     | 2.17                     | 0.44              |
| 13:m:107:ARG:HD2  | 13:m:113:ARG:HG3  | 2.00                     | 0.44              |
| 24:v:96:SER:O     | 24:v:445:GLN:NE2  | 2.50                     | 0.44              |
| 25:A:39:G:H2'     | 25:A:40:U:C6      | 2.53                     | 0.44              |
| 25:A:1047:G:H2'   | 25:A:1110:G:N1    | 2.32                     | 0.44              |
| 25:A:2136:G:H22   | 25:A:2156:G:H1'   | 1.82                     | 0.44              |
| 27:C:16:VAL:HG22  | 27:C:206:GLY:HA3  | 1.98                     | 0.44              |
| 32:I:42:ARG:NH1   | 33:J:120:ALA:HA   | 2.32                     | 0.44              |
| 1:a:19:A:H2'      | 1:a:20:U:C6       | 2.52                     | 0.44              |
| 1:a:270:A:H2'     | 1:a:271:C:C6      | 2.51                     | 0.44              |
| 1:a:425:G:H2'     | 1:a:426:U:C6      | 2.53                     | 0.44              |
| 1:a:1277:C:H1'    | 1:a:1282:C:C2     | 2.53                     | 0.44              |
| 1:a:1410:A:H2'    | 1:a:1411:C:C6     | 2.52                     | 0.44              |
| 4:d:25:VAL:HG23   | 4:d:26:ARG:HG3    | 1.99                     | 0.44              |
| 6:f:42:TRP:CE2    | 6:f:102:MET:HG3   | 2.52                     | 0.44              |
| 7:g:51:ALA:O      | 7:g:55:GLY:N      | 2.39                     | 0.44              |
| 10:j:65:TYR:HB3   | 14:n:96:LEU:HD11  | 2.00                     | 0.44              |
| 25:A:2449:H2U:H2' | 25:A:2449:H2U:H61 | 1.78                     | 0.44              |
| 30:F:144:ASP:OD1  | 30:F:145:LYS:N    | 2.51                     | 0.44              |
| 1:a:834:U:H2'     | 1:a:835:U:C6      | 2.52                     | 0.44              |
| 1:a:1014:A:H2     | 19:s:34:TRP:CE2   | 2.35                     | 0.44              |
| 1:a:1077:G:N1     | 1:a:1080:A:OP2    | 2.47                     | 0.44              |
| 1:a:1360:A:H2'    | 1:a:1360:A:N3     | 2.33                     | 0.44              |
| 15:o:80:GLN:O     | 15:o:83:GLU:HG2   | 2.17                     | 0.44              |
| 17:q:7:THR:OG1    | 17:q:60:GLU:OE2   | 2.25                     | 0.44              |
| 19:s:19:VAL:O     | 19:s:23:VAL:HG23  | 2.17                     | 0.44              |
| 25:A:863:A:H2'    | 25:A:864:G:C8     | 2.52                     | 0.44              |
| 25:A:1092:C:H2'   | 25:A:1093:G:O4'   | 2.17                     | 0.44              |
| 25:A:1182:G:H2'   | 25:A:1183:U:O4'   | 2.18                     | 0.44              |
| 25:A:1850:G:H2'   | 25:A:1851:U:C6    | 2.52                     | 0.44              |
| 25:A:1853:A:N3    | 25:A:2233:U:O2'   | 2.43                     | 0.44              |
| 25:A:2478:A:H1'   | 25:A:2528:U:O2'   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:F:114:PHE:HE2  | 51:3:44:PHE:HE1  | 1.66                     | 0.44              |
| 1:a:150:U:H2'     | 1:a:151:A:C8     | 2.46                     | 0.44              |
| 1:a:1298:U:H5     | 7:g:114:LYS:HZ3  | 1.64                     | 0.44              |
| 7:g:49:THR:HG22   | 7:g:53:ARG:NE    | 2.32                     | 0.44              |
| 30:F:152:LEU:HD23 | 30:F:153:ASP:N   | 2.33                     | 0.44              |
| 1:a:493:A:H2'     | 1:a:494:G:C8     | 2.53                     | 0.44              |
| 5:e:41:ASP:OD1    | 5:e:42:GLY:N     | 2.48                     | 0.44              |
| 11:k:60:PRO:HG3   | 11:k:91:PRO:HB2  | 1.99                     | 0.44              |
| 25:A:1597:A:H5''  | 25:A:1598:A:H5'  | 1.99                     | 0.44              |
| 25:A:2700:A:H2'   | 25:A:2701:U:C6   | 2.53                     | 0.44              |
| 26:B:5:U:H2'      | 26:B:6:G:H8      | 1.82                     | 0.44              |
| 1:a:1376:U:H2'    | 1:a:1377:A:C8    | 2.52                     | 0.44              |
| 6:f:18:VAL:O      | 6:f:21:MET:HG2   | 2.16                     | 0.44              |
| 7:g:134:ALA:HA    | 7:g:137:LYS:HG2  | 1.99                     | 0.44              |
| 11:k:13:ARG:HA    | 11:k:13:ARG:HD3  | 1.74                     | 0.44              |
| 25:A:5:A:H2'      | 25:A:6:A:C8      | 2.53                     | 0.44              |
| 25:A:65:U:H2'     | 25:A:66:C:H6     | 1.82                     | 0.44              |
| 25:A:1537:G:N1    | 25:A:1538:G:N3   | 2.66                     | 0.44              |
| 25:A:2292:U:H2'   | 25:A:2293:G:C8   | 2.52                     | 0.44              |
| 1:a:933:G:N7      | 7:g:3:ARG:NE     | 2.65                     | 0.44              |
| 3:c:150:LYS:HB2   | 3:c:169:ARG:HG3  | 1.99                     | 0.44              |
| 5:e:13:GLU:HB3    | 5:e:39:VAL:HG12  | 2.00                     | 0.44              |
| 16:p:44:SER:N     | 16:p:47:GLU:OE2  | 2.46                     | 0.44              |
| 25:A:871:U:H2'    | 25:A:872:U:C6    | 2.52                     | 0.44              |
| 25:A:891:G:H2'    | 25:A:892:A:H8    | 1.81                     | 0.44              |
| 25:A:947:A:H2'    | 25:A:948:C:C6    | 2.53                     | 0.44              |
| 25:A:1069:A:O2'   | 25:A:1072:C:OP1  | 2.22                     | 0.44              |
| 27:C:107:PRO:HG2  | 27:C:110:LEU:HB2 | 2.00                     | 0.44              |
| 30:F:70:ALA:N     | 30:F:83:TYR:O    | 2.48                     | 0.44              |
| 32:I:1:MET:HB3    | 32:I:2:ALA:H     | 1.51                     | 0.44              |
| 39:Q:18:LEU:HD13  | 39:Q:25:ARG:HG2  | 2.00                     | 0.44              |
| 1:a:303:A:H2'     | 1:a:304:U:O4'    | 2.18                     | 0.44              |
| 1:a:1034:G:H2'    | 1:a:1034:G:N3    | 2.33                     | 0.44              |
| 1:a:1207:2MG:H2'  | 1:a:1208:C:C6    | 2.53                     | 0.44              |
| 1:a:1251:A:H2'    | 1:a:1252:A:C8    | 2.53                     | 0.44              |
| 1:a:1313:U:OP1    | 19:s:5:LEU:HB3   | 2.18                     | 0.44              |
| 1:a:1495:U:O2'    | 25:A:1919:A:N1   | 2.42                     | 0.44              |
| 18:r:30:LYS:HE2   | 18:r:68:LEU:HD21 | 2.00                     | 0.44              |
| 20:t:35:VAL:O     | 20:t:39:ILE:HG13 | 2.18                     | 0.44              |
| 25:A:2130:U:H2'   | 25:A:2131:U:H5'' | 2.00                     | 0.44              |
| 25:A:2154:A:H2'   | 25:A:2155:U:C6   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:A:2589:A:H2'   | 25:A:2590:A:H8    | 1.83                     | 0.44              |
| 27:C:3:VAL:HG22   | 27:C:19:VAL:HG22  | 2.00                     | 0.44              |
| 27:C:145:GLU:HB2  | 27:C:188:CYS:HB3  | 2.00                     | 0.44              |
| 1:a:335:C:H2'     | 1:a:336:A:H8      | 1.82                     | 0.43              |
| 1:a:929:G:O6      | 1:a:1389:C:N4     | 2.51                     | 0.43              |
| 1:a:1530:G:H2'    | 1:a:1531:A:C8     | 2.52                     | 0.43              |
| 2:b:37:LYS:O      | 2:b:37:LYS:HD3    | 2.18                     | 0.43              |
| 4:d:171:LEU:HD23  | 4:d:182:PHE:HA    | 2.00                     | 0.43              |
| 6:f:61:LEU:HD12   | 6:f:62:MET:H      | 1.82                     | 0.43              |
| 7:g:66:LEU:HD22   | 7:g:100:ALA:HB1   | 1.99                     | 0.43              |
| 14:n:64:CYS:HB2   | 14:n:80:SER:OG    | 2.18                     | 0.43              |
| 25:A:863:A:H2'    | 25:A:864:G:H8     | 1.83                     | 0.43              |
| 25:A:1857:G:N2    | 25:A:1884:G:O2'   | 2.43                     | 0.43              |
| 25:A:2170:A:H2'   | 25:A:2171:A:O4'   | 2.18                     | 0.43              |
| 25:A:2514:U:H2'   | 25:A:2515:C:C6    | 2.53                     | 0.43              |
| 1:a:144:G:C6      | 1:a:179:A:C6      | 3.06                     | 0.43              |
| 1:a:944:G:N1      | 1:a:1338:G:OP2    | 2.45                     | 0.43              |
| 9:i:47:VAL:HA     | 9:i:50:GLN:OE1    | 2.17                     | 0.43              |
| 11:k:116:ILE:HD13 | 11:k:116:ILE:HA   | 1.90                     | 0.43              |
| 24:v:7:LEU:HA     | 24:v:10:VAL:HG12  | 1.99                     | 0.43              |
| 24:v:14:ARG:HG2   | 24:v:276:ALA:HB3  | 2.00                     | 0.43              |
| 24:v:155:LEU:HD21 | 24:v:168:PRO:HG3  | 2.00                     | 0.43              |
| 25:A:956:G:H2'    | 25:A:957:C:H2'    | 2.00                     | 0.43              |
| 25:A:1223:G:OP1   | 42:T:68:ARG:NH1   | 2.51                     | 0.43              |
| 30:F:134:GLU:CD   | 30:F:136:ILE:HG12 | 2.43                     | 0.43              |
| 30:F:162:SER:OG   | 30:F:163:ASP:N    | 2.49                     | 0.43              |
| 34:L:9:GLU:OE1    | 34:L:9:GLU:N      | 2.51                     | 0.43              |
| 1:a:538:G:H2'     | 1:a:539:A:H8      | 1.83                     | 0.43              |
| 1:a:674:G:H21     | 11:k:118:HIS:HB2  | 1.83                     | 0.43              |
| 13:m:70:ARG:HD2   | 13:m:71:ARG:N     | 2.32                     | 0.43              |
| 22:x:41:C:H2'     | 22:x:42:C:C6      | 2.53                     | 0.43              |
| 24:v:334:VAL:HG21 | 24:v:384:MET:HG2  | 2.00                     | 0.43              |
| 24:v:349:MET:HB3  | 24:v:356:VAL:HA   | 2.00                     | 0.43              |
| 25:A:1063:G:N2    | 33:J:136:MET:SD   | 2.91                     | 0.43              |
| 25:A:1434:A:H2'   | 25:A:1435:G:H8    | 1.83                     | 0.43              |
| 1:a:704:A:C5      | 1:a:705:G:C8      | 3.06                     | 0.43              |
| 1:a:978:A:N6      | 1:a:1318:A:N7     | 2.66                     | 0.43              |
| 1:a:1120:C:H2'    | 1:a:1121:U:C6     | 2.51                     | 0.43              |
| 1:a:1219:A:H2'    | 1:a:1220:G:H8     | 1.81                     | 0.43              |
| 1:a:1357:A:N6     | 1:a:1365:G:N1     | 2.36                     | 0.43              |
| 9:i:43:THR:O      | 9:i:47:VAL:HG23   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:t:8:LYS:O      | 20:t:12:ILE:HG12  | 2.18                     | 0.43              |
| 24:v:173:ILE:HD11 | 24:v:227:LEU:HD13 | 2.00                     | 0.43              |
| 24:v:476:CYS:HB3  | 24:v:482:PHE:HD1  | 1.83                     | 0.43              |
| 25:A:84:A:N1      | 25:A:98:G:O2'     | 2.45                     | 0.43              |
| 25:A:277:G:N3     | 25:A:278:A:N6     | 2.66                     | 0.43              |
| 25:A:1031:G:O2'   | 25:A:1032:A:OP1   | 2.31                     | 0.43              |
| 25:A:1064:C:N4    | 25:A:1065:U:O4    | 2.51                     | 0.43              |
| 25:A:1068:G:H21   | 25:A:1095:A:H4'   | 1.82                     | 0.43              |
| 25:A:1907:G:C6    | 25:A:1923:U:O2    | 2.71                     | 0.43              |
| 25:A:2152:G:H2'   | 25:A:2153:C:O4'   | 2.18                     | 0.43              |
| 29:E:18:THR:HG23  | 29:E:200:LEU:HD12 | 1.99                     | 0.43              |
| 39:Q:76:LYS:HE3   | 39:Q:76:LYS:HB3   | 1.83                     | 0.43              |
| 1:a:91:U:H2'      | 1:a:92:U:C2       | 2.54                     | 0.43              |
| 1:a:1012:A:N6     | 1:a:1018:G:O6     | 2.52                     | 0.43              |
| 1:a:1130:A:N6     | 1:a:1144:G:H21    | 2.17                     | 0.43              |
| 13:m:64:VAL:HG13  | 13:m:68:ASP:OD2   | 2.18                     | 0.43              |
| 17:q:76:VAL:HG12  | 17:q:77:ARG:HG2   | 2.00                     | 0.43              |
| 22:x:23:A:H8      | 22:x:23:A:O5'     | 2.01                     | 0.43              |
| 24:v:454:LYS:HE2  | 24:v:460:GLU:OE1  | 2.18                     | 0.43              |
| 24:v:508:MET:C    | 24:v:512:ARG:HH21 | 2.26                     | 0.43              |
| 25:A:299:A:N3     | 25:A:319:G:O2'    | 2.44                     | 0.43              |
| 25:A:636:G:N7     | 36:N:109:LYS:HE2  | 2.33                     | 0.43              |
| 25:A:811:U:H2'    | 36:N:21:ARG:HA    | 2.00                     | 0.43              |
| 25:A:1031:G:HO2'  | 25:A:1032:A:P     | 2.40                     | 0.43              |
| 25:A:1914:C:H2'   | 25:A:1915:3TD:H6  | 2.00                     | 0.43              |
| 1:a:553:A:H2'     | 1:a:554:A:H8      | 1.83                     | 0.43              |
| 1:a:565:U:OP2     | 1:a:566:G:O2'     | 2.26                     | 0.43              |
| 1:a:946:A:O2'     | 1:a:1333:A:N3     | 2.48                     | 0.43              |
| 1:a:1315:U:O2     | 1:a:1360:A:H2     | 2.02                     | 0.43              |
| 11:k:52:PHE:HD2   | 11:k:56:ARG:HG3   | 1.84                     | 0.43              |
| 13:m:3:ARG:HH22   | 13:m:7:ILE:N      | 2.17                     | 0.43              |
| 25:A:271:G:H1'    | 25:A:272:A:C8     | 2.54                     | 0.43              |
| 25:A:651:G:H5'    | 55:7:19:LYS:HG3   | 2.01                     | 0.43              |
| 25:A:1682:G:H2'   | 25:A:1683:U:H6    | 1.83                     | 0.43              |
| 25:A:2051:A:H8    | 25:A:2051:A:OP2   | 2.01                     | 0.43              |
| 25:A:2579:C:O2'   | 28:D:136:ASN:ND2  | 2.52                     | 0.43              |
| 26:B:114:C:H2'    | 26:B:115:A:C8     | 2.52                     | 0.43              |
| 27:C:132:MET:HE2  | 27:C:188:CYS:HB2  | 2.00                     | 0.43              |
| 29:E:188:MET:HE1  | 29:E:196:VAL:HG21 | 2.00                     | 0.43              |
| 30:F:64:LYS:HG3   | 30:F:65:PRO:HD2   | 2.01                     | 0.43              |
| 32:I:8:LYS:O      | 32:I:11:ILE:HG22  | 2.19                     | 0.43              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 39:Q:99:TYR:OH     | 39:Q:111:ARG:NH1 | 2.52                     | 0.43              |
| 1:a:985:C:H2'      | 1:a:986:U:C6     | 2.53                     | 0.43              |
| 1:a:1354:U:H2'     | 1:a:1355:G:H8    | 1.83                     | 0.43              |
| 4:d:28:ILE:HD12    | 4:d:34:ILE:HD11  | 2.00                     | 0.43              |
| 7:g:66:LEU:O       | 7:g:70:ARG:HG2   | 2.18                     | 0.43              |
| 7:g:116:MET:SD     | 7:g:119:ARG:HD2  | 2.59                     | 0.43              |
| 25:A:1794:A:H2'    | 25:A:1795:C:H6   | 1.83                     | 0.43              |
| 25:A:2108:A:N6     | 25:A:2182:U:O2   | 2.50                     | 0.43              |
| 25:A:2163:A:OP1    | 25:A:2171:A:N6   | 2.49                     | 0.43              |
| 25:A:2172:U:O2'    | 25:A:2174:C:OP1  | 2.25                     | 0.43              |
| 25:A:2552:OMU:HM22 | 25:A:2553:G:C8   | 2.53                     | 0.43              |
| 25:A:2684:U:O4'    | 35:M:70:ARG:NH1  | 2.52                     | 0.43              |
| 30:F:64:LYS:HD3    | 51:3:5:ILE:HG13  | 2.01                     | 0.43              |
| 1:a:184:G:H2'      | 1:a:185:U:C6     | 2.54                     | 0.43              |
| 1:a:715:A:H2'      | 1:a:716:A:C8     | 2.53                     | 0.43              |
| 1:a:916:U:H2'      | 1:a:917:G:H8     | 1.83                     | 0.43              |
| 1:a:1125:U:HO2'    | 1:a:1126:U:P     | 2.40                     | 0.43              |
| 1:a:1128:C:H2'     | 1:a:1129:C:C6    | 2.53                     | 0.43              |
| 11:k:37:ARG:NH1    | 11:k:83:GLU:OE2  | 2.51                     | 0.43              |
| 11:k:47:ALA:O      | 11:k:50:SER:OG   | 2.37                     | 0.43              |
| 25:A:151:C:H2'     | 25:A:152:A:H8    | 1.84                     | 0.43              |
| 25:A:1542:U:H2'    | 25:A:1543:G:O4'  | 2.18                     | 0.43              |
| 25:A:1605:C:N4     | 25:A:1606:C:H41  | 2.17                     | 0.43              |
| 25:A:1734:G:H2'    | 25:A:1735:A:H8   | 1.83                     | 0.43              |
| 25:A:2813:A:C4     | 25:A:2814:A:C8   | 3.07                     | 0.43              |
| 1:a:79:G:OP2       | 1:a:79:G:H8      | 2.02                     | 0.43              |
| 1:a:185:U:H2'      | 1:a:186:C:C6     | 2.54                     | 0.43              |
| 1:a:580:C:H2'      | 1:a:581:G:O4'    | 2.18                     | 0.43              |
| 1:a:678:U:H2'      | 1:a:679:C:H6     | 1.83                     | 0.43              |
| 1:a:766:A:OP2      | 1:a:812:G:N2     | 2.52                     | 0.43              |
| 1:a:1452:C:H4'     | 1:a:1453:G:N3    | 2.34                     | 0.43              |
| 7:g:15:ASP:OD1     | 7:g:20:SER:N     | 2.26                     | 0.43              |
| 19:s:10:PHE:CE2    | 19:s:37:ARG:HD2  | 2.50                     | 0.43              |
| 25:A:895:U:C2      | 25:A:897:C:N4    | 2.87                     | 0.43              |
| 25:A:1063:G:N1     | 33:J:136:MET:HE1 | 2.33                     | 0.43              |
| 25:A:2566:A:N1     | 35:M:28:SER:OG   | 2.41                     | 0.43              |
| 26:B:74:U:O2       | 46:X:29:ILE:HD13 | 2.19                     | 0.43              |
| 1:a:678:U:H2'      | 1:a:679:C:C6     | 2.54                     | 0.43              |
| 1:a:859:G:H2'      | 1:a:860:A:H8     | 1.84                     | 0.43              |
| 1:a:1173:U:H2'     | 1:a:1174:G:C8    | 2.48                     | 0.43              |
| 1:a:1179:A:H2'     | 1:a:1180:A:C8    | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:f:10:VAL:HA    | 6:f:84:VAL:HA    | 2.01                     | 0.43              |
| 25:A:703:U:H2'   | 25:A:704:G:O4'   | 2.19                     | 0.43              |
| 25:A:1168:G:H2'  | 25:A:1169:A:C8   | 2.54                     | 0.43              |
| 25:A:1929:G:OP2  | 25:A:1929:G:N2   | 2.48                     | 0.43              |
| 25:A:1966:A:N3   | 25:A:2592:G:O2'  | 2.48                     | 0.43              |
| 25:A:2150:C:H2'  | 25:A:2151:U:O4'  | 2.19                     | 0.43              |
| 25:A:2190:G:H2'  | 25:A:2191:A:H8   | 1.84                     | 0.43              |
| 38:P:103:ARG:HE  | 38:P:110:MET:HE2 | 1.84                     | 0.43              |
| 1:a:689:C:C2     | 1:a:690:G:C8     | 3.07                     | 0.42              |
| 7:g:46:ALA:HB2   | 7:g:117:ALA:HA   | 2.02                     | 0.42              |
| 11:k:74:VAL:O    | 11:k:74:VAL:HG12 | 2.19                     | 0.42              |
| 22:x:19:G:C8     | 25:A:2112:G:H1'  | 2.54                     | 0.42              |
| 24:v:23:ASP:CA   | 58:v:601:G4P:O1B | 2.67                     | 0.42              |
| 24:v:298:GLY:N   | 24:v:379:PHE:O   | 2.52                     | 0.42              |
| 25:A:475:C:O2    | 25:A:479:A:N6    | 2.49                     | 0.42              |
| 25:A:801:G:C8    | 29:E:50:ALA:HB2  | 2.54                     | 0.42              |
| 25:A:2030:6MZ:C2 | 25:A:2499:C:H5'' | 2.49                     | 0.42              |
| 32:I:80:THR:O    | 32:I:82:ILE:HG23 | 2.19                     | 0.42              |
| 37:O:21:ALA:HB2  | 37:O:97:GLN:HG2  | 2.01                     | 0.42              |
| 1:a:472:U:H2'    | 1:a:473:U:C6     | 2.55                     | 0.42              |
| 1:a:524:G:H2'    | 1:a:525:C:C6     | 2.54                     | 0.42              |
| 1:a:950:U:OP2    | 13:m:101:ARG:NE  | 2.41                     | 0.42              |
| 1:a:986:U:H2'    | 1:a:987:G:C8     | 2.54                     | 0.42              |
| 1:a:1058:G:OP1   | 3:c:199:LYS:HE3  | 2.19                     | 0.42              |
| 1:a:1115:U:H2'   | 1:a:1116:U:C6    | 2.55                     | 0.42              |
| 2:b:140:GLU:O    | 2:b:144:LEU:HD23 | 2.17                     | 0.42              |
| 11:k:18:ASP:N    | 11:k:18:ASP:OD1  | 2.51                     | 0.42              |
| 24:v:374:GLN:HG2 | 24:v:422:GLU:HA  | 2.01                     | 0.42              |
| 25:A:1107:G:H2'  | 25:A:1108:U:C6   | 2.55                     | 0.42              |
| 25:A:1405:U:H2'  | 25:A:1406:U:C6   | 2.54                     | 0.42              |
| 30:F:116:GLY:C   | 30:F:178:ARG:HD3 | 2.45                     | 0.42              |
| 36:N:3:LEU:HD23  | 36:N:3:LEU:HA    | 1.88                     | 0.42              |
| 1:a:323:U:H2'    | 1:a:324:G:O4'    | 2.19                     | 0.42              |
| 1:a:377:G:H2'    | 1:a:378:G:H8     | 1.84                     | 0.42              |
| 1:a:1191:A:OP1   | 3:c:4:LYS:NZ     | 2.38                     | 0.42              |
| 4:d:50:ASP:O     | 4:d:54:GLN:HG3   | 2.18                     | 0.42              |
| 7:g:15:ASP:OD1   | 7:g:15:ASP:N     | 2.50                     | 0.42              |
| 7:g:49:THR:O     | 7:g:53:ARG:NE    | 2.49                     | 0.42              |
| 24:v:281:PRO:HB3 | 24:v:290:GLU:HB3 | 2.01                     | 0.42              |
| 24:v:299:PHE:O   | 24:v:299:PHE:CG  | 2.72                     | 0.42              |
| 25:A:277:G:H1'   | 25:A:278:A:C5    | 2.54                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:A:1405:U:H2'  | 25:A:1406:U:H6    | 1.84                     | 0.42              |
| 25:A:1882:U:H2'  | 25:A:1883:U:H6    | 1.85                     | 0.42              |
| 34:L:60:ASP:OD2  | 34:L:61:LYS:HG3   | 2.19                     | 0.42              |
| 42:T:87:GLN:HG2  | 42:T:88:GLY:H     | 1.84                     | 0.42              |
| 45:W:38:GLY:H    | 45:W:62:GLU:CD    | 2.27                     | 0.42              |
| 56:8:27:CYS:SG   | 56:8:33:HIS:HB2   | 2.59                     | 0.42              |
| 1:a:672:U:H2'    | 1:a:673:A:C8      | 2.55                     | 0.42              |
| 1:a:1072:G:H2'   | 1:a:1073:U:H6     | 1.85                     | 0.42              |
| 1:a:1306:A:H61   | 1:a:1331:G:H1'    | 1.84                     | 0.42              |
| 1:a:1342:C:C4'   | 9:i:126:GLN:HE21  | 2.32                     | 0.42              |
| 3:c:64:ILE:HG22  | 3:c:99:ALA:HA     | 2.01                     | 0.42              |
| 3:c:83:ASP:OD1   | 3:c:83:ASP:N      | 2.50                     | 0.42              |
| 25:A:358:U:H2'   | 25:A:359:G:C8     | 2.54                     | 0.42              |
| 25:A:536:G:OP2   | 60:A:3401:HOH:O   | 2.22                     | 0.42              |
| 25:A:1168:G:H2'  | 25:A:1169:A:H8    | 1.83                     | 0.42              |
| 25:A:1370:C:N4   | 60:A:3421:HOH:O   | 2.44                     | 0.42              |
| 27:C:31:ALA:HB3  | 27:C:32:PRO:HD3   | 2.00                     | 0.42              |
| 30:F:122:PHE:HD2 | 30:F:163:ASP:HB3  | 1.85                     | 0.42              |
| 32:I:37:LYS:O    | 32:I:41:LEU:N     | 2.48                     | 0.42              |
| 1:a:212:G:C4     | 1:a:213:G:C8      | 3.07                     | 0.42              |
| 1:a:602:A:H2'    | 1:a:603:U:C6      | 2.55                     | 0.42              |
| 1:a:1229:A:OP1   | 13:m:113:ARG:HD3  | 2.19                     | 0.42              |
| 1:a:1392:G:H5'   | 1:a:1531:A:H5''   | 2.01                     | 0.42              |
| 4:d:88:GLU:HG2   | 4:d:188:ARG:HB2   | 2.01                     | 0.42              |
| 4:d:124:MET:HE3  | 4:d:124:MET:HB3   | 1.76                     | 0.42              |
| 10:j:10:LEU:HD21 | 10:j:22:THR:HG22  | 2.01                     | 0.42              |
| 17:q:11:ARG:HD2  | 17:q:12:VAL:O     | 2.20                     | 0.42              |
| 24:v:127:MET:HG3 | 24:v:162:LEU:HD13 | 2.01                     | 0.42              |
| 25:A:1808:A:H3'  | 25:A:1809:A:C8    | 2.54                     | 0.42              |
| 25:A:2070:A:H2'  | 25:A:2071:A:C8    | 2.55                     | 0.42              |
| 42:T:51:VAL:HG13 | 42:T:51:VAL:O     | 2.20                     | 0.42              |
| 1:a:321:A:H2'    | 1:a:322:C:C6      | 2.55                     | 0.42              |
| 1:a:949:A:H2'    | 1:a:950:U:H6      | 1.82                     | 0.42              |
| 1:a:1015:G:H1'   | 1:a:1218:C:O2'    | 2.20                     | 0.42              |
| 1:a:1057:G:H2'   | 1:a:1058:G:H8     | 1.85                     | 0.42              |
| 1:a:1124:G:O6    | 1:a:1150:A:N6     | 2.53                     | 0.42              |
| 1:a:1157:A:N6    | 1:a:1178:G:H1'    | 2.35                     | 0.42              |
| 1:a:1171:A:H2'   | 1:a:1172:C:C6     | 2.55                     | 0.42              |
| 2:b:114:LEU:HD13 | 2:b:144:LEU:HB3   | 2.01                     | 0.42              |
| 11:k:35:THR:HG22 | 11:k:41:ALA:HA    | 2.01                     | 0.42              |
| 13:m:10:PRO:HD2  | 13:m:18:ALA:HB1   | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:t:57:ILE:H    | 20:t:57:ILE:HD12 | 1.84                     | 0.42              |
| 24:v:94:ASP:OD1  | 24:v:94:ASP:N    | 2.51                     | 0.42              |
| 29:E:87:ALA:O    | 29:E:88:ARG:HD3  | 2.19                     | 0.42              |
| 31:G:90:VAL:HG12 | 31:G:160:LYS:HA  | 2.00                     | 0.42              |
| 35:M:105:ARG:NH2 | 40:R:34:GLU:HB3  | 2.34                     | 0.42              |
| 1:a:34:C:H2'     | 1:a:35:G:H8      | 1.84                     | 0.42              |
| 1:a:328:C:H4'    | 1:a:329:A:H5'    | 2.01                     | 0.42              |
| 1:a:564:C:OP2    | 12:l:12:ARG:NH2  | 2.36                     | 0.42              |
| 1:a:695:A:H2'    | 1:a:696:A:C8     | 2.55                     | 0.42              |
| 1:a:1239:A:H1'   | 1:a:1241:G:C5    | 2.55                     | 0.42              |
| 2:b:130:THR:O    | 2:b:131:LYS:HG2  | 2.20                     | 0.42              |
| 5:e:85:VAL:HG11  | 5:e:147:MET:HG3  | 2.01                     | 0.42              |
| 7:g:72:THR:HA    | 7:g:96:ARG:NH1   | 2.35                     | 0.42              |
| 10:j:8:ILE:HG23  | 10:j:98:VAL:HG13 | 2.01                     | 0.42              |
| 13:m:4:ILE:HG22  | 13:m:9:ILE:HG12  | 2.01                     | 0.42              |
| 24:v:21:HIS:CD2  | 24:v:122:ARG:HB2 | 2.54                     | 0.42              |
| 24:v:410:LYS:HD2 | 24:v:410:LYS:C   | 2.45                     | 0.42              |
| 25:A:891:G:H2'   | 25:A:892:A:C8    | 2.54                     | 0.42              |
| 25:A:1149:G:H2'  | 25:A:1150:C:C6   | 2.54                     | 0.42              |
| 27:C:75:PRO:O    | 27:C:97:LYS:HG2  | 2.20                     | 0.42              |
| 1:a:838:G:C6     | 1:a:849:G:C6     | 3.07                     | 0.42              |
| 1:a:979:C:O2     | 14:n:59:ARG:HG2  | 2.19                     | 0.42              |
| 1:a:1015:G:H2'   | 1:a:1016:A:C8    | 2.55                     | 0.42              |
| 3:c:6:HIS:HD2    | 3:c:8:ASN:H      | 1.68                     | 0.42              |
| 25:A:848:C:H2'   | 25:A:849:A:C8    | 2.51                     | 0.42              |
| 25:A:876:C:H2'   | 25:A:877:A:O4'   | 2.20                     | 0.42              |
| 25:A:1295:C:C2   | 25:A:1296:G:C8   | 3.08                     | 0.42              |
| 25:A:1532:A:H2'  | 25:A:1533:C:C6   | 2.55                     | 0.42              |
| 25:A:2233:U:H2'  | 25:A:2234:G:C8   | 2.54                     | 0.42              |
| 50:2:24:LEU:HD11 | 50:2:54:MET:HE3  | 2.00                     | 0.42              |
| 1:a:322:C:O2'    | 20:t:18:ARG:HB2  | 2.19                     | 0.42              |
| 1:a:634:C:H2'    | 1:a:635:A:C8     | 2.55                     | 0.42              |
| 1:a:978:A:N6     | 1:a:1316:G:H21   | 2.18                     | 0.42              |
| 1:a:1148:U:H2'   | 1:a:1149:C:O4'   | 2.19                     | 0.42              |
| 1:a:1384:C:H2'   | 1:a:1385:G:C8    | 2.54                     | 0.42              |
| 2:b:205:ASP:OD1  | 2:b:206:ALA:N    | 2.53                     | 0.42              |
| 4:d:105:MET:SD   | 4:d:180:GLY:HA3  | 2.59                     | 0.42              |
| 13:m:20:THR:HG23 | 13:m:26:GLY:HA2  | 2.02                     | 0.42              |
| 22:x:28:G:H2'    | 22:x:29:G:C8     | 2.55                     | 0.42              |
| 24:v:10:VAL:CG2  | 24:v:361:PRO:HG2 | 2.50                     | 0.42              |
| 25:A:1071:G:O2'  | 25:A:1072:C:O4'  | 2.14                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 25:A:1113:U:H2'  | 25:A:1114:C:H6     | 1.84                     | 0.42              |
| 25:A:1532:A:H2'  | 25:A:1533:C:H6     | 1.85                     | 0.42              |
| 25:A:2683:C:H4'  | 28:D:13:ARG:NH2    | 2.35                     | 0.42              |
| 40:R:15:GLN:N    | 40:R:15:GLN:OE1    | 2.53                     | 0.42              |
| 1:a:82:G:H2'     | 1:a:83:C:C6        | 2.55                     | 0.42              |
| 1:a:950:U:H3'    | 13:m:101:ARG:NH2   | 2.33                     | 0.42              |
| 1:a:1436:U:H2'   | 1:a:1437:A:C8      | 2.54                     | 0.42              |
| 10:j:9:ARG:HB2   | 10:j:99:GLN:HE21   | 1.84                     | 0.42              |
| 13:m:5:ALA:HB3   | 13:m:22:ILE:HG12   | 2.02                     | 0.42              |
| 24:v:173:ILE:CD1 | 24:v:227:LEU:HD13  | 2.50                     | 0.42              |
| 24:v:525:GLN:N   | 24:v:525:GLN:OE1   | 2.52                     | 0.42              |
| 25:A:581:C:H2'   | 25:A:582:A:H8      | 1.85                     | 0.42              |
| 32:I:97:LYS:HE3  | 32:I:126:LEU:O     | 2.19                     | 0.42              |
| 35:M:17:ARG:CZ   | 35:M:47:ILE:HD11   | 2.49                     | 0.42              |
| 1:a:390:U:H2'    | 1:a:391:G:C8       | 2.54                     | 0.41              |
| 1:a:451:A:H1'    | 1:a:452:A:C2       | 2.55                     | 0.41              |
| 1:a:806:C:H2'    | 1:a:807:A:H8       | 1.85                     | 0.41              |
| 1:a:986:U:H2'    | 1:a:987:G:H8       | 1.85                     | 0.41              |
| 1:a:1086:U:H3    | 1:a:1099:G:N2      | 2.09                     | 0.41              |
| 2:b:84:ALA:HA    | 2:b:87:CYS:HB3     | 2.02                     | 0.41              |
| 11:k:126:LYS:HZ3 | 21:u:37:PHE:HD2    | 1.68                     | 0.41              |
| 25:A:78:U:H2'    | 25:A:79:C:C6       | 2.55                     | 0.41              |
| 25:A:172:A:H2'   | 25:A:173:A:C8      | 2.53                     | 0.41              |
| 25:A:568:U:H1'   | 25:A:2030:6MZ:H9C1 | 2.02                     | 0.41              |
| 25:A:878:A:H3'   | 25:A:879:G:H8      | 1.85                     | 0.41              |
| 25:A:1912:A:H62  | 25:A:1917:PSU:HN3  | 1.68                     | 0.41              |
| 25:A:2191:A:H2'  | 25:A:2192:U:C6     | 2.55                     | 0.41              |
| 25:A:2619:C:O2   | 28:D:161:MET:HE1   | 2.19                     | 0.41              |
| 40:R:6:LYS:HE2   | 40:R:6:LYS:HB3     | 1.84                     | 0.41              |
| 45:W:24:LYS:HB2  | 45:W:24:LYS:HE2    | 1.68                     | 0.41              |
| 1:a:184:G:H2'    | 1:a:185:U:H6       | 1.84                     | 0.41              |
| 1:a:235:C:H2'    | 1:a:236:A:H8       | 1.84                     | 0.41              |
| 1:a:460:A:H2'    | 1:a:461:A:H8       | 1.85                     | 0.41              |
| 1:a:532:A:H61    | 3:c:193:TYR:HD1    | 1.68                     | 0.41              |
| 1:a:978:A:C5     | 1:a:1319:A:C2      | 3.08                     | 0.41              |
| 1:a:979:C:O2     | 1:a:979:C:H2'      | 2.19                     | 0.41              |
| 4:d:160:GLU:O    | 4:d:163:GLU:HG2    | 2.20                     | 0.41              |
| 9:i:15:SER:OG    | 9:i:70:GLY:HA3     | 2.20                     | 0.41              |
| 10:j:80:THR:HB   | 10:j:83:THR:HG22   | 2.02                     | 0.41              |
| 25:A:363:G:H2'   | 25:A:364:C:H6      | 1.85                     | 0.41              |
| 25:A:2513:A:H2'  | 25:A:2514:U:C6     | 2.55                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:B:3:C:H2'     | 26:B:4:C:H6       | 1.86                     | 0.41              |
| 32:I:48:ALA:HB3  | 32:I:51:TYR:CE1   | 2.52                     | 0.41              |
| 32:I:93:ALA:O    | 32:I:97:LYS:NZ    | 2.53                     | 0.41              |
| 1:a:193:C:H2'    | 1:a:194:C:C6      | 2.55                     | 0.41              |
| 1:a:938:A:N3     | 1:a:1376:U:O2'    | 2.43                     | 0.41              |
| 1:a:1064:G:H5'   | 1:a:1066:C:H5'    | 2.02                     | 0.41              |
| 1:a:1184:G:C2    | 1:a:1185:G:C8     | 3.08                     | 0.41              |
| 1:a:1205:U:O2'   | 3:c:195:VAL:HG13  | 2.20                     | 0.41              |
| 1:a:1306:A:N6    | 1:a:1331:G:H1'    | 2.35                     | 0.41              |
| 1:a:1402:4OC:H2' | 1:a:1403:C:O4'    | 2.20                     | 0.41              |
| 2:b:12:ALA:HB1   | 2:b:209:ALA:HA    | 2.02                     | 0.41              |
| 7:g:65:ALA:HB2   | 7:g:128:ALA:HB2   | 2.01                     | 0.41              |
| 7:g:73:VAL:HG22  | 7:g:88:PRO:HB2    | 2.01                     | 0.41              |
| 12:l:73:ASN:OD1  | 12:l:105:SER:OG   | 2.28                     | 0.41              |
| 24:v:115:ALA:HA  | 24:v:154:LEU:HD21 | 2.02                     | 0.41              |
| 24:v:144:LEU:O   | 24:v:144:LEU:HD23 | 2.21                     | 0.41              |
| 25:A:286:U:C2    | 25:A:287:G:C8     | 3.08                     | 0.41              |
| 25:A:580:U:H2'   | 25:A:581:C:C6     | 2.54                     | 0.41              |
| 25:A:895:U:H2'   | 25:A:897:C:C5     | 2.55                     | 0.41              |
| 25:A:2285:C:OP2  | 53:5:6:ARG:HD3    | 2.20                     | 0.41              |
| 25:A:2411:A:H2'  | 25:A:2412:A:C8    | 2.55                     | 0.41              |
| 26:B:112:G:H2'   | 26:B:113:C:H6     | 1.85                     | 0.41              |
| 35:M:20:MET:O    | 35:M:41:ILE:HA    | 2.20                     | 0.41              |
| 46:X:63:ILE:O    | 46:X:63:ILE:HG13  | 2.21                     | 0.41              |
| 1:a:950:U:P      | 13:m:101:ARG:HH21 | 2.44                     | 0.41              |
| 1:a:1049:U:H5    | 14:n:2:ALA:HA     | 1.86                     | 0.41              |
| 8:h:88:ARG:NH2   | 8:h:91:GLU:OE2    | 2.53                     | 0.41              |
| 25:A:722:A:H2'   | 25:A:723:C:H6     | 1.85                     | 0.41              |
| 25:A:2138:G:N2   | 25:A:2154:A:C4    | 2.88                     | 0.41              |
| 33:J:36:MET:HG3  | 33:J:36:MET:O     | 2.19                     | 0.41              |
| 37:O:2:LEU:HD12  | 37:O:68:PHE:CE1   | 2.55                     | 0.41              |
| 37:O:41:LEU:HG   | 37:O:96:ILE:HG13  | 2.02                     | 0.41              |
| 48:Z:11:ARG:HG3  | 48:Z:12:PRO:HD2   | 2.02                     | 0.41              |
| 1:a:95:C:H2'     | 1:a:96:U:C6       | 2.55                     | 0.41              |
| 1:a:946:A:H2'    | 1:a:947:G:C8      | 2.55                     | 0.41              |
| 1:a:1106:G:OP1   | 3:c:172:ARG:NH2   | 2.47                     | 0.41              |
| 1:a:1107:C:C4    | 1:a:1108:G:C8     | 3.08                     | 0.41              |
| 1:a:1176:A:H2'   | 1:a:1177:G:C8     | 2.55                     | 0.41              |
| 1:a:1319:A:H8    | 1:a:1323:G:N7     | 2.19                     | 0.41              |
| 1:a:1371:G:H2'   | 1:a:1372:U:H6     | 1.83                     | 0.41              |
| 2:b:144:LEU:O    | 2:b:148:LEU:HD23  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:d:85:ASN:OD1    | 4:d:87:GLY:N      | 2.53                     | 0.41              |
| 5:e:65:GLU:OE1    | 5:e:68:ARG:NH2    | 2.46                     | 0.41              |
| 8:h:11:LEU:HG     | 8:h:75:ILE:HD11   | 2.01                     | 0.41              |
| 14:n:20:TYR:HE2   | 14:n:52:PRO:HD2   | 1.85                     | 0.41              |
| 22:x:25:C:C2      | 22:x:26:A:C8      | 3.09                     | 0.41              |
| 24:v:331:LEU:HD23 | 24:v:331:LEU:H    | 1.85                     | 0.41              |
| 25:A:3:U:H2'      | 25:A:4:U:H6       | 1.86                     | 0.41              |
| 25:A:592:A:C2     | 55:7:4:ILE:HD11   | 2.56                     | 0.41              |
| 25:A:1102:C:C2    | 25:A:1103:A:C8    | 3.09                     | 0.41              |
| 25:A:1360:G:C8    | 25:A:1361:G:C8    | 3.08                     | 0.41              |
| 26:B:33:G:C2      | 26:B:50:A:C2      | 3.08                     | 0.41              |
| 33:J:71:THR:OG1   | 33:J:72:LYS:N     | 2.53                     | 0.41              |
| 33:J:100:LYS:HA   | 33:J:139:VAL:H    | 1.84                     | 0.41              |
| 40:R:62:ARG:NH1   | 40:R:71:GLU:OE2   | 2.53                     | 0.41              |
| 46:X:62:THR:OG1   | 46:X:69:GLU:HG3   | 2.20                     | 0.41              |
| 1:a:19:A:H2'      | 1:a:20:U:H6       | 1.84                     | 0.41              |
| 1:a:1201:A:H4'    | 1:a:1202:U:H5''   | 2.02                     | 0.41              |
| 5:e:77:ASN:HD22   | 5:e:82:GLN:NE2    | 2.18                     | 0.41              |
| 7:g:135:VAL:O     | 7:g:139:GLU:OE1   | 2.39                     | 0.41              |
| 9:i:21:ILE:CD1    | 9:i:63:LEU:HG     | 2.50                     | 0.41              |
| 13:m:19:LEU:HD11  | 13:m:60:VAL:HG21  | 2.02                     | 0.41              |
| 22:x:33:U:O4'     | 22:x:37:MIA:H161  | 2.21                     | 0.41              |
| 24:v:89:THR:O     | 24:v:89:THR:OG1   | 2.37                     | 0.41              |
| 24:v:230:GLU:O    | 24:v:234:VAL:HG23 | 2.20                     | 0.41              |
| 25:A:1710:G:H2'   | 25:A:1711:A:H8    | 1.84                     | 0.41              |
| 32:I:19:ALA:HB2   | 32:I:69:PHE:HZ    | 1.86                     | 0.41              |
| 1:a:496:A:H5'     | 1:a:497:G:OP2     | 2.21                     | 0.41              |
| 1:a:1048:G:H5''   | 14:n:3:LYS:HG2    | 2.02                     | 0.41              |
| 1:a:1246:A:C6     | 1:a:1292:G:C6     | 3.09                     | 0.41              |
| 3:c:7:PRO:HD2     | 3:c:184:TYR:CD2   | 2.56                     | 0.41              |
| 3:c:157:LEU:HD12  | 3:c:164:ARG:HG3   | 2.02                     | 0.41              |
| 4:d:161:LEU:O     | 4:d:164:GLN:HG3   | 2.20                     | 0.41              |
| 13:m:59:GLU:HA    | 13:m:59:GLU:OE2   | 2.21                     | 0.41              |
| 25:A:306:U:H2'    | 25:A:307:G:O4'    | 2.21                     | 0.41              |
| 25:A:376:G:H2'    | 25:A:377:G:H8     | 1.86                     | 0.41              |
| 25:A:492:A:H2'    | 25:A:493:G:O4'    | 2.20                     | 0.41              |
| 25:A:936:A:H2'    | 25:A:937:C:C6     | 2.55                     | 0.41              |
| 25:A:2149:U:H2'   | 25:A:2150:C:H6    | 1.86                     | 0.41              |
| 25:A:2584:U:H2'   | 25:A:2585:U:H2'   | 2.02                     | 0.41              |
| 25:A:2591:C:H2'   | 25:A:2592:G:H8    | 1.86                     | 0.41              |
| 26:B:44:G:H1'     | 26:B:47:C:N4      | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:F:4:LEU:HA     | 30:F:7:TYR:HB3    | 2.02                     | 0.41              |
| 40:R:31:TRP:CE3   | 40:R:38:LYS:HG3   | 2.56                     | 0.41              |
| 1:a:21:G:H2'      | 1:a:22:G:H8       | 1.85                     | 0.41              |
| 1:a:82:G:O2'      | 1:a:83:C:O4'      | 2.34                     | 0.41              |
| 1:a:413:G:N2      | 1:a:429:U:OP2     | 2.48                     | 0.41              |
| 4:d:12:SER:O      | 4:d:16:GLY:N      | 2.52                     | 0.41              |
| 5:e:81:LEU:HD22   | 5:e:147:MET:HE3   | 2.03                     | 0.41              |
| 22:x:52:G:C2      | 22:x:53:G:C8      | 3.09                     | 0.41              |
| 24:v:407:LEU:HD12 | 24:v:407:LEU:HA   | 1.86                     | 0.41              |
| 25:A:1505:A:H2'   | 25:A:1506:U:C6    | 2.56                     | 0.41              |
| 25:A:2020:A:H5'   | 52:4:9:THR:CG2    | 2.50                     | 0.41              |
| 25:A:2419:U:H4'   | 53:5:22:THR:HG21  | 2.02                     | 0.41              |
| 28:D:25:THR:HG21  | 28:D:193:VAL:HG22 | 2.03                     | 0.41              |
| 1:a:184:G:N2      | 1:a:194:C:O2      | 2.53                     | 0.41              |
| 1:a:981:U:H5''    | 14:n:6:MET:SD     | 2.61                     | 0.41              |
| 1:a:1026:G:H2'    | 1:a:1027:C:C6     | 2.56                     | 0.41              |
| 1:a:1038:C:H2'    | 1:a:1039:G:C8     | 2.56                     | 0.41              |
| 1:a:1060:U:H2'    | 1:a:1061:G:H8     | 1.86                     | 0.41              |
| 1:a:1204:A:H8     | 1:a:1204:A:O5'    | 2.03                     | 0.41              |
| 1:a:1217:C:P      | 14:n:9:ARG:HH21   | 2.43                     | 0.41              |
| 2:b:20:THR:O      | 2:b:23:TRP:CD1    | 2.72                     | 0.41              |
| 2:b:59:LYS:HB3    | 2:b:63:ARG:NH1    | 2.35                     | 0.41              |
| 3:c:64:ILE:O      | 3:c:100:GLN:HB3   | 2.20                     | 0.41              |
| 3:c:115:LEU:HD23  | 3:c:115:LEU:H     | 1.86                     | 0.41              |
| 3:c:154:SER:CB    | 3:c:165:THR:HG22  | 2.49                     | 0.41              |
| 12:l:5:ASN:ND2    | 17:q:36:LYS:HE2   | 2.35                     | 0.41              |
| 13:m:83:LEU:HD23  | 13:m:83:LEU:HA    | 1.94                     | 0.41              |
| 15:o:8:THR:O      | 15:o:12:VAL:HG22  | 2.20                     | 0.41              |
| 18:r:42:SER:O     | 18:r:46:GLY:N     | 2.53                     | 0.41              |
| 25:A:671:C:H2'    | 25:A:672:C:C6     | 2.56                     | 0.41              |
| 25:A:880:G:H3'    | 25:A:881:G:C8     | 2.56                     | 0.41              |
| 25:A:1065:U:H2'   | 25:A:1066:U:C6    | 2.56                     | 0.41              |
| 25:A:1281:G:H2'   | 25:A:1282:U:C6    | 2.56                     | 0.41              |
| 25:A:1319:C:O2'   | 25:A:1320:C:H5'   | 2.21                     | 0.41              |
| 25:A:1495:A:N3    | 25:A:1578:U:O2'   | 2.45                     | 0.41              |
| 25:A:1585:C:H2'   | 25:A:1586:A:O4'   | 2.21                     | 0.41              |
| 25:A:2131:U:H5'   | 25:A:2132:U:H5''  | 2.03                     | 0.41              |
| 25:A:2182:U:H2'   | 25:A:2183:A:C8    | 2.56                     | 0.41              |
| 27:C:155:ALA:HB2  | 27:C:162:VAL:HG13 | 2.02                     | 0.41              |
| 29:E:106:LYS:HG2  | 29:E:200:LEU:HD13 | 2.01                     | 0.41              |
| 30:F:29:PRO:HB3   | 30:F:160:ALA:HB2  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:I:23:LEU:HD23  | 32:I:91:ALA:HB1   | 2.03                     | 0.41              |
| 33:J:8:TYR:HB3    | 33:J:60:THR:HA    | 2.02                     | 0.41              |
| 39:Q:53:THR:HB    | 39:Q:65:THR:OG1   | 2.21                     | 0.41              |
| 40:R:43:PHE:CE2   | 40:R:63:LYS:HD3   | 2.56                     | 0.41              |
| 45:W:19:LYS:HE3   | 45:W:19:LYS:HB2   | 1.85                     | 0.41              |
| 1:a:1097:C:H2'    | 1:a:1098:C:C6     | 2.56                     | 0.41              |
| 1:a:1141:C:H2'    | 1:a:1142:G:C8     | 2.55                     | 0.41              |
| 1:a:1497:G:H1'    | 1:a:1518:MA6:H2   | 2.03                     | 0.41              |
| 14:n:17:ALA:HA    | 14:n:55:SER:O     | 2.21                     | 0.41              |
| 21:u:11:PRO:HG2   | 21:u:14:VAL:HG23  | 2.02                     | 0.41              |
| 24:v:320:VAL:HG12 | 24:v:361:PRO:HA   | 2.03                     | 0.41              |
| 25:A:288:U:C2     | 25:A:289:G:C8     | 3.08                     | 0.41              |
| 25:A:712:G:H2'    | 25:A:713:G:O4'    | 2.21                     | 0.41              |
| 25:A:851:C:H2'    | 25:A:852:U:C6     | 2.56                     | 0.41              |
| 25:A:852:U:H2'    | 25:A:853:C:C6     | 2.56                     | 0.41              |
| 25:A:1262:A:N3    | 52:4:7:LYS:HE3    | 2.36                     | 0.41              |
| 25:A:1716:U:H2'   | 25:A:1717:A:H8    | 1.86                     | 0.41              |
| 25:A:2108:A:H2'   | 25:A:2109:U:O4'   | 2.22                     | 0.41              |
| 25:A:2114:A:H3'   | 25:A:2115:G:H8    | 1.86                     | 0.41              |
| 27:C:262:ARG:HG3  | 27:C:263:THR:HG23 | 2.02                     | 0.41              |
| 28:D:89:GLU:HA    | 28:D:89:GLU:OE2   | 2.21                     | 0.41              |
| 32:I:34:THR:HA    | 32:I:37:LYS:HB2   | 2.03                     | 0.41              |
| 1:a:436:C:H2'     | 1:a:437:U:C6      | 2.56                     | 0.40              |
| 1:a:1135:U:H3'    | 1:a:1137:C:N4     | 2.35                     | 0.40              |
| 3:c:132:ARG:CZ    | 3:c:136:ARG:HH22  | 2.33                     | 0.40              |
| 3:c:173:VAL:HG12  | 3:c:175:LEU:HD12  | 2.02                     | 0.40              |
| 7:g:34:GLY:C      | 7:g:35:LYS:HD2    | 2.46                     | 0.40              |
| 18:r:26:ILE:H     | 18:r:26:ILE:HD12  | 1.86                     | 0.40              |
| 19:s:50:ALA:HB1   | 19:s:57:HIS:HB3   | 2.02                     | 0.40              |
| 25:A:539:G:H5'    | 34:L:9:GLU:OE2    | 2.21                     | 0.40              |
| 25:A:1005:C:O2'   | 34:L:30:THR:HG21  | 2.21                     | 0.40              |
| 25:A:1790:C:H2'   | 25:A:1791:A:N7    | 2.36                     | 0.40              |
| 25:A:2111:U:H1'   | 25:A:2118:U:H4'   | 2.02                     | 0.40              |
| 25:A:2230:G:H2'   | 25:A:2231:U:C6    | 2.55                     | 0.40              |
| 25:A:2233:U:H2'   | 25:A:2234:G:H8    | 1.86                     | 0.40              |
| 25:A:2705:A:O2'   | 25:A:2852:G:OP1   | 2.38                     | 0.40              |
| 25:A:2804:U:H2'   | 25:A:2805:C:C6    | 2.56                     | 0.40              |
| 25:A:2865:U:OP2   | 25:A:2866:U:O2'   | 2.33                     | 0.40              |
| 26:B:29:A:H2'     | 26:B:30:C:H6      | 1.86                     | 0.40              |
| 26:B:46:A:C5      | 26:B:47:C:C5      | 3.09                     | 0.40              |
| 30:F:103:LEU:O    | 30:F:107:ALA:HB3  | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 32:I:121:SER:OG  | 32:I:122:GLN:N   | 2.54                     | 0.40              |
| 34:L:15:TRP:HB3  | 34:L:137:PRO:HB3 | 2.03                     | 0.40              |
| 39:Q:7:ARG:HA    | 39:Q:10:ARG:HE   | 1.85                     | 0.40              |
| 1:a:1377:A:OP1   | 7:g:95:ARG:NH2   | 2.50                     | 0.40              |
| 2:b:130:THR:O    | 2:b:132:LYS:N    | 2.55                     | 0.40              |
| 3:c:67:THR:HA    | 3:c:102:ASN:HB2  | 2.03                     | 0.40              |
| 10:j:9:ARG:O     | 10:j:99:GLN:HG2  | 2.21                     | 0.40              |
| 22:x:13:C:N4     | 22:x:22:G:H1     | 2.19                     | 0.40              |
| 25:A:365:U:H2'   | 25:A:366:C:C6    | 2.56                     | 0.40              |
| 25:A:893:C:H2'   | 25:A:894:U:O4'   | 2.20                     | 0.40              |
| 25:A:1790:C:H2'  | 25:A:1791:A:C8   | 2.56                     | 0.40              |
| 25:A:2399:G:C6   | 25:A:2418:A:C6   | 3.09                     | 0.40              |
| 25:A:2680:U:O2'  | 25:A:2681:C:H5'  | 2.21                     | 0.40              |
| 31:G:173:GLU:HA  | 31:G:173:GLU:OE2 | 2.20                     | 0.40              |
| 33:J:28:LEU:HD11 | 33:J:35:ILE:HA   | 2.03                     | 0.40              |
| 45:W:5:ILE:HD11  | 45:W:67:VAL:HG23 | 2.02                     | 0.40              |
| 54:6:3:ARG:HA    | 54:6:3:ARG:HD3   | 1.83                     | 0.40              |
| 1:a:708:C:H2'    | 1:a:709:U:H6     | 1.86                     | 0.40              |
| 11:k:122:ARG:HA  | 11:k:123:PRO:HD3 | 1.92                     | 0.40              |
| 12:l:83:ARG:NH1  | 12:l:84:GLY:O    | 2.54                     | 0.40              |
| 13:m:33:ILE:HD11 | 13:m:63:PHE:CE2  | 2.56                     | 0.40              |
| 13:m:76:SER:O    | 13:m:79:ARG:HG3  | 2.21                     | 0.40              |
| 25:A:272:A:H2'   | 25:A:273:G:H8    | 1.86                     | 0.40              |
| 25:A:379:G:N1    | 25:A:396:G:C6    | 2.89                     | 0.40              |
| 25:A:1084:A:O2'  | 25:A:1085:A:O4'  | 2.35                     | 0.40              |
| 25:A:1410:G:H2'  | 25:A:1411:U:C6   | 2.56                     | 0.40              |
| 25:A:1775:U:O4   | 25:A:1789:A:H2   | 2.05                     | 0.40              |
| 25:A:2143:C:C2   | 25:A:2144:G:C8   | 3.09                     | 0.40              |
| 25:A:2340:A:H2'  | 25:A:2341:G:H8   | 1.87                     | 0.40              |
| 26:B:34:A:H4'    | 26:B:35:C:H5     | 1.86                     | 0.40              |
| 26:B:117:G:H2'   | 26:B:118:C:C6    | 2.56                     | 0.40              |
| 43:U:88:ARG:HD2  | 43:U:88:ARG:HA   | 1.90                     | 0.40              |
| 44:V:34:VAL:HG23 | 44:V:81:LYS:HB3  | 2.03                     | 0.40              |
| 53:5:35:GLU:OE2  | 53:5:48:ILE:HD12 | 2.20                     | 0.40              |
| 2:b:217:VAL:O    | 2:b:220:THR:HG22 | 2.21                     | 0.40              |
| 4:d:19:LEU:HB2   | 4:d:21:LEU:HG    | 2.02                     | 0.40              |
| 6:f:9:MET:HE1    | 18:r:65:LEU:CD1  | 2.52                     | 0.40              |
| 7:g:72:THR:HB    | 7:g:96:ARG:HH22  | 1.86                     | 0.40              |
| 22:x:46:G7M:H8   | 22:x:46:G7M:H2'  | 1.90                     | 0.40              |
| 24:v:98:ASP:O    | 24:v:100:TYR:CA  | 2.67                     | 0.40              |
| 24:v:349:MET:C   | 24:v:351:GLY:H   | 2.30                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:v:494:ALA:HB3 | 24:v:504:ILE:HD12 | 2.04                     | 0.40              |
| 25:A:874:G:C2    | 25:A:875:G:C8     | 3.10                     | 0.40              |
| 25:A:993:G:H1'   | 42:T:91:GLN:NE2   | 2.35                     | 0.40              |
| 25:A:1438:U:H2'  | 25:A:1439:A:H8    | 1.86                     | 0.40              |
| 25:A:1509:A:O2'  | 25:A:1510:G:H8    | 2.04                     | 0.40              |
| 25:A:2138:G:C2   | 25:A:2139:U:C2    | 3.10                     | 0.40              |
| 25:A:2480:C:H2'  | 25:A:2481:G:H5'   | 2.02                     | 0.40              |
| 30:F:32:GLU:C    | 30:F:96:MET:HE1   | 2.47                     | 0.40              |
| 38:P:1:MET:HE3   | 38:P:1:MET:HB2    | 1.90                     | 0.40              |
| 1:a:516:PSU:H2'  | 1:a:517:G:C8      | 2.57                     | 0.40              |
| 1:a:620:C:C2     | 1:a:621:A:C8      | 3.10                     | 0.40              |
| 1:a:661:G:H2'    | 1:a:662:U:C6      | 2.56                     | 0.40              |
| 1:a:951:G:C6     | 1:a:1231:G:C6     | 3.10                     | 0.40              |
| 1:a:958:A:O2'    | 1:a:959:A:O4'     | 2.28                     | 0.40              |
| 1:a:1227:A:OP1   | 19:s:80:TYR:OH    | 2.20                     | 0.40              |
| 18:r:50:LYS:H    | 18:r:50:LYS:HG2   | 1.70                     | 0.40              |
| 25:A:146:A:H2'   | 25:A:147:C:C6     | 2.56                     | 0.40              |
| 25:A:2305:U:H3   | 30:F:151:GLY:HA3  | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | b     | 222/241 (92%) | 195 (88%) | 27 (12%) | 0        | 100         | 100 |
| 3   | c     | 204/233 (88%) | 191 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 4   | d     | 203/206 (98%) | 200 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 5   | e     | 154/167 (92%) | 145 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 6   | f     | 101/131 (77%) | 95 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 7   | g     | 150/156 (96%) | 144 (96%) | 6 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 8   | h     | 127/130 (98%) | 125 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 9   | i     | 125/130 (96%) | 118 (94%) | 6 (5%)   | 1 (1%)   | 16          | 50  |
| 10  | j     | 96/103 (93%)  | 90 (94%)  | 5 (5%)   | 1 (1%)   | 12          | 45  |
| 11  | k     | 113/129 (88%) | 106 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 12  | l     | 118/124 (95%) | 108 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 13  | m     | 113/118 (96%) | 105 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 14  | n     | 98/101 (97%)  | 95 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 15  | o     | 86/89 (97%)   | 82 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 16  | p     | 79/82 (96%)   | 76 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 17  | q     | 77/84 (92%)   | 72 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 18  | r     | 52/75 (69%)   | 47 (90%)  | 5 (10%)  | 0        | 100         | 100 |
| 19  | s     | 81/92 (88%)   | 76 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 20  | t     | 84/87 (97%)   | 81 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 21  | u     | 53/71 (75%)   | 52 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 24  | v     | 489/529 (92%) | 412 (84%) | 73 (15%) | 4 (1%)   | 16          | 50  |
| 27  | C     | 269/273 (98%) | 256 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 28  | D     | 206/209 (99%) | 198 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 29  | E     | 199/201 (99%) | 196 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 30  | F     | 175/179 (98%) | 163 (93%) | 12 (7%)  | 0        | 100         | 100 |
| 31  | G     | 174/177 (98%) | 164 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 32  | I     | 129/165 (78%) | 103 (80%) | 26 (20%) | 0        | 100         | 100 |
| 33  | J     | 139/142 (98%) | 121 (87%) | 17 (12%) | 1 (1%)   | 18          | 52  |
| 34  | L     | 140/142 (99%) | 137 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 35  | M     | 121/123 (98%) | 114 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 36  | N     | 142/144 (99%) | 138 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 37  | O     | 132/136 (97%) | 126 (96%) | 5 (4%)   | 1 (1%)   | 16          | 50  |
| 38  | P     | 116/127 (91%) | 111 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 39  | Q     | 114/117 (97%) | 110 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 40  | R     | 112/115 (97%) | 105 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 41  | S     | 115/118 (98%) | 114 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 42  | T     | 101/103 (98%) | 97 (96%)  | 4 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 43  | U     | 108/110 (98%)   | 103 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 44  | V     | 91/100 (91%)    | 85 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 45  | W     | 100/104 (96%)   | 94 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 46  | X     | 92/94 (98%)     | 87 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 47  | Y     | 74/85 (87%)     | 72 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 48  | Z     | 75/78 (96%)     | 74 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 49  | 1     | 59/63 (94%)     | 57 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 50  | 2     | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 51  | 3     | 46/70 (66%)     | 43 (94%)   | 3 (6%)   | 0        | 100         | 100 |
| 52  | 4     | 53/57 (93%)     | 53 (100%)  | 0        | 0        | 100         | 100 |
| 53  | 5     | 49/55 (89%)     | 47 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 54  | 6     | 44/46 (96%)     | 42 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 55  | 7     | 62/65 (95%)     | 58 (94%)   | 3 (5%)   | 1 (2%)   | 7           | 36  |
| 56  | 8     | 36/38 (95%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| All | All   | 6154/6573 (94%) | 5773 (94%) | 372 (6%) | 9 (0%)   | 49          | 79  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | v     | 99  | THR  |
| 10  | j     | 57  | VAL  |
| 24  | v     | 18  | ILE  |
| 24  | v     | 97  | GLU  |
| 33  | J     | 33  | VAL  |
| 37  | O     | 83  | GLY  |
| 9   | i     | 13  | LYS  |
| 24  | v     | 320 | VAL  |
| 55  | 7     | 32  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | b     | 186/199 (94%)  | 186 (100%) | 0        | 100         | 100 |
| 3   | c     | 170/190 (90%)  | 170 (100%) | 0        | 100         | 100 |
| 4   | d     | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 5   | e     | 119/126 (94%)  | 119 (100%) | 0        | 100         | 100 |
| 6   | f     | 90/112 (80%)   | 90 (100%)  | 0        | 100         | 100 |
| 7   | g     | 125/129 (97%)  | 125 (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     | 89/98 (91%)    | 89 (100%)  | 0        | 100         | 100 |
| 12  | l     | 101/103 (98%)  | 101 (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     | 47/65 (72%)    | 47 (100%)  | 0        | 100         | 100 |
| 19  | s     | 72/79 (91%)    | 72 (100%)  | 0        | 100         | 100 |
| 20  | t     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 21  | u     | 48/61 (79%)    | 48 (100%)  | 0        | 100         | 100 |
| 24  | v     | 421/453 (93%)  | 420 (100%) | 1 (0%)   | 87          | 89  |
| 27  | C     | 216/218 (99%)  | 216 (100%) | 0        | 100         | 100 |
| 28  | D     | 163/163 (100%) | 163 (100%) | 0        | 100         | 100 |
| 29  | E     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 30  | F     | 148/150 (99%)  | 148 (100%) | 0        | 100         | 100 |
| 31  | G     | 137/138 (99%)  | 137 (100%) | 0        | 100         | 100 |
| 32  | I     | 100/123 (81%)  | 100 (100%) | 0        | 100         | 100 |
| 33  | J     | 109/110 (99%)  | 109 (100%) | 0        | 100         | 100 |
| 34  | L     | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 35  | M     | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 36  | N     | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 37  | O     | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 38  | P     | 98/103 (95%)    | 98 (100%)   | 0        | 100         | 100 |
| 39  | Q     | 86/87 (99%)     | 86 (100%)   | 0        | 100         | 100 |
| 40  | R     | 99/100 (99%)    | 99 (100%)   | 0        | 100         | 100 |
| 41  | S     | 89/90 (99%)     | 89 (100%)   | 0        | 100         | 100 |
| 42  | T     | 84/84 (100%)    | 84 (100%)   | 0        | 100         | 100 |
| 43  | U     | 93/93 (100%)    | 93 (100%)   | 0        | 100         | 100 |
| 44  | V     | 80/84 (95%)     | 80 (100%)   | 0        | 100         | 100 |
| 45  | W     | 83/85 (98%)     | 83 (100%)   | 0        | 100         | 100 |
| 46  | X     | 78/78 (100%)    | 78 (100%)   | 0        | 100         | 100 |
| 47  | Y     | 58/63 (92%)     | 58 (100%)   | 0        | 100         | 100 |
| 48  | Z     | 67/68 (98%)     | 67 (100%)   | 0        | 100         | 100 |
| 49  | 1     | 54/55 (98%)     | 54 (100%)   | 0        | 100         | 100 |
| 50  | 2     | 48/49 (98%)     | 48 (100%)   | 0        | 100         | 100 |
| 51  | 3     | 44/62 (71%)     | 44 (100%)   | 0        | 100         | 100 |
| 52  | 4     | 46/48 (96%)     | 46 (100%)   | 0        | 100         | 100 |
| 53  | 5     | 46/49 (94%)     | 46 (100%)   | 0        | 100         | 100 |
| 54  | 6     | 38/38 (100%)    | 38 (100%)   | 0        | 100         | 100 |
| 55  | 7     | 51/52 (98%)     | 51 (100%)   | 0        | 100         | 100 |
| 56  | 8     | 34/34 (100%)    | 34 (100%)   | 0        | 100         | 100 |
| All | All   | 5134/5375 (96%) | 5133 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | v     | 97  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 51  | ASN  |
| 2   | b     | 109 | GLN  |
| 2   | b     | 122 | GLN  |
| 4   | d     | 40  | GLN  |
| 4   | d     | 116 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | d     | 136 | GLN  |
| 4   | d     | 198 | HIS  |
| 5   | e     | 43  | ASN  |
| 5   | e     | 70  | ASN  |
| 5   | e     | 77  | ASN  |
| 5   | e     | 83  | HIS  |
| 5   | e     | 97  | GLN  |
| 6   | f     | 58  | HIS  |
| 6   | f     | 63  | ASN  |
| 7   | g     | 52  | GLN  |
| 7   | g     | 86  | GLN  |
| 7   | g     | 97  | ASN  |
| 8   | h     | 67  | GLN  |
| 8   | h     | 76  | GLN  |
| 9   | i     | 32  | GLN  |
| 9   | i     | 75  | GLN  |
| 9   | i     | 110 | GLN  |
| 10  | j     | 70  | HIS  |
| 11  | k     | 15  | GLN  |
| 11  | k     | 28  | ASN  |
| 11  | k     | 29  | ASN  |
| 11  | k     | 40  | ASN  |
| 14  | n     | 35  | ASN  |
| 14  | n     | 71  | HIS  |
| 15  | o     | 20  | ASN  |
| 15  | o     | 51  | HIS  |
| 16  | p     | 9   | HIS  |
| 17  | q     | 9   | GLN  |
| 18  | r     | 31  | ASN  |
| 20  | t     | 20  | HIS  |
| 20  | t     | 21  | ASN  |
| 20  | t     | 70  | ASN  |
| 21  | u     | 9   | ASN  |
| 21  | u     | 56  | HIS  |
| 24  | v     | 21  | HIS  |
| 24  | v     | 85  | ASN  |
| 24  | v     | 225 | GLN  |
| 24  | v     | 226 | GLN  |
| 24  | v     | 262 | ASN  |
| 24  | v     | 333 | GLN  |
| 24  | v     | 445 | GLN  |
| 27  | C     | 25  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | C     | 53  | HIS  |
| 27  | C     | 86  | ASN  |
| 27  | C     | 143 | ASN  |
| 27  | C     | 226 | ASN  |
| 27  | C     | 239 | ASN  |
| 28  | D     | 130 | GLN  |
| 28  | D     | 134 | HIS  |
| 28  | D     | 136 | ASN  |
| 29  | E     | 41  | GLN  |
| 29  | E     | 92  | HIS  |
| 29  | E     | 97  | ASN  |
| 30  | F     | 81  | GLN  |
| 31  | G     | 20  | ASN  |
| 31  | G     | 22  | GLN  |
| 31  | G     | 143 | GLN  |
| 32  | I     | 6   | GLN  |
| 34  | L     | 47  | HIS  |
| 34  | L     | 76  | HIS  |
| 34  | L     | 80  | HIS  |
| 34  | L     | 128 | ASN  |
| 34  | L     | 130 | HIS  |
| 36  | N     | 4   | ASN  |
| 38  | P     | 9   | GLN  |
| 38  | P     | 11  | ASN  |
| 39  | Q     | 38  | GLN  |
| 40  | R     | 66  | ASN  |
| 41  | S     | 72  | ASN  |
| 42  | T     | 11  | GLN  |
| 42  | T     | 91  | GLN  |
| 43  | U     | 57  | ASN  |
| 43  | U     | 61  | ASN  |
| 44  | V     | 91  | GLN  |
| 44  | V     | 92  | ASN  |
| 46  | X     | 5   | ASN  |
| 46  | X     | 12  | GLN  |
| 47  | Y     | 50  | ASN  |
| 51  | 3     | 20  | ASN  |
| 53  | 5     | 45  | GLN  |
| 56  | 8     | 13  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | a     | 1526/1542 (98%) | 220 (14%)         | 0               |
| 22  | x     | 72/76 (94%)     | 24 (33%)          | 0               |
| 23  | z     | 7/21 (33%)      | 1 (14%)           | 0               |
| 25  | A     | 2897/2904 (99%) | 376 (12%)         | 14 (0%)         |
| 26  | B     | 119/120 (99%)   | 11 (9%)           | 1 (0%)          |
| All | All   | 4621/4663 (99%) | 632 (13%)         | 15 (0%)         |

All (632) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 4   | U    |
| 1   | a     | 5   | U    |
| 1   | a     | 6   | G    |
| 1   | a     | 8   | A    |
| 1   | a     | 32  | A    |
| 1   | a     | 39  | G    |
| 1   | a     | 44  | A    |
| 1   | a     | 47  | C    |
| 1   | a     | 48  | C    |
| 1   | a     | 51  | A    |
| 1   | a     | 71  | A    |
| 1   | a     | 74  | A    |
| 1   | a     | 77  | A    |
| 1   | a     | 79  | G    |
| 1   | a     | 80  | A    |
| 1   | a     | 82  | G    |
| 1   | a     | 85  | U    |
| 1   | a     | 86  | G    |
| 1   | a     | 87  | C    |
| 1   | a     | 92  | U    |
| 1   | a     | 93  | U    |
| 1   | a     | 94  | G    |
| 1   | a     | 95  | C    |
| 1   | a     | 121 | U    |
| 1   | a     | 130 | A    |
| 1   | a     | 131 | A    |
| 1   | a     | 163 | C    |
| 1   | a     | 174 | A    |
| 1   | a     | 184 | G    |
| 1   | a     | 189 | A    |
| 1   | a     | 197 | A    |
| 1   | a     | 208 | U    |
| 1   | a     | 209 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 210 | C    |
| 1   | a     | 211 | G    |
| 1   | a     | 212 | G    |
| 1   | a     | 240 | G    |
| 1   | a     | 245 | U    |
| 1   | a     | 247 | G    |
| 1   | a     | 251 | G    |
| 1   | a     | 266 | G    |
| 1   | a     | 267 | C    |
| 1   | a     | 269 | C    |
| 1   | a     | 280 | C    |
| 1   | a     | 281 | G    |
| 1   | a     | 289 | G    |
| 1   | a     | 321 | A    |
| 1   | a     | 328 | C    |
| 1   | a     | 344 | A    |
| 1   | a     | 345 | C    |
| 1   | a     | 347 | G    |
| 1   | a     | 352 | C    |
| 1   | a     | 354 | G    |
| 1   | a     | 367 | U    |
| 1   | a     | 372 | C    |
| 1   | a     | 373 | A    |
| 1   | a     | 384 | G    |
| 1   | a     | 406 | G    |
| 1   | a     | 408 | A    |
| 1   | a     | 411 | A    |
| 1   | a     | 412 | A    |
| 1   | a     | 413 | G    |
| 1   | a     | 414 | A    |
| 1   | a     | 415 | A    |
| 1   | a     | 421 | U    |
| 1   | a     | 422 | C    |
| 1   | a     | 423 | G    |
| 1   | a     | 424 | G    |
| 1   | a     | 428 | G    |
| 1   | a     | 429 | U    |
| 1   | a     | 448 | A    |
| 1   | a     | 451 | A    |
| 1   | a     | 462 | G    |
| 1   | a     | 467 | U    |
| 1   | a     | 468 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 478 | A    |
| 1   | a     | 479 | U    |
| 1   | a     | 481 | G    |
| 1   | a     | 482 | A    |
| 1   | a     | 484 | G    |
| 1   | a     | 486 | U    |
| 1   | a     | 490 | C    |
| 1   | a     | 495 | A    |
| 1   | a     | 496 | A    |
| 1   | a     | 497 | G    |
| 1   | a     | 509 | A    |
| 1   | a     | 511 | C    |
| 1   | a     | 518 | C    |
| 1   | a     | 521 | G    |
| 1   | a     | 527 | G7M  |
| 1   | a     | 532 | A    |
| 1   | a     | 547 | A    |
| 1   | a     | 564 | C    |
| 1   | a     | 573 | A    |
| 1   | a     | 575 | G    |
| 1   | a     | 576 | C    |
| 1   | a     | 577 | G    |
| 1   | a     | 588 | G    |
| 1   | a     | 633 | G    |
| 1   | a     | 650 | G    |
| 1   | a     | 656 | G    |
| 1   | a     | 665 | A    |
| 1   | a     | 673 | A    |
| 1   | a     | 703 | G    |
| 1   | a     | 723 | U    |
| 1   | a     | 724 | G    |
| 1   | a     | 755 | G    |
| 1   | a     | 777 | A    |
| 1   | a     | 792 | A    |
| 1   | a     | 793 | U    |
| 1   | a     | 794 | A    |
| 1   | a     | 815 | A    |
| 1   | a     | 817 | C    |
| 1   | a     | 818 | G    |
| 1   | a     | 821 | G    |
| 1   | a     | 829 | G    |
| 1   | a     | 851 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 890  | G    |
| 1   | a     | 914  | A    |
| 1   | a     | 926  | G    |
| 1   | a     | 929  | G    |
| 1   | a     | 930  | C    |
| 1   | a     | 934  | C    |
| 1   | a     | 935  | A    |
| 1   | a     | 960  | U    |
| 1   | a     | 966  | 2MG  |
| 1   | a     | 969  | A    |
| 1   | a     | 975  | A    |
| 1   | a     | 976  | G    |
| 1   | a     | 977  | A    |
| 1   | a     | 978  | A    |
| 1   | a     | 980  | C    |
| 1   | a     | 992  | U    |
| 1   | a     | 993  | G    |
| 1   | a     | 994  | A    |
| 1   | a     | 1003 | G    |
| 1   | a     | 1004 | A    |
| 1   | a     | 1009 | U    |
| 1   | a     | 1017 | U    |
| 1   | a     | 1022 | A    |
| 1   | a     | 1024 | G    |
| 1   | a     | 1027 | C    |
| 1   | a     | 1028 | C    |
| 1   | a     | 1029 | U    |
| 1   | a     | 1030 | U    |
| 1   | a     | 1032 | G    |
| 1   | a     | 1033 | G    |
| 1   | a     | 1035 | A    |
| 1   | a     | 1041 | G    |
| 1   | a     | 1042 | A    |
| 1   | a     | 1044 | A    |
| 1   | a     | 1045 | C    |
| 1   | a     | 1053 | G    |
| 1   | a     | 1065 | U    |
| 1   | a     | 1094 | G    |
| 1   | a     | 1095 | U    |
| 1   | a     | 1101 | A    |
| 1   | a     | 1130 | A    |
| 1   | a     | 1136 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1137 | C    |
| 1   | a     | 1138 | G    |
| 1   | a     | 1139 | G    |
| 1   | a     | 1152 | A    |
| 1   | a     | 1159 | U    |
| 1   | a     | 1167 | A    |
| 1   | a     | 1193 | G    |
| 1   | a     | 1196 | A    |
| 1   | a     | 1197 | A    |
| 1   | a     | 1204 | A    |
| 1   | a     | 1206 | G    |
| 1   | a     | 1213 | A    |
| 1   | a     | 1227 | A    |
| 1   | a     | 1238 | A    |
| 1   | a     | 1258 | G    |
| 1   | a     | 1260 | G    |
| 1   | a     | 1266 | G    |
| 1   | a     | 1267 | C    |
| 1   | a     | 1274 | A    |
| 1   | a     | 1275 | A    |
| 1   | a     | 1280 | A    |
| 1   | a     | 1285 | A    |
| 1   | a     | 1287 | A    |
| 1   | a     | 1300 | G    |
| 1   | a     | 1301 | U    |
| 1   | a     | 1302 | C    |
| 1   | a     | 1304 | G    |
| 1   | a     | 1305 | G    |
| 1   | a     | 1319 | A    |
| 1   | a     | 1320 | C    |
| 1   | a     | 1321 | U    |
| 1   | a     | 1332 | A    |
| 1   | a     | 1335 | U    |
| 1   | a     | 1340 | A    |
| 1   | a     | 1346 | A    |
| 1   | a     | 1357 | A    |
| 1   | a     | 1360 | A    |
| 1   | a     | 1361 | G    |
| 1   | a     | 1362 | A    |
| 1   | a     | 1363 | A    |
| 1   | a     | 1370 | G    |
| 1   | a     | 1378 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1379 | G    |
| 1   | a     | 1388 | C    |
| 1   | a     | 1397 | C    |
| 1   | a     | 1398 | A    |
| 1   | a     | 1402 | 4OC  |
| 1   | a     | 1419 | G    |
| 1   | a     | 1441 | A    |
| 1   | a     | 1446 | A    |
| 1   | a     | 1448 | C    |
| 1   | a     | 1452 | C    |
| 1   | a     | 1454 | G    |
| 1   | a     | 1474 | U    |
| 1   | a     | 1475 | G    |
| 1   | a     | 1499 | A    |
| 1   | a     | 1503 | A    |
| 1   | a     | 1506 | U    |
| 1   | a     | 1517 | G    |
| 1   | a     | 1529 | G    |
| 1   | a     | 1530 | G    |
| 22  | x     | 9    | A    |
| 22  | x     | 10   | G    |
| 22  | x     | 11   | C    |
| 22  | x     | 19   | G    |
| 22  | x     | 20   | U    |
| 22  | x     | 21   | A    |
| 22  | x     | 24   | G    |
| 22  | x     | 26   | A    |
| 22  | x     | 29   | G    |
| 22  | x     | 30   | G    |
| 22  | x     | 34   | G    |
| 22  | x     | 35   | A    |
| 22  | x     | 37   | MIA  |
| 22  | x     | 38   | A    |
| 22  | x     | 44   | G    |
| 22  | x     | 46   | G7M  |
| 22  | x     | 48   | C    |
| 22  | x     | 52   | G    |
| 22  | x     | 55   | PSU  |
| 22  | x     | 56   | C    |
| 22  | x     | 58   | A    |
| 22  | x     | 60   | U    |
| 22  | x     | 73   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | x     | 76  | A    |
| 23  | z     | 17  | U    |
| 25  | A     | 4   | U    |
| 25  | A     | 6   | A    |
| 25  | A     | 10  | A    |
| 25  | A     | 34  | U    |
| 25  | A     | 35  | G    |
| 25  | A     | 45  | G    |
| 25  | A     | 51  | G    |
| 25  | A     | 71  | A    |
| 25  | A     | 74  | A    |
| 25  | A     | 75  | G    |
| 25  | A     | 84  | A    |
| 25  | A     | 100 | U    |
| 25  | A     | 101 | A    |
| 25  | A     | 118 | A    |
| 25  | A     | 120 | U    |
| 25  | A     | 139 | U    |
| 25  | A     | 141 | G    |
| 25  | A     | 142 | A    |
| 25  | A     | 165 | A    |
| 25  | A     | 181 | A    |
| 25  | A     | 196 | A    |
| 25  | A     | 199 | A    |
| 25  | A     | 215 | G    |
| 25  | A     | 216 | A    |
| 25  | A     | 221 | A    |
| 25  | A     | 222 | A    |
| 25  | A     | 233 | A    |
| 25  | A     | 248 | G    |
| 25  | A     | 269 | C    |
| 25  | A     | 271 | G    |
| 25  | A     | 275 | C    |
| 25  | A     | 277 | G    |
| 25  | A     | 278 | A    |
| 25  | A     | 279 | A    |
| 25  | A     | 281 | C    |
| 25  | A     | 285 | G    |
| 25  | A     | 288 | U    |
| 25  | A     | 291 | G    |
| 25  | A     | 311 | A    |
| 25  | A     | 329 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | A     | 330 | A    |
| 25  | A     | 346 | A    |
| 25  | A     | 353 | C    |
| 25  | A     | 362 | A    |
| 25  | A     | 367 | G    |
| 25  | A     | 386 | G    |
| 25  | A     | 396 | G    |
| 25  | A     | 404 | A    |
| 25  | A     | 405 | U    |
| 25  | A     | 411 | G    |
| 25  | A     | 412 | A    |
| 25  | A     | 428 | A    |
| 25  | A     | 435 | C    |
| 25  | A     | 481 | G    |
| 25  | A     | 491 | G    |
| 25  | A     | 504 | A    |
| 25  | A     | 505 | A    |
| 25  | A     | 509 | C    |
| 25  | A     | 510 | C    |
| 25  | A     | 530 | G    |
| 25  | A     | 531 | C    |
| 25  | A     | 532 | A    |
| 25  | A     | 545 | U    |
| 25  | A     | 546 | U    |
| 25  | A     | 547 | A    |
| 25  | A     | 549 | G    |
| 25  | A     | 563 | A    |
| 25  | A     | 573 | U    |
| 25  | A     | 575 | A    |
| 25  | A     | 603 | A    |
| 25  | A     | 615 | U    |
| 25  | A     | 627 | A    |
| 25  | A     | 631 | A    |
| 25  | A     | 637 | A    |
| 25  | A     | 645 | C    |
| 25  | A     | 646 | U    |
| 25  | A     | 647 | G    |
| 25  | A     | 653 | U    |
| 25  | A     | 654 | A    |
| 25  | A     | 655 | A    |
| 25  | A     | 686 | U    |
| 25  | A     | 710 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | A     | 714 | U    |
| 25  | A     | 715 | A    |
| 25  | A     | 717 | C    |
| 25  | A     | 729 | G    |
| 25  | A     | 730 | A    |
| 25  | A     | 740 | C    |
| 25  | A     | 747 | 5MU  |
| 25  | A     | 748 | G    |
| 25  | A     | 764 | A    |
| 25  | A     | 775 | G    |
| 25  | A     | 776 | G    |
| 25  | A     | 782 | A    |
| 25  | A     | 784 | G    |
| 25  | A     | 785 | G    |
| 25  | A     | 789 | A    |
| 25  | A     | 805 | G    |
| 25  | A     | 812 | C    |
| 25  | A     | 827 | U    |
| 25  | A     | 828 | U    |
| 25  | A     | 830 | G    |
| 25  | A     | 846 | U    |
| 25  | A     | 859 | G    |
| 25  | A     | 878 | A    |
| 25  | A     | 879 | G    |
| 25  | A     | 888 | C    |
| 25  | A     | 891 | G    |
| 25  | A     | 895 | U    |
| 25  | A     | 896 | A    |
| 25  | A     | 897 | C    |
| 25  | A     | 907 | G    |
| 25  | A     | 910 | A    |
| 25  | A     | 915 | C    |
| 25  | A     | 927 | A    |
| 25  | A     | 931 | U    |
| 25  | A     | 938 | G    |
| 25  | A     | 946 | C    |
| 25  | A     | 957 | C    |
| 25  | A     | 961 | C    |
| 25  | A     | 974 | G    |
| 25  | A     | 983 | A    |
| 25  | A     | 990 | A    |
| 25  | A     | 996 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | A     | 1005 | C    |
| 25  | A     | 1009 | A    |
| 25  | A     | 1012 | U    |
| 25  | A     | 1013 | C    |
| 25  | A     | 1026 | G    |
| 25  | A     | 1032 | A    |
| 25  | A     | 1033 | U    |
| 25  | A     | 1039 | A    |
| 25  | A     | 1045 | C    |
| 25  | A     | 1046 | A    |
| 25  | A     | 1047 | G    |
| 25  | A     | 1059 | G    |
| 25  | A     | 1060 | U    |
| 25  | A     | 1061 | U    |
| 25  | A     | 1062 | G    |
| 25  | A     | 1064 | C    |
| 25  | A     | 1065 | U    |
| 25  | A     | 1067 | A    |
| 25  | A     | 1068 | G    |
| 25  | A     | 1069 | A    |
| 25  | A     | 1070 | A    |
| 25  | A     | 1071 | G    |
| 25  | A     | 1076 | C    |
| 25  | A     | 1081 | U    |
| 25  | A     | 1082 | U    |
| 25  | A     | 1084 | A    |
| 25  | A     | 1085 | A    |
| 25  | A     | 1087 | G    |
| 25  | A     | 1088 | A    |
| 25  | A     | 1090 | A    |
| 25  | A     | 1097 | U    |
| 25  | A     | 1103 | A    |
| 25  | A     | 1104 | C    |
| 25  | A     | 1106 | G    |
| 25  | A     | 1111 | A    |
| 25  | A     | 1112 | G    |
| 25  | A     | 1132 | U    |
| 25  | A     | 1135 | C    |
| 25  | A     | 1142 | A    |
| 25  | A     | 1212 | G    |
| 25  | A     | 1250 | G    |
| 25  | A     | 1253 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | A     | 1255 | U    |
| 25  | A     | 1256 | G    |
| 25  | A     | 1257 | C    |
| 25  | A     | 1268 | A    |
| 25  | A     | 1271 | G    |
| 25  | A     | 1272 | A    |
| 25  | A     | 1288 | G    |
| 25  | A     | 1300 | G    |
| 25  | A     | 1301 | A    |
| 25  | A     | 1329 | U    |
| 25  | A     | 1338 | G    |
| 25  | A     | 1365 | A    |
| 25  | A     | 1379 | U    |
| 25  | A     | 1383 | A    |
| 25  | A     | 1386 | C    |
| 25  | A     | 1416 | G    |
| 25  | A     | 1428 | C    |
| 25  | A     | 1452 | G    |
| 25  | A     | 1459 | G    |
| 25  | A     | 1482 | G    |
| 25  | A     | 1493 | C    |
| 25  | A     | 1497 | U    |
| 25  | A     | 1509 | A    |
| 25  | A     | 1510 | G    |
| 25  | A     | 1515 | A    |
| 25  | A     | 1524 | G    |
| 25  | A     | 1535 | A    |
| 25  | A     | 1536 | C    |
| 25  | A     | 1537 | G    |
| 25  | A     | 1566 | A    |
| 25  | A     | 1569 | A    |
| 25  | A     | 1578 | U    |
| 25  | A     | 1584 | U    |
| 25  | A     | 1585 | C    |
| 25  | A     | 1606 | C    |
| 25  | A     | 1608 | A    |
| 25  | A     | 1647 | U    |
| 25  | A     | 1648 | U    |
| 25  | A     | 1674 | G    |
| 25  | A     | 1676 | A    |
| 25  | A     | 1715 | G    |
| 25  | A     | 1729 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | A     | 1730 | C    |
| 25  | A     | 1733 | G    |
| 25  | A     | 1738 | G    |
| 25  | A     | 1744 | A    |
| 25  | A     | 1757 | A    |
| 25  | A     | 1764 | C    |
| 25  | A     | 1773 | A    |
| 25  | A     | 1800 | C    |
| 25  | A     | 1801 | A    |
| 25  | A     | 1808 | A    |
| 25  | A     | 1816 | C    |
| 25  | A     | 1829 | A    |
| 25  | A     | 1848 | A    |
| 25  | A     | 1858 | A    |
| 25  | A     | 1866 | A    |
| 25  | A     | 1872 | A    |
| 25  | A     | 1879 | C    |
| 25  | A     | 1907 | G    |
| 25  | A     | 1913 | A    |
| 25  | A     | 1914 | C    |
| 25  | A     | 1922 | G    |
| 25  | A     | 1926 | U    |
| 25  | A     | 1927 | A    |
| 25  | A     | 1930 | G    |
| 25  | A     | 1937 | A    |
| 25  | A     | 1938 | A    |
| 25  | A     | 1955 | U    |
| 25  | A     | 1966 | A    |
| 25  | A     | 1967 | C    |
| 25  | A     | 1970 | A    |
| 25  | A     | 1971 | U    |
| 25  | A     | 1972 | G    |
| 25  | A     | 1991 | U    |
| 25  | A     | 1993 | U    |
| 25  | A     | 2021 | C    |
| 25  | A     | 2023 | C    |
| 25  | A     | 2031 | A    |
| 25  | A     | 2033 | A    |
| 25  | A     | 2034 | U    |
| 25  | A     | 2043 | C    |
| 25  | A     | 2044 | C    |
| 25  | A     | 2055 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | A     | 2056 | G    |
| 25  | A     | 2060 | A    |
| 25  | A     | 2061 | G    |
| 25  | A     | 2069 | G7M  |
| 25  | A     | 2093 | G    |
| 25  | A     | 2096 | C    |
| 25  | A     | 2098 | U    |
| 25  | A     | 2100 | G    |
| 25  | A     | 2108 | A    |
| 25  | A     | 2110 | G    |
| 25  | A     | 2111 | U    |
| 25  | A     | 2112 | G    |
| 25  | A     | 2113 | U    |
| 25  | A     | 2114 | A    |
| 25  | A     | 2118 | U    |
| 25  | A     | 2119 | A    |
| 25  | A     | 2123 | G    |
| 25  | A     | 2131 | U    |
| 25  | A     | 2132 | U    |
| 25  | A     | 2133 | G    |
| 25  | A     | 2136 | G    |
| 25  | A     | 2145 | C    |
| 25  | A     | 2146 | C    |
| 25  | A     | 2147 | A    |
| 25  | A     | 2157 | G    |
| 25  | A     | 2161 | C    |
| 25  | A     | 2162 | G    |
| 25  | A     | 2164 | C    |
| 25  | A     | 2165 | C    |
| 25  | A     | 2167 | U    |
| 25  | A     | 2170 | A    |
| 25  | A     | 2172 | U    |
| 25  | A     | 2173 | A    |
| 25  | A     | 2174 | C    |
| 25  | A     | 2176 | A    |
| 25  | A     | 2178 | C    |
| 25  | A     | 2180 | U    |
| 25  | A     | 2190 | G    |
| 25  | A     | 2192 | U    |
| 25  | A     | 2198 | A    |
| 25  | A     | 2204 | G    |
| 25  | A     | 2211 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | A     | 2225 | A    |
| 25  | A     | 2238 | G    |
| 25  | A     | 2239 | G    |
| 25  | A     | 2252 | G    |
| 25  | A     | 2266 | A    |
| 25  | A     | 2279 | G    |
| 25  | A     | 2283 | C    |
| 25  | A     | 2287 | A    |
| 25  | A     | 2288 | A    |
| 25  | A     | 2305 | U    |
| 25  | A     | 2308 | G    |
| 25  | A     | 2309 | A    |
| 25  | A     | 2310 | C    |
| 25  | A     | 2322 | A    |
| 25  | A     | 2325 | G    |
| 25  | A     | 2333 | A    |
| 25  | A     | 2334 | U    |
| 25  | A     | 2335 | A    |
| 25  | A     | 2345 | G    |
| 25  | A     | 2350 | C    |
| 25  | A     | 2361 | G    |
| 25  | A     | 2383 | G    |
| 25  | A     | 2385 | C    |
| 25  | A     | 2401 | U    |
| 25  | A     | 2402 | U    |
| 25  | A     | 2406 | A    |
| 25  | A     | 2424 | C    |
| 25  | A     | 2425 | A    |
| 25  | A     | 2429 | G    |
| 25  | A     | 2441 | U    |
| 25  | A     | 2447 | G    |
| 25  | A     | 2448 | A    |
| 25  | A     | 2469 | A    |
| 25  | A     | 2470 | G    |
| 25  | A     | 2474 | U    |
| 25  | A     | 2476 | A    |
| 25  | A     | 2477 | U    |
| 25  | A     | 2492 | U    |
| 25  | A     | 2502 | G    |
| 25  | A     | 2504 | PSU  |
| 25  | A     | 2505 | G    |
| 25  | A     | 2518 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | A     | 2520 | C    |
| 25  | A     | 2529 | G    |
| 25  | A     | 2547 | A    |
| 25  | A     | 2566 | A    |
| 25  | A     | 2567 | G    |
| 25  | A     | 2576 | G    |
| 25  | A     | 2585 | U    |
| 25  | A     | 2602 | A    |
| 25  | A     | 2609 | U    |
| 25  | A     | 2613 | U    |
| 25  | A     | 2615 | U    |
| 25  | A     | 2629 | U    |
| 25  | A     | 2630 | G    |
| 25  | A     | 2661 | G    |
| 25  | A     | 2663 | G    |
| 25  | A     | 2669 | G    |
| 25  | A     | 2689 | U    |
| 25  | A     | 2690 | U    |
| 25  | A     | 2714 | G    |
| 25  | A     | 2718 | G    |
| 25  | A     | 2726 | A    |
| 25  | A     | 2729 | G    |
| 25  | A     | 2733 | A    |
| 25  | A     | 2744 | G    |
| 25  | A     | 2748 | A    |
| 25  | A     | 2751 | G    |
| 25  | A     | 2765 | A    |
| 25  | A     | 2778 | A    |
| 25  | A     | 2797 | U    |
| 25  | A     | 2798 | U    |
| 25  | A     | 2800 | A    |
| 25  | A     | 2820 | A    |
| 25  | A     | 2821 | A    |
| 25  | A     | 2836 | U    |
| 25  | A     | 2849 | U    |
| 25  | A     | 2861 | U    |
| 25  | A     | 2873 | A    |
| 25  | A     | 2880 | C    |
| 25  | A     | 2884 | U    |
| 25  | A     | 2885 | G    |
| 25  | A     | 2886 | A    |
| 25  | A     | 2902 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | B     | 4   | C    |
| 26  | B     | 35  | C    |
| 26  | B     | 42  | C    |
| 26  | B     | 44  | G    |
| 26  | B     | 45  | A    |
| 26  | B     | 56  | G    |
| 26  | B     | 66  | A    |
| 26  | B     | 68  | C    |
| 26  | B     | 89  | U    |
| 26  | B     | 91  | C    |
| 26  | B     | 109 | A    |

All (15) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | A     | 3    | U    |
| 25  | A     | 277  | G    |
| 25  | A     | 784  | G    |
| 25  | A     | 1026 | G    |
| 25  | A     | 1031 | G    |
| 25  | A     | 1081 | U    |
| 25  | A     | 1084 | A    |
| 25  | A     | 1111 | A    |
| 25  | A     | 1328 | A    |
| 25  | A     | 1583 | A    |
| 25  | A     | 2189 | U    |
| 25  | A     | 2191 | A    |
| 25  | A     | 2473 | U    |
| 25  | A     | 2799 | A    |
| 26  | B     | 3    | C    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5MC  | a     | 967  | 1     | 19,22,23     | 1.62 | 3 (15%)  | 26,32,35    | 1.12 | 2 (7%)   |
| 25  | 6MZ  | A     | 1618 | 25    | 22,25,26     | 1.45 | 5 (22%)  | 29,36,39    | 2.27 | 9 (31%)  |
| 1   | MA6  | a     | 1519 | 1     | 23,26,27     | 1.50 | 5 (21%)  | 33,38,41    | 2.43 | 14 (42%) |
| 22  | PSU  | x     | 32   | 22    | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.02 | 3 (14%)  |
| 22  | PSU  | x     | 39   | 22    | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 2.12 | 4 (19%)  |
| 25  | PSU  | A     | 746  | 57,25 | 18,21,22     | 1.39 | 3 (16%)  | 21,30,33    | 2.06 | 4 (19%)  |
| 25  | 5MU  | A     | 1939 | 25    | 19,22,23     | 1.37 | 5 (26%)  | 27,32,35    | 2.16 | 6 (22%)  |
| 25  | OMC  | A     | 2498 | 57,25 | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.96 | 1 (4%)   |
| 25  | PSU  | A     | 1917 | 25    | 18,21,22     | 1.44 | 3 (16%)  | 21,30,33    | 2.05 | 3 (14%)  |
| 1   | 4OC  | a     | 1402 | 1     | 20,23,24     | 0.76 | 0        | 25,32,35    | 0.94 | 1 (4%)   |
| 22  | G7M  | x     | 46   | 22    | 23,26,27     | 2.37 | 5 (21%)  | 34,39,42    | 3.07 | 11 (32%) |
| 25  | 6MZ  | A     | 2030 | 25    | 22,25,26     | 1.44 | 5 (22%)  | 29,36,39    | 2.37 | 10 (34%) |
| 25  | 5MC  | A     | 1962 | 25    | 19,22,23     | 1.43 | 3 (15%)  | 26,32,35    | 1.13 | 2 (7%)   |
| 1   | 5MC  | a     | 1407 | 1     | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.15 | 3 (11%)  |
| 25  | PSU  | A     | 2504 | 25    | 18,21,22     | 1.37 | 3 (16%)  | 21,30,33    | 2.01 | 4 (19%)  |
| 22  | 5MU  | x     | 54   | 22    | 19,22,23     | 1.37 | 5 (26%)  | 27,32,35    | 2.00 | 6 (22%)  |
| 1   | MA6  | a     | 1518 | 1     | 23,26,27     | 1.48 | 4 (17%)  | 33,38,41    | 2.44 | 14 (42%) |
| 1   | PSU  | a     | 516  | 1     | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 37  | 4D4  | O     | 81   | 37    | 9,11,12      | 2.73 | 3 (33%)  | 7,13,15     | 0.92 | 0        |
| 11  | IAS  | k     | 119  | 11    | 6,7,8        | 0.98 | 0        | 3,8,10      | 1.51 | 1 (33%)  |
| 25  | OMU  | A     | 2552 | 25    | 19,22,23     | 1.26 | 3 (15%)  | 25,31,34    | 1.84 | 5 (20%)  |
| 1   | 2MG  | a     | 966  | 1     | 23,26,27     | 1.25 | 4 (17%)  | 33,38,41    | 2.19 | 7 (21%)  |
| 37  | MS6  | O     | 82   | 37    | 5,7,8        | 0.51 | 0        | 2,7,9       | 1.12 | 0        |
| 1   | G7M  | a     | 527  | 1     | 23,26,27     | 1.56 | 3 (13%)  | 34,39,42    | 1.77 | 5 (14%)  |
| 25  | 2MA  | A     | 2503 | 25    | 22,25,26     | 1.51 | 4 (18%)  | 32,37,40    | 2.31 | 8 (25%)  |
| 22  | MIA  | x     | 37   | 22    | 28,31,32     | 2.37 | 6 (21%)  | 38,44,47    | 2.77 | 14 (36%) |
| 25  | 1MG  | A     | 745  | 25    | 23,26,27     | 1.18 | 3 (13%)  | 33,39,42    | 1.74 | 5 (15%)  |
| 25  | PSU  | A     | 2580 | 25    | 18,21,22     | 1.41 | 4 (22%)  | 21,30,33    | 2.12 | 4 (19%)  |
| 25  | H2U  | A     | 2449 | 25    | 18,21,22     | 1.04 | 2 (11%)  | 19,30,33    | 1.00 | 2 (10%)  |
| 22  | PSU  | x     | 55   | 22    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 2.00 | 3 (14%)  |
| 1   | 2MG  | a     | 1516 | 1     | 23,26,27     | 1.25 | 3 (13%)  | 33,38,41    | 2.15 | 7 (21%)  |
| 1   | 2MG  | a     | 1207 | 1     | 23,26,27     | 1.24 | 4 (17%)  | 33,38,41    | 2.23 | 8 (24%)  |
| 25  | 3TD  | A     | 1915 | 25    | 19,22,23     | 4.26 | 7 (36%)  | 23,32,35    | 1.82 | 3 (13%)  |
| 28  | MEQ  | D     | 150  | 28    | 8,9,10       | 0.51 | 0        | 5,10,12     | 0.22 | 0        |
| 25  | G7M  | A     | 2069 | 25    | 23,26,27     | 1.55 | 3 (13%)  | 34,39,42    | 1.72 | 5 (14%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | UR3  | a     | 1498 | 1    | 19,22,23     | 0.98 | 0        | 26,32,35    | 1.74 | 2 (7%)   |
| 25  | 5MU  | A     | 747  | 25   | 19,22,23     | 1.38 | 4 (21%)  | 27,32,35    | 2.21 | 6 (22%)  |
| 25  | PSU  | A     | 955  | 25   | 18,21,22     | 1.43 | 4 (22%)  | 21,30,33    | 2.08 | 3 (14%)  |
| 25  | 2MG  | A     | 2445 | 25   | 23,26,27     | 1.27 | 4 (17%)  | 33,38,41    | 2.21 | 8 (24%)  |
| 25  | PSU  | A     | 2457 | 25   | 18,21,22     | 1.39 | 3 (16%)  | 21,30,33    | 2.14 | 5 (23%)  |
| 25  | PSU  | A     | 2604 | 25   | 18,21,22     | 1.40 | 4 (22%)  | 21,30,33    | 2.03 | 4 (19%)  |
| 12  | D2T  | l     | 89   | 12   | 8,9,10       | 2.35 | 1 (12%)  | 6,11,13     | 2.23 | 2 (33%)  |
| 22  | 4SU  | x     | 8    | 22   | 18,21,22     | 1.83 | 5 (27%)  | 25,30,33    | 2.34 | 5 (20%)  |
| 25  | PSU  | A     | 1911 | 25   | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 25  | OMG  | A     | 2251 | 25   | 23,26,27     | 1.19 | 3 (13%)  | 32,38,41    | 1.97 | 5 (15%)  |
| 25  | PSU  | A     | 2605 | 25   | 18,21,22     | 1.39 | 3 (16%)  | 21,30,33    | 2.04 | 4 (19%)  |
| 25  | 2MG  | A     | 1835 | 25   | 23,26,27     | 1.27 | 4 (17%)  | 33,38,41    | 2.16 | 6 (18%)  |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | 5MC  | a     | 967  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | 6MZ  | A     | 1618 | 25    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | MA6  | a     | 1519 | 1     | -       | 3/11/29/30 | 0/3/3/3 |
| 22  | PSU  | x     | 32   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | PSU  | x     | 39   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | PSU  | A     | 746  | 57,25 | -       | 1/7/25/26  | 0/2/2/2 |
| 25  | 5MU  | A     | 1939 | 25    | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | OMC  | A     | 2498 | 57,25 | -       | 1/9/27/28  | 0/2/2/2 |
| 25  | PSU  | A     | 1917 | 25    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | a     | 1402 | 1     | -       | 3/9/29/30  | 0/2/2/2 |
| 22  | G7M  | x     | 46   | 22    | -       | 1/7/25/26  | 0/3/3/3 |
| 25  | 6MZ  | A     | 2030 | 25    | -       | 2/9/27/28  | 0/3/3/3 |
| 25  | 5MC  | A     | 1962 | 25    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | a     | 1407 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | PSU  | A     | 2504 | 25    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 5MU  | x     | 54   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | a     | 1518 | 1     | -       | 1/11/29/30 | 0/3/3/3 |
| 1   | PSU  | a     | 516  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 37  | 4D4  | O     | 81   | 37    | -       | 8/11/12/14 | -       |
| 11  | IAS  | k     | 119  | 11    | -       | 0/7/7/8    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 25  | OMU  | A     | 2552 | 25   | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | 2MG  | a     | 966  | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 37  | MS6  | O     | 82   | 37   | -       | 3/4/6/8    | -       |
| 1   | G7M  | a     | 527  | 1    | -       | 1/7/25/26  | 0/3/3/3 |
| 25  | 2MA  | A     | 2503 | 25   | -       | 0/7/25/26  | 0/3/3/3 |
| 22  | MIA  | x     | 37   | 22   | -       | 4/15/33/34 | 0/3/3/3 |
| 25  | 1MG  | A     | 745  | 25   | -       | 0/7/25/26  | 0/3/3/3 |
| 25  | PSU  | A     | 2580 | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | H2U  | A     | 2449 | 25   | -       | 0/7/38/39  | 0/2/2/2 |
| 22  | PSU  | x     | 55   | 22   | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | a     | 1516 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 2MG  | a     | 1207 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 25  | 3TD  | A     | 1915 | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | MEQ  | D     | 150  | 28   | -       | 2/8/9/11   | -       |
| 25  | G7M  | A     | 2069 | 25   | -       | 3/7/25/26  | 0/3/3/3 |
| 1   | UR3  | a     | 1498 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | 5MU  | A     | 747  | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | PSU  | A     | 955  | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | 2MG  | A     | 2445 | 25   | -       | 0/9/27/28  | 0/3/3/3 |
| 25  | PSU  | A     | 2457 | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | PSU  | A     | 2604 | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 12  | D2T  | l     | 89   | 12   | -       | 1/7/12/14  | -       |
| 22  | 4SU  | x     | 8    | 22   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | PSU  | A     | 1911 | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | OMG  | A     | 2251 | 25   | -       | 0/9/27/28  | 0/3/3/3 |
| 25  | PSU  | A     | 2605 | 25   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | 2MG  | A     | 1835 | 25   | -       | 0/9/27/28  | 0/3/3/3 |

All (146) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | A     | 1915 | 3TD  | C6-C5   | 12.62 | 1.49        | 1.35     |
| 25  | A     | 1915 | 3TD  | C2-N1   | 9.92  | 1.49        | 1.37     |
| 22  | x     | 46   | G7M  | C8-N7   | 7.82  | 1.46        | 1.33     |
| 22  | x     | 37   | MIA  | C2-S10  | -7.34 | 1.69        | 1.75     |
| 22  | x     | 37   | MIA  | C13-C14 | 6.78  | 1.52        | 1.32     |
| 37  | O     | 81   | 4D4  | CZ-NE   | 6.41  | 1.45        | 1.33     |
| 12  | l     | 89   | D2T  | CB-CA   | -5.99 | 1.52        | 1.54     |
| 25  | A     | 1915 | 3TD  | C6-N1   | 5.90  | 1.46        | 1.36     |
| 1   | a     | 1407 | 5MC  | C5-C4   | 5.88  | 1.48        | 1.44     |
| 1   | a     | 967  | 5MC  | C5-C4   | 5.79  | 1.48        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 25  | A     | 2069 | G7M  | C5-N7  | -5.12 | 1.33        | 1.39     |
| 25  | A     | 1915 | 3TD  | C2-N3  | 5.08  | 1.49        | 1.38     |
| 1   | a     | 527  | G7M  | C5-N7  | -5.04 | 1.33        | 1.39     |
| 22  | x     | 8    | 4SU  | C4-S4  | -4.98 | 1.59        | 1.68     |
| 25  | A     | 1962 | 5MC  | C5-C4  | 4.95  | 1.47        | 1.44     |
| 22  | x     | 37   | MIA  | C5-C4  | 4.76  | 1.47        | 1.39     |
| 1   | a     | 1518 | MA6  | C5-C4  | 4.62  | 1.47        | 1.39     |
| 1   | a     | 1519 | MA6  | C5-C4  | 4.58  | 1.47        | 1.39     |
| 25  | A     | 2503 | 2MA  | C5-C4  | 4.57  | 1.47        | 1.39     |
| 22  | x     | 46   | G7M  | C5-N7  | -4.39 | 1.34        | 1.39     |
| 25  | A     | 1618 | 6MZ  | C5-C4  | 4.38  | 1.46        | 1.39     |
| 25  | A     | 2030 | 6MZ  | C5-C4  | 4.22  | 1.46        | 1.39     |
| 22  | x     | 46   | G7M  | C8-N9  | 4.17  | 1.47        | 1.35     |
| 37  | O     | 81   | 4D4  | CZ-NH2 | 3.80  | 1.45        | 1.32     |
| 22  | x     | 46   | G7M  | C5-C4  | 3.77  | 1.47        | 1.38     |
| 22  | x     | 55   | PSU  | C6-C5  | 3.54  | 1.39        | 1.35     |
| 22  | x     | 8    | 4SU  | C4-N3  | -3.33 | 1.34        | 1.37     |
| 25  | A     | 1911 | PSU  | C6-C5  | 3.32  | 1.39        | 1.35     |
| 25  | A     | 1917 | PSU  | C6-C5  | 3.27  | 1.38        | 1.35     |
| 22  | x     | 32   | PSU  | C6-C5  | 3.25  | 1.38        | 1.35     |
| 25  | A     | 2504 | PSU  | C6-C5  | 3.23  | 1.38        | 1.35     |
| 25  | A     | 745  | 1MG  | C5-C4  | 3.20  | 1.47        | 1.38     |
| 1   | a     | 527  | G7M  | C5-C4  | 3.18  | 1.46        | 1.38     |
| 1   | a     | 516  | PSU  | C6-C5  | 3.16  | 1.38        | 1.35     |
| 22  | x     | 39   | PSU  | C6-C5  | 3.15  | 1.38        | 1.35     |
| 1   | a     | 1207 | 2MG  | C5-C4  | 3.09  | 1.47        | 1.38     |
| 25  | A     | 2251 | OMG  | C5-C4  | 3.09  | 1.47        | 1.38     |
| 1   | a     | 966  | 2MG  | C5-C4  | 3.07  | 1.47        | 1.38     |
| 25  | A     | 1835 | 2MG  | C5-C4  | 3.07  | 1.47        | 1.38     |
| 1   | a     | 1516 | 2MG  | C5-C4  | 3.06  | 1.47        | 1.38     |
| 25  | A     | 2457 | PSU  | C6-C5  | 3.06  | 1.38        | 1.35     |
| 25  | A     | 955  | PSU  | C6-C5  | 2.99  | 1.38        | 1.35     |
| 25  | A     | 2069 | G7M  | C5-C4  | 2.98  | 1.45        | 1.38     |
| 25  | A     | 955  | PSU  | C4-N3  | -2.98 | 1.33        | 1.38     |
| 25  | A     | 2605 | PSU  | C6-C5  | 2.97  | 1.38        | 1.35     |
| 25  | A     | 2605 | PSU  | C4-N3  | -2.96 | 1.33        | 1.38     |
| 25  | A     | 2445 | 2MG  | C5-C4  | 2.94  | 1.46        | 1.38     |
| 22  | x     | 37   | MIA  | C5-C6  | 2.94  | 1.49        | 1.41     |
| 25  | A     | 746  | PSU  | C6-C5  | 2.91  | 1.38        | 1.35     |
| 25  | A     | 2604 | PSU  | C6-C5  | 2.91  | 1.38        | 1.35     |
| 25  | A     | 2552 | OMU  | C4-N3  | -2.91 | 1.33        | 1.38     |
| 1   | a     | 1519 | MA6  | C5-C6  | 2.89  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | a     | 967  | 5MC  | C6-C5 | 2.88  | 1.39        | 1.34     |
| 25  | A     | 2580 | PSU  | C6-C5 | 2.85  | 1.38        | 1.35     |
| 25  | A     | 747  | 5MU  | C4-N3 | -2.82 | 1.33        | 1.38     |
| 25  | A     | 746  | PSU  | C4-N3 | -2.82 | 1.33        | 1.38     |
| 25  | A     | 1915 | 3TD  | C4-N3 | 2.80  | 1.46        | 1.40     |
| 25  | A     | 2457 | PSU  | C4-N3 | -2.79 | 1.33        | 1.38     |
| 1   | a     | 1518 | MA6  | C5-C6 | 2.77  | 1.48        | 1.41     |
| 22  | x     | 54   | 5MU  | C6-C5 | 2.76  | 1.39        | 1.34     |
| 1   | a     | 1407 | 5MC  | C6-C5 | 2.76  | 1.39        | 1.34     |
| 25  | A     | 2030 | 6MZ  | C5-C6 | 2.75  | 1.48        | 1.41     |
| 25  | A     | 1939 | 5MU  | C4-N3 | -2.75 | 1.33        | 1.38     |
| 25  | A     | 2604 | PSU  | C4-N3 | -2.75 | 1.33        | 1.38     |
| 25  | A     | 1911 | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 25  | A     | 1835 | 2MG  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 25  | A     | 2504 | PSU  | C4-N3 | -2.69 | 1.33        | 1.38     |
| 22  | x     | 8    | 4SU  | C5-C4 | -2.69 | 1.39        | 1.42     |
| 25  | A     | 2503 | 2MA  | C5-C6 | 2.69  | 1.48        | 1.41     |
| 25  | A     | 1917 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 25  | A     | 2449 | H2U  | C2-N3 | -2.67 | 1.33        | 1.38     |
| 25  | A     | 2580 | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 22  | x     | 32   | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 25  | A     | 1939 | 5MU  | C6-N1 | -2.64 | 1.33        | 1.38     |
| 1   | a     | 516  | PSU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 22  | x     | 39   | PSU  | C4-N3 | -2.63 | 1.33        | 1.38     |
| 25  | A     | 2445 | 2MG  | C6-N1 | -2.63 | 1.33        | 1.38     |
| 25  | A     | 1618 | 6MZ  | C5-C6 | 2.62  | 1.48        | 1.41     |
| 22  | x     | 55   | PSU  | C4-N3 | -2.62 | 1.33        | 1.38     |
| 25  | A     | 2069 | G7M  | C6-N1 | -2.59 | 1.34        | 1.38     |
| 25  | A     | 1915 | 3TD  | O2-C2 | -2.59 | 1.18        | 1.23     |
| 25  | A     | 747  | 5MU  | C6-N1 | -2.57 | 1.33        | 1.38     |
| 25  | A     | 2251 | OMG  | C6-N1 | -2.57 | 1.34        | 1.38     |
| 25  | A     | 2449 | H2U  | C4-N3 | -2.56 | 1.33        | 1.37     |
| 22  | x     | 54   | 5MU  | C4-N3 | -2.56 | 1.34        | 1.38     |
| 1   | a     | 1516 | 2MG  | C6-N1 | -2.54 | 1.34        | 1.38     |
| 1   | a     | 527  | G7M  | C6-N1 | -2.54 | 1.34        | 1.38     |
| 1   | a     | 966  | 2MG  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 25  | A     | 1939 | 5MU  | C6-C5 | 2.51  | 1.38        | 1.34     |
| 25  | A     | 1962 | 5MC  | C6-N1 | -2.48 | 1.33        | 1.38     |
| 1   | a     | 1519 | MA6  | C8-N7 | 2.47  | 1.36        | 1.31     |
| 1   | a     | 1207 | 2MG  | C6-N1 | -2.46 | 1.34        | 1.38     |
| 25  | A     | 747  | 5MU  | C6-C5 | 2.46  | 1.38        | 1.34     |
| 25  | A     | 2503 | 2MA  | C5-N7 | -2.44 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | A     | 1962 | 5MC  | C6-C5   | 2.41  | 1.38        | 1.34     |
| 25  | A     | 1618 | 6MZ  | C5-N7   | -2.41 | 1.34        | 1.39     |
| 25  | A     | 2552 | OMU  | C2-N3   | -2.40 | 1.33        | 1.38     |
| 25  | A     | 2030 | 6MZ  | C5-N7   | -2.38 | 1.34        | 1.39     |
| 25  | A     | 2445 | 2MG  | C5-N7   | -2.35 | 1.34        | 1.39     |
| 25  | A     | 2580 | PSU  | O4'-C1' | -2.33 | 1.40        | 1.43     |
| 22  | x     | 46   | G7M  | C6-N1   | -2.33 | 1.34        | 1.38     |
| 25  | A     | 745  | 1MG  | C5-N7   | -2.30 | 1.34        | 1.39     |
| 37  | O     | 81   | 4D4  | CZ-NH1  | -2.30 | 1.25        | 1.34     |
| 25  | A     | 1835 | 2MG  | C5-N7   | -2.29 | 1.34        | 1.39     |
| 25  | A     | 955  | PSU  | C2-N3   | -2.29 | 1.33        | 1.37     |
| 25  | A     | 747  | 5MU  | C2-N3   | -2.28 | 1.34        | 1.38     |
| 25  | A     | 2503 | 2MA  | C8-N7   | 2.25  | 1.36        | 1.31     |
| 25  | A     | 2030 | 6MZ  | C8-N7   | 2.24  | 1.36        | 1.31     |
| 1   | a     | 1407 | 5MC  | C6-N1   | -2.24 | 1.34        | 1.38     |
| 22  | x     | 37   | MIA  | C5-N7   | -2.24 | 1.35        | 1.39     |
| 1   | a     | 1518 | MA6  | C5-N7   | -2.23 | 1.35        | 1.39     |
| 22  | x     | 37   | MIA  | C8-N7   | 2.23  | 1.36        | 1.31     |
| 25  | A     | 1939 | 5MU  | C2-N3   | -2.23 | 1.34        | 1.38     |
| 1   | a     | 1519 | MA6  | C5-N7   | -2.22 | 1.35        | 1.39     |
| 25  | A     | 2605 | PSU  | C2-N3   | -2.20 | 1.33        | 1.37     |
| 22  | x     | 54   | 5MU  | C4-C5   | 2.20  | 1.48        | 1.44     |
| 1   | a     | 1518 | MA6  | C8-N7   | 2.19  | 1.35        | 1.31     |
| 22  | x     | 54   | 5MU  | C6-N1   | -2.16 | 1.34        | 1.38     |
| 25  | A     | 1618 | 6MZ  | C8-N7   | 2.16  | 1.35        | 1.31     |
| 22  | x     | 54   | 5MU  | C2-N1   | 2.16  | 1.41        | 1.38     |
| 25  | A     | 1835 | 2MG  | C2-N3   | 2.16  | 1.36        | 1.32     |
| 25  | A     | 2552 | OMU  | C5-C4   | -2.15 | 1.39        | 1.43     |
| 25  | A     | 2251 | OMG  | C5-N7   | -2.15 | 1.34        | 1.39     |
| 1   | a     | 966  | 2MG  | C2-N3   | 2.14  | 1.36        | 1.32     |
| 1   | a     | 1207 | 2MG  | C5-N7   | -2.14 | 1.34        | 1.39     |
| 1   | a     | 967  | 5MC  | C6-N1   | -2.13 | 1.34        | 1.38     |
| 1   | a     | 1516 | 2MG  | C5-N7   | -2.13 | 1.34        | 1.39     |
| 25  | A     | 745  | 1MG  | C2-N1   | 2.13  | 1.41        | 1.37     |
| 22  | x     | 8    | 4SU  | C2-N1   | 2.12  | 1.41        | 1.38     |
| 25  | A     | 2030 | 6MZ  | C4-N9   | -2.10 | 1.33        | 1.37     |
| 1   | a     | 966  | 2MG  | C5-N7   | -2.09 | 1.34        | 1.39     |
| 25  | A     | 1939 | 5MU  | C4-C5   | 2.08  | 1.48        | 1.44     |
| 25  | A     | 1915 | 3TD  | O4-C4   | -2.08 | 1.18        | 1.23     |
| 25  | A     | 746  | PSU  | C2-N3   | -2.08 | 1.34        | 1.37     |
| 1   | a     | 1207 | 2MG  | C2-N3   | 2.08  | 1.35        | 1.32     |
| 22  | x     | 8    | 4SU  | C2-N3   | -2.07 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 25  | A     | 2580 | PSU  | C2-N1 | -2.07 | 1.34        | 1.36     |
| 25  | A     | 1618 | 6MZ  | C4-N9 | -2.06 | 1.33        | 1.37     |
| 25  | A     | 2604 | PSU  | C2-N3 | -2.06 | 1.34        | 1.37     |
| 25  | A     | 2604 | PSU  | C2-N1 | -2.02 | 1.34        | 1.36     |
| 25  | A     | 2445 | 2MG  | C2-N3 | 2.02  | 1.35        | 1.32     |
| 1   | a     | 1519 | MA6  | C4-N9 | -2.02 | 1.33        | 1.37     |
| 25  | A     | 1917 | PSU  | C2-N3 | -2.02 | 1.34        | 1.37     |
| 25  | A     | 955  | PSU  | C2-N1 | -2.01 | 1.34        | 1.36     |
| 25  | A     | 2457 | PSU  | C2-N3 | -2.01 | 1.34        | 1.37     |
| 25  | A     | 2504 | PSU  | C2-N3 | -2.00 | 1.34        | 1.37     |

All (232) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | A     | 2503 | 2MA  | C5-C4-N3    | -8.35 | 118.38      | 127.18   |
| 22  | x     | 37   | MIA  | C12-C13-C14 | -8.18 | 112.33      | 127.01   |
| 22  | x     | 46   | G7M  | CN7-N7-C8   | -8.05 | 112.61      | 124.79   |
| 22  | x     | 37   | MIA  | C5-C4-N3    | -7.97 | 118.78      | 127.18   |
| 1   | a     | 1207 | 2MG  | C2-N3-C4    | 7.22  | 121.03      | 112.00   |
| 25  | A     | 2445 | 2MG  | C2-N3-C4    | 7.20  | 121.00      | 112.00   |
| 22  | x     | 8    | 4SU  | C4-N3-C2    | -7.18 | 120.44      | 127.31   |
| 25  | A     | 1835 | 2MG  | C2-N3-C4    | 7.08  | 120.86      | 112.00   |
| 1   | a     | 966  | 2MG  | C2-N3-C4    | 7.07  | 120.84      | 112.00   |
| 1   | a     | 1516 | 2MG  | C2-N3-C4    | 6.98  | 120.73      | 112.00   |
| 1   | a     | 1498 | UR3  | C4-N3-C2    | -6.87 | 119.05      | 124.58   |
| 22  | x     | 46   | G7M  | N9-C8-N7    | -6.84 | 95.87       | 112.48   |
| 22  | x     | 46   | G7M  | C8-N7-C5    | 6.71  | 116.17      | 107.78   |
| 25  | A     | 2457 | PSU  | N1-C2-N3    | 6.62  | 122.15      | 115.17   |
| 25  | A     | 746  | PSU  | N1-C2-N3    | 6.60  | 122.13      | 115.17   |
| 22  | x     | 39   | PSU  | N1-C2-N3    | 6.58  | 122.11      | 115.17   |
| 25  | A     | 1917 | PSU  | N1-C2-N3    | 6.57  | 122.10      | 115.17   |
| 25  | A     | 2503 | 2MA  | N3-C4-N9    | 6.50  | 135.23      | 126.99   |
| 25  | A     | 955  | PSU  | N1-C2-N3    | 6.48  | 122.01      | 115.17   |
| 25  | A     | 2580 | PSU  | N1-C2-N3    | 6.48  | 122.00      | 115.17   |
| 22  | x     | 46   | G7M  | N9-C4-N3    | 6.44  | 138.83      | 125.95   |
| 22  | x     | 55   | PSU  | N1-C2-N3    | 6.41  | 121.93      | 115.17   |
| 1   | a     | 516  | PSU  | N1-C2-N3    | 6.39  | 121.91      | 115.17   |
| 22  | x     | 32   | PSU  | N1-C2-N3    | 6.37  | 121.88      | 115.17   |
| 25  | A     | 1835 | 2MG  | C5-C4-N3    | -6.35 | 118.29      | 128.39   |
| 25  | A     | 2604 | PSU  | N1-C2-N3    | 6.35  | 121.86      | 115.17   |
| 25  | A     | 1911 | PSU  | N1-C2-N3    | 6.32  | 121.83      | 115.17   |
| 25  | A     | 2605 | PSU  | N1-C2-N3    | 6.28  | 121.79      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25  | A     | 2504 | PSU  | N1-C2-N3  | 6.25  | 121.76      | 115.17   |
| 25  | A     | 2445 | 2MG  | C5-C4-N3  | -6.24 | 118.46      | 128.39   |
| 25  | A     | 2251 | OMG  | C5-C4-N3  | -6.21 | 118.51      | 128.39   |
| 1   | a     | 1207 | 2MG  | C5-C4-N3  | -6.17 | 118.57      | 128.39   |
| 1   | a     | 966  | 2MG  | C5-C4-N3  | -6.12 | 118.65      | 128.39   |
| 22  | x     | 37   | MIA  | N3-C4-N9  | 6.12  | 134.75      | 126.99   |
| 25  | A     | 1618 | 6MZ  | C5-C4-N3  | -5.99 | 118.47      | 126.72   |
| 1   | a     | 1516 | 2MG  | C5-C4-N3  | -5.98 | 118.87      | 128.39   |
| 22  | x     | 8    | 4SU  | C5-C4-N3  | 5.93  | 120.27      | 114.75   |
| 25  | A     | 2030 | 6MZ  | C5-C4-N3  | -5.85 | 118.67      | 126.72   |
| 1   | a     | 1518 | MA6  | C5-C4-N3  | -5.78 | 118.76      | 126.72   |
| 1   | a     | 527  | G7M  | N9-C4-N3  | 5.71  | 137.37      | 125.95   |
| 25  | A     | 1915 | 3TD  | N1-C2-N3  | 5.68  | 120.26      | 116.13   |
| 22  | x     | 46   | G7M  | C5-C4-N3  | -5.67 | 117.44      | 128.15   |
| 1   | a     | 1519 | MA6  | C5-C4-N3  | -5.62 | 118.98      | 126.72   |
| 1   | a     | 527  | G7M  | C5-C4-N3  | -5.58 | 117.61      | 128.15   |
| 25  | A     | 745  | 1MG  | C5-C4-N3  | -5.49 | 119.65      | 128.39   |
| 25  | A     | 747  | 5MU  | C4-N3-C2  | -5.41 | 120.25      | 127.34   |
| 25  | A     | 1939 | 5MU  | C4-N3-C2  | -5.33 | 120.36      | 127.34   |
| 25  | A     | 747  | 5MU  | N3-C2-N1  | 5.28  | 121.77      | 114.89   |
| 25  | A     | 2069 | G7M  | N9-C4-N3  | 5.28  | 136.51      | 125.95   |
| 25  | A     | 2069 | G7M  | C5-C4-N3  | -5.21 | 118.31      | 128.15   |
| 25  | A     | 2251 | OMG  | C2-N3-C4  | 5.05  | 121.00      | 112.30   |
| 25  | A     | 1939 | 5MU  | N3-C2-N1  | 5.04  | 121.45      | 114.89   |
| 25  | A     | 2030 | 6MZ  | C9-N6-C6  | -4.98 | 118.23      | 122.85   |
| 25  | A     | 2552 | OMU  | C4-N3-C2  | -4.94 | 120.48      | 126.61   |
| 22  | x     | 54   | 5MU  | N3-C2-N1  | 4.85  | 121.21      | 114.89   |
| 25  | A     | 1835 | 2MG  | N9-C4-N3  | 4.84  | 135.64      | 125.95   |
| 22  | x     | 54   | 5MU  | C4-N3-C2  | -4.76 | 121.09      | 127.34   |
| 1   | a     | 527  | G7M  | C2-N3-C4  | 4.75  | 120.48      | 112.30   |
| 25  | A     | 1618 | 6MZ  | N3-C4-N9  | 4.72  | 135.20      | 127.17   |
| 1   | a     | 1519 | MA6  | C9-N6-C6  | -4.67 | 108.64      | 120.52   |
| 22  | x     | 46   | G7M  | C2-N3-C4  | 4.66  | 120.33      | 112.30   |
| 25  | A     | 2445 | 2MG  | N9-C4-N3  | 4.63  | 135.21      | 125.95   |
| 1   | a     | 1519 | MA6  | C10-N6-C6 | -4.61 | 108.78      | 120.52   |
| 25  | A     | 2069 | G7M  | C2-N3-C4  | 4.61  | 120.24      | 112.30   |
| 1   | a     | 1518 | MA6  | N3-C4-N9  | 4.61  | 135.00      | 127.17   |
| 1   | a     | 966  | 2MG  | N9-C4-N3  | 4.60  | 135.14      | 125.95   |
| 25  | A     | 2251 | OMG  | N9-C4-N3  | 4.55  | 135.05      | 125.95   |
| 1   | a     | 1207 | 2MG  | N9-C4-N3  | 4.49  | 134.92      | 125.95   |
| 22  | x     | 39   | PSU  | C4-N3-C2  | -4.44 | 120.26      | 126.37   |
| 25  | A     | 747  | 5MU  | C5-C4-N3  | 4.43  | 119.18      | 115.32   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | A     | 2030 | 6MZ  | N3-C4-N9    | 4.43  | 134.70      | 127.17   |
| 1   | a     | 1518 | MA6  | C10-N6-C6   | -4.43 | 109.26      | 120.52   |
| 25  | A     | 747  | 5MU  | O4-C4-C5    | -4.42 | 119.86      | 124.92   |
| 22  | x     | 8    | 4SU  | N3-C2-N1    | 4.40  | 120.62      | 114.89   |
| 25  | A     | 2552 | OMU  | N3-C2-N1    | 4.39  | 120.61      | 114.89   |
| 25  | A     | 1939 | 5MU  | C5-C4-N3    | 4.38  | 119.13      | 115.32   |
| 25  | A     | 1915 | 3TD  | C4-N3-C2    | -4.37 | 119.99      | 124.61   |
| 25  | A     | 746  | PSU  | C4-N3-C2    | -4.33 | 120.41      | 126.37   |
| 25  | A     | 745  | 1MG  | C2-N3-C4    | 4.31  | 121.67      | 111.98   |
| 25  | A     | 2457 | PSU  | C4-N3-C2    | -4.30 | 120.44      | 126.37   |
| 22  | x     | 46   | G7M  | C8-N9-C4    | 4.28  | 117.69      | 107.09   |
| 22  | x     | 37   | MIA  | C16-C14-C13 | -4.27 | 109.85      | 122.66   |
| 1   | a     | 1516 | 2MG  | N9-C4-N3    | 4.26  | 134.48      | 125.95   |
| 25  | A     | 1911 | PSU  | C4-N3-C2    | -4.25 | 120.52      | 126.37   |
| 25  | A     | 2605 | PSU  | C4-N3-C2    | -4.22 | 120.55      | 126.37   |
| 25  | A     | 745  | 1MG  | N9-C4-N3    | 4.17  | 134.29      | 125.95   |
| 22  | x     | 8    | 4SU  | C5-C4-S4    | -4.14 | 119.58      | 124.31   |
| 1   | a     | 1519 | MA6  | C2-N1-C6    | 4.13  | 121.93      | 111.83   |
| 25  | A     | 1618 | 6MZ  | C9-N6-C6    | -4.13 | 119.02      | 122.85   |
| 1   | a     | 1518 | MA6  | C9-N6-C6    | -4.11 | 110.06      | 120.52   |
| 1   | a     | 1518 | MA6  | C2-N1-C6    | 4.11  | 121.87      | 111.83   |
| 25  | A     | 2504 | PSU  | C4-N3-C2    | -4.10 | 120.72      | 126.37   |
| 25  | A     | 1939 | 5MU  | O4-C4-C5    | -4.10 | 120.23      | 124.92   |
| 1   | a     | 1519 | MA6  | N3-C4-N9    | 4.09  | 134.13      | 127.17   |
| 25  | A     | 955  | PSU  | C4-N3-C2    | -4.07 | 120.77      | 126.37   |
| 25  | A     | 2580 | PSU  | C4-N3-C2    | -4.07 | 120.77      | 126.37   |
| 25  | A     | 2604 | PSU  | C4-N3-C2    | -4.04 | 120.80      | 126.37   |
| 1   | a     | 516  | PSU  | C4-N3-C2    | -4.04 | 120.80      | 126.37   |
| 22  | x     | 32   | PSU  | C4-N3-C2    | -4.03 | 120.82      | 126.37   |
| 22  | x     | 54   | 5MU  | C5-C4-N3    | 4.00  | 118.80      | 115.32   |
| 22  | x     | 54   | 5MU  | O4-C4-C5    | -3.99 | 120.36      | 124.92   |
| 25  | A     | 2580 | PSU  | O2-C2-N1    | -3.95 | 118.72      | 122.79   |
| 25  | A     | 2030 | 6MZ  | C6-C5-N7    | 3.94  | 136.72      | 132.43   |
| 22  | x     | 46   | G7M  | C1'-N9-C8   | -3.91 | 113.53      | 126.74   |
| 25  | A     | 1939 | 5MU  | C5-C6-N1    | -3.91 | 119.06      | 123.31   |
| 1   | a     | 516  | PSU  | O2-C2-N1    | -3.90 | 118.77      | 122.79   |
| 25  | A     | 1917 | PSU  | O2-C2-N1    | -3.88 | 118.78      | 122.79   |
| 25  | A     | 2552 | OMU  | C5-C4-N3    | 3.87  | 120.22      | 114.80   |
| 22  | x     | 55   | PSU  | C4-N3-C2    | -3.87 | 121.05      | 126.37   |
| 25  | A     | 1917 | PSU  | C4-N3-C2    | -3.87 | 121.05      | 126.37   |
| 1   | a     | 1519 | MA6  | C4-C5-N7    | -3.85 | 106.18      | 110.58   |
| 25  | A     | 2030 | 6MZ  | C2-N3-C4    | 3.85  | 121.22      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | x     | 37   | MIA  | C4-C5-N7    | -3.84 | 106.19      | 110.58   |
| 25  | A     | 2030 | 6MZ  | C4-C5-N7    | -3.79 | 106.25      | 110.58   |
| 25  | A     | 1618 | 6MZ  | C2-N3-C4    | 3.77  | 121.04      | 111.83   |
| 22  | x     | 37   | MIA  | C15-C14-C13 | -3.73 | 111.46      | 122.66   |
| 25  | A     | 2457 | PSU  | O2-C2-N1    | -3.72 | 118.95      | 122.79   |
| 25  | A     | 747  | 5MU  | C5-C6-N1    | -3.69 | 119.31      | 123.31   |
| 22  | x     | 37   | MIA  | C6-C5-N7    | 3.66  | 136.41      | 132.43   |
| 22  | x     | 39   | PSU  | O2-C2-N1    | -3.65 | 119.02      | 122.79   |
| 25  | A     | 2604 | PSU  | O2-C2-N1    | -3.64 | 119.03      | 122.79   |
| 1   | a     | 1518 | MA6  | C2-N3-C4    | 3.64  | 120.72      | 111.83   |
| 1   | a     | 1519 | MA6  | C2-N3-C4    | 3.63  | 120.70      | 111.83   |
| 1   | a     | 1518 | MA6  | C4-C5-N7    | -3.63 | 106.44      | 110.58   |
| 25  | A     | 746  | PSU  | O2-C2-N1    | -3.59 | 119.08      | 122.79   |
| 22  | x     | 32   | PSU  | O2-C2-N1    | -3.59 | 119.09      | 122.79   |
| 22  | x     | 46   | G7M  | CN7-N7-C5   | 3.55  | 131.22      | 126.80   |
| 25  | A     | 1911 | PSU  | O2-C2-N1    | -3.52 | 119.16      | 122.79   |
| 25  | A     | 1618 | 6MZ  | C4-C5-N7    | -3.51 | 106.57      | 110.58   |
| 22  | x     | 55   | PSU  | O2-C2-N1    | -3.50 | 119.18      | 122.79   |
| 1   | a     | 967  | 5MC  | C5-C6-N1    | -3.47 | 119.54      | 123.31   |
| 1   | a     | 1518 | MA6  | N1-C6-N6    | 3.47  | 121.08      | 116.86   |
| 25  | A     | 2503 | 2MA  | C4-C5-N7    | -3.45 | 106.64      | 110.58   |
| 22  | x     | 37   | MIA  | C2-N3-C4    | 3.42  | 121.26      | 112.29   |
| 25  | A     | 1618 | 6MZ  | C6-C5-N7    | 3.40  | 136.13      | 132.43   |
| 22  | x     | 37   | MIA  | C11-S10-C2  | -3.38 | 99.71       | 102.25   |
| 25  | A     | 955  | PSU  | O2-C2-N1    | -3.36 | 119.32      | 122.79   |
| 25  | A     | 2030 | 6MZ  | N1-C2-N3    | -3.35 | 123.51      | 128.58   |
| 1   | a     | 1407 | 5MC  | C5-C6-N1    | -3.33 | 119.69      | 123.31   |
| 25  | A     | 2504 | PSU  | O2-C2-N1    | -3.33 | 119.35      | 122.79   |
| 1   | a     | 1516 | 2MG  | C6-C5-N7    | 3.30  | 136.30      | 130.29   |
| 12  | l     | 89   | D2T  | CB1-SB-CB   | 3.30  | 108.29      | 102.36   |
| 1   | a     | 1498 | UR3  | C5-C4-N3    | 3.28  | 119.36      | 115.04   |
| 12  | l     | 89   | D2T  | OD2-CG-CB   | 3.25  | 120.17      | 113.15   |
| 1   | a     | 1207 | 2MG  | C6-C5-N7    | 3.25  | 136.21      | 130.29   |
| 25  | A     | 1618 | 6MZ  | N1-C2-N3    | -3.22 | 123.71      | 128.58   |
| 22  | x     | 54   | 5MU  | C5-C6-N1    | -3.20 | 119.84      | 123.31   |
| 25  | A     | 2251 | OMG  | C6-C5-N7    | 3.19  | 136.09      | 130.29   |
| 1   | a     | 1518 | MA6  | N1-C2-N3    | -3.18 | 123.77      | 128.58   |
| 25  | A     | 2605 | PSU  | O2-C2-N1    | -3.16 | 119.53      | 122.79   |
| 25  | A     | 1962 | 5MC  | C5-C6-N1    | -3.16 | 119.88      | 123.31   |
| 1   | a     | 1519 | MA6  | N1-C2-N3    | -3.14 | 123.82      | 128.58   |
| 25  | A     | 1939 | 5MU  | O2-C2-N1    | -3.08 | 118.79      | 122.80   |
| 25  | A     | 2445 | 2MG  | C6-C5-N7    | 3.08  | 135.89      | 130.29   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | a     | 966  | 2MG  | C6-C5-N7    | 3.07  | 135.88      | 130.29   |
| 25  | A     | 2552 | OMU  | O4-C4-C5    | -3.06 | 119.88      | 125.16   |
| 1   | a     | 1519 | MA6  | C10-N6-C9   | -2.89 | 106.90      | 116.18   |
| 25  | A     | 1835 | 2MG  | C6-C5-N7    | 2.86  | 135.50      | 130.29   |
| 1   | a     | 1518 | MA6  | C4-N9-C8    | 2.84  | 108.72      | 105.74   |
| 25  | A     | 2503 | 2MA  | N6-C6-N1    | 2.79  | 120.79      | 117.03   |
| 25  | A     | 2030 | 6MZ  | C4-N9-C8    | 2.78  | 108.65      | 105.74   |
| 22  | x     | 37   | MIA  | C5-N7-C8    | 2.75  | 107.77      | 103.45   |
| 25  | A     | 2030 | 6MZ  | C5-N7-C8    | 2.73  | 107.74      | 103.45   |
| 1   | a     | 967  | 5MC  | C5-C4-N3    | -2.73 | 118.96      | 121.75   |
| 1   | a     | 1519 | MA6  | N1-C6-N6    | 2.72  | 120.18      | 116.86   |
| 1   | a     | 1407 | 5MC  | C5-C4-N3    | -2.72 | 118.97      | 121.75   |
| 25  | A     | 1618 | 6MZ  | C4-N9-C8    | 2.71  | 108.58      | 105.74   |
| 25  | A     | 1962 | 5MC  | C5-C4-N3    | -2.67 | 119.01      | 121.75   |
| 1   | a     | 1518 | MA6  | C5-N7-C8    | 2.66  | 107.63      | 103.45   |
| 25  | A     | 2503 | 2MA  | C2-N1-C6    | 2.63  | 122.14      | 118.10   |
| 1   | a     | 1516 | 2MG  | C4-C5-N7    | -2.63 | 106.51      | 110.67   |
| 22  | x     | 37   | MIA  | C4-N9-C8    | 2.62  | 108.49      | 105.74   |
| 1   | a     | 1519 | MA6  | C5-N7-C8    | 2.61  | 107.55      | 103.45   |
| 1   | a     | 1207 | 2MG  | C4-C5-N7    | -2.60 | 106.56      | 110.67   |
| 25  | A     | 2251 | OMG  | C4-C5-N7    | -2.58 | 106.59      | 110.67   |
| 25  | A     | 745  | 1MG  | C6-C5-N7    | 2.55  | 135.04      | 129.36   |
| 25  | A     | 2069 | G7M  | O6-C6-C5    | -2.55 | 122.32      | 128.01   |
| 22  | x     | 46   | G7M  | O6-C6-C5    | -2.54 | 122.35      | 128.01   |
| 25  | A     | 2445 | 2MG  | C4-C5-N7    | -2.51 | 106.69      | 110.67   |
| 25  | A     | 745  | 1MG  | C4-C5-N7    | -2.51 | 106.70      | 110.67   |
| 25  | A     | 747  | 5MU  | O2-C2-N1    | -2.49 | 119.55      | 122.80   |
| 25  | A     | 2503 | 2MA  | C5-N7-C8    | 2.49  | 107.36      | 103.45   |
| 1   | a     | 1518 | MA6  | C5-C6-N6    | -2.49 | 121.39      | 125.33   |
| 11  | k     | 119  | IAS  | OD1-CG-CB   | -2.49 | 118.14      | 125.38   |
| 25  | A     | 1618 | 6MZ  | C5-N7-C8    | 2.48  | 107.36      | 103.45   |
| 1   | a     | 966  | 2MG  | C4-C5-N7    | -2.48 | 106.74      | 110.67   |
| 25  | A     | 2503 | 2MA  | C4-N9-C8    | 2.48  | 108.34      | 105.74   |
| 22  | x     | 54   | 5MU  | O2-C2-N1    | -2.45 | 119.61      | 122.80   |
| 25  | A     | 2498 | OMC  | O2-C2-N3    | -2.44 | 118.48      | 122.33   |
| 1   | a     | 527  | G7M  | O6-C6-C5    | -2.43 | 122.58      | 128.01   |
| 1   | a     | 1519 | MA6  | C4-N9-C8    | 2.43  | 108.29      | 105.74   |
| 22  | x     | 37   | MIA  | C2-N1-C6    | 2.43  | 122.15      | 117.54   |
| 25  | A     | 2580 | PSU  | O4'-C1'-C2' | 2.42  | 108.49      | 105.15   |
| 1   | a     | 1518 | MA6  | C10-N6-C9   | -2.39 | 108.49      | 116.18   |
| 1   | a     | 516  | PSU  | O4'-C1'-C2' | 2.38  | 108.44      | 105.15   |
| 25  | A     | 1915 | 3TD  | C6-C5-C4    | 2.38  | 119.78      | 118.19   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | a     | 1207 | 2MG  | N1-C2-N2    | 2.35  | 118.96      | 116.56   |
| 25  | A     | 1835 | 2MG  | C4-C5-N7    | -2.34 | 106.95      | 110.67   |
| 22  | x     | 37   | MIA  | N3-C2-N1    | -2.34 | 122.72      | 127.00   |
| 25  | A     | 2457 | PSU  | O4'-C1'-C2' | 2.30  | 108.34      | 105.15   |
| 25  | A     | 2552 | OMU  | O2-C2-N1    | -2.29 | 119.82      | 122.80   |
| 25  | A     | 2449 | H2U  | O2-C2-N1    | -2.27 | 120.37      | 123.10   |
| 25  | A     | 2030 | 6MZ  | N9-C8-N7    | -2.27 | 110.72      | 113.94   |
| 1   | a     | 1402 | 4OC  | C6-C5-C4    | 2.26  | 119.72      | 117.00   |
| 22  | x     | 39   | PSU  | C5-C6-N1    | -2.26 | 119.01      | 122.14   |
| 25  | A     | 2457 | PSU  | C5-C6-N1    | -2.23 | 119.04      | 122.14   |
| 1   | a     | 527  | G7M  | C5-C6-N1    | 2.21  | 116.42      | 111.84   |
| 22  | x     | 8    | 4SU  | O2-C2-N1    | -2.21 | 119.93      | 122.80   |
| 25  | A     | 2449 | H2U  | C5-C6-N1    | -2.19 | 104.89      | 111.52   |
| 25  | A     | 746  | PSU  | C5-C6-N1    | -2.19 | 119.10      | 122.14   |
| 1   | a     | 966  | 2MG  | O6-C6-C5    | -2.18 | 120.77      | 126.53   |
| 25  | A     | 2445 | 2MG  | O6-C6-C5    | -2.18 | 120.78      | 126.53   |
| 25  | A     | 1911 | PSU  | C5-C6-N1    | -2.16 | 119.14      | 122.14   |
| 1   | a     | 1407 | 5MC  | O2-C2-N3    | -2.15 | 118.94      | 122.33   |
| 25  | A     | 2504 | PSU  | C5-C6-N1    | -2.15 | 119.16      | 122.14   |
| 1   | a     | 1207 | 2MG  | O6-C6-C5    | -2.14 | 120.88      | 126.53   |
| 25  | A     | 2069 | G7M  | C5-C6-N1    | 2.14  | 116.26      | 111.84   |
| 25  | A     | 2445 | 2MG  | N1-C2-N2    | 2.12  | 118.72      | 116.56   |
| 25  | A     | 1835 | 2MG  | O6-C6-C5    | -2.12 | 120.94      | 126.53   |
| 1   | a     | 966  | 2MG  | N1-C2-N2    | 2.10  | 118.71      | 116.56   |
| 25  | A     | 2605 | PSU  | C5-C6-N1    | -2.09 | 119.24      | 122.14   |
| 1   | a     | 1518 | MA6  | N9-C8-N7    | -2.09 | 110.97      | 113.94   |
| 1   | a     | 1519 | MA6  | C6-C5-N7    | 2.09  | 136.76      | 133.43   |
| 1   | a     | 1516 | 2MG  | N1-C2-N2    | 2.07  | 118.68      | 116.56   |
| 25  | A     | 2604 | PSU  | C5-C6-N1    | -2.06 | 119.29      | 122.14   |
| 1   | a     | 1516 | 2MG  | O6-C6-C5    | -2.06 | 121.11      | 126.53   |
| 1   | a     | 1207 | 2MG  | C2-N1-C6    | -2.05 | 122.07      | 124.55   |
| 25  | A     | 2503 | 2MA  | C6-C5-N7    | 2.03  | 136.01      | 132.09   |
| 22  | x     | 46   | G7M  | C5-C6-N1    | 2.02  | 116.02      | 111.84   |
| 25  | A     | 2445 | 2MG  | CM2-N2-C2   | -2.01 | 119.33      | 123.65   |
| 22  | x     | 37   | MIA  | N9-C8-N7    | -2.00 | 111.09      | 113.94   |
| 1   | a     | 1519 | MA6  | N9-C8-N7    | -2.00 | 111.09      | 113.94   |

There are no chirality outliers.

All (39) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | a     | 1519 | MA6  | C5-C6-N6-C9 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | a     | 1519 | MA6  | N1-C6-N6-C9     |
| 22  | x     | 37   | MIA  | C12-C13-C14-C15 |
| 37  | O     | 81   | 4D4  | C-CA-CB-OB      |
| 37  | O     | 81   | 4D4  | C-CA-CB-CG      |
| 37  | O     | 81   | 4D4  | N-CA-CB-OB      |
| 37  | O     | 81   | 4D4  | N-CA-CB-CG      |
| 37  | O     | 81   | 4D4  | OB-CB-CG-CD     |
| 37  | O     | 81   | 4D4  | NE-CD-CG-CB     |
| 25  | A     | 1917 | PSU  | C2'-C1'-C5-C4   |
| 37  | O     | 82   | MS6  | C-CA-CB-CG      |
| 1   | a     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 22  | x     | 55   | PSU  | C4'-C5'-O5'-P   |
| 22  | x     | 37   | MIA  | N1-C6-N6-C12    |
| 1   | a     | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 25  | A     | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 1   | a     | 966  | 2MG  | C3'-C4'-C5'-O5' |
| 25  | A     | 2069 | G7M  | C3'-C4'-C5'-O5' |
| 1   | a     | 1519 | MA6  | C5-C6-N6-C10    |
| 22  | x     | 37   | MIA  | C5-C6-N6-C12    |
| 37  | O     | 82   | MS6  | CB-CG-SD-CE     |
| 1   | a     | 1518 | MA6  | C5-C6-N6-C9     |
| 28  | D     | 150  | MEQ  | OE1-CD-CG-CB    |
| 12  | l     | 89   | D2T  | CG-CB-SB-CB1    |
| 37  | O     | 81   | 4D4  | CA-CB-CG-CD     |
| 1   | a     | 966  | 2MG  | O4'-C4'-C5'-O5' |
| 28  | D     | 150  | MEQ  | NE2-CD-CG-CB    |
| 25  | A     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 25  | A     | 2552 | OMU  | C3'-C2'-O2'-CM2 |
| 1   | a     | 1402 | 4OC  | C3'-C2'-O2'-CM2 |
| 25  | A     | 746  | PSU  | O4'-C1'-C5-C6   |
| 1   | a     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 22  | x     | 46   | G7M  | O4'-C4'-C5'-O5' |
| 22  | x     | 37   | MIA  | C4'-C5'-O5'-P   |
| 37  | O     | 82   | MS6  | N-CA-CB-CG      |
| 25  | A     | 2069 | G7M  | C4'-C5'-O5'-P   |
| 37  | O     | 81   | 4D4  | O-C-CA-CB       |
| 25  | A     | 2498 | OMC  | C2'-C1'-N1-C2   |
| 25  | A     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |

There are no ring outliers.

19 monomers are involved in 32 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | a     | 1519 | MA6  | 2       | 0            |
| 25  | A     | 2498 | OMC  | 1       | 0            |
| 25  | A     | 1917 | PSU  | 1       | 0            |
| 1   | a     | 1402 | 4OC  | 3       | 0            |
| 22  | x     | 46   | G7M  | 2       | 0            |
| 25  | A     | 2030 | 6MZ  | 3       | 0            |
| 22  | x     | 54   | 5MU  | 1       | 0            |
| 1   | a     | 1518 | MA6  | 4       | 0            |
| 1   | a     | 516  | PSU  | 1       | 0            |
| 25  | A     | 2552 | OMU  | 1       | 0            |
| 1   | a     | 966  | 2MG  | 2       | 0            |
| 25  | A     | 2503 | 2MA  | 1       | 0            |
| 22  | x     | 37   | MIA  | 2       | 0            |
| 25  | A     | 2449 | H2U  | 1       | 0            |
| 1   | a     | 1516 | 2MG  | 3       | 0            |
| 1   | a     | 1207 | 2MG  | 1       | 0            |
| 25  | A     | 1915 | 3TD  | 1       | 0            |
| 25  | A     | 2457 | PSU  | 1       | 0            |
| 12  | l     | 89   | D2T  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 387 ligands modelled in this entry, 386 are monoatomic - leaving 1 for Mogul analysis.

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 |
| 58  | G4P  | v     | 601 | 57   | 36,38,38     | 1.50 | 5 (13%)  | 56,61,61    | 2.00 | 13 (23%) |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 58  | G4P  | v     | 601 | 57   | -       | 5/27/43/43 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 58  | v     | 601 | G4P  | C6-N1  | -4.37 | 1.30        | 1.38     |
| 58  | v     | 601 | G4P  | C5-N7  | -3.02 | 1.33        | 1.39     |
| 58  | v     | 601 | G4P  | C2-N1  | -2.88 | 1.30        | 1.37     |
| 58  | v     | 601 | G4P  | C8-N9  | -2.43 | 1.32        | 1.37     |
| 58  | v     | 601 | G4P  | PA-O3A | -2.34 | 1.57        | 1.59     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 58  | v     | 601 | G4P  | C5-C4-N3    | -7.23 | 116.89      | 128.39   |
| 58  | v     | 601 | G4P  | N9-C4-N3    | 5.76  | 137.47      | 125.95   |
| 58  | v     | 601 | G4P  | C2-N3-C4    | 5.63  | 121.99      | 112.30   |
| 58  | v     | 601 | G4P  | C6-C5-N7    | 3.22  | 136.15      | 130.29   |
| 58  | v     | 601 | G4P  | C5-C6-N1    | 2.87  | 120.55      | 113.25   |
| 58  | v     | 601 | G4P  | O6-C6-C5    | -2.72 | 119.36      | 126.53   |
| 58  | v     | 601 | G4P  | C2-N1-C6    | -2.62 | 120.36      | 125.11   |
| 58  | v     | 601 | G4P  | C4-C5-N7    | -2.40 | 106.86      | 110.67   |
| 58  | v     | 601 | G4P  | O3D-PD-O2D  | 2.26  | 116.27      | 107.80   |
| 58  | v     | 601 | G4P  | C8-N7-C5    | 2.26  | 108.28      | 104.26   |
| 58  | v     | 601 | G4P  | O4'-C1'-N9  | -2.09 | 103.62      | 108.36   |
| 58  | v     | 601 | G4P  | C2'-C3'-C4' | -2.06 | 99.64       | 103.24   |
| 58  | v     | 601 | G4P  | N9-C8-N7    | -2.05 | 109.59      | 113.40   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

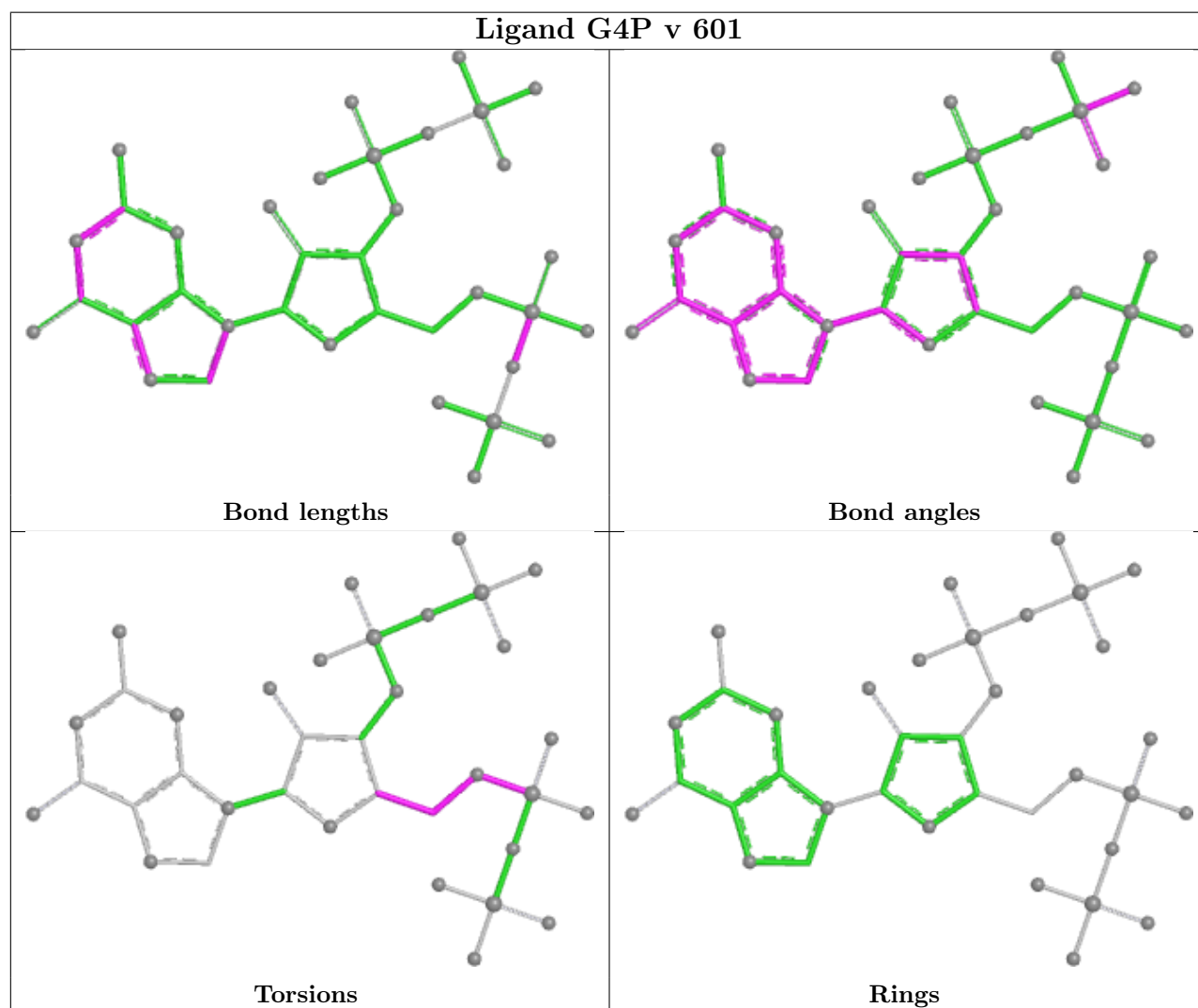
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 58  | v     | 601 | G4P  | C5'-O5'-PA-O3A  |
| 58  | v     | 601 | G4P  | C5'-O5'-PA-O2A  |
| 58  | v     | 601 | G4P  | O4'-C4'-C5'-O5' |
| 58  | v     | 601 | G4P  | C3'-C4'-C5'-O5' |
| 58  | v     | 601 | G4P  | C4'-C5'-O5'-PA  |

There are no ring outliers.

1 monomer is involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 58  | v     | 601 | G4P  | 8       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

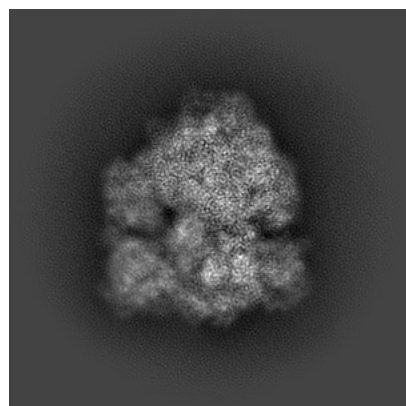
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29624. These allow visual inspection of the internal detail of the map and identification of artifacts.

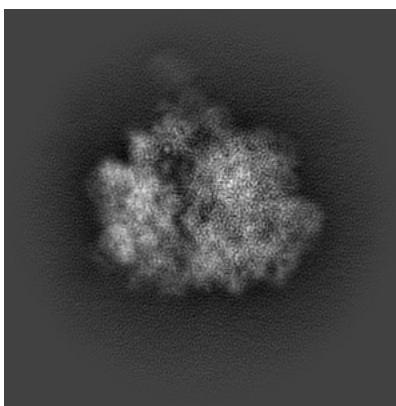
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

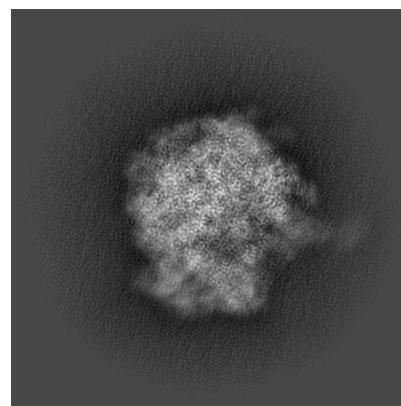
#### 6.1.1 Primary map



X

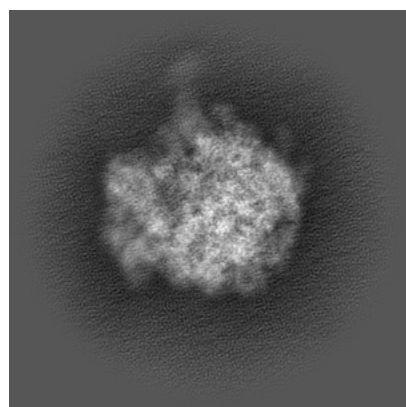


Y

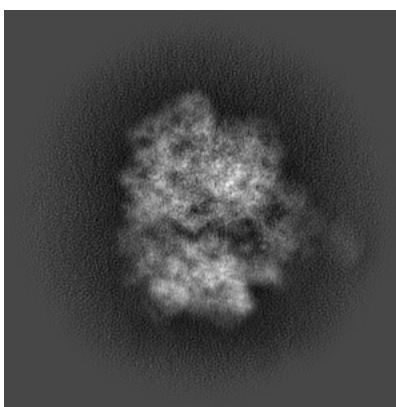


Z

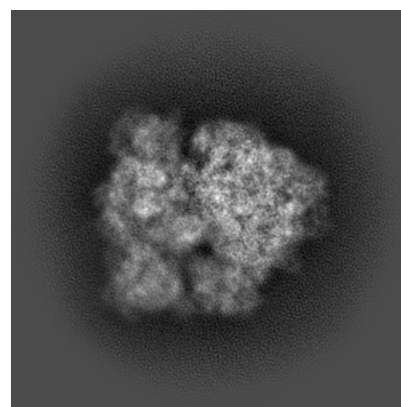
#### 6.1.2 Raw map



X



Y

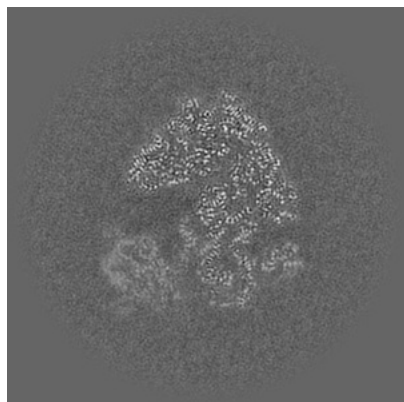


Z

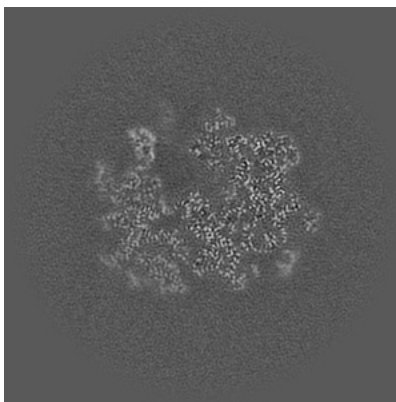
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

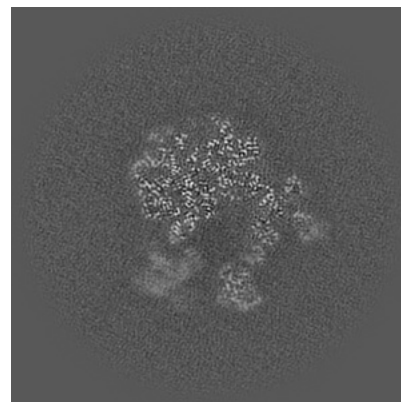
### 6.2.1 Primary map



X Index: 256

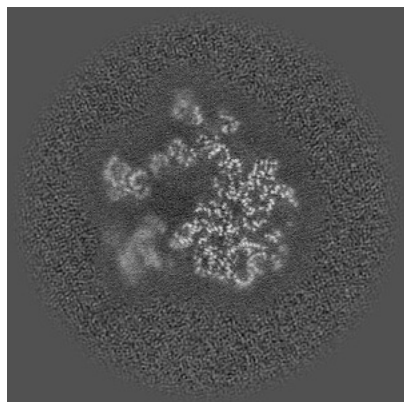


Y Index: 256

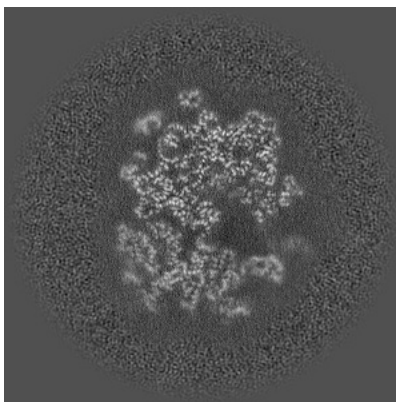


Z Index: 256

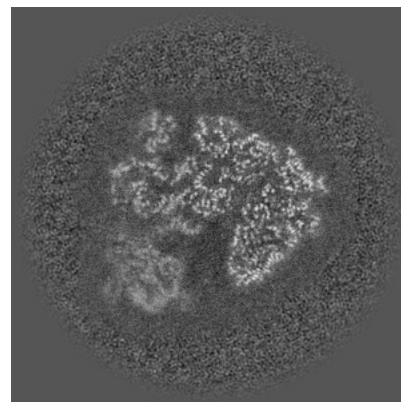
### 6.2.2 Raw map



X Index: 256



Y Index: 256

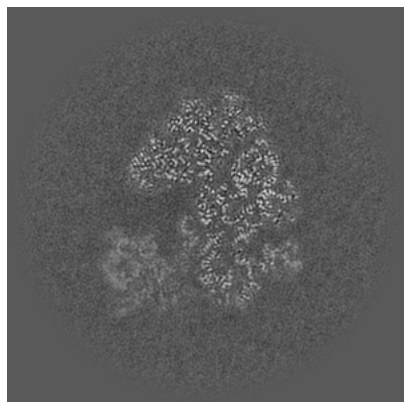


Z Index: 256

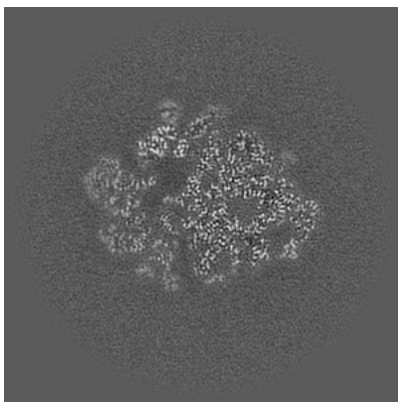
The images above show central slices of the map in three orthogonal directions.

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

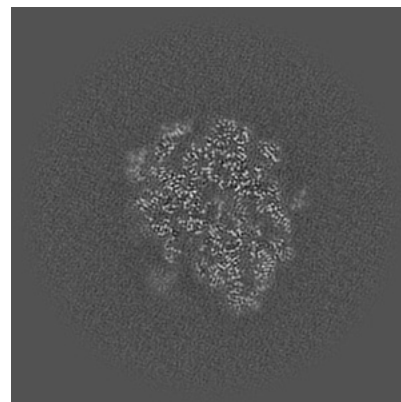
### 6.3.1 Primary map



X Index: 254

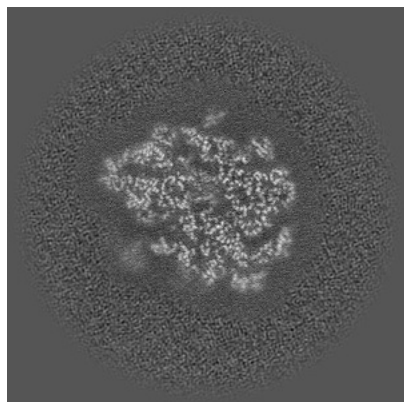


Y Index: 280

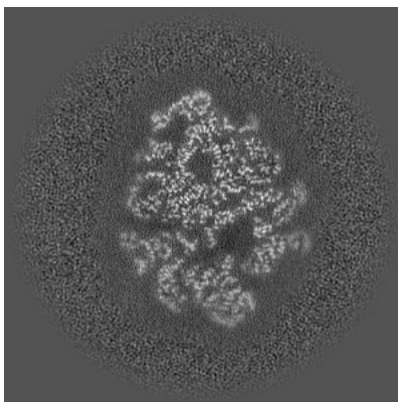


Z Index: 290

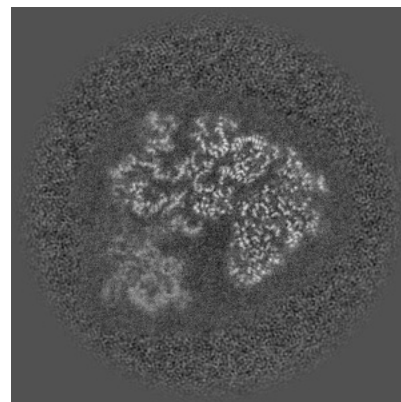
### 6.3.2 Raw map



X Index: 290



Y Index: 279

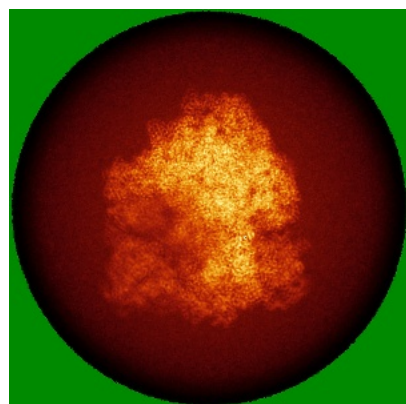


Z Index: 254

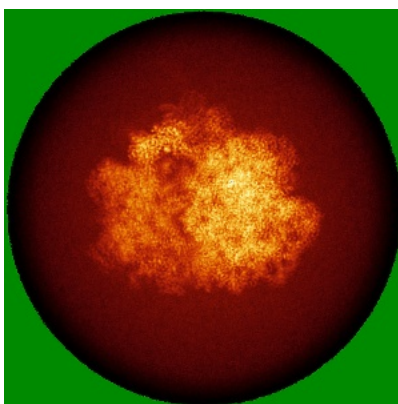
The images above show the largest variance slices of the map in three orthogonal directions.

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

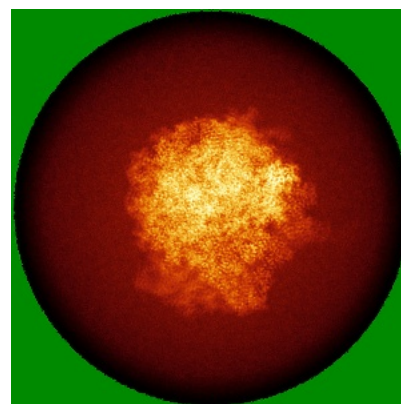
### 6.4.1 Primary map



X

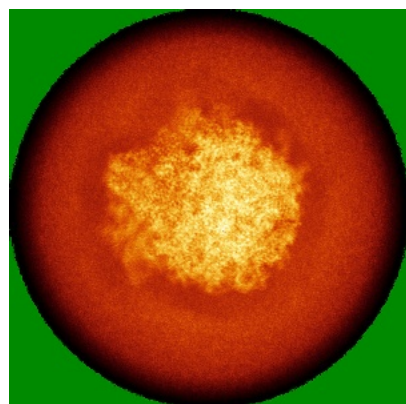


Y

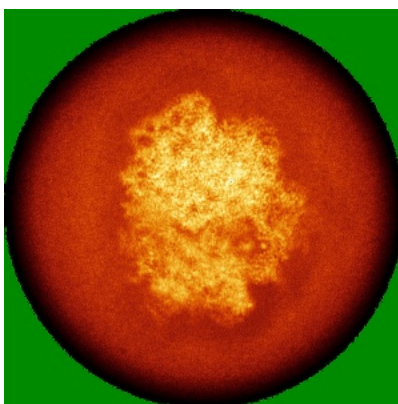


Z

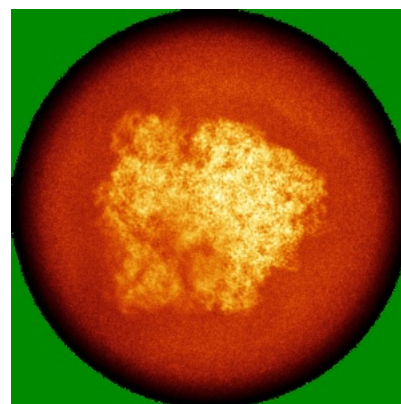
### 6.4.2 Raw map



X



Y

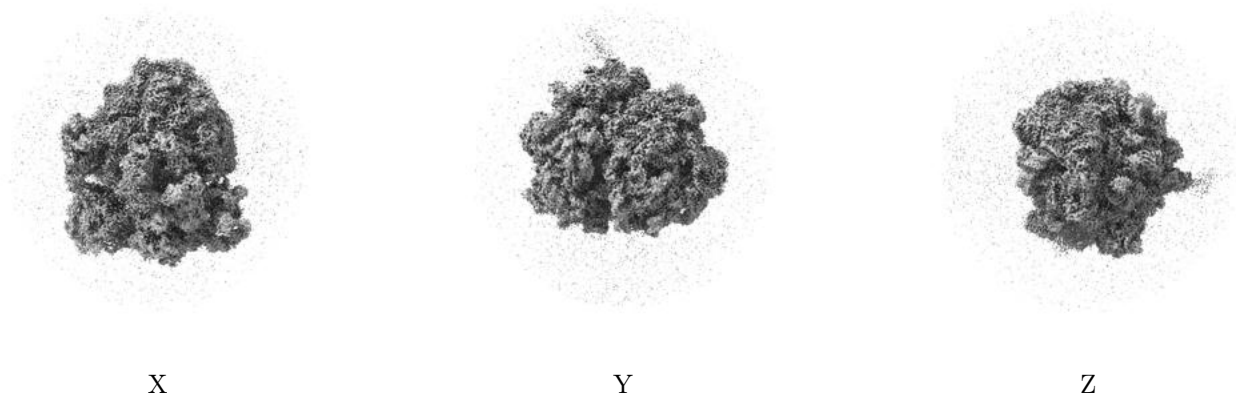


Z

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.

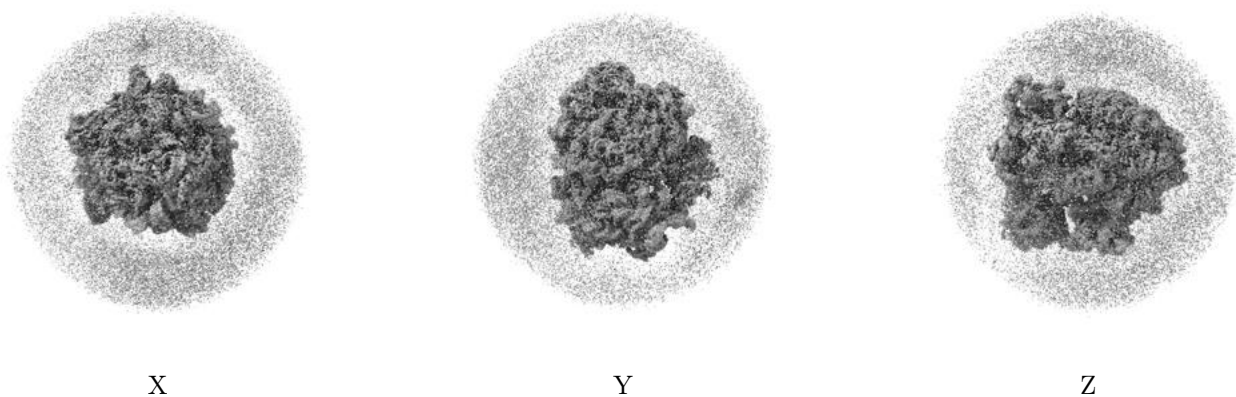
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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



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.

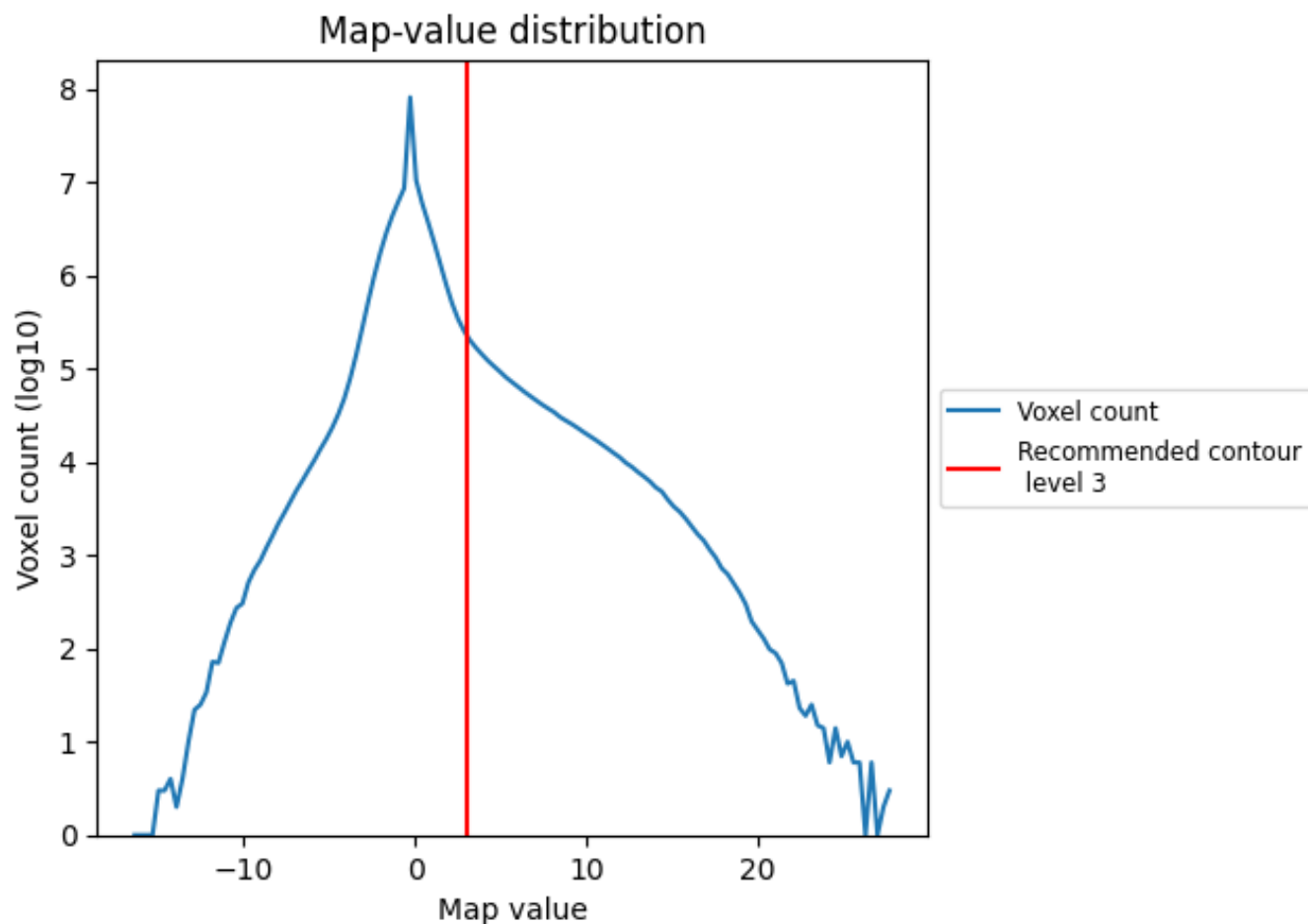
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

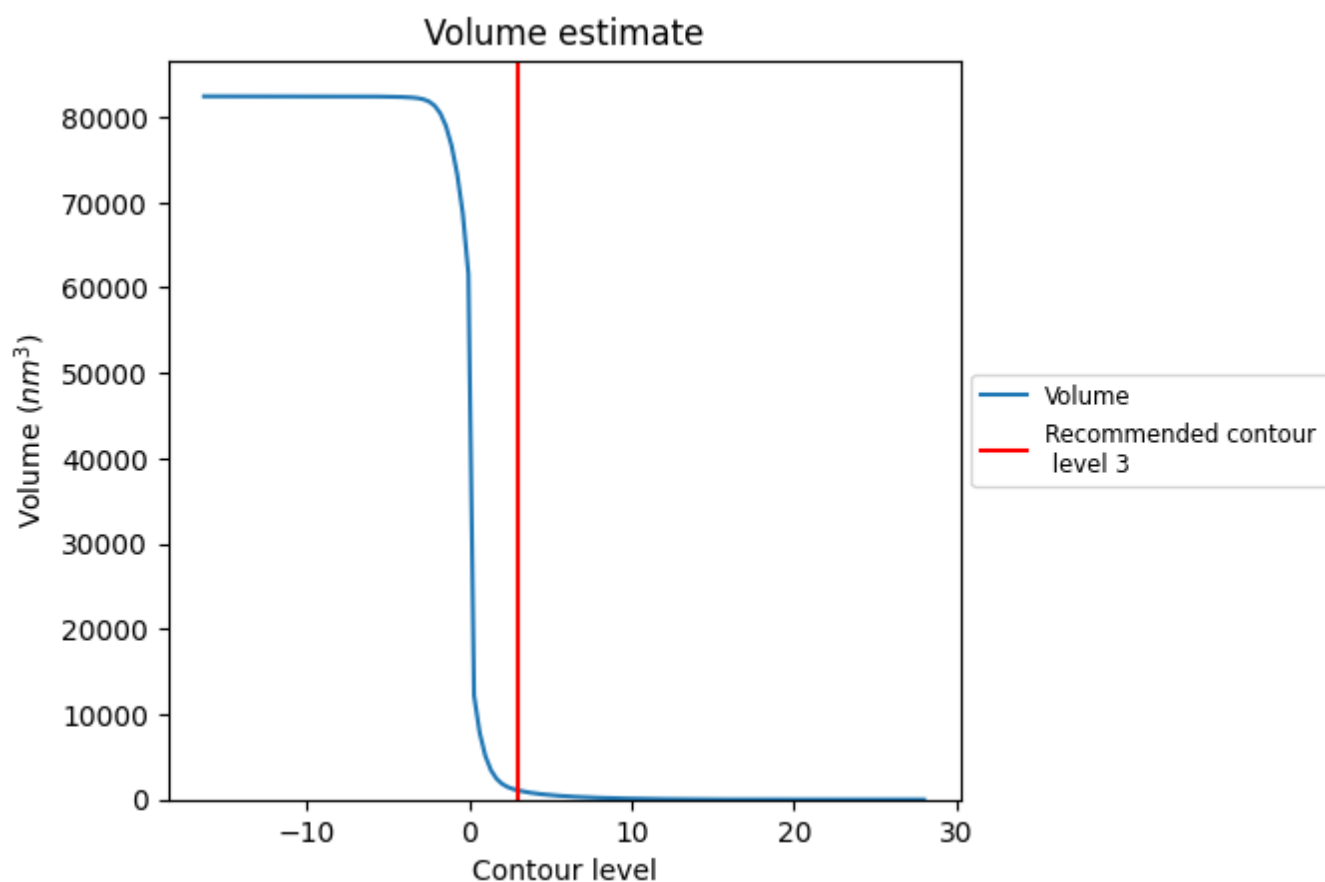
This section contains the results of statistical analysis of the map.

### 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.

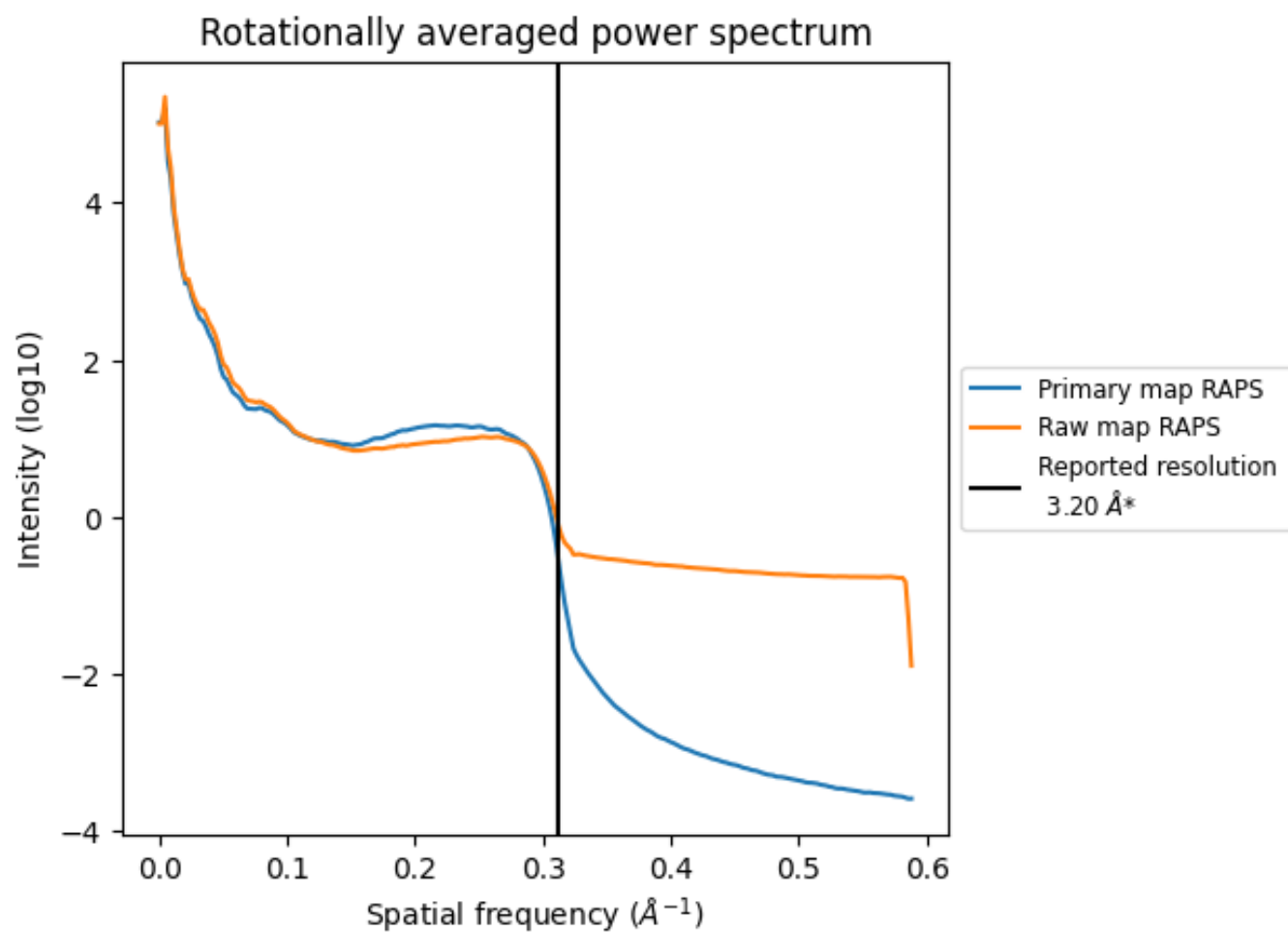
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1076 nm<sup>3</sup>; this corresponds to an approximate mass of 972 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 ⓘ

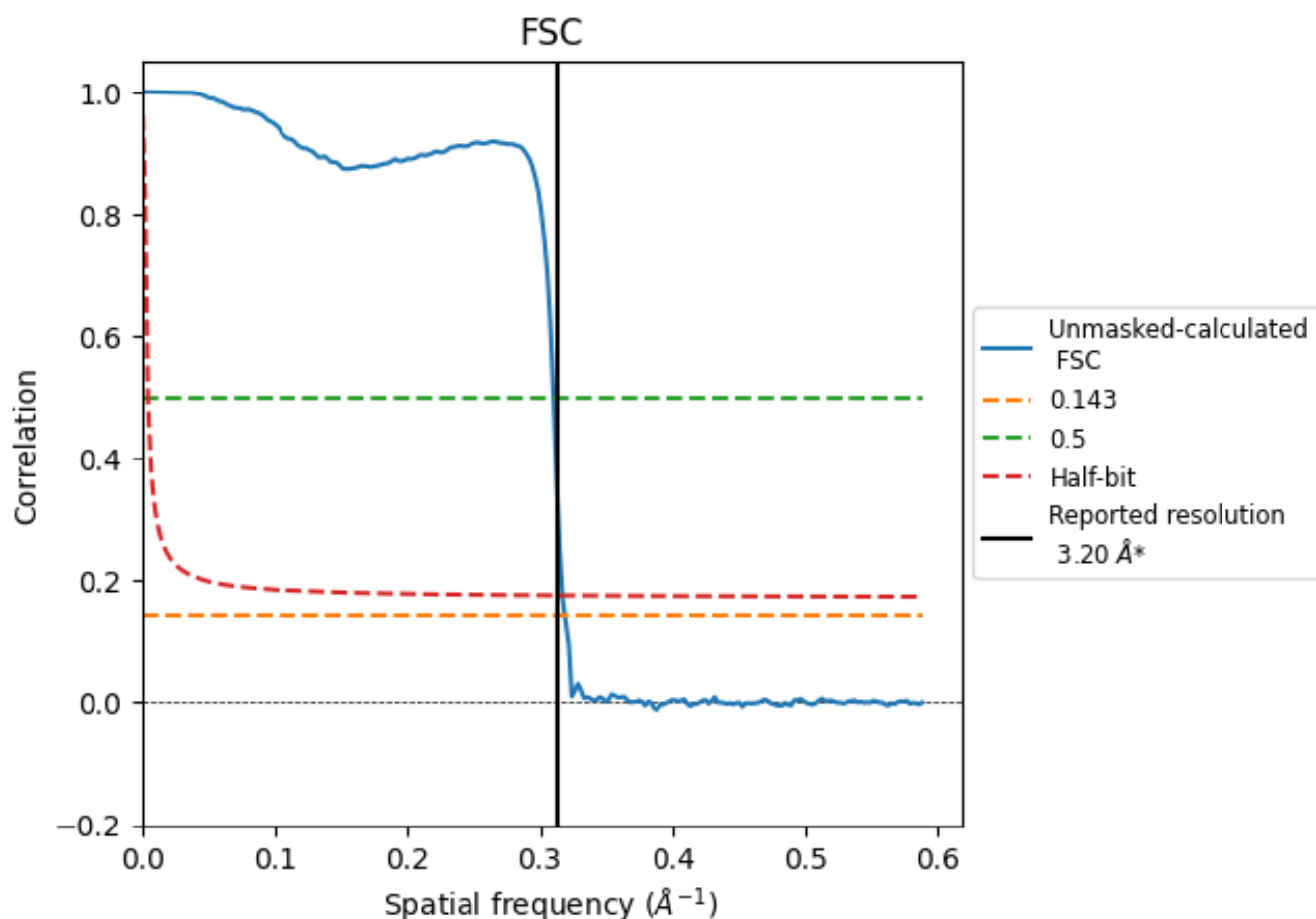


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

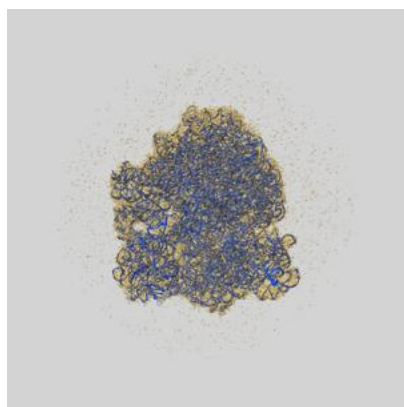
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.20                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.14                               | 3.22 | 3.16     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

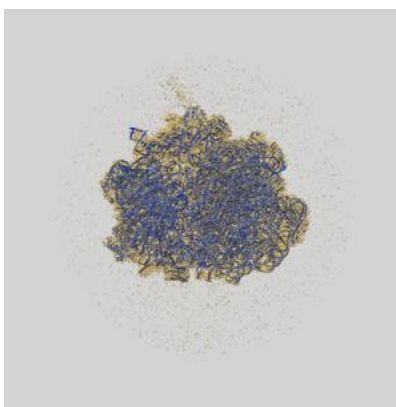
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29624 and PDB model 8FZF. Per-residue inclusion information can be found in section [3](#) on page [17](#).

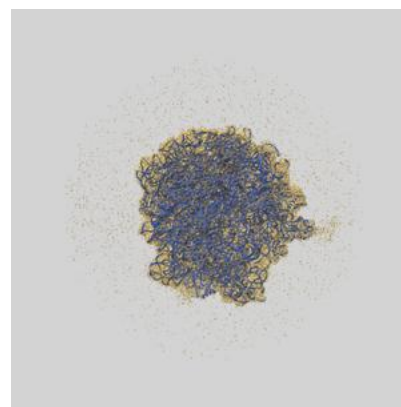
### 9.1 Map-model overlay [i](#)



X



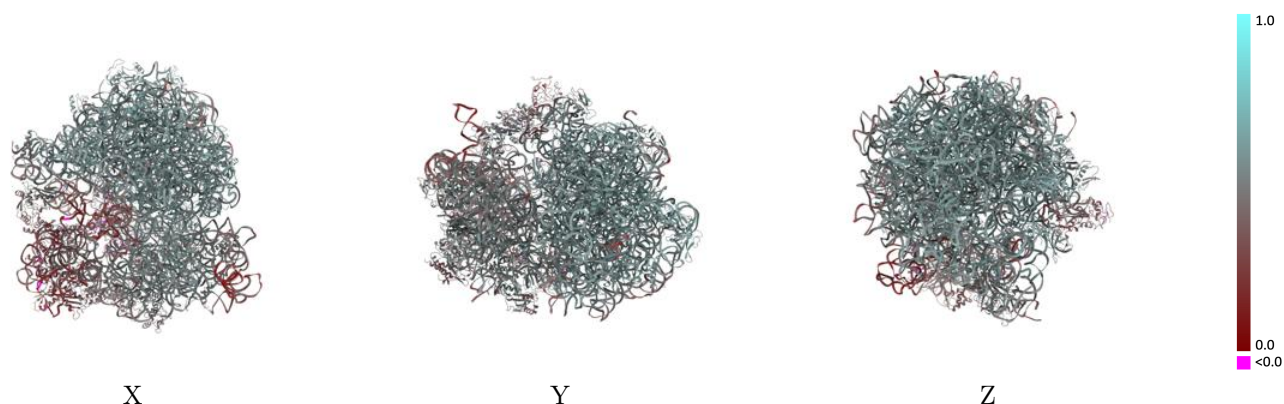
Y



Z

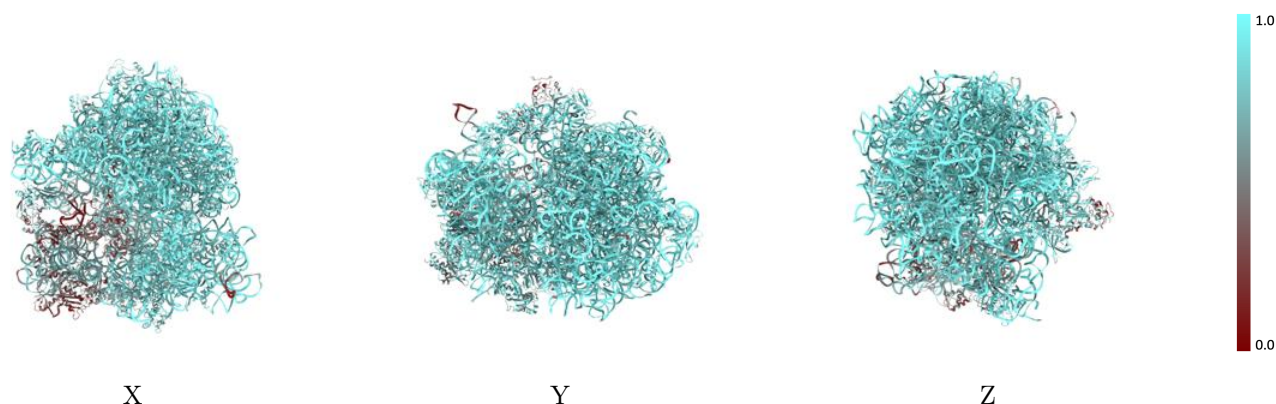
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



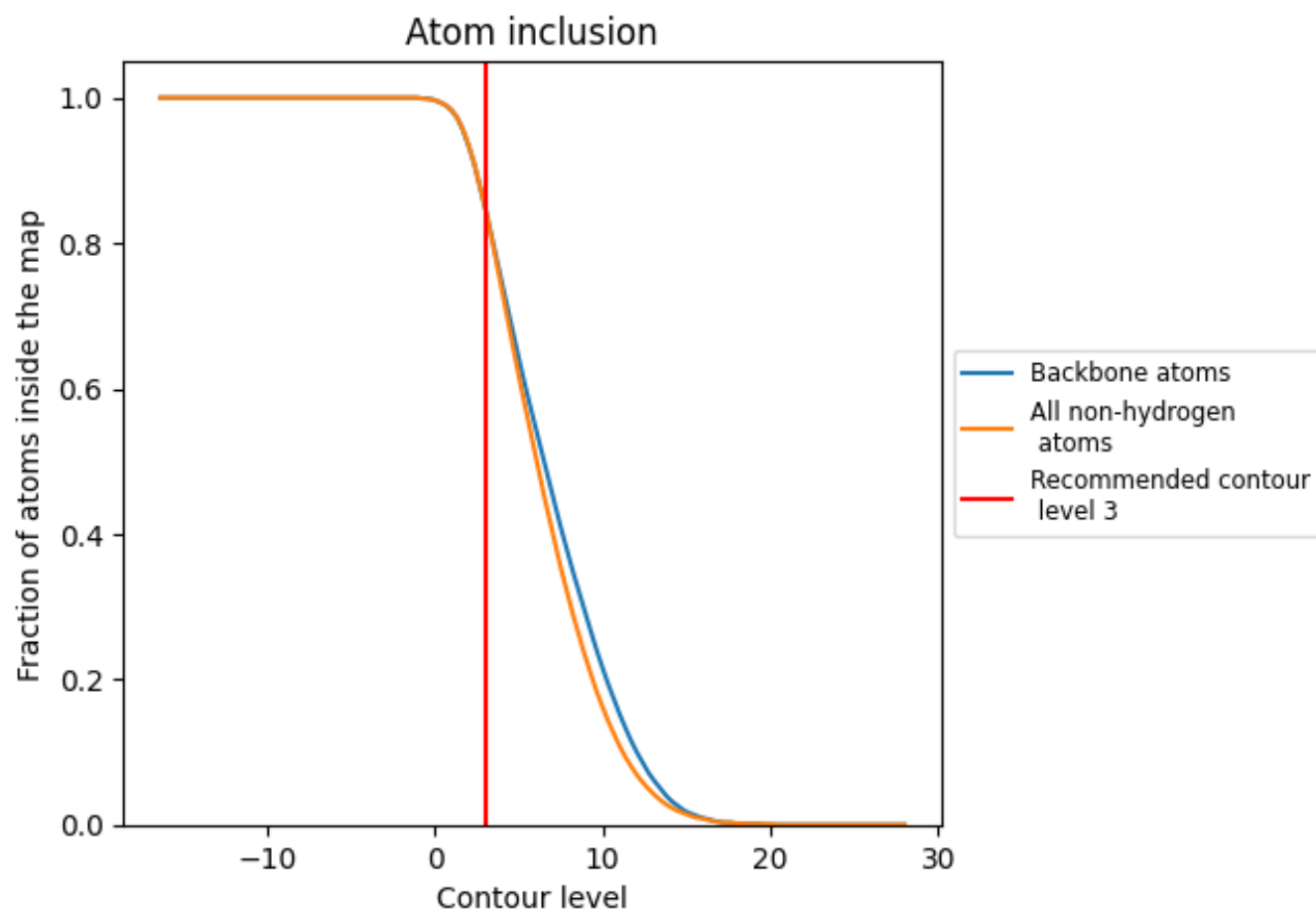
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8500   |  0.4990   |
| 1     |  0.8780   |  0.5530   |
| 2     |  0.8760   |  0.5690   |
| 3     |  0.5550   |  0.4030   |
| 4     |  0.9260   |  0.5790   |
| 5     |  0.8090   |  0.5430   |
| 6     |  0.9160   |  0.5940   |
| 7     |  0.9110   |  0.5860   |
| 8     |  0.9180   |  0.5840   |
| A     |  0.9190   |  0.5310   |
| B     |  0.9170   |  0.4930   |
| C     |  0.8950   |  0.5810   |
| D     |  0.8990   |  0.5800   |
| E     |  0.8650   |  0.5670   |
| F     |  0.7330  |  0.4450  |
| G     |  0.8470 |  0.5300 |
| I     |  0.4290 |  0.3140 |
| J     |  0.3130 |  0.2330 |
| L     |  0.9100 |  0.5860 |
| M     |  0.8570 |  0.5760 |
| N     |  0.8970 |  0.5720 |
| O     |  0.8210 |  0.5520 |
| P     |  0.9420 |  0.5920 |
| Q     |  0.8620 |  0.5310 |
| R     |  0.8490 |  0.5710 |
| S     |  0.9540 |  0.5980 |
| T     |  0.9250 |  0.5730 |
| U     |  0.8850 |  0.5740 |
| V     |  0.8640 |  0.5630 |
| W     |  0.8660 |  0.5430 |
| X     |  0.8580 |  0.5530 |
| Y     |  0.8850 |  0.5840 |
| Z     |  0.9020 |  0.5730 |
| a     |  0.8510 |  0.4510 |
| b     |  0.6130 |  0.4070 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| c     |  0.3900   |  0.3840   |
| d     |  0.8010   |  0.4920   |
| e     |  0.8080   |  0.5130   |
| f     |  0.7550   |  0.4610   |
| g     |  0.3300   |  0.2960   |
| h     |  0.8200   |  0.5080   |
| i     |  0.5800   |  0.3700   |
| j     |  0.4380   |  0.3200   |
| k     |  0.7320   |  0.4910   |
| l     |  0.7870   |  0.5300   |
| m     |  0.4120   |  0.3400   |
| n     |  0.4930   |  0.3780   |
| o     |  0.8150   |  0.4890   |
| p     |  0.8280   |  0.5120   |
| q     |  0.8180   |  0.5150   |
| r     |  0.8150   |  0.5080   |
| s     |  0.4130   |  0.2980   |
| t     |  0.7880  |  0.4880  |
| u     |  0.4420 |  0.4010 |
| v     |  0.9510 |  0.5130 |
| x     |  0.6210 |  0.3410 |
| z     |  0.5660 |  0.4570 |