



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:02 AM UTC

PDB ID : 9GUP / pdb\_00009gup  
EMDB ID : EMD-51615  
Title : 30S mRNA delivery complex (open head)  
Authors : Rahil, H.; Weixlbaumer, A.; Webster, M.W.  
Deposited on : 2024-09-20  
Resolution : 2.80 Å(reported)

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:

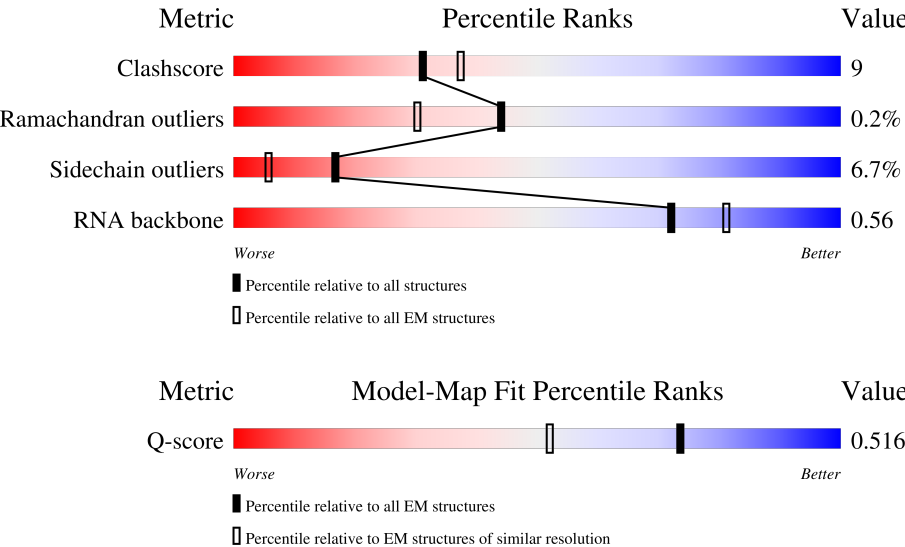
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 2.80 Å.

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



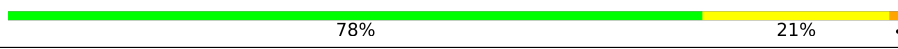
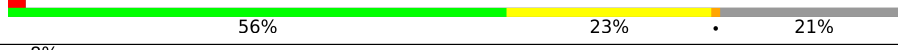
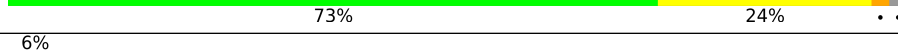
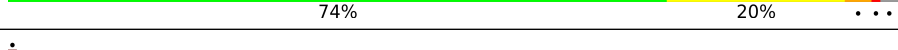
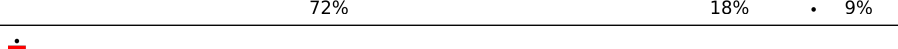
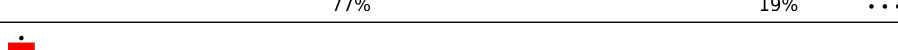
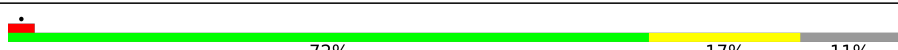
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11806 ( 2.30 - 3.30 )                                    |

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     | 1541   |  |
| 2   | B     | 557    |  |
| 3   | C     | 241    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 233    |    |
| 5   | E     | 206    |    |
| 6   | F     | 156    |    |
| 7   | G     | 131    |    |
| 8   | H     | 156    |    |
| 9   | I     | 130    |    |
| 10  | J     | 130    |    |
| 11  | K     | 103    |    |
| 12  | L     | 129    |    |
| 13  | M     | 124    |    |
| 14  | N     | 118    |    |
| 15  | O     | 101    |  |
| 16  | P     | 89     |  |
| 17  | Q     | 82     |  |
| 18  | R     | 84     |  |
| 19  | S     | 75     |  |
| 20  | T     | 92     |  |
| 21  | U     | 87     |  |
| 22  | V     | 71     |  |
| 23  | X     | 53     |  |

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 53689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | A     | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33023 | 14736 | 6046 | 10702 | 1539 |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1148  | 708 | 201 | 238 | 1 |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1116 | 317 | 324 | 8 |         |       |

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | D     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1046 | 310 | 293 | 4 |         |       |

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S5.

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

- Molecule 7 is a protein called Small ribosomal subunit protein bS6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 848   | 536 | 153 | 152 | 7 |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1176  | 732 | 226 | 214 | 4 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | I     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1031  | 639 | 207 | 182 | 3 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 504 | 155 | 148 | 1 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 951   | 588 | 195 | 163 | 5 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 552 | 179 | 157 | 3 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 19  | S     | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 554   | 350 | 104 | 99 | 1 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 424 | 126 | 111 | 2 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | U     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 22  | V     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 590   | 366 | 125 | 98 | 1 |         |       |

- Molecule 23 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 23  | X     | 17       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 365   | 163 | 65 | 120 | 17 |         |       |

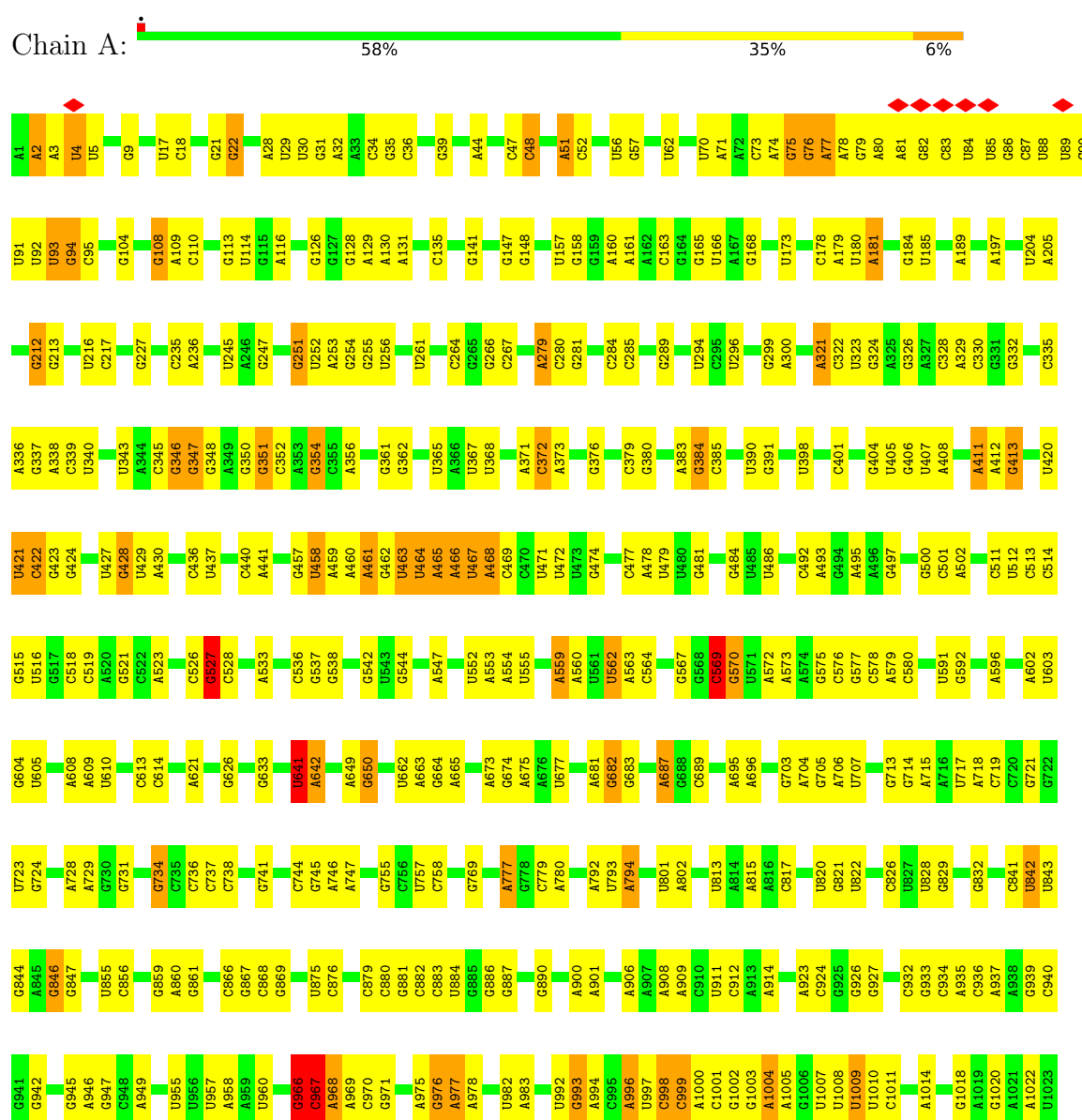
- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

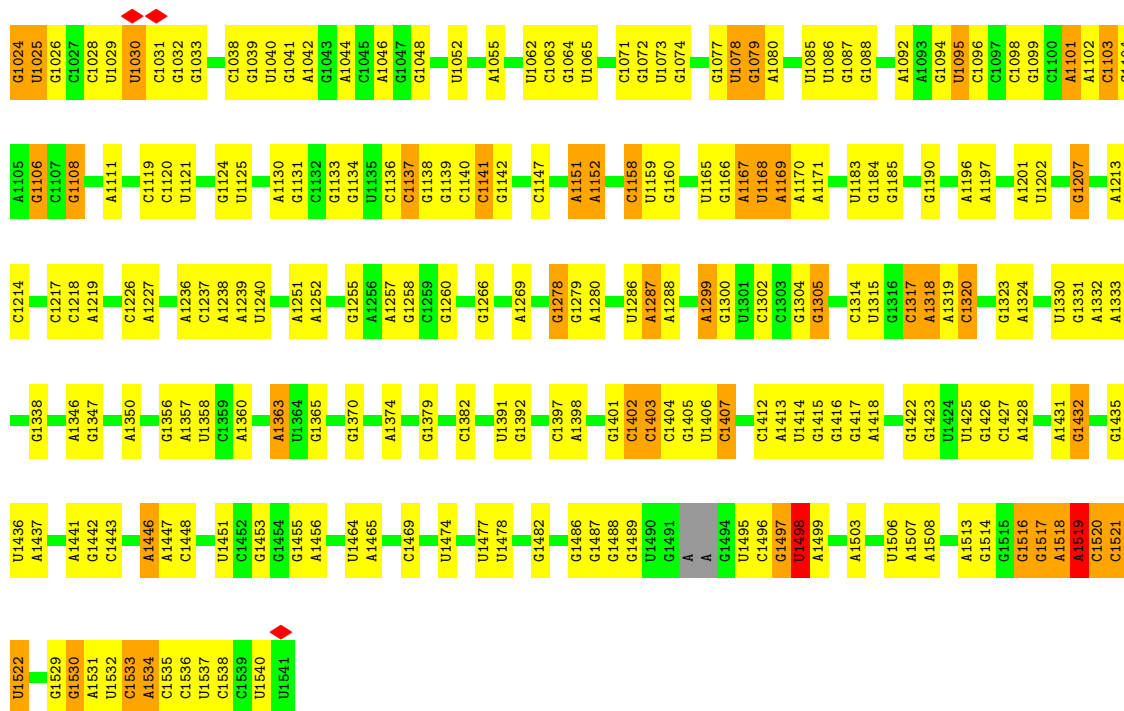
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | A     | 86       | Total | Mg | 0       |
|     |       |          | 86    | 86 |         |

### 3 Residue-property plots

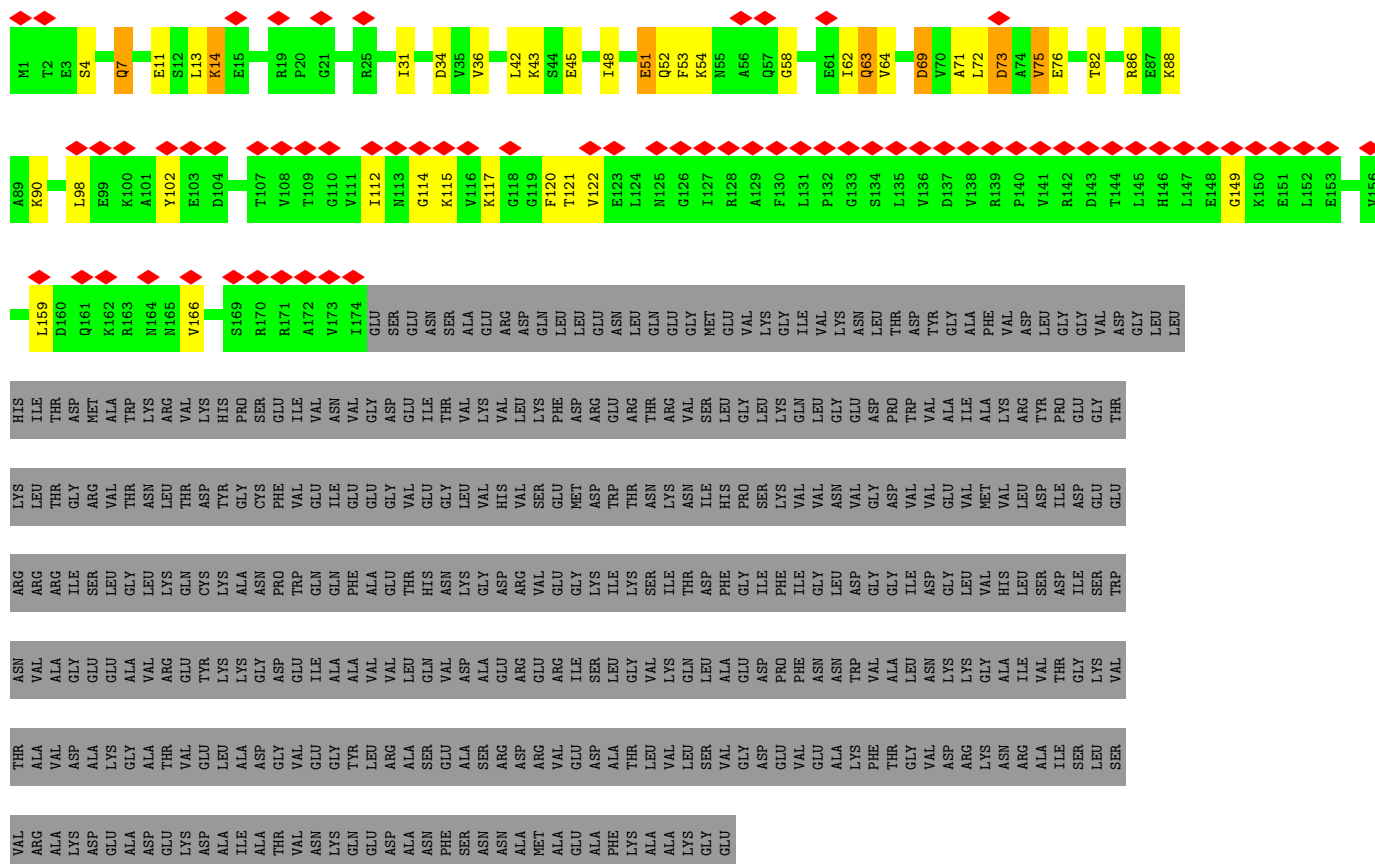
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

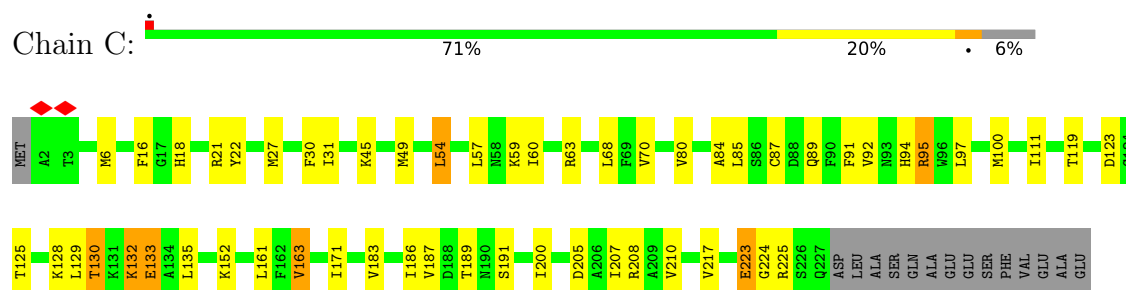




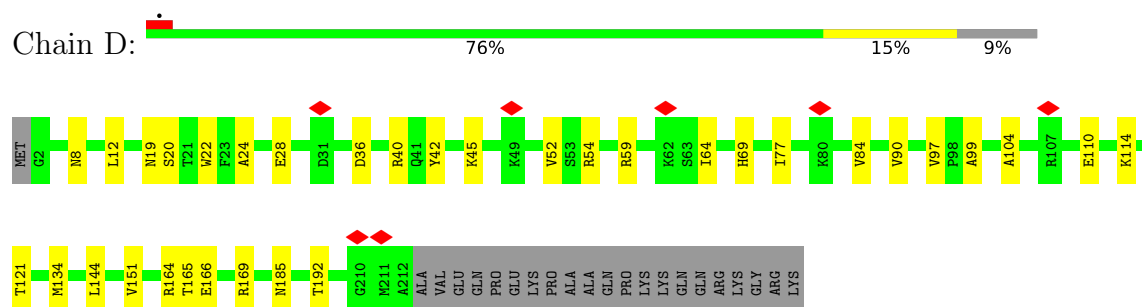
• Molecule 2: 30S ribosomal protein S1



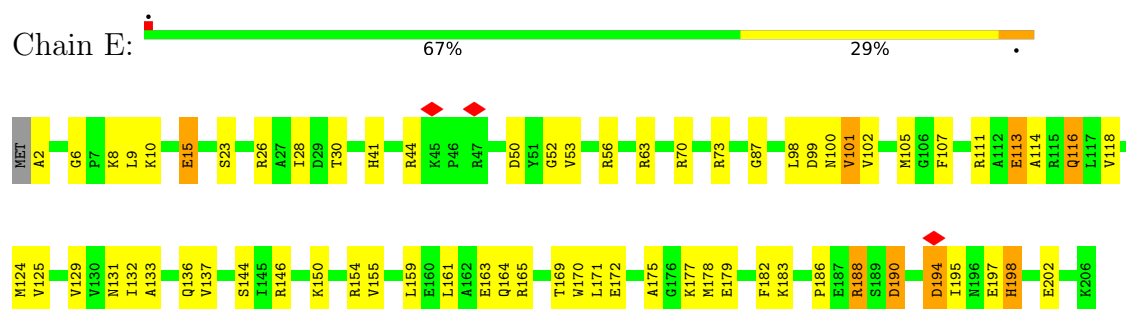
- Molecule 3: 30S ribosomal protein S2



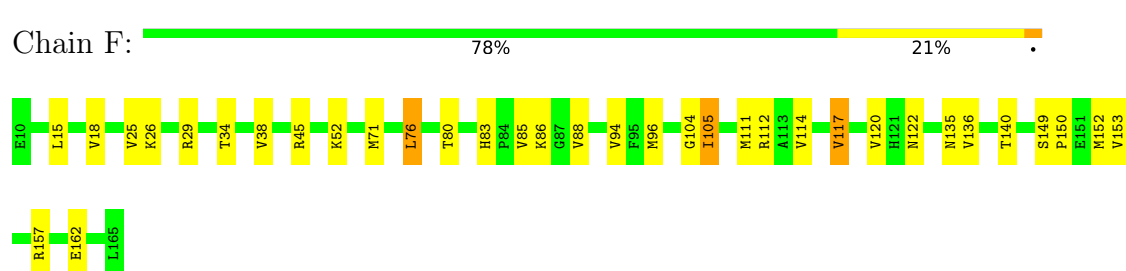
- Molecule 4: Small ribosomal subunit protein uS3



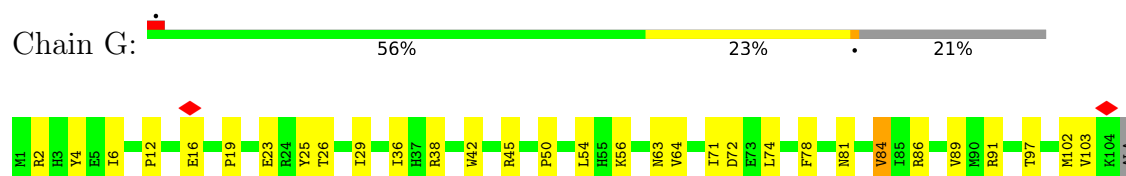
- Molecule 5: Small ribosomal subunit protein uS4



- Molecule 6: 30S ribosomal protein S5



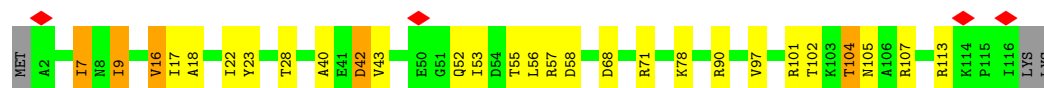
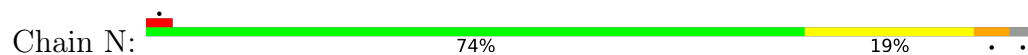
- Molecule 7: Small ribosomal subunit protein bS6



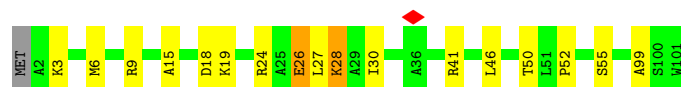
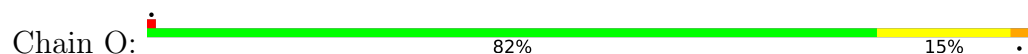




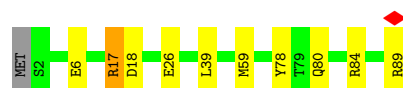
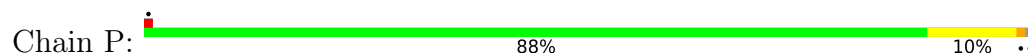
- Molecule 14: 30S ribosomal protein S13



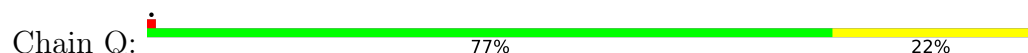
- Molecule 15: 30S ribosomal protein S14



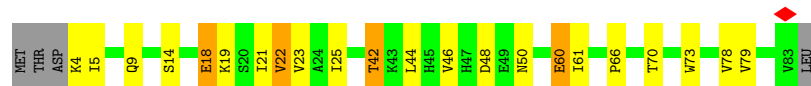
- Molecule 16: Small ribosomal subunit protein uS15



- Molecule 17: 30S ribosomal protein S16



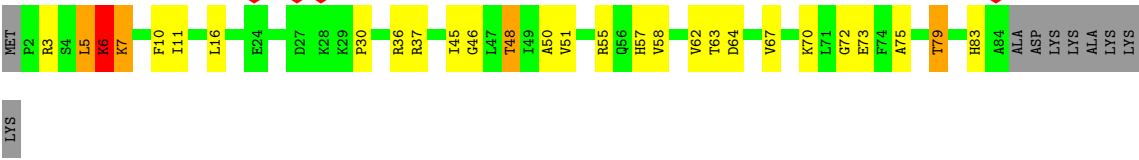
- Molecule 18: 30S ribosomal protein S17



- Molecule 19: 30S ribosomal protein S18



- Molecule 20: 30S ribosomal protein S19



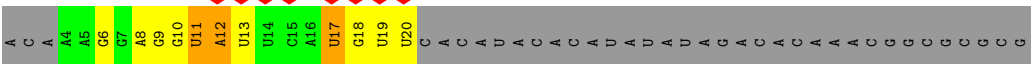
• Molecule 21: 30S ribosomal protein S20



• Molecule 22: 30S ribosomal protein S21



• Molecule 23: mRNA



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 52113                                   | 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 ( $e^-/\text{\AA}^2$ ) | 49.95                                   | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 7.196                                   | Depositor |
| Minimum map value                    | -2.451                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.151                                   | Depositor |
| Recommended contour level            | 0.745                                   | Depositor |
| Map size (Å)                         | 503.99997, 503.99997, 503.99997         | wwPDB     |
| Map dimensions                       | 600, 600, 600                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.84, 0.84, 0.84                        | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, MA6, 2MG, PSU, G7M, UR3, D2T, 5MC, MG

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.34         | 2/36692 (0.0%) | 0.37        | 9/57230 (0.0%)  |
| 2   | B     | 0.20         | 0/1157         | 0.43        | 0/1574          |
| 3   | C     | 0.29         | 0/1796         | 0.46        | 0/2420          |
| 4   | D     | 0.24         | 0/1680         | 0.38        | 0/2263          |
| 5   | E     | 0.26         | 0/1665         | 0.38        | 0/2227          |
| 6   | F     | 0.24         | 0/1165         | 0.36        | 0/1568          |
| 7   | G     | 0.27         | 0/867          | 0.41        | 0/1171          |
| 8   | H     | 0.20         | 0/1190         | 0.37        | 0/1595          |
| 9   | I     | 0.25         | 0/989          | 0.37        | 0/1326          |
| 10  | J     | 0.29         | 0/1043         | 0.40        | 0/1387          |
| 11  | K     | 0.33         | 0/818          | 0.73        | 3/1105 (0.3%)   |
| 12  | L     | 0.23         | 0/893          | 0.38        | 0/1205          |
| 13  | M     | 0.32         | 0/954          | 0.55        | 2/1279 (0.2%)   |
| 14  | N     | 0.22         | 0/900          | 0.32        | 0/1204          |
| 15  | O     | 0.24         | 0/817          | 0.30        | 0/1088          |
| 16  | P     | 0.24         | 0/722          | 0.35        | 0/964           |
| 17  | Q     | 0.31         | 0/659          | 0.35        | 0/884           |
| 18  | R     | 0.24         | 0/657          | 0.32        | 0/881           |
| 19  | S     | 0.27         | 0/563          | 0.37        | 0/754           |
| 20  | T     | 0.30         | 0/680          | 0.57        | 2/915 (0.2%)    |
| 21  | U     | 0.26         | 0/676          | 0.32        | 0/895           |
| 22  | V     | 0.19         | 0/598          | 0.31        | 0/792           |
| 23  | X     | 0.16         | 0/408          | 0.35        | 0/634           |
| All | All   | 0.31         | 2/57589 (0.0%) | 0.38        | 16/85361 (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 |
|-----|-------|---------------------|---------------------|
| 11  | K     | 0                   | 1                   |
| 13  | M     | 0                   | 1                   |
| 20  | T     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1108 | G    | O3'-P | -5.43 | 1.53        | 1.61     |
| 1   | A     | 527  | G7M  | O3'-P | 5.38  | 1.61        | 1.56     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 11  | K     | 39   | PRO  | CB-CA-C     | -15.30 | 92.21       | 111.64   |
| 1   | A     | 641  | U    | C2'-C3'-O3' | 12.34  | 128.00      | 109.50   |
| 20  | T     | 7    | LYS  | N-CA-C      | -9.78  | 101.11      | 113.43   |
| 20  | T     | 6    | LYS  | CB-CA-C     | -7.52  | 95.46       | 110.42   |
| 1   | A     | 527  | G7M  | OP1-P-O3'   | 6.84   | 120.25      | 105.20   |
| 11  | K     | 38   | GLY  | CA-C-N      | 6.77   | 127.17      | 119.93   |
| 11  | K     | 38   | GLY  | C-N-CA      | 6.77   | 127.17      | 119.93   |
| 13  | M     | 44   | LYS  | N-CA-CB     | -6.47  | 101.76      | 110.23   |
| 1   | A     | 813  | U    | C1'-C2'-O2' | -5.99  | 99.42       | 108.40   |
| 1   | A     | 1106 | G    | C1'-C2'-O2' | -5.77  | 99.74       | 108.40   |
| 1   | A     | 570  | G    | C4'-C3'-O3' | -5.73  | 104.41      | 113.00   |
| 13  | M     | 44   | LYS  | CB-CA-C     | 5.55   | 117.37      | 109.38   |
| 1   | A     | 1403 | C    | C1'-C2'-O2' | -5.43  | 100.25      | 108.40   |
| 1   | A     | 1522 | U    | C2'-C3'-O3' | -5.35  | 105.67      | 113.70   |
| 1   | A     | 563  | A    | C4'-C3'-O3' | -5.26  | 105.10      | 113.00   |
| 1   | A     | 569  | C    | C2'-C3'-O3' | -5.17  | 105.95      | 113.70   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 11  | K     | 38  | GLY  | Peptide   |
| 13  | M     | 44  | LYS  | Peptide   |
| 20  | T     | 5   | LEU  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 33023 | 0        | 16643    | 453     | 0            |
| 2   | B     | 1148  | 0        | 948      | 39      | 0            |
| 3   | C     | 1765  | 0        | 1792     | 41      | 0            |
| 4   | D     | 1653  | 0        | 1727     | 18      | 0            |
| 5   | E     | 1643  | 0        | 1707     | 43      | 0            |
| 6   | F     | 1152  | 0        | 1196     | 25      | 0            |
| 7   | G     | 848   | 0        | 846      | 14      | 0            |
| 8   | H     | 1176  | 0        | 1233     | 29      | 0            |
| 9   | I     | 979   | 0        | 1031     | 16      | 0            |
| 10  | J     | 1031  | 0        | 1076     | 23      | 0            |
| 11  | K     | 808   | 0        | 845      | 14      | 0            |
| 12  | L     | 877   | 0        | 887      | 20      | 0            |
| 13  | M     | 951   | 0        | 1012     | 15      | 0            |
| 14  | N     | 891   | 0        | 952      | 15      | 0            |
| 15  | O     | 805   | 0        | 844      | 14      | 0            |
| 16  | P     | 714   | 0        | 734      | 7       | 0            |
| 17  | Q     | 649   | 0        | 666      | 11      | 0            |
| 18  | R     | 648   | 0        | 691      | 13      | 0            |
| 19  | S     | 554   | 0        | 573      | 11      | 0            |
| 20  | T     | 663   | 0        | 688      | 23      | 0            |
| 21  | U     | 670   | 0        | 719      | 16      | 0            |
| 22  | V     | 590   | 0        | 629      | 24      | 0            |
| 23  | X     | 365   | 0        | 182      | 11      | 0            |
| 24  | A     | 86    | 0        | 0        | 0       | 0            |
| All | All   | 53689 | 0        | 37621    | 791     | 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 9.

All (791) 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) |
|----------------|-----------------|--------------------------|-------------------|
| 2:B:53:PHE:CD2 | 2:B:62:ILE:HD12 | 1.61                     | 1.34              |
| 2:B:53:PHE:HD2 | 2:B:62:ILE:CD1  | 1.41                     | 1.33              |
| 2:B:53:PHE:CD2 | 2:B:62:ILE:CD1  | 2.18                     | 1.25              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:75:VAL:O     | 2:B:76:GLU:HG3   | 1.50                     | 1.09              |
| 2:B:53:PHE:HD2   | 2:B:62:ILE:HD12  | 0.86                     | 1.03              |
| 1:A:966:2MG:H5'' | 1:A:966:2MG:H8   | 1.20                     | 1.01              |
| 1:A:75:G:H4'     | 1:A:75:G:OP1     | 1.68                     | 0.91              |
| 1:A:966:2MG:H5'' | 1:A:966:2MG:C8   | 2.04                     | 0.91              |
| 12:L:89:PRO:HB3  | 22:V:32:VAL:HG21 | 1.51                     | 0.90              |
| 1:A:75:G:C5'     | 1:A:75:G:H8      | 1.88                     | 0.86              |
| 7:G:26:THR:HG23  | 7:G:36:ILE:HG13  | 1.58                     | 0.86              |
| 2:B:75:VAL:O     | 2:B:76:GLU:CG    | 2.24                     | 0.84              |
| 1:A:1533:C:OP2   | 1:A:1533:C:H2'   | 1.79                     | 0.82              |
| 1:A:421:U:H5''   | 1:A:422:C:H5     | 1.44                     | 0.82              |
| 1:A:346:G:H3'    | 1:A:346:G:N3     | 1.97                     | 0.80              |
| 4:D:36:ASP:OD1   | 4:D:59:ARG:NH1   | 2.15                     | 0.79              |
| 3:C:27:MET:HG2   | 3:C:189:THR:HA   | 1.63                     | 0.79              |
| 1:A:1520:C:H5''  | 1:A:1520:C:H6    | 1.47                     | 0.78              |
| 5:E:124:MET:HE3  | 5:E:146:ARG:HE   | 1.48                     | 0.78              |
| 1:A:420:U:H2'    | 1:A:422:C:C5     | 2.19                     | 0.78              |
| 1:A:1423:G:H1    | 1:A:1477:U:H3    | 1.31                     | 0.78              |
| 2:B:75:VAL:C     | 2:B:76:GLU:HG3   | 2.08                     | 0.77              |
| 1:A:1382:C:H5'   | 8:H:79:ARG:HH21  | 1.50                     | 0.76              |
| 20:T:70:LYS:HB2  | 20:T:73:GLU:HG3  | 1.67                     | 0.76              |
| 1:A:465:A:N3     | 1:A:465:A:H2'    | 2.01                     | 0.75              |
| 5:E:102:VAL:HG13 | 5:E:114:ALA:HB1  | 1.68                     | 0.75              |
| 1:A:1147:C:O2'   | 10:J:7:TYR:OH    | 2.05                     | 0.75              |
| 1:A:1350:A:O2'   | 8:H:33:ASP:OD1   | 2.05                     | 0.74              |
| 1:A:1520:C:H5''  | 1:A:1520:C:C6    | 2.23                     | 0.73              |
| 5:E:101:VAL:HG21 | 5:E:137:VAL:HG21 | 1.70                     | 0.73              |
| 1:A:468:A:H3'    | 1:A:469:C:H6     | 1.54                     | 0.73              |
| 1:A:458:U:H5''   | 1:A:458:U:H6     | 1.54                     | 0.73              |
| 1:A:664:G:H22    | 1:A:741:G:H1     | 1.34                     | 0.73              |
| 1:A:407:U:O2'    | 5:E:113:GLU:OE1  | 2.06                     | 0.73              |
| 1:A:1240:U:OP1   | 8:H:119:ARG:NH2  | 2.22                     | 0.73              |
| 2:B:43:LYS:HG3   | 3:C:16:PHE:HB3   | 1.70                     | 0.72              |
| 1:A:1363:A:O2'   | 1:A:1365:G:N7    | 2.20                     | 0.72              |
| 2:B:53:PHE:CD2   | 2:B:62:ILE:HD13  | 2.22                     | 0.72              |
| 1:A:75:G:H8      | 1:A:75:G:H5'     | 1.53                     | 0.72              |
| 3:C:119:THR:O    | 3:C:123:ASP:HB2  | 1.89                     | 0.72              |
| 1:A:1374:A:OP1   | 8:H:36:LYS:NZ    | 2.19                     | 0.72              |
| 1:A:3:A:H5''     | 1:A:4:U:H5'      | 1.72                     | 0.72              |
| 1:A:77:A:O5'     | 1:A:77:A:H8      | 1.72                     | 0.72              |
| 2:B:112:ILE:O    | 2:B:149:GLY:N    | 2.16                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 20:T:36:ARG:NH2   | 20:T:75:ALA:O    | 2.23                     | 0.72              |
| 2:B:75:VAL:HG22   | 2:B:76:GLU:HG3   | 1.72                     | 0.71              |
| 1:A:423:G:H5''    | 1:A:423:G:N3     | 2.06                     | 0.71              |
| 1:A:562:U:H1'     | 13:M:12:ARG:HB3  | 1.70                     | 0.71              |
| 1:A:421:U:H3'     | 1:A:422:C:C6     | 2.26                     | 0.71              |
| 1:A:1403:C:O5'    | 1:A:1403:C:H6    | 1.73                     | 0.71              |
| 8:H:113:ASP:OD2   | 8:H:122:ASN:ND2  | 2.23                     | 0.71              |
| 1:A:467:U:H3'     | 1:A:467:U:O2     | 1.92                     | 0.70              |
| 2:B:114:GLY:O     | 2:B:121:THR:N    | 2.24                     | 0.70              |
| 1:A:75:G:C5'      | 1:A:75:G:C8      | 2.73                     | 0.70              |
| 21:U:35:VAL:HG21  | 21:U:54:MET:HG2  | 1.72                     | 0.70              |
| 1:A:826:C:O2      | 9:I:16:ASN:ND2   | 2.24                     | 0.70              |
| 1:A:458:U:H3      | 1:A:474:G:H1     | 1.40                     | 0.70              |
| 13:M:99:ARG:NH1   | 13:M:105:SER:O   | 2.26                     | 0.69              |
| 1:A:713:G:H2'     | 1:A:714:G:C8     | 2.28                     | 0.69              |
| 10:J:118:LEU:HD22 | 10:J:124:ARG:HG2 | 1.75                     | 0.69              |
| 1:A:126:G:OP1     | 1:A:605:U:O2'    | 2.09                     | 0.69              |
| 1:A:933:G:N7      | 8:H:3:ARG:NH1    | 2.40                     | 0.69              |
| 14:N:68:ASP:OD1   | 14:N:71:ARG:NH1  | 2.26                     | 0.69              |
| 1:A:468:A:H3'     | 1:A:469:C:C6     | 2.29                     | 0.68              |
| 21:U:15:GLU:OE2   | 21:U:19:LYS:NZ   | 2.27                     | 0.67              |
| 1:A:1158:C:H5'    | 3:C:132:LYS:HD3  | 1.77                     | 0.67              |
| 1:A:261:U:OP2     | 21:U:74:ARG:NH2  | 2.28                     | 0.67              |
| 1:A:421:U:H5''    | 1:A:422:C:C5     | 2.27                     | 0.67              |
| 2:B:53:PHE:CE2    | 2:B:62:ILE:CD1   | 2.78                     | 0.67              |
| 1:A:641:U:H1'     | 1:A:642:A:N7     | 2.10                     | 0.66              |
| 10:J:52:LEU:HD11  | 10:J:63:LEU:HD11 | 1.77                     | 0.66              |
| 1:A:492:C:H2'     | 1:A:493:A:C8     | 2.31                     | 0.66              |
| 1:A:526:C:C4      | 1:A:527:G7M:H1'  | 2.31                     | 0.66              |
| 20:T:46:GLY:N     | 20:T:62:VAL:O    | 2.26                     | 0.66              |
| 1:A:946:A:H2'     | 1:A:947:G:C8     | 2.30                     | 0.66              |
| 5:E:100:ASN:OD1   | 5:E:111:ARG:NH1  | 2.29                     | 0.65              |
| 1:A:255:G:H2'     | 1:A:256:U:C6     | 2.30                     | 0.65              |
| 3:C:60:ILE:HG12   | 3:C:63:ARG:HH21  | 1.62                     | 0.65              |
| 1:A:227:G:O2'     | 17:Q:63:GLN:OE1  | 2.13                     | 0.65              |
| 1:A:75:G:H5'      | 1:A:75:G:C8      | 2.31                     | 0.65              |
| 1:A:79:G:H2'      | 1:A:80:A:C8      | 2.33                     | 0.64              |
| 2:B:4:SER:OG      | 2:B:7:GLN:NE2    | 2.31                     | 0.64              |
| 2:B:73:ASP:OD1    | 2:B:73:ASP:N     | 2.30                     | 0.64              |
| 22:V:29:LEU:HA    | 22:V:32:VAL:HG22 | 1.80                     | 0.64              |
| 1:A:347:G:H8      | 1:A:347:G:OP2    | 1.81                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1530:G:H2'    | 1:A:1531:A:C8    | 2.32                     | 0.64              |
| 6:F:83:HIS:HD2    | 9:I:99:LEU:HD12  | 1.62                     | 0.64              |
| 10:J:116:VAL:HG13 | 11:K:62:ARG:HH11 | 1.61                     | 0.64              |
| 1:A:1533:C:OP2    | 1:A:1533:C:H6    | 1.80                     | 0.64              |
| 1:A:890:G:O2'     | 1:A:906:A:N6     | 2.31                     | 0.64              |
| 2:B:159:LEU:HA    | 2:B:166:VAL:HA   | 1.80                     | 0.63              |
| 20:T:50:ALA:HB1   | 20:T:57:HIS:HB3  | 1.80                     | 0.63              |
| 1:A:356:A:N3      | 1:A:368:U:O2'    | 2.29                     | 0.63              |
| 4:D:20:SER:OG     | 4:D:22:TRP:NE1   | 2.31                     | 0.63              |
| 13:M:71:GLY:O     | 13:M:99:ARG:NH2  | 2.32                     | 0.63              |
| 1:A:1536:C:C2     | 23:X:10:G:N2     | 2.67                     | 0.62              |
| 3:C:97:LEU:HB2    | 3:C:100:MET:HG3  | 1.81                     | 0.62              |
| 7:G:2:ARG:HG2     | 7:G:91:ARG:HH21  | 1.63                     | 0.62              |
| 1:A:1356:G:H2'    | 1:A:1357:A:C8    | 2.34                     | 0.62              |
| 9:I:11:LEU:HD22   | 9:I:75:ILE:HD11  | 1.80                     | 0.62              |
| 15:O:6:MET:SD     | 15:O:9:ARG:NH1   | 2.72                     | 0.62              |
| 8:H:113:ASP:N     | 8:H:113:ASP:OD1  | 2.30                     | 0.62              |
| 1:A:717:U:O3'     | 12:L:119:ASN:ND2 | 2.33                     | 0.62              |
| 1:A:673:A:H2'     | 1:A:674:G:C8     | 2.34                     | 0.62              |
| 1:A:746:A:H2'     | 1:A:747:A:C8     | 2.35                     | 0.62              |
| 1:A:467:U:O2      | 1:A:467:U:C3'    | 2.47                     | 0.62              |
| 1:A:626:G:OP1     | 17:Q:35:ARG:NH2  | 2.33                     | 0.62              |
| 8:H:111:ARG:NH2   | 8:H:126:ASP:OD2  | 2.29                     | 0.62              |
| 20:T:5:LEU:C      | 20:T:7:LYS:H     | 2.07                     | 0.62              |
| 2:B:53:PHE:CE2    | 2:B:62:ILE:HD13  | 2.35                     | 0.61              |
| 5:E:194:ASP:OD1   | 5:E:194:ASP:N    | 2.21                     | 0.61              |
| 1:A:1251:A:H2'    | 1:A:1252:A:C8    | 2.35                     | 0.61              |
| 1:A:946:A:H2'     | 1:A:947:G:H8     | 1.65                     | 0.60              |
| 1:A:1239:A:H62    | 1:A:1299:A:H62   | 1.48                     | 0.60              |
| 12:L:76:GLU:O     | 12:L:76:GLU:HG2  | 1.99                     | 0.60              |
| 22:V:4:ILE:HG13   | 22:V:19:PHE:HA   | 1.83                     | 0.60              |
| 11:K:54:SER:OG    | 11:K:57:VAL:O    | 2.14                     | 0.60              |
| 1:A:859:G:H2'     | 1:A:860:A:H8     | 1.66                     | 0.60              |
| 1:A:1488:G:H2'    | 1:A:1489:G:H8    | 1.67                     | 0.60              |
| 17:Q:6:LEU:HB3    | 17:Q:17:TYR:HB3  | 1.82                     | 0.60              |
| 1:A:993:G:H2'     | 1:A:993:G:N3     | 2.16                     | 0.60              |
| 1:A:1516:2MG:H2'  | 1:A:1518:MA6:OP2 | 2.01                     | 0.60              |
| 2:B:69:ASP:OD1    | 2:B:69:ASP:N     | 2.35                     | 0.60              |
| 1:A:77:A:H2'      | 1:A:78:A:C8      | 2.37                     | 0.59              |
| 1:A:463:U:H5''    | 1:A:463:U:C6     | 2.37                     | 0.59              |
| 1:A:999:C:H2'     | 1:A:1000:A:C8    | 2.36                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1005:A:OP2    | 1:A:1024:G:N2    | 2.26                     | 0.59              |
| 1:A:1537:U:H2'    | 1:A:1538:C:C6    | 2.36                     | 0.59              |
| 3:C:129:LEU:HD13  | 3:C:133:GLU:HB2  | 1.83                     | 0.59              |
| 5:E:202:GLU:OE2   | 6:F:112:ARG:NH1  | 2.35                     | 0.59              |
| 1:A:1062:U:H2'    | 1:A:1063:C:C6    | 2.38                     | 0.59              |
| 1:A:465:A:H3'     | 1:A:466:A:C8     | 2.38                     | 0.59              |
| 1:A:1537:U:H2'    | 1:A:1538:C:H6    | 1.67                     | 0.59              |
| 3:C:27:MET:HG3    | 3:C:27:MET:O     | 2.03                     | 0.59              |
| 4:D:77:ILE:HA     | 4:D:84:VAL:HG23  | 1.84                     | 0.59              |
| 6:F:150:PRO:HA    | 6:F:153:VAL:HG12 | 1.85                     | 0.59              |
| 1:A:216:U:H1'     | 1:A:466:A:H61    | 1.69                     | 0.58              |
| 1:A:1111:A:O2'    | 3:C:133:GLU:OE1  | 2.20                     | 0.58              |
| 1:A:1427:C:H2'    | 1:A:1428:A:H8    | 1.68                     | 0.58              |
| 6:F:114:VAL:HG11  | 6:F:140:THR:HG21 | 1.85                     | 0.58              |
| 1:A:1518:MA6:H103 | 1:A:1519:MA6:N6  | 2.18                     | 0.58              |
| 1:A:1130:A:H2'    | 1:A:1131:G:H8    | 1.68                     | 0.58              |
| 1:A:1397:C:OP2    | 6:F:29:ARG:NH2   | 2.37                     | 0.58              |
| 6:F:83:HIS:CD2    | 9:I:99:LEU:HD12  | 2.38                     | 0.58              |
| 1:A:966:2MG:HM23  | 1:A:967:5MC:H1'  | 1.85                     | 0.58              |
| 8:H:138:ARG:NH1   | 8:H:139:GLU:OE2  | 2.37                     | 0.58              |
| 1:A:75:G:H2'      | 1:A:76:G:O4'     | 2.04                     | 0.58              |
| 1:A:859:G:H2'     | 1:A:860:A:C8     | 2.39                     | 0.58              |
| 1:A:1535:C:H2'    | 1:A:1536:C:C6    | 2.38                     | 0.58              |
| 1:A:714:G:H2'     | 1:A:715:A:C8     | 2.39                     | 0.58              |
| 1:A:1519:MA6:N7   | 1:A:1519:MA6:H93 | 2.19                     | 0.58              |
| 2:B:43:LYS:NZ     | 3:C:205:ASP:OD2  | 2.36                     | 0.58              |
| 8:H:136:LYS:NZ    | 8:H:140:ASP:OD1  | 2.36                     | 0.58              |
| 10:J:116:VAL:HG13 | 11:K:62:ARG:NH1  | 2.19                     | 0.58              |
| 1:A:421:U:H3'     | 1:A:422:C:H6     | 1.68                     | 0.57              |
| 1:A:477:C:H2'     | 1:A:478:A:C8     | 2.39                     | 0.57              |
| 2:B:117:LYS:O     | 23:X:18:G:N2     | 2.33                     | 0.57              |
| 1:A:147:G:H2'     | 1:A:148:G:C8     | 2.38                     | 0.57              |
| 1:A:1488:G:H2'    | 1:A:1489:G:C8    | 2.38                     | 0.57              |
| 4:D:19:ASN:OD1    | 4:D:54:ARG:NH1   | 2.37                     | 0.57              |
| 5:E:159:LEU:O     | 5:E:163:GLU:HG2  | 2.03                     | 0.57              |
| 15:O:52:PRO:O     | 15:O:55:SER:OG   | 2.22                     | 0.57              |
| 1:A:466:A:H8      | 1:A:466:A:OP2    | 1.86                     | 0.57              |
| 5:E:172:GLU:HB3   | 5:E:183:LYS:HD3  | 1.85                     | 0.57              |
| 1:A:79:G:H2'      | 1:A:80:A:H8      | 1.68                     | 0.57              |
| 12:L:111:THR:CG2  | 22:V:3:VAL:HG12  | 2.34                     | 0.57              |
| 1:A:376:G:H5''    | 17:Q:5:ARG:HD2   | 1.87                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:164:ARG:NE    | 4:D:166:GLU:OE2  | 2.36                     | 0.57              |
| 1:A:1102:A:O2'    | 1:A:1103:C:H5'   | 2.05                     | 0.57              |
| 1:A:1534:A:C1'    | 22:V:58:LYS:HG3  | 2.34                     | 0.57              |
| 1:A:1217:C:P      | 15:O:9:ARG:HH21  | 2.28                     | 0.57              |
| 2:B:54:LYS:HB3    | 2:B:58:GLY:HA2   | 1.87                     | 0.56              |
| 19:S:74:HIS:HD2   | 19:S:75:GLN:H    | 1.53                     | 0.56              |
| 1:A:1518:MA6:N7   | 1:A:1518:MA6:H93 | 2.21                     | 0.56              |
| 1:A:1323:G:H2'    | 1:A:1324:A:C8    | 2.40                     | 0.56              |
| 3:C:30:PHE:HE1    | 3:C:49:MET:HE1   | 1.69                     | 0.56              |
| 12:L:17:SER:HA    | 12:L:79:ILE:HA   | 1.87                     | 0.56              |
| 22:V:29:LEU:O     | 22:V:32:VAL:HG22 | 2.04                     | 0.56              |
| 1:A:744:C:H2'     | 1:A:745:G:H8     | 1.69                     | 0.56              |
| 1:A:1414:U:H2'    | 1:A:1415:G:H8    | 1.71                     | 0.56              |
| 1:A:87:C:H2'      | 1:A:88:U:C6      | 2.41                     | 0.56              |
| 1:A:408:A:O3'     | 5:E:23:SER:OG    | 2.22                     | 0.56              |
| 12:L:111:THR:HG22 | 22:V:3:VAL:HG12  | 1.87                     | 0.56              |
| 1:A:1532:U:C2'    | 1:A:1533:C:H5'   | 2.36                     | 0.56              |
| 2:B:69:ASP:OD1    | 2:B:86:ARG:NH1   | 2.29                     | 0.56              |
| 14:N:42:ASP:OD1   | 14:N:42:ASP:N    | 2.38                     | 0.56              |
| 1:A:93:U:H2'      | 1:A:94:G:H5''    | 1.87                     | 0.56              |
| 1:A:346:G:N3      | 1:A:346:G:C3'    | 2.68                     | 0.56              |
| 1:A:255:G:H2'     | 1:A:256:U:H6     | 1.71                     | 0.55              |
| 1:A:1405:G:O2'    | 1:A:1518:MA6:O2' | 2.24                     | 0.55              |
| 1:A:1486:G:H2'    | 1:A:1487:G:C8    | 2.42                     | 0.55              |
| 12:L:16:VAL:O     | 12:L:17:SER:OG   | 2.23                     | 0.55              |
| 1:A:1239:A:H62    | 1:A:1299:A:N6    | 2.04                     | 0.55              |
| 1:A:544:G:OP1     | 5:E:56:ARG:NH1   | 2.39                     | 0.55              |
| 5:E:98:LEU:O      | 5:E:102:VAL:HG12 | 2.07                     | 0.55              |
| 3:C:18:HIS:H      | 3:C:189:THR:HG22 | 1.71                     | 0.55              |
| 1:A:1497:G:C2'    | 1:A:1498:UR3:H5' | 2.36                     | 0.55              |
| 7:G:4:TYR:CD2     | 7:G:71:ILE:HG13  | 2.42                     | 0.55              |
| 11:K:66:GLU:HB3   | 15:O:99:ALA:HB2  | 1.88                     | 0.55              |
| 21:U:28:MET:SD    | 21:U:67:ILE:HD12 | 2.47                     | 0.55              |
| 11:K:26:VAL:HG23  | 11:K:36:VAL:HG11 | 1.87                     | 0.55              |
| 1:A:1071:C:H2'    | 1:A:1072:G:H8    | 1.72                     | 0.55              |
| 3:C:94:HIS:O      | 3:C:95:ARG:C     | 2.50                     | 0.55              |
| 1:A:77:A:H8       | 1:A:77:A:P       | 2.30                     | 0.54              |
| 1:A:1255:G:O2'    | 1:A:1258:G:N3    | 2.37                     | 0.54              |
| 16:P:26:GLU:OE1   | 16:P:26:GLU:N    | 2.38                     | 0.54              |
| 1:A:542:G:OP1     | 5:E:10:LYS:NZ    | 2.39                     | 0.54              |
| 1:A:662:U:H2'     | 1:A:663:A:C8     | 2.42                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1305:G:H21   | 1:A:1332:A:H2    | 1.53                     | 0.54              |
| 1:A:350:G:H2'    | 1:A:351:G:C8     | 2.42                     | 0.54              |
| 1:A:413:G:N2     | 1:A:428:G:H1'    | 2.23                     | 0.54              |
| 15:O:24:ARG:NH1  | 15:O:55:SER:OG   | 2.41                     | 0.54              |
| 6:F:105:ILE:HD11 | 6:F:112:ARG:HA   | 1.88                     | 0.54              |
| 22:V:51:SER:HA   | 22:V:54:LYS:HE3  | 1.90                     | 0.54              |
| 1:A:946:A:O2'    | 1:A:1333:A:N3    | 2.40                     | 0.54              |
| 1:A:405:U:O4     | 5:E:2:ALA:N      | 2.41                     | 0.54              |
| 1:A:422:C:OP2    | 1:A:422:C:H2'    | 2.08                     | 0.54              |
| 1:A:977:A:H3'    | 1:A:977:A:N3     | 2.23                     | 0.54              |
| 1:A:996:A:H2'    | 1:A:997:U:O4'    | 2.08                     | 0.54              |
| 1:A:1320:C:C2    | 20:T:72:GLY:HA3  | 2.42                     | 0.54              |
| 1:A:1412:C:H2'   | 1:A:1413:A:C8    | 2.42                     | 0.54              |
| 5:E:99:ASP:OD2   | 5:E:133:ALA:HB1  | 2.08                     | 0.54              |
| 1:A:204:U:H2'    | 1:A:205:A:O4'    | 2.08                     | 0.54              |
| 1:A:1535:C:H2'   | 1:A:1536:C:H6    | 1.73                     | 0.54              |
| 4:D:134:MET:HB2  | 4:D:151:VAL:HG21 | 1.89                     | 0.54              |
| 7:G:29:ILE:HD13  | 7:G:64:VAL:HG11  | 1.90                     | 0.54              |
| 7:G:50:PRO:HD3   | 19:S:75:GLN:HB2  | 1.89                     | 0.54              |
| 19:S:37:GLY:O    | 19:S:63:ARG:NH2  | 2.40                     | 0.54              |
| 21:U:42:GLY:HA2  | 21:U:86:LEU:HD11 | 1.91                     | 0.54              |
| 1:A:474:G:C8     | 1:A:474:G:H5''   | 2.42                     | 0.53              |
| 1:A:958:A:C5     | 20:T:55:ARG:NH1  | 2.76                     | 0.53              |
| 1:A:967:5MC:H5'' | 1:A:968:A:H2'    | 1.89                     | 0.53              |
| 1:A:1078:U:O2'   | 1:A:1079:G:OP1   | 2.25                     | 0.53              |
| 1:A:958:A:C4     | 20:T:55:ARG:HD3  | 2.43                     | 0.53              |
| 6:F:34:THR:HG22  | 6:F:52:LYS:HG3   | 1.89                     | 0.53              |
| 23:X:17:U:H3'    | 23:X:18:G:H8     | 1.72                     | 0.53              |
| 1:A:56:U:H2'     | 1:A:57:G:C8      | 2.43                     | 0.53              |
| 1:A:745:G:H2'    | 1:A:746:A:C8     | 2.44                     | 0.53              |
| 2:B:69:ASP:O     | 2:B:86:ARG:NH1   | 2.42                     | 0.53              |
| 1:A:74:A:H2'     | 1:A:75:G:C4'     | 2.38                     | 0.53              |
| 14:N:90:ARG:HB2  | 14:N:97:VAL:HG23 | 1.90                     | 0.53              |
| 18:R:25:ILE:HB   | 18:R:42:THR:HG23 | 1.90                     | 0.53              |
| 1:A:413:G:H21    | 1:A:428:G:H1'    | 1.73                     | 0.53              |
| 3:C:95:ARG:CZ    | 3:C:95:ARG:HB3   | 2.37                     | 0.53              |
| 8:H:5:ARG:HG2    | 8:H:6:VAL:H      | 1.74                     | 0.53              |
| 1:A:380:G:N2     | 1:A:383:A:OP2    | 2.38                     | 0.53              |
| 1:A:1004:A:OP1   | 1:A:1025:U:N3    | 2.39                     | 0.53              |
| 1:A:17:U:H2'     | 1:A:18:C:C6      | 2.44                     | 0.53              |
| 3:C:207:ILE:HA   | 3:C:210:VAL:HG22 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:26:ARG:HH21   | 5:E:30:THR:HG22   | 1.73                     | 0.53              |
| 1:A:401:C:O2'     | 1:A:621:A:N3      | 2.32                     | 0.52              |
| 1:A:683:G:H1      | 1:A:707:U:H3      | 1.58                     | 0.52              |
| 2:B:45:GLU:OE2    | 3:C:208:ARG:HG3   | 2.08                     | 0.52              |
| 16:P:78:TYR:OH    | 16:P:89:ARG:O     | 2.18                     | 0.52              |
| 17:Q:5:ARG:HH12   | 17:Q:24:SER:HA    | 1.74                     | 0.52              |
| 21:U:39:ILE:HD11  | 21:U:83:ILE:HG13  | 1.91                     | 0.52              |
| 1:A:74:A:H2'      | 1:A:75:G:O4'      | 2.09                     | 0.52              |
| 1:A:1403:C:O5'    | 1:A:1403:C:C6     | 2.60                     | 0.52              |
| 5:E:15:GLU:OE1    | 5:E:63:ARG:NH1    | 2.43                     | 0.52              |
| 1:A:1014:A:C2     | 1:A:1219:A:H1'    | 2.45                     | 0.52              |
| 1:A:1431:A:H2     | 1:A:1469:C:H41    | 1.57                     | 0.52              |
| 11:K:36:VAL:HG22  | 11:K:38:GLY:H     | 1.74                     | 0.52              |
| 1:A:1347:G:O6     | 10:J:12:ARG:NH2   | 2.43                     | 0.52              |
| 3:C:129:LEU:HB3   | 3:C:133:GLU:CG    | 2.40                     | 0.52              |
| 1:A:75:G:H8       | 1:A:75:G:H5''     | 1.69                     | 0.52              |
| 10:J:21:ILE:HG12  | 10:J:63:LEU:HD22  | 1.91                     | 0.52              |
| 1:A:89:U:H2'      | 1:A:90:C:C6       | 2.45                     | 0.52              |
| 1:A:1052:U:O2'    | 1:A:1055:A:OP2    | 2.18                     | 0.52              |
| 1:A:1078:U:H1'    | 6:F:135:ASN:HD21  | 1.76                     | 0.52              |
| 1:A:1391:U:H2'    | 1:A:1392:G:C8     | 2.45                     | 0.52              |
| 12:L:22:HIS:HB2   | 12:L:33:THR:HG23  | 1.92                     | 0.52              |
| 1:A:77:A:C8       | 1:A:77:A:OP2      | 2.63                     | 0.51              |
| 1:A:1498:UR3:H5'' | 1:A:1519:MA6:H102 | 1.91                     | 0.51              |
| 13:M:110:ARG:HB2  | 13:M:119:VAL:HG21 | 1.92                     | 0.51              |
| 6:F:45:ARG:HH21   | 6:F:71:MET:HE3    | 1.75                     | 0.51              |
| 7:G:19:PRO:O      | 7:G:23:GLU:HG2    | 2.10                     | 0.51              |
| 1:A:463:U:H2'     | 1:A:463:U:O2      | 2.09                     | 0.51              |
| 3:C:68:LEU:HD11   | 3:C:92:VAL:HG23   | 1.92                     | 0.51              |
| 5:E:190:ASP:OD1   | 5:E:190:ASP:N     | 2.44                     | 0.51              |
| 12:L:110:ILE:HG22 | 22:V:19:PHE:CE1   | 2.45                     | 0.51              |
| 1:A:81:A:H2'      | 1:A:82:G:C8       | 2.46                     | 0.51              |
| 1:A:110:C:O2'     | 17:Q:25:ARG:O     | 2.28                     | 0.51              |
| 7:G:86:ARG:NH1    | 19:S:64:TYR:O     | 2.43                     | 0.51              |
| 1:A:337:G:H2'     | 1:A:338:A:C8      | 2.45                     | 0.51              |
| 6:F:76:LEU:HD11   | 6:F:120:VAL:HG22  | 1.92                     | 0.51              |
| 5:E:198:HIS:CD2   | 5:E:198:HIS:H     | 2.27                     | 0.51              |
| 11:K:3:ASN:OD1    | 11:K:4:GLN:N      | 2.42                     | 0.51              |
| 1:A:514:C:H2'     | 1:A:515:G:H8      | 1.75                     | 0.51              |
| 6:F:38:VAL:HG12   | 6:F:117:VAL:HG11  | 1.93                     | 0.51              |
| 1:A:501:C:H2'     | 1:A:502:A:H8      | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1029:U:O2'   | 1:A:1032:G:O6    | 2.23                     | 0.51              |
| 6:F:85:VAL:HG23  | 6:F:96:MET:HE3   | 1.92                     | 0.51              |
| 1:A:160:A:H2'    | 1:A:161:A:O4'    | 2.10                     | 0.51              |
| 1:A:758:C:H4'    | 1:A:880:C:H4'    | 1.92                     | 0.51              |
| 5:E:175:ALA:O    | 5:E:178:MET:HG2  | 2.11                     | 0.50              |
| 1:A:216:U:H1'    | 1:A:466:A:N6     | 2.25                     | 0.50              |
| 2:B:115:LYS:HA   | 2:B:120:PHE:HA   | 1.94                     | 0.50              |
| 5:E:87:GLY:HA3   | 5:E:197:GLU:HG3  | 1.92                     | 0.50              |
| 14:N:9:ILE:HG23  | 14:N:18:ALA:HB1  | 1.92                     | 0.50              |
| 1:A:235:C:H2'    | 1:A:236:A:C8     | 2.46                     | 0.50              |
| 1:A:347:G:OP2    | 1:A:347:G:C8     | 2.63                     | 0.50              |
| 1:A:958:A:N7     | 20:T:55:ARG:NH1  | 2.59                     | 0.50              |
| 2:B:75:VAL:O     | 2:B:75:VAL:CG2   | 2.60                     | 0.50              |
| 9:I:112:THR:HG23 | 9:I:115:ALA:H    | 1.76                     | 0.50              |
| 16:P:39:LEU:HD12 | 16:P:59:MET:HE1  | 1.93                     | 0.50              |
| 1:A:1226:C:P     | 14:N:90:ARG:HH22 | 2.34                     | 0.50              |
| 1:A:1314:C:H2'   | 1:A:1315:U:C6    | 2.47                     | 0.50              |
| 1:A:56:U:H2'     | 1:A:57:G:H8      | 1.75                     | 0.50              |
| 1:A:923:A:H2'    | 1:A:924:C:C6     | 2.46                     | 0.50              |
| 1:A:1048:G:H5''  | 15:O:3:LYS:HD2   | 1.94                     | 0.50              |
| 1:A:1305:G:N2    | 1:A:1331:G:O2'   | 2.32                     | 0.50              |
| 3:C:111:ILE:HD12 | 3:C:152:LYS:HA   | 1.94                     | 0.50              |
| 1:A:135:C:N3     | 17:Q:1:MET:HB2   | 2.27                     | 0.50              |
| 1:A:216:U:H2'    | 1:A:217:C:C6     | 2.46                     | 0.50              |
| 2:B:31:ILE:HG12  | 2:B:36:VAL:HG13  | 1.94                     | 0.50              |
| 1:A:1071:C:H2'   | 1:A:1072:G:C8    | 2.47                     | 0.50              |
| 1:A:1391:U:H2'   | 1:A:1392:G:H8    | 1.77                     | 0.50              |
| 17:Q:4:ILE:HB    | 17:Q:67:ILE:HD13 | 1.94                     | 0.50              |
| 1:A:1134:G:O6    | 1:A:1141:C:N4    | 2.45                     | 0.49              |
| 1:A:1098:C:O2'   | 22:V:71:TYR:OXT  | 2.23                     | 0.49              |
| 1:A:1106:G:O2'   | 4:D:169:ARG:NH1  | 2.41                     | 0.49              |
| 4:D:110:GLU:HB2  | 4:D:144:LEU:HD12 | 1.93                     | 0.49              |
| 1:A:945:G:C2     | 1:A:946:A:C8     | 3.01                     | 0.49              |
| 1:A:1427:C:H2'   | 1:A:1428:A:C8    | 2.46                     | 0.49              |
| 1:A:1464:U:H2'   | 1:A:1465:A:H8    | 1.77                     | 0.49              |
| 10:J:65:ILE:HD13 | 10:J:79:ILE:HG23 | 1.94                     | 0.49              |
| 8:H:57:SER:HB3   | 8:H:60:GLU:HB2   | 1.93                     | 0.49              |
| 7:G:12:PRO:HB3   | 7:G:56:LYS:O     | 2.11                     | 0.49              |
| 14:N:104:THR:OG1 | 14:N:105:ASN:N   | 2.46                     | 0.49              |
| 12:L:114:THR:O   | 19:S:73:ARG:NH1  | 2.46                     | 0.49              |
| 8:H:63:GLU:O     | 8:H:67:GLU:HG3   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:68:ASN:O     | 8:H:138:ARG:NH2  | 2.45                     | 0.49              |
| 10:J:30:ILE:HG12 | 10:J:65:ILE:HB   | 1.95                     | 0.49              |
| 1:A:251:G:H4'    | 1:A:252:U:O5'    | 2.11                     | 0.49              |
| 1:A:518:C:H5'    | 1:A:519:C:C6     | 2.47                     | 0.49              |
| 1:A:744:C:H2'    | 1:A:745:G:C8     | 2.46                     | 0.49              |
| 1:A:1119:C:H2'   | 1:A:1120:C:H6    | 1.76                     | 0.49              |
| 3:C:129:LEU:HB3  | 3:C:133:GLU:HG2  | 1.94                     | 0.49              |
| 6:F:157:ARG:NH2  | 9:I:43:GLU:OE1   | 2.46                     | 0.49              |
| 13:M:67:ILE:HD13 | 13:M:74:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:562:U:C5     | 13:M:15:LYS:HG2  | 2.48                     | 0.49              |
| 1:A:1534:A:N9    | 22:V:58:LYS:HG3  | 2.28                     | 0.49              |
| 8:H:69:VAL:HG21  | 8:H:104:ILE:HD11 | 1.94                     | 0.49              |
| 12:L:18:ASP:HB2  | 12:L:37:ARG:HH21 | 1.78                     | 0.49              |
| 1:A:235:C:H2'    | 1:A:236:A:H8     | 1.77                     | 0.48              |
| 1:A:460:A:H2'    | 1:A:461:A:C8     | 2.47                     | 0.48              |
| 1:A:465:A:H3'    | 1:A:466:A:H8     | 1.78                     | 0.48              |
| 1:A:826:C:H5'    | 9:I:13:ARG:CZ    | 2.43                     | 0.48              |
| 1:A:868:C:H2'    | 1:A:869:G:O4'    | 2.12                     | 0.48              |
| 1:A:949:A:N7     | 14:N:105:ASN:ND2 | 2.61                     | 0.48              |
| 1:A:1007:U:OP1   | 15:O:19:LYS:NZ   | 2.41                     | 0.48              |
| 1:A:1498:UR3:OP2 | 1:A:1498:UR3:H6  | 2.13                     | 0.48              |
| 21:U:67:ILE:HG12 | 21:U:71:LYS:HD3  | 1.94                     | 0.48              |
| 1:A:745:G:H2'    | 1:A:746:A:H8     | 1.78                     | 0.48              |
| 1:A:1279:G:C8    | 1:A:1279:G:H3'   | 2.48                     | 0.48              |
| 20:T:5:LEU:C     | 20:T:7:LYS:N     | 2.71                     | 0.48              |
| 1:A:677:U:O2     | 1:A:777:A:O2'    | 2.31                     | 0.48              |
| 1:A:932:C:H5''   | 8:H:4:ARG:HD3    | 1.94                     | 0.48              |
| 6:F:80:THR:HG23  | 6:F:122:ASN:O    | 2.13                     | 0.48              |
| 11:K:52:LEU:HD21 | 11:K:59:LYS:HA   | 1.95                     | 0.48              |
| 15:O:46:LEU:O    | 15:O:50:THR:HG23 | 2.14                     | 0.48              |
| 1:A:80:A:C6      | 1:A:81:A:N6      | 2.82                     | 0.48              |
| 1:A:89:U:H2'     | 1:A:90:C:H6      | 1.77                     | 0.48              |
| 1:A:1314:C:H2'   | 1:A:1315:U:H6    | 1.79                     | 0.48              |
| 1:A:1403:C:H2'   | 1:A:1404:C:C6    | 2.48                     | 0.48              |
| 1:A:1152:A:OP1   | 11:K:70:HIS:ND1  | 2.43                     | 0.48              |
| 14:N:7:ILE:HD11  | 14:N:22:ILE:HG12 | 1.95                     | 0.48              |
| 15:O:41:ARG:NH2  | 20:T:6:LYS:O     | 2.46                     | 0.48              |
| 1:A:523:A:N6     | 13:M:87:VAL:HG12 | 2.29                     | 0.48              |
| 1:A:923:A:H2'    | 1:A:924:C:H6     | 1.77                     | 0.48              |
| 1:A:976:G:OP2    | 1:A:1358:U:O2'   | 2.31                     | 0.48              |
| 1:A:1402:4OC:H6  | 1:A:1402:4OC:O5' | 2.14                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:384:G:H2'     | 1:A:385:C:C6     | 2.48                     | 0.48              |
| 5:E:6:GLY:O       | 5:E:8:LYS:NZ     | 2.42                     | 0.48              |
| 1:A:180:U:H2'     | 1:A:181:A:H5'    | 1.96                     | 0.48              |
| 1:A:734:G:O2'     | 19:S:60:LYS:HD3  | 2.14                     | 0.48              |
| 1:A:957:U:H4'     | 20:T:79:THR:HG23 | 1.94                     | 0.48              |
| 22:V:7:ARG:O      | 22:V:10:GLU:HG2  | 2.13                     | 0.48              |
| 1:A:1426:G:H1     | 1:A:1474:U:H3    | 1.60                     | 0.48              |
| 1:A:1530:G:H2'    | 1:A:1531:A:H8    | 1.77                     | 0.48              |
| 1:A:113:G:H1'     | 1:A:354:G:H5'    | 1.96                     | 0.48              |
| 1:A:1010:U:H2'    | 1:A:1011:C:H6    | 1.79                     | 0.48              |
| 1:A:1074:G:O2'    | 1:A:1101:A:N1    | 2.40                     | 0.48              |
| 22:V:29:LEU:O     | 22:V:32:VAL:CG2  | 2.61                     | 0.48              |
| 1:A:371:A:H2'     | 1:A:372:C:O4'    | 2.14                     | 0.47              |
| 1:A:1183:U:O2'    | 1:A:1185:G:OP2   | 2.31                     | 0.47              |
| 8:H:16:PRO:HB3    | 10:J:46:MET:HE2  | 1.95                     | 0.47              |
| 1:A:820:U:H4'     | 1:A:821:G:OP2    | 2.14                     | 0.47              |
| 1:A:883:C:H2'     | 1:A:884:U:C6     | 2.49                     | 0.47              |
| 1:A:999:C:C3'     | 1:A:999:C:C6     | 2.97                     | 0.47              |
| 1:A:1077:G:N1     | 1:A:1080:A:OP2   | 2.43                     | 0.47              |
| 1:A:1540:U:C2     | 23:X:6:G:C2      | 3.02                     | 0.47              |
| 1:A:728:A:H2'     | 1:A:729:A:C8     | 2.48                     | 0.47              |
| 1:A:1124:G:N2     | 1:A:1125:U:O4    | 2.38                     | 0.47              |
| 1:A:1141:C:O2'    | 1:A:1142:G:H8    | 1.96                     | 0.47              |
| 1:A:1279:G:C8     | 1:A:1279:G:C3'   | 2.97                     | 0.47              |
| 12:L:89:PRO:HA    | 22:V:29:LEU:HD22 | 1.96                     | 0.47              |
| 2:B:11:GLU:O      | 2:B:14:LYS:HG3   | 2.14                     | 0.47              |
| 13:M:33:VAL:HG22  | 13:M:79:VAL:HG12 | 1.97                     | 0.47              |
| 22:V:29:LEU:HA    | 22:V:32:VAL:CG2  | 2.43                     | 0.47              |
| 1:A:500:G:H2'     | 1:A:501:C:C6     | 2.50                     | 0.47              |
| 1:A:1519:MA6:H5'' | 1:A:1520:C:O4'   | 2.15                     | 0.47              |
| 22:V:29:LEU:CA    | 22:V:32:VAL:HG22 | 2.45                     | 0.47              |
| 1:A:87:C:H2'      | 1:A:88:U:H6      | 1.78                     | 0.47              |
| 1:A:254:G:N2      | 18:R:18:GLU:OE2  | 2.44                     | 0.47              |
| 1:A:335:C:H2'     | 1:A:336:A:H8     | 1.79                     | 0.47              |
| 1:A:536:C:H2'     | 1:A:537:G:H8     | 1.80                     | 0.47              |
| 1:A:1102:A:C2'    | 1:A:1103:C:H5'   | 2.45                     | 0.47              |
| 2:B:52:GLN:O      | 2:B:90:LYS:NZ    | 2.37                     | 0.47              |
| 6:F:111:MET:HE2   | 6:F:111:MET:HB3  | 1.75                     | 0.47              |
| 11:K:7:ARG:NH1    | 11:K:73:LEU:HD21 | 2.29                     | 0.47              |
| 4:D:69:HIS:HA     | 4:D:104:ALA:O    | 2.14                     | 0.47              |
| 21:U:35:VAL:HG22  | 21:U:50:ALA:HB1  | 1.96                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:427:U:OP2   | 1:A:428:G:O2'    | 2.28                     | 0.47              |
| 1:A:1266:G:N2   | 1:A:1269:A:OP2   | 2.36                     | 0.47              |
| 1:A:1319:A:P    | 20:T:3:ARG:HD2   | 2.54                     | 0.47              |
| 7:G:45:ARG:O    | 7:G:56:LYS:HA    | 2.14                     | 0.47              |
| 1:A:21:G:H2'    | 1:A:22:G:C8      | 2.50                     | 0.47              |
| 1:A:955:U:O2    | 20:T:83:HIS:HE1  | 1.98                     | 0.47              |
| 1:A:966:2MG:C8  | 1:A:966:2MG:C5'  | 2.90                     | 0.47              |
| 1:A:1137:C:H1'  | 1:A:1138:G:N2    | 2.30                     | 0.47              |
| 1:A:1477:U:H2'  | 1:A:1478:U:C6    | 2.50                     | 0.47              |
| 12:L:87:LYS:HG3 | 12:L:115:PRO:HD3 | 1.96                     | 0.47              |
| 1:A:35:G:H2'    | 1:A:36:C:C6      | 2.49                     | 0.46              |
| 1:A:1008:U:H2'  | 1:A:1009:U:C6    | 2.50                     | 0.46              |
| 1:A:1319:A:OP2  | 20:T:3:ARG:HD2   | 2.15                     | 0.46              |
| 8:H:116:MET:HA  | 8:H:119:ARG:HE   | 1.80                     | 0.46              |
| 9:I:32:LEU:O    | 9:I:36:ILE:HG13  | 2.14                     | 0.46              |
| 10:J:41:ARG:HD3 | 10:J:43:THR:HB   | 1.97                     | 0.46              |
| 10:J:88:MET:HE3 | 10:J:88:MET:HB2  | 1.84                     | 0.46              |
| 18:R:19:LYS:NZ  | 18:R:50:ASN:H    | 2.12                     | 0.46              |
| 20:T:6:LYS:O    | 20:T:6:LYS:HG3   | 2.14                     | 0.46              |
| 1:A:801:U:H2'   | 1:A:802:A:H8     | 1.81                     | 0.46              |
| 1:A:982:U:H4'   | 1:A:983:A:O4'    | 2.14                     | 0.46              |
| 1:A:999:C:C6    | 1:A:999:C:H3'    | 2.49                     | 0.46              |
| 1:A:436:C:H2'   | 1:A:437:U:C6     | 2.50                     | 0.46              |
| 1:A:1495:U:H2'  | 1:A:1496:C:C6    | 2.50                     | 0.46              |
| 3:C:21:ARG:HG3  | 3:C:22:TYR:CE2   | 2.51                     | 0.46              |
| 5:E:105:MET:HE2 | 5:E:105:MET:HB3  | 1.75                     | 0.46              |
| 10:J:88:MET:SD  | 10:J:95:ARG:NE   | 2.89                     | 0.46              |
| 1:A:536:C:H2'   | 1:A:537:G:C8     | 2.50                     | 0.46              |
| 1:A:1040:U:H2'  | 1:A:1041:G:C8    | 2.51                     | 0.46              |
| 3:C:125:THR:HA  | 3:C:128:LYS:NZ   | 2.30                     | 0.46              |
| 16:P:6:GLU:OE1  | 16:P:6:GLU:N     | 2.43                     | 0.46              |
| 23:X:11:U:H1'   | 23:X:12:A:OP2    | 2.14                     | 0.46              |
| 1:A:501:C:H2'   | 1:A:502:A:C8     | 2.50                     | 0.46              |
| 1:A:1008:U:H2'  | 1:A:1009:U:H6    | 1.80                     | 0.46              |
| 1:A:1435:G:H2'  | 1:A:1436:U:C6    | 2.51                     | 0.46              |
| 4:D:114:LYS:HB2 | 4:D:185:ASN:ND2  | 2.30                     | 0.46              |
| 1:A:62:U:O2'    | 1:A:379:C:O2     | 2.34                     | 0.46              |
| 5:E:50:ASP:OD1  | 5:E:50:ASP:N     | 2.39                     | 0.46              |
| 11:K:39:PRO:HA  | 11:K:73:LEU:O    | 2.15                     | 0.46              |
| 1:A:104:G:N7    | 21:U:9:LYS:NZ    | 2.54                     | 0.46              |
| 1:A:736:C:H2'   | 1:A:737:C:H6     | 1.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:16:VAL:HG13 | 14:N:17:ILE:HD12 | 1.97                     | 0.46              |
| 18:R:44:LEU:HD23 | 18:R:73:TRP:CD1  | 2.50                     | 0.46              |
| 1:A:294:U:OP1    | 1:A:610:U:O2'    | 2.28                     | 0.46              |
| 1:A:390:U:H2'    | 1:A:391:G:H8     | 1.81                     | 0.46              |
| 1:A:866:C:C4     | 1:A:867:G:H1'    | 2.51                     | 0.46              |
| 1:A:1004:A:H2'   | 1:A:1005:A:O4'   | 2.15                     | 0.46              |
| 2:B:112:ILE:HA   | 2:B:122:VAL:HA   | 1.97                     | 0.46              |
| 4:D:8:ASN:O      | 4:D:12:LEU:HG    | 2.16                     | 0.46              |
| 6:F:25:VAL:HG12  | 6:F:26:LYS:H     | 1.81                     | 0.46              |
| 1:A:706:A:O2'    | 12:L:33:THR:HG21 | 2.16                     | 0.46              |
| 1:A:1166:G:O2'   | 1:A:1169:A:N6    | 2.45                     | 0.46              |
| 1:A:1422:G:H1    | 1:A:1478:U:H3    | 1.64                     | 0.46              |
| 7:G:38:ARG:HB3   | 7:G:63:ASN:HB3   | 1.98                     | 0.46              |
| 20:T:11:ILE:HD13 | 20:T:16:LEU:HD13 | 1.98                     | 0.46              |
| 1:A:75:G:C8      | 1:A:75:G:C4'     | 3.00                     | 0.45              |
| 1:A:299:G:H2'    | 1:A:300:A:C8     | 2.51                     | 0.45              |
| 1:A:769:G:H4'    | 1:A:1513:A:H4'   | 1.98                     | 0.45              |
| 1:A:932:C:H2'    | 1:A:933:G:C8     | 2.51                     | 0.45              |
| 1:A:1436:U:H2'   | 1:A:1437:A:H8    | 1.81                     | 0.45              |
| 5:E:116:GLN:HG2  | 5:E:154:ARG:HH22 | 1.81                     | 0.45              |
| 5:E:188:ARG:NH2  | 5:E:195:ILE:O    | 2.49                     | 0.45              |
| 1:A:875:U:O2'    | 9:I:15:ARG:NH1   | 2.48                     | 0.45              |
| 1:A:736:C:H2'    | 1:A:737:C:C6     | 2.50                     | 0.45              |
| 1:A:1330:U:H4'   | 14:N:23:TYR:CE2  | 2.51                     | 0.45              |
| 3:C:128:LYS:H    | 3:C:128:LYS:HD2  | 1.82                     | 0.45              |
| 11:K:50:THR:HG23 | 11:K:64:GLN:HG2  | 1.99                     | 0.45              |
| 1:A:81:A:H2'     | 1:A:82:G:H8      | 1.81                     | 0.45              |
| 1:A:440:C:C2     | 1:A:441:A:C8     | 3.05                     | 0.45              |
| 1:A:1101:A:H5''  | 3:C:171:ILE:HD11 | 1.98                     | 0.45              |
| 1:A:1455:G:H2'   | 1:A:1456:A:H8    | 1.82                     | 0.45              |
| 1:A:1532:U:O2'   | 1:A:1533:C:H5'   | 2.16                     | 0.45              |
| 5:E:50:ASP:O     | 5:E:53:VAL:HG22  | 2.17                     | 0.45              |
| 5:E:161:LEU:O    | 5:E:165:ARG:HG3  | 2.16                     | 0.45              |
| 14:N:40:ALA:O    | 14:N:43:VAL:HG12 | 2.15                     | 0.45              |
| 1:A:404:G:O6     | 5:E:2:ALA:N      | 2.49                     | 0.45              |
| 1:A:1319:A:C8    | 1:A:1323:G:C5    | 3.05                     | 0.45              |
| 4:D:64:ILE:HG22  | 4:D:97:VAL:HG23  | 1.99                     | 0.45              |
| 14:N:107:ARG:NH2 | 14:N:113:ARG:HA  | 2.32                     | 0.45              |
| 1:A:1151:A:HO2'  | 1:A:1152:A:H8    | 1.61                     | 0.45              |
| 8:H:93:PRO:HA    | 8:H:96:ARG:HD2   | 1.99                     | 0.45              |
| 23:X:11:U:H4'    | 23:X:12:A:O5'    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:73:C:H2'     | 1:A:74:A:O4'     | 2.16                     | 0.45              |
| 1:A:544:G:OP2    | 5:E:63:ARG:NH2   | 2.49                     | 0.45              |
| 5:E:102:VAL:HG23 | 5:E:107:PHE:HB2  | 1.98                     | 0.45              |
| 22:V:29:LEU:C    | 22:V:32:VAL:HG22 | 2.41                     | 0.45              |
| 1:A:591:U:H2'    | 1:A:592:G:H8     | 1.81                     | 0.45              |
| 1:A:1086:U:H2'   | 1:A:1087:G:H8    | 1.82                     | 0.45              |
| 6:F:136:VAL:O    | 6:F:140:THR:HG22 | 2.17                     | 0.45              |
| 8:H:53:ARG:HH22  | 8:H:121:ALA:HB1  | 1.80                     | 0.45              |
| 16:P:17:ARG:HD2  | 16:P:17:ARG:O    | 2.16                     | 0.45              |
| 17:Q:18:GLN:HE21 | 17:Q:35:ARG:NH2  | 2.15                     | 0.45              |
| 1:A:855:U:H2'    | 1:A:856:C:H6     | 1.82                     | 0.45              |
| 1:A:881:G:P      | 13:M:9:ARG:HH22  | 2.39                     | 0.45              |
| 1:A:1436:U:H2'   | 1:A:1437:A:C8    | 2.51                     | 0.45              |
| 16:P:80:GLN:HE22 | 16:P:84:ARG:NE   | 2.15                     | 0.45              |
| 1:A:34:C:H2'     | 1:A:35:G:H8      | 1.82                     | 0.45              |
| 1:A:160:A:N6     | 1:A:347:G:H1'    | 2.32                     | 0.45              |
| 1:A:826:C:H5'    | 9:I:13:ARG:NH2   | 2.31                     | 0.45              |
| 1:A:1158:C:C4    | 1:A:1160:G:C8    | 3.05                     | 0.45              |
| 1:A:1317:C:O2    | 20:T:37:ARG:NH2  | 2.50                     | 0.45              |
| 1:A:1318:A:H5'   | 20:T:10:PHE:CD1  | 2.51                     | 0.45              |
| 1:A:1498:UR3:H4' | 1:A:1519:MA6:N1  | 2.32                     | 0.45              |
| 5:E:170:TRP:CD2  | 5:E:186:PRO:HB3  | 2.53                     | 0.45              |
| 10:J:23:PRO:HA   | 10:J:61:LEU:HD23 | 1.98                     | 0.45              |
| 21:U:62:ALA:HA   | 21:U:67:ILE:O    | 2.17                     | 0.45              |
| 1:A:2:A:H8       | 1:A:2:A:OP2      | 2.00                     | 0.44              |
| 1:A:254:G:OP1    | 18:R:70:THR:HG22 | 2.17                     | 0.44              |
| 1:A:324:G:N2     | 1:A:326:G:H3'    | 2.32                     | 0.44              |
| 18:R:14:SER:HB3  | 18:R:22:VAL:CG1  | 2.48                     | 0.44              |
| 1:A:161:A:N1     | 1:A:347:G:O2'    | 2.49                     | 0.44              |
| 1:A:458:U:H6     | 1:A:458:U:C5'    | 2.26                     | 0.44              |
| 1:A:689:C:OP1    | 12:L:29:ASN:ND2  | 2.46                     | 0.44              |
| 1:A:1078:U:HO2'  | 1:A:1079:G:P     | 2.41                     | 0.44              |
| 1:A:1217:C:OP1   | 15:O:9:ARG:NE    | 2.37                     | 0.44              |
| 1:A:1320:C:O2    | 20:T:72:GLY:HA3  | 2.17                     | 0.44              |
| 2:B:53:PHE:HD2   | 2:B:62:ILE:HD11  | 1.61                     | 0.44              |
| 5:E:41:HIS:HB3   | 5:E:44:ARG:HE    | 1.82                     | 0.44              |
| 5:E:177:LYS:HD2  | 5:E:177:LYS:HA   | 1.74                     | 0.44              |
| 12:L:35:THR:OG1  | 12:L:36:ASP:N    | 2.51                     | 0.44              |
| 1:A:613:C:H2'    | 1:A:614:C:C6     | 2.52                     | 0.44              |
| 1:A:978:A:C5     | 1:A:1319:A:C2    | 3.05                     | 0.44              |
| 1:A:1287:A:H2'   | 1:A:1288:A:C8    | 2.52                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1536:C:H2'    | 1:A:1537:U:C6    | 2.53                     | 0.44              |
| 18:R:9:GLN:HE21   | 18:R:60:GLU:HG3  | 1.83                     | 0.44              |
| 1:A:569:C:H5''    | 1:A:570:G:OP1    | 2.18                     | 0.44              |
| 1:A:879:C:H2'     | 1:A:880:C:C6     | 2.52                     | 0.44              |
| 1:A:886:G:H2'     | 1:A:887:G:O4'    | 2.18                     | 0.44              |
| 1:A:1519:MA6:H8   | 1:A:1519:MA6:C5' | 2.47                     | 0.44              |
| 3:C:54:LEU:HD12   | 3:C:54:LEU:HA    | 1.84                     | 0.44              |
| 3:C:133:GLU:CD    | 3:C:133:GLU:H    | 2.24                     | 0.44              |
| 19:S:74:HIS:CD2   | 19:S:75:GLN:H    | 2.33                     | 0.44              |
| 1:A:474:G:H5''    | 1:A:474:G:H8     | 1.82                     | 0.44              |
| 1:A:538:G:OP2     | 13:M:112:GLN:HG3 | 2.17                     | 0.44              |
| 1:A:695:A:H2'     | 1:A:696:A:C8     | 2.53                     | 0.44              |
| 3:C:89:GLN:NE2    | 3:C:225:ARG:HD2  | 2.32                     | 0.44              |
| 3:C:95:ARG:NH2    | 3:C:97:LEU:HD23  | 2.33                     | 0.44              |
| 23:X:8:A:H2'      | 23:X:9:G:C8      | 2.53                     | 0.44              |
| 1:A:1072:G:H2'    | 1:A:1073:U:C6    | 2.52                     | 0.44              |
| 1:A:1356:G:H2'    | 1:A:1357:A:H8    | 1.79                     | 0.44              |
| 1:A:1413:A:H2     | 1:A:1487:G:H22   | 1.64                     | 0.44              |
| 3:C:30:PHE:CE1    | 3:C:49:MET:HE1   | 2.50                     | 0.44              |
| 3:C:84:ALA:HA     | 3:C:87:CYS:SG    | 2.58                     | 0.44              |
| 8:H:79:ARG:HA     | 8:H:84:THR:HA    | 1.99                     | 0.44              |
| 18:R:48:ASP:OD1   | 18:R:48:ASP:N    | 2.49                     | 0.44              |
| 1:A:361:G:H2'     | 1:A:362:G:O4'    | 2.18                     | 0.44              |
| 1:A:1279:G:H3'    | 1:A:1279:G:H8    | 1.83                     | 0.44              |
| 5:E:171:LEU:HD23  | 5:E:182:PHE:HA   | 2.00                     | 0.44              |
| 10:J:40:GLY:O     | 10:J:45:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:178:C:C2      | 1:A:179:A:C8     | 3.06                     | 0.44              |
| 1:A:184:G:H2'     | 1:A:185:U:C6     | 2.53                     | 0.44              |
| 2:B:98:LEU:HD23   | 2:B:98:LEU:HA    | 1.84                     | 0.44              |
| 10:J:123:ARG:NH1  | 10:J:124:ARG:O   | 2.48                     | 0.44              |
| 13:M:72:HIS:HA    | 13:M:99:ARG:HH22 | 1.83                     | 0.44              |
| 21:U:31:PHE:O     | 21:U:35:VAL:HG23 | 2.18                     | 0.44              |
| 3:C:223:GLU:HG3   | 3:C:224:GLY:N    | 2.33                     | 0.43              |
| 6:F:15:LEU:HD23   | 6:F:15:LEU:H     | 1.82                     | 0.43              |
| 9:I:10:MET:HG3    | 9:I:27:MET:SD    | 2.58                     | 0.43              |
| 10:J:84:THR:HG23  | 10:J:98:LEU:HD13 | 1.99                     | 0.43              |
| 1:A:1442:G:H2'    | 1:A:1443:C:C6    | 2.53                     | 0.43              |
| 2:B:13:LEU:HD23   | 2:B:13:LEU:HA    | 1.87                     | 0.43              |
| 12:L:116:ILE:HD12 | 22:V:31:GLU:HG2  | 2.00                     | 0.43              |
| 15:O:26:GLU:HG3   | 15:O:27:LEU:N    | 2.33                     | 0.43              |
| 1:A:264:C:O2'     | 18:R:66:PRO:O    | 2.36                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:413:G:H1'   | 1:A:428:G:H21    | 1.83                     | 0.43              |
| 1:A:467:U:O2    | 1:A:467:U:H5''   | 2.17                     | 0.43              |
| 1:A:999:C:H6    | 1:A:999:C:C5'    | 2.30                     | 0.43              |
| 1:A:1534:A:H2'  | 1:A:1535:C:O4'   | 2.17                     | 0.43              |
| 16:P:18:ASP:OD1 | 16:P:18:ASP:N    | 2.49                     | 0.43              |
| 1:A:681:A:H2'   | 1:A:682:G:O4'    | 2.18                     | 0.43              |
| 1:A:911:U:H2'   | 1:A:912:C:C6     | 2.53                     | 0.43              |
| 1:A:1038:C:H2'  | 1:A:1039:G:H8    | 1.83                     | 0.43              |
| 22:V:32:VAL:O   | 22:V:36:GLU:HG3  | 2.18                     | 0.43              |
| 1:A:180:U:C2'   | 1:A:181:A:H5'    | 2.48                     | 0.43              |
| 1:A:335:C:H2'   | 1:A:336:A:C8     | 2.54                     | 0.43              |
| 1:A:552:U:C2    | 1:A:553:A:C8     | 3.07                     | 0.43              |
| 1:A:936:C:C2    | 1:A:937:A:C8     | 3.06                     | 0.43              |
| 1:A:996:A:N7    | 1:A:1046:A:O2'   | 2.50                     | 0.43              |
| 1:A:1001:C:H2'  | 1:A:1002:G:H8    | 1.83                     | 0.43              |
| 3:C:59:LYS:HE3  | 3:C:59:LYS:HB2   | 1.92                     | 0.43              |
| 9:I:66:PHE:CD2  | 9:I:67:GLN:HG3   | 2.53                     | 0.43              |
| 1:A:579:A:H2'   | 1:A:580:C:C6     | 2.54                     | 0.43              |
| 2:B:63:GLN:HG2  | 2:B:64:VAL:H     | 1.84                     | 0.43              |
| 1:A:462:G:H3'   | 1:A:463:U:H6     | 1.84                     | 0.43              |
| 1:A:471:U:H2'   | 1:A:472:U:C6     | 2.54                     | 0.43              |
| 1:A:512:U:OP1   | 5:E:44:ARG:NH2   | 2.52                     | 0.43              |
| 1:A:1496:C:H2'  | 1:A:1497:G:O4'   | 2.19                     | 0.43              |
| 21:U:2:ALA:HB3  | 21:U:8:LYS:HG2   | 2.01                     | 0.43              |
| 1:A:687:A:C2    | 1:A:704:A:C5     | 3.07                     | 0.43              |
| 6:F:86:LYS:HE3  | 6:F:86:LYS:HB3   | 1.89                     | 0.43              |
| 10:J:17:ALA:HB2 | 10:J:67:VAL:HG13 | 2.01                     | 0.43              |
| 20:T:63:THR:OG1 | 20:T:64:ASP:N    | 2.50                     | 0.43              |
| 1:A:390:U:H2'   | 1:A:391:G:C8     | 2.53                     | 0.43              |
| 1:A:1040:U:H2'  | 1:A:1041:G:H8    | 1.83                     | 0.43              |
| 1:A:1095:U:H2'  | 1:A:1096:C:C6    | 2.54                     | 0.43              |
| 1:A:1278:G:H4'  | 1:A:1279:G:O5'   | 2.18                     | 0.43              |
| 11:K:85:ASP:O   | 11:K:89:ARG:HG2  | 2.19                     | 0.43              |
| 1:A:842:U:H4'   | 1:A:846:G:C6     | 2.54                     | 0.43              |
| 1:A:1401:G:H2'  | 1:A:1402:4OC:O4' | 2.19                     | 0.43              |
| 1:A:1521:C:H2'  | 1:A:1522:U:C6    | 2.53                     | 0.43              |
| 13:M:44:LYS:HE3 | 13:M:44:LYS:HB2  | 1.71                     | 0.43              |
| 1:A:253:A:H2'   | 1:A:254:G:C8     | 2.54                     | 0.42              |
| 1:A:538:G:H5''  | 13:M:111:LYS:HB2 | 2.01                     | 0.42              |
| 1:A:608:A:H2'   | 1:A:609:A:O4'    | 2.19                     | 0.42              |
| 1:A:757:U:OP1   | 1:A:822:U:O2'    | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1120:C:H2'   | 1:A:1121:U:H6    | 1.84                     | 0.42              |
| 1:A:1319:A:C8    | 1:A:1323:G:C6    | 3.07                     | 0.42              |
| 20:T:30:PRO:HA   | 20:T:48:THR:HG23 | 2.02                     | 0.42              |
| 23:X:19:U:H2'    | 23:X:20:U:O4'    | 2.18                     | 0.42              |
| 1:A:719:C:O2'    | 19:S:39:ILE:O    | 2.32                     | 0.42              |
| 1:A:1236:A:H2'   | 1:A:1237:C:C6    | 2.54                     | 0.42              |
| 1:A:1416:G:H2'   | 1:A:1417:G:O4'   | 2.18                     | 0.42              |
| 4:D:20:SER:HG    | 4:D:22:TRP:NE1   | 2.16                     | 0.42              |
| 1:A:1137:C:O2    | 1:A:1138:G:N2    | 2.52                     | 0.42              |
| 5:E:70:ARG:CD    | 5:E:73:ARG:HH21  | 2.32                     | 0.42              |
| 7:G:42:TRP:HZ2   | 19:S:24:LYS:HD2  | 1.84                     | 0.42              |
| 1:A:91:U:C2'     | 1:A:92:U:H5'     | 2.48                     | 0.42              |
| 1:A:279:A:H5''   | 1:A:281:G:O4'    | 2.18                     | 0.42              |
| 1:A:362:G:N2     | 1:A:365:U:OP2    | 2.46                     | 0.42              |
| 1:A:1010:U:H2'   | 1:A:1011:C:C6    | 2.53                     | 0.42              |
| 5:E:102:VAL:HA   | 5:E:105:MET:HG2  | 2.01                     | 0.42              |
| 8:H:16:PRO:HG3   | 10:J:46:MET:HE2  | 2.00                     | 0.42              |
| 15:O:15:ALA:HA   | 15:O:18:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:204:U:C2     | 1:A:205:A:C8     | 3.08                     | 0.42              |
| 1:A:384:G:H2'    | 1:A:385:C:H6     | 1.84                     | 0.42              |
| 1:A:1029:U:H4'   | 1:A:1030:U:H5    | 1.85                     | 0.42              |
| 3:C:57:LEU:HD13  | 3:C:217:VAL:HG13 | 2.01                     | 0.42              |
| 18:R:21:ILE:HG13 | 18:R:46:VAL:HB   | 2.00                     | 0.42              |
| 1:A:321:A:H2'    | 1:A:322:C:C6     | 2.55                     | 0.42              |
| 1:A:1403:C:H2'   | 1:A:1404:C:H6    | 1.83                     | 0.42              |
| 1:A:1418:A:N6    | 1:A:1482:G:O2'   | 2.50                     | 0.42              |
| 7:G:81:ASN:HB3   | 7:G:84:VAL:HG23  | 2.02                     | 0.42              |
| 15:O:26:GLU:O    | 15:O:30:ILE:HG22 | 2.19                     | 0.42              |
| 18:R:46:VAL:HG21 | 18:R:61:ILE:HG21 | 2.02                     | 0.42              |
| 1:A:337:G:H2'    | 1:A:338:A:H8     | 1.85                     | 0.42              |
| 1:A:1201:A:H4'   | 1:A:1202:U:H5''  | 2.02                     | 0.42              |
| 1:A:1425:U:H2'   | 1:A:1426:G:H8    | 1.84                     | 0.42              |
| 1:A:1536:C:C2    | 23:X:10:G:C2     | 3.08                     | 0.42              |
| 2:B:69:ASP:H     | 2:B:86:ARG:NH1   | 2.18                     | 0.42              |
| 5:E:177:LYS:HB3  | 5:E:179:GLU:HG2  | 2.01                     | 0.42              |
| 6:F:153:VAL:HG11 | 9:I:99:LEU:HD22  | 2.02                     | 0.42              |
| 6:F:162:GLU:CD   | 6:F:162:GLU:H    | 2.27                     | 0.42              |
| 8:H:16:PRO:CB    | 10:J:46:MET:HE2  | 2.49                     | 0.42              |
| 12:L:16:VAL:HG23 | 12:L:17:SER:H    | 1.85                     | 0.42              |
| 14:N:52:GLN:O    | 14:N:55:THR:OG1  | 2.33                     | 0.42              |
| 1:A:1507:A:H2'   | 1:A:1508:A:C8    | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:51:GLU:HA    | 2:B:54:LYS:HD2   | 2.00                     | 0.42              |
| 3:C:84:ALA:CB    | 3:C:91:PHE:HB3   | 2.49                     | 0.42              |
| 4:D:20:SER:HB2   | 4:D:40:ARG:HH22  | 1.85                     | 0.42              |
| 1:A:846:G:H2'    | 1:A:847:G:C8     | 2.54                     | 0.42              |
| 1:A:970:C:N4     | 10:J:130:ARG:OXT | 2.53                     | 0.42              |
| 1:A:1236:A:H4'   | 1:A:1304:G:H4'   | 2.01                     | 0.42              |
| 1:A:1323:G:H2'   | 1:A:1324:A:H8    | 1.81                     | 0.42              |
| 1:A:1406:U:H2'   | 1:A:1407:5MC:O4' | 2.20                     | 0.42              |
| 21:U:24:ARG:HA   | 21:U:24:ARG:HD3  | 1.80                     | 0.42              |
| 22:V:32:VAL:HG23 | 22:V:33:ARG:N    | 2.35                     | 0.42              |
| 1:A:704:A:C4     | 1:A:705:G:C8     | 3.08                     | 0.42              |
| 1:A:932:C:OP2    | 8:H:3:ARG:HD3    | 2.20                     | 0.42              |
| 1:A:996:A:C2     | 1:A:997:U:H1'    | 2.55                     | 0.42              |
| 1:A:1446:A:O2'   | 1:A:1447:A:H5'   | 2.20                     | 0.42              |
| 2:B:75:VAL:O     | 2:B:75:VAL:HG22  | 2.19                     | 0.42              |
| 1:A:846:G:H2'    | 1:A:847:G:H8     | 1.85                     | 0.41              |
| 1:A:908:A:H2'    | 1:A:909:A:H8     | 1.84                     | 0.41              |
| 1:A:1130:A:H2'   | 1:A:1131:G:C8    | 2.51                     | 0.41              |
| 1:A:1455:G:H2'   | 1:A:1456:A:C8    | 2.55                     | 0.41              |
| 1:A:28:A:O2'     | 1:A:296:U:OP1    | 2.30                     | 0.41              |
| 1:A:108:G:H5''   | 1:A:109:A:H5''   | 2.02                     | 0.41              |
| 1:A:284:C:H2'    | 1:A:285:C:H6     | 1.86                     | 0.41              |
| 1:A:1317:C:OP2   | 15:O:28:LYS:HD3  | 2.21                     | 0.41              |
| 1:A:1431:A:O2'   | 1:A:1432:G:H5'   | 2.20                     | 0.41              |
| 3:C:6:MET:HE3    | 3:C:6:MET:HB2    | 1.90                     | 0.41              |
| 19:S:70:TYR:HB2  | 19:S:74:HIS:CE1  | 2.55                     | 0.41              |
| 1:A:554:A:H2'    | 1:A:555:U:C6     | 2.55                     | 0.41              |
| 1:A:559:A:H4'    | 1:A:560:A:H3'    | 2.03                     | 0.41              |
| 1:A:674:G:H2'    | 1:A:675:A:C8     | 2.55                     | 0.41              |
| 1:A:737:C:H2'    | 1:A:738:C:C6     | 2.55                     | 0.41              |
| 1:A:998:C:H2'    | 1:A:999:C:H5'    | 2.01                     | 0.41              |
| 4:D:24:ALA:HB1   | 4:D:28:GLU:HG2   | 2.01                     | 0.41              |
| 5:E:9:LEU:HD23   | 5:E:9:LEU:HA     | 1.88                     | 0.41              |
| 7:G:25:TYR:CE2   | 7:G:78:PHE:HE1   | 2.38                     | 0.41              |
| 9:I:87:LYS:HG3   | 9:I:125:ILE:HD11 | 2.03                     | 0.41              |
| 21:U:27:MET:HE3  | 21:U:27:MET:HB3  | 1.84                     | 0.41              |
| 1:A:1497:G:H1'   | 1:A:1518:MA6:H2  | 2.03                     | 0.41              |
| 6:F:149:SER:OG   | 6:F:152:MET:HG2  | 2.20                     | 0.41              |
| 10:J:19:VAL:HG13 | 10:J:65:ILE:HG12 | 2.02                     | 0.41              |
| 17:Q:19:VAL:HG21 | 17:Q:52:LEU:HD11 | 2.02                     | 0.41              |
| 1:A:779:C:H2'    | 1:A:780:A:O4'    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1315:U:O2'   | 1:A:1360:A:N3    | 2.53                     | 0.41              |
| 8:H:140:ASP:HA   | 8:H:143:ARG:NH1  | 2.34                     | 0.41              |
| 14:N:78:LYS:HD2  | 14:N:78:LYS:HA   | 1.92                     | 0.41              |
| 19:S:32:TYR:O    | 19:S:40:VAL:HG12 | 2.21                     | 0.41              |
| 1:A:513:C:H2'    | 1:A:514:C:C6     | 2.56                     | 0.41              |
| 1:A:1165:U:H2'   | 1:A:1166:G:O4'   | 2.20                     | 0.41              |
| 2:B:71:ALA:HB3   | 2:B:88:LYS:HB2   | 2.03                     | 0.41              |
| 3:C:68:LEU:HB3   | 3:C:161:LEU:HD22 | 2.01                     | 0.41              |
| 3:C:187:VAL:HG22 | 3:C:191:SER:HB2  | 2.01                     | 0.41              |
| 13:M:110:ARG:HA  | 13:M:110:ARG:HD2 | 1.79                     | 0.41              |
| 23:X:10:G:H2'    | 23:X:11:U:C6     | 2.55                     | 0.41              |
| 1:A:602:A:H2'    | 1:A:603:U:C6     | 2.56                     | 0.41              |
| 1:A:603:U:H2'    | 1:A:604:G:H8     | 1.86                     | 0.41              |
| 1:A:860:A:H2'    | 1:A:861:G:O4'    | 2.21                     | 0.41              |
| 1:A:1442:G:H2'   | 1:A:1443:C:H6    | 1.85                     | 0.41              |
| 4:D:45:LYS:HB3   | 4:D:45:LYS:HE3   | 1.87                     | 0.41              |
| 9:I:7:ILE:O      | 9:I:11:LEU:HG    | 2.21                     | 0.41              |
| 18:R:22:VAL:HA   | 18:R:44:LEU:O    | 2.20                     | 0.41              |
| 1:A:1086:U:O5'   | 1:A:1086:U:O2    | 2.39                     | 0.41              |
| 9:I:67:GLN:C     | 9:I:69:LYS:H     | 2.29                     | 0.41              |
| 1:A:212:G:C2     | 1:A:213:G:C8     | 3.09                     | 0.41              |
| 1:A:212:G:C4     | 1:A:213:G:C8     | 3.08                     | 0.41              |
| 1:A:407:U:H2'    | 1:A:408:A:C8     | 2.56                     | 0.41              |
| 1:A:463:U:H3'    | 1:A:464:U:H6     | 1.85                     | 0.41              |
| 1:A:603:U:H2'    | 1:A:604:G:C8     | 2.56                     | 0.41              |
| 1:A:1025:U:H4'   | 1:A:1026:G:H5'   | 2.02                     | 0.41              |
| 1:A:1167:A:H4'   | 1:A:1168:U:OP2   | 2.19                     | 0.41              |
| 1:A:1404:C:H2'   | 1:A:1405:G:C8    | 2.56                     | 0.41              |
| 2:B:42:LEU:HB2   | 2:B:82:THR:HG21  | 2.03                     | 0.41              |
| 5:E:118:VAL:HG11 | 5:E:133:ALA:HA   | 2.03                     | 0.41              |
| 8:H:25:LYS:HE2   | 8:H:25:LYS:HB2   | 1.91                     | 0.41              |
| 13:M:76:GLU:OE1  | 13:M:76:GLU:N    | 2.54                     | 0.41              |
| 1:A:31:G:O2'     | 1:A:48:C:N4      | 2.54                     | 0.41              |
| 1:A:128:G:H2'    | 1:A:129:A:C8     | 2.56                     | 0.41              |
| 1:A:411:A:H4'    | 1:A:412:A:H5'    | 2.02                     | 0.41              |
| 1:A:458:U:H2'    | 1:A:459:A:C8     | 2.55                     | 0.41              |
| 1:A:792:A:H1'    | 1:A:794:A:N7     | 2.36                     | 0.41              |
| 1:A:1041:G:H2'   | 1:A:1042:A:C8    | 2.56                     | 0.41              |
| 1:A:1417:G:H2'   | 1:A:1482:G:N2    | 2.35                     | 0.41              |
| 3:C:70:VAL:O     | 3:C:163:VAL:HA   | 2.20                     | 0.41              |
| 3:C:85:LEU:HD23  | 3:C:85:LEU:HA    | 1.83                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:130:THR:C    | 3:C:132:LYS:H     | 2.28                     | 0.41              |
| 3:C:186:ILE:HD13 | 3:C:200:ILE:HB    | 2.03                     | 0.41              |
| 5:E:52:GLY:O     | 5:E:56:ARG:HG2    | 2.21                     | 0.41              |
| 8:H:45:SER:O     | 8:H:49:THR:HG22   | 2.21                     | 0.41              |
| 21:U:54:MET:HE2  | 21:U:54:MET:HB2   | 1.97                     | 0.41              |
| 1:A:321:A:H2'    | 1:A:322:C:H6      | 1.85                     | 0.40              |
| 1:A:468:A:H5''   | 1:A:469:C:H5      | 1.86                     | 0.40              |
| 1:A:526:C:C5     | 1:A:527:G7M:H1'   | 2.55                     | 0.40              |
| 1:A:900:A:H2'    | 1:A:901:A:C8      | 2.56                     | 0.40              |
| 1:A:1003:G:N2    | 1:A:1005:A:O5'    | 2.53                     | 0.40              |
| 1:A:1064:G:H1'   | 1:A:1190:G:N2     | 2.35                     | 0.40              |
| 1:A:1513:A:H2'   | 1:A:1514:G:C8     | 2.56                     | 0.40              |
| 18:R:19:LYS:HZ2  | 18:R:50:ASN:H     | 1.69                     | 0.40              |
| 1:A:421:U:H3'    | 1:A:422:C:C5      | 2.56                     | 0.40              |
| 4:D:42:TYR:OH    | 4:D:90:VAL:HG11   | 2.20                     | 0.40              |
| 6:F:104:GLY:O    | 6:F:122:ASN:HA    | 2.21                     | 0.40              |
| 6:F:111:MET:HA   | 6:F:114:VAL:HG12  | 2.02                     | 0.40              |
| 7:G:6:ILE:HG12   | 7:G:89:VAL:HG12   | 2.04                     | 0.40              |
| 17:Q:80:LYS:HB3  | 17:Q:80:LYS:HE2   | 1.89                     | 0.40              |
| 1:A:29:U:O2'     | 1:A:30:U:H5'      | 2.21                     | 0.40              |
| 1:A:51:A:N7      | 1:A:114:U:O2'     | 2.54                     | 0.40              |
| 1:A:466:A:H2'    | 1:A:468:A:C2      | 2.56                     | 0.40              |
| 1:A:1000:A:O5'   | 1:A:1000:A:H8     | 2.04                     | 0.40              |
| 1:A:1152:A:P     | 11:K:72:ARG:HH22  | 2.45                     | 0.40              |
| 1:A:1517:G:H2'   | 1:A:1518:MA6:C8   | 2.52                     | 0.40              |
| 8:H:113:ASP:HB2  | 8:H:119:ARG:HG3   | 2.03                     | 0.40              |
| 10:J:36:GLU:HA   | 10:J:45:ARG:HD3   | 2.04                     | 0.40              |
| 14:N:53:ILE:O    | 14:N:57:ARG:HG3   | 2.21                     | 0.40              |
| 1:A:339:C:H2'    | 1:A:340:U:H6      | 1.86                     | 0.40              |
| 1:A:422:C:H4'    | 1:A:423:G:C5'     | 2.51                     | 0.40              |
| 1:A:1315:U:O2    | 1:A:1360:A:H2     | 2.04                     | 0.40              |
| 1:A:1464:U:H2'   | 1:A:1465:A:C8     | 2.56                     | 0.40              |
| 4:D:64:ILE:O     | 4:D:99:ALA:HA     | 2.21                     | 0.40              |
| 5:E:150:LYS:NZ   | 5:E:178:MET:HB2   | 2.36                     | 0.40              |
| 8:H:92:ARG:O     | 8:H:96:ARG:HG3    | 2.21                     | 0.40              |
| 12:L:34:ILE:HD12 | 12:L:74:VAL:HG11  | 2.04                     | 0.40              |
| 12:L:87:LYS:HB2  | 12:L:113:VAL:HG13 | 2.04                     | 0.40              |
| 20:T:45:ILE:HD11 | 20:T:67:VAL:CG2   | 2.51                     | 0.40              |
| 21:U:48:GLN:HE21 | 21:U:52:ASN:HD21  | 1.69                     | 0.40              |
| 22:V:11:PRO:HG2  | 22:V:14:VAL:HG23  | 2.03                     | 0.40              |
| 22:V:69:ARG:NE   | 22:V:71:TYR:O     | 2.52                     | 0.40              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 23:X:17:U:H3'  | 23:X:18:G:C8     | 2.52                     | 0.40              |
| 1:A:323:U:H2'  | 1:A:324:G:O4'    | 2.22                     | 0.40              |
| 1:A:649:A:H2'  | 1:A:650:G:O4'    | 2.21                     | 0.40              |
| 1:A:939:G:H2'  | 1:A:940:C:C6     | 2.57                     | 0.40              |
| 1:A:978:A:C4   | 1:A:1319:A:C2    | 3.09                     | 0.40              |
| 1:A:1088:G:H5' | 22:V:70:LEU:HD23 | 2.04                     | 0.40              |
| 1:A:1218:C:H2' | 1:A:1219:A:C8    | 2.56                     | 0.40              |
| 1:A:1447:A:OP1 | 1:A:1448:C:N4    | 2.40                     | 0.40              |
| 1:A:1530:G:O6  | 22:V:46:LYS:NZ   | 2.46                     | 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     | 172/557 (31%) | 158 (92%) | 14 (8%) | 0        | 100         | 100 |
| 3   | C     | 224/241 (93%) | 214 (96%) | 10 (4%) | 0        | 100         | 100 |
| 4   | D     | 209/233 (90%) | 204 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 5   | E     | 203/206 (98%) | 199 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 6   | F     | 154/156 (99%) | 152 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 7   | G     | 102/131 (78%) | 100 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 8   | H     | 148/156 (95%) | 140 (95%) | 6 (4%)  | 2 (1%)   | 9           | 30  |
| 9   | I     | 127/130 (98%) | 122 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 10  | J     | 126/130 (97%) | 118 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 11  | K     | 99/103 (96%)  | 96 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 12  | L     | 115/129 (89%) | 109 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 13  | M     | 119/124 (96%) | 113 (95%) | 5 (4%)  | 1 (1%)   | 16          | 44  |
| 14  | N     | 113/118 (96%) | 110 (97%) | 3 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 15  | O     | 98/101 (97%)    | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 16  | P     | 86/89 (97%)     | 84 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 17  | Q     | 80/82 (98%)     | 78 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 18  | R     | 78/84 (93%)     | 75 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 19  | S     | 65/75 (87%)     | 63 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 20  | T     | 81/92 (88%)     | 80 (99%)   | 0       | 1 (1%)   | 10          | 34  |
| 21  | U     | 84/87 (97%)     | 84 (100%)  | 0       | 0        | 100         | 100 |
| 22  | V     | 68/71 (96%)     | 67 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| All | All   | 2551/3095 (82%) | 2463 (97%) | 84 (3%) | 4 (0%)   | 44          | 72  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 5   | ARG  |
| 8   | H     | 6   | VAL  |
| 20  | T     | 6   | LYS  |
| 13  | M     | 45  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | B     | 86/461 (19%)   | 75 (87%)  | 11 (13%) | 4           | 15 |
| 3   | C     | 187/199 (94%)  | 175 (94%) | 12 (6%)  | 16          | 44 |
| 4   | D     | 172/190 (90%)  | 168 (98%) | 4 (2%)   | 44          | 78 |
| 5   | E     | 172/173 (99%)  | 154 (90%) | 18 (10%) | 6           | 22 |
| 6   | F     | 119/119 (100%) | 113 (95%) | 6 (5%)   | 22          | 54 |
| 7   | G     | 91/112 (81%)   | 83 (91%)  | 8 (9%)   | 9           | 29 |
| 8   | H     | 124/129 (96%)  | 115 (93%) | 9 (7%)   | 13          | 38 |
| 9   | I     | 104/105 (99%)  | 102 (98%) | 2 (2%)   | 50          | 81 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 10  | J     | 106/107 (99%)   | 99 (93%)   | 7 (7%)   | 15          | 43 |
| 11  | K     | 88/90 (98%)     | 81 (92%)   | 7 (8%)   | 11          | 34 |
| 12  | L     | 90/99 (91%)     | 87 (97%)   | 3 (3%)   | 33          | 69 |
| 13  | M     | 102/103 (99%)   | 92 (90%)   | 10 (10%) | 7           | 25 |
| 14  | N     | 93/96 (97%)     | 83 (89%)   | 10 (11%) | 6           | 21 |
| 15  | O     | 83/84 (99%)     | 81 (98%)   | 2 (2%)   | 43          | 77 |
| 16  | P     | 76/77 (99%)     | 75 (99%)   | 1 (1%)   | 61          | 86 |
| 17  | Q     | 65/65 (100%)    | 59 (91%)   | 6 (9%)   | 8           | 27 |
| 18  | R     | 74/78 (95%)     | 65 (88%)   | 9 (12%)  | 5           | 16 |
| 19  | S     | 58/65 (89%)     | 57 (98%)   | 1 (2%)   | 53          | 83 |
| 20  | T     | 72/79 (91%)     | 68 (94%)   | 4 (6%)   | 19          | 50 |
| 21  | U     | 65/66 (98%)     | 59 (91%)   | 6 (9%)   | 8           | 27 |
| 22  | V     | 60/61 (98%)     | 56 (93%)   | 4 (7%)   | 15          | 42 |
| All | All   | 2087/2558 (82%) | 1947 (93%) | 140 (7%) | 17          | 42 |

All (140) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 7   | GLN  |
| 2   | B     | 14  | LYS  |
| 2   | B     | 34  | ASP  |
| 2   | B     | 48  | ILE  |
| 2   | B     | 51  | GLU  |
| 2   | B     | 63  | GLN  |
| 2   | B     | 69  | ASP  |
| 2   | B     | 72  | LEU  |
| 2   | B     | 73  | ASP  |
| 2   | B     | 75  | VAL  |
| 2   | B     | 102 | TYR  |
| 3   | C     | 31  | ILE  |
| 3   | C     | 45  | LYS  |
| 3   | C     | 54  | LEU  |
| 3   | C     | 80  | VAL  |
| 3   | C     | 95  | ARG  |
| 3   | C     | 130 | THR  |
| 3   | C     | 132 | LYS  |
| 3   | C     | 133 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 135 | LEU  |
| 3   | C     | 163 | VAL  |
| 3   | C     | 183 | VAL  |
| 3   | C     | 223 | GLU  |
| 4   | D     | 52  | VAL  |
| 4   | D     | 121 | THR  |
| 4   | D     | 165 | THR  |
| 4   | D     | 192 | THR  |
| 5   | E     | 15  | GLU  |
| 5   | E     | 28  | ILE  |
| 5   | E     | 101 | VAL  |
| 5   | E     | 113 | GLU  |
| 5   | E     | 116 | GLN  |
| 5   | E     | 125 | VAL  |
| 5   | E     | 129 | VAL  |
| 5   | E     | 131 | ASN  |
| 5   | E     | 132 | ILE  |
| 5   | E     | 136 | GLN  |
| 5   | E     | 144 | SER  |
| 5   | E     | 155 | VAL  |
| 5   | E     | 164 | GLN  |
| 5   | E     | 169 | THR  |
| 5   | E     | 188 | ARG  |
| 5   | E     | 190 | ASP  |
| 5   | E     | 194 | ASP  |
| 5   | E     | 198 | HIS  |
| 6   | F     | 18  | VAL  |
| 6   | F     | 76  | LEU  |
| 6   | F     | 88  | VAL  |
| 6   | F     | 94  | VAL  |
| 6   | F     | 105 | ILE  |
| 6   | F     | 117 | VAL  |
| 7   | G     | 16  | GLU  |
| 7   | G     | 54  | LEU  |
| 7   | G     | 72  | ASP  |
| 7   | G     | 74  | LEU  |
| 7   | G     | 84  | VAL  |
| 7   | G     | 97  | THR  |
| 7   | G     | 102 | MET  |
| 7   | G     | 103 | VAL  |
| 8   | H     | 12  | ILE  |
| 8   | H     | 56  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 58  | GLU  |
| 8   | H     | 59  | LEU  |
| 8   | H     | 75  | VAL  |
| 8   | H     | 79  | ARG  |
| 8   | H     | 91  | VAL  |
| 8   | H     | 113 | ASP  |
| 8   | H     | 146 | GLU  |
| 9   | I     | 62  | THR  |
| 9   | I     | 110 | VAL  |
| 10  | J     | 15  | SER  |
| 10  | J     | 22  | LYS  |
| 10  | J     | 29  | VAL  |
| 10  | J     | 58  | VAL  |
| 10  | J     | 67  | VAL  |
| 10  | J     | 95  | ARG  |
| 10  | J     | 105 | THR  |
| 11  | K     | 5   | ARG  |
| 11  | K     | 20  | GLN  |
| 11  | K     | 36  | VAL  |
| 11  | K     | 37  | ARG  |
| 11  | K     | 66  | GLU  |
| 11  | K     | 77  | VAL  |
| 11  | K     | 98  | VAL  |
| 12  | L     | 76  | GLU  |
| 12  | L     | 96  | THR  |
| 12  | L     | 108 | THR  |
| 13  | M     | 4   | VAL  |
| 13  | M     | 10  | LYS  |
| 13  | M     | 15  | LYS  |
| 13  | M     | 16  | VAL  |
| 13  | M     | 34  | CYS  |
| 13  | M     | 44  | LYS  |
| 13  | M     | 55  | VAL  |
| 13  | M     | 75  | GLN  |
| 13  | M     | 87  | VAL  |
| 13  | M     | 107 | VAL  |
| 14  | N     | 7   | ILE  |
| 14  | N     | 9   | ILE  |
| 14  | N     | 16  | VAL  |
| 14  | N     | 28  | THR  |
| 14  | N     | 42  | ASP  |
| 14  | N     | 56  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 58  | ASP  |
| 14  | N     | 101 | ARG  |
| 14  | N     | 102 | THR  |
| 14  | N     | 104 | THR  |
| 15  | O     | 26  | GLU  |
| 15  | O     | 28  | LYS  |
| 16  | P     | 17  | ARG  |
| 17  | Q     | 3   | THR  |
| 17  | Q     | 18  | GLN  |
| 17  | Q     | 21  | VAL  |
| 17  | Q     | 46  | LYS  |
| 17  | Q     | 48  | GLU  |
| 17  | Q     | 69  | ASP  |
| 18  | R     | 4   | LYS  |
| 18  | R     | 5   | ILE  |
| 18  | R     | 18  | GLU  |
| 18  | R     | 22  | VAL  |
| 18  | R     | 23  | VAL  |
| 18  | R     | 42  | THR  |
| 18  | R     | 60  | GLU  |
| 18  | R     | 78  | VAL  |
| 18  | R     | 79  | VAL  |
| 19  | S     | 26  | ILE  |
| 20  | T     | 48  | THR  |
| 20  | T     | 51  | VAL  |
| 20  | T     | 58  | VAL  |
| 20  | T     | 79  | THR  |
| 21  | U     | 3   | ASN  |
| 21  | U     | 5   | LYS  |
| 21  | U     | 14  | SER  |
| 21  | U     | 60  | ARG  |
| 21  | U     | 64  | LYS  |
| 21  | U     | 67  | ILE  |
| 22  | V     | 3   | VAL  |
| 22  | V     | 44  | GLU  |
| 22  | V     | 59  | LYS  |
| 22  | V     | 63  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 7   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 63  | GLN  |
| 4   | D     | 3   | GLN  |
| 4   | D     | 123 | GLN  |
| 4   | D     | 190 | HIS  |
| 5   | E     | 40  | GLN  |
| 5   | E     | 54  | GLN  |
| 5   | E     | 116 | GLN  |
| 5   | E     | 136 | GLN  |
| 5   | E     | 198 | HIS  |
| 6   | F     | 135 | ASN  |
| 7   | G     | 46  | GLN  |
| 7   | G     | 52  | ASN  |
| 7   | G     | 58  | HIS  |
| 7   | G     | 63  | ASN  |
| 8   | H     | 9   | GLN  |
| 8   | H     | 130 | ASN  |
| 10  | J     | 4   | ASN  |
| 10  | J     | 37  | GLN  |
| 10  | J     | 75  | GLN  |
| 12  | L     | 15  | GLN  |
| 12  | L     | 101 | ASN  |
| 14  | N     | 12  | HIS  |
| 15  | O     | 35  | ASN  |
| 15  | O     | 66  | GLN  |
| 16  | P     | 35  | GLN  |
| 16  | P     | 80  | GLN  |
| 18  | R     | 9   | GLN  |
| 18  | R     | 51  | ASN  |
| 19  | S     | 74  | HIS  |
| 20  | T     | 14  | HIS  |
| 21  | U     | 13  | GLN  |
| 21  | U     | 48  | GLN  |
| 21  | U     | 61  | GLN  |
| 21  | U     | 70  | ASN  |
| 22  | V     | 64  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1537/1541 (99%) | 240 (15%)         | 10 (0%)         |
| 23  | X     | 16/53 (30%)     | 3 (18%)           | 1 (6%)          |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| All | All   | 1553/1594 (97%) | 243 (15%)         | 11 (0%)         |

All (243) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | A    |
| 1   | A     | 4   | U    |
| 1   | A     | 5   | U    |
| 1   | A     | 9   | G    |
| 1   | A     | 22  | G    |
| 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     | 52  | C    |
| 1   | A     | 70  | U    |
| 1   | A     | 71  | A    |
| 1   | A     | 75  | G    |
| 1   | A     | 76  | G    |
| 1   | A     | 77  | A    |
| 1   | A     | 83  | C    |
| 1   | A     | 84  | U    |
| 1   | A     | 85  | U    |
| 1   | A     | 86  | G    |
| 1   | A     | 93  | U    |
| 1   | A     | 94  | G    |
| 1   | A     | 95  | C    |
| 1   | A     | 108 | G    |
| 1   | A     | 116 | A    |
| 1   | A     | 130 | A    |
| 1   | A     | 131 | A    |
| 1   | A     | 141 | G    |
| 1   | A     | 157 | U    |
| 1   | A     | 158 | G    |
| 1   | A     | 163 | C    |
| 1   | A     | 165 | G    |
| 1   | A     | 166 | U    |
| 1   | A     | 168 | G    |
| 1   | A     | 173 | U    |
| 1   | A     | 181 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 189 | A    |
| 1   | A     | 197 | A    |
| 1   | A     | 212 | G    |
| 1   | A     | 245 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 279 | A    |
| 1   | A     | 280 | C    |
| 1   | A     | 289 | G    |
| 1   | A     | 321 | A    |
| 1   | A     | 328 | C    |
| 1   | A     | 329 | A    |
| 1   | A     | 330 | C    |
| 1   | A     | 332 | G    |
| 1   | A     | 343 | U    |
| 1   | A     | 345 | C    |
| 1   | A     | 346 | G    |
| 1   | A     | 347 | G    |
| 1   | A     | 348 | G    |
| 1   | A     | 351 | 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     | 398 | U    |
| 1   | A     | 406 | G    |
| 1   | A     | 411 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 421 | U    |
| 1   | A     | 422 | C    |
| 1   | A     | 424 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 457 | G    |
| 1   | A     | 458 | U    |
| 1   | A     | 461 | A    |
| 1   | A     | 463 | U    |
| 1   | A     | 464 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 465 | A    |
| 1   | A     | 466 | A    |
| 1   | A     | 467 | U    |
| 1   | A     | 468 | A    |
| 1   | A     | 479 | U    |
| 1   | A     | 481 | G    |
| 1   | A     | 484 | G    |
| 1   | A     | 486 | U    |
| 1   | A     | 495 | A    |
| 1   | A     | 497 | G    |
| 1   | A     | 511 | C    |
| 1   | A     | 521 | G    |
| 1   | A     | 527 | G7M  |
| 1   | A     | 528 | C    |
| 1   | A     | 533 | A    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 562 | U    |
| 1   | A     | 564 | C    |
| 1   | A     | 567 | G    |
| 1   | A     | 569 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | C    |
| 1   | A     | 577 | G    |
| 1   | A     | 578 | C    |
| 1   | A     | 596 | A    |
| 1   | A     | 633 | G    |
| 1   | A     | 642 | A    |
| 1   | A     | 650 | G    |
| 1   | A     | 665 | A    |
| 1   | A     | 682 | G    |
| 1   | A     | 687 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 718 | A    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |
| 1   | A     | 731 | G    |
| 1   | A     | 734 | G    |
| 1   | A     | 755 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 777  | A    |
| 1   | A     | 793  | U    |
| 1   | A     | 794  | A    |
| 1   | A     | 815  | A    |
| 1   | A     | 817  | C    |
| 1   | A     | 828  | U    |
| 1   | A     | 829  | G    |
| 1   | A     | 832  | G    |
| 1   | A     | 841  | C    |
| 1   | A     | 842  | U    |
| 1   | A     | 843  | U    |
| 1   | A     | 844  | G    |
| 1   | A     | 846  | G    |
| 1   | A     | 876  | C    |
| 1   | A     | 882  | C    |
| 1   | A     | 914  | A    |
| 1   | A     | 926  | G    |
| 1   | A     | 927  | G    |
| 1   | A     | 934  | C    |
| 1   | A     | 935  | A    |
| 1   | A     | 942  | G    |
| 1   | A     | 960  | U    |
| 1   | A     | 966  | 2MG  |
| 1   | A     | 967  | 5MC  |
| 1   | A     | 968  | A    |
| 1   | A     | 969  | A    |
| 1   | A     | 971  | G    |
| 1   | A     | 975  | A    |
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 994  | A    |
| 1   | A     | 996  | A    |
| 1   | A     | 998  | C    |
| 1   | A     | 999  | C    |
| 1   | A     | 1004 | A    |
| 1   | A     | 1009 | U    |
| 1   | A     | 1018 | G    |
| 1   | A     | 1020 | G    |
| 1   | A     | 1022 | A    |
| 1   | A     | 1024 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1025 | U    |
| 1   | A     | 1028 | C    |
| 1   | A     | 1030 | U    |
| 1   | A     | 1031 | C    |
| 1   | A     | 1033 | G    |
| 1   | A     | 1044 | A    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1079 | G    |
| 1   | A     | 1085 | U    |
| 1   | A     | 1092 | A    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1099 | G    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1103 | C    |
| 1   | A     | 1104 | G    |
| 1   | A     | 1108 | G    |
| 1   | A     | 1133 | G    |
| 1   | A     | 1136 | C    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1140 | C    |
| 1   | A     | 1141 | C    |
| 1   | A     | 1151 | A    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1158 | C    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1167 | A    |
| 1   | A     | 1168 | U    |
| 1   | A     | 1169 | A    |
| 1   | A     | 1170 | A    |
| 1   | A     | 1171 | A    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1196 | A    |
| 1   | A     | 1197 | A    |
| 1   | A     | 1207 | 2MG  |
| 1   | A     | 1213 | A    |
| 1   | A     | 1214 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1257 | A    |
| 1   | A     | 1260 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1278 | G    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1286 | U    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1299 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1302 | C    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1318 | A    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1370 | G    |
| 1   | A     | 1379 | G    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1432 | G    |
| 1   | A     | 1441 | A    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1451 | U    |
| 1   | A     | 1453 | G    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1498 | UR3  |
| 1   | A     | 1499 | A    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1519 | MA6  |
| 1   | A     | 1520 | C    |
| 1   | A     | 1521 | C    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1533 | C    |
| 1   | A     | 1534 | A    |
| 23  | X     | 12   | A    |
| 23  | X     | 13   | U    |
| 23  | X     | 17   | U    |

All (11) RNA pucker outliers are listed below:

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
|-----|-------|-----|------|

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 422  | C    |
| 1   | A     | 428  | G    |
| 1   | A     | 429  | U    |
| 1   | A     | 463  | U    |
| 1   | A     | 467  | U    |
| 1   | A     | 575  | G    |
| 1   | A     | 641  | U    |
| 1   | A     | 966  | 2MG  |
| 1   | A     | 1078 | U    |
| 1   | A     | 1167 | A    |
| 23  | X     | 11   | U    |

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

12 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   | PSU  | A     | 516  | 1,24 | 18,21,22     | 0.92 | 1 (5%)   | 21,30,33    | 0.70 | 0        |
| 1   | 2MG  | A     | 1207 | 1    | 23,26,27     | 1.50 | 5 (21%)  | 33,38,41    | 2.35 | 10 (30%) |
| 1   | 5MC  | A     | 1407 | 1    | 19,22,23     | 1.74 | 2 (10%)  | 26,32,35    | 1.71 | 6 (23%)  |
| 13  | D2T  | M     | 89   | 13   | 8,9,10       | 2.36 | 1 (12%)  | 6,11,13     | 2.31 | 2 (33%)  |
| 1   | G7M  | A     | 527  | 1    | 23,26,27     | 0.72 | 1 (4%)   | 34,39,42    | 0.95 | 1 (2%)   |
| 1   | 2MG  | A     | 1516 | 1    | 23,26,27     | 1.32 | 4 (17%)  | 33,38,41    | 2.30 | 7 (21%)  |
| 1   | 2MG  | A     | 966  | 1    | 23,26,27     | 1.30 | 4 (17%)  | 33,38,41    | 2.38 | 11 (33%) |
| 1   | MA6  | A     | 1519 | 1    | 23,26,27     | 1.52 | 5 (21%)  | 33,38,41    | 2.45 | 16 (48%) |
| 1   | UR3  | A     | 1498 | 1    | 19,22,23     | 1.10 | 2 (10%)  | 26,32,35    | 2.12 | 7 (26%)  |
| 1   | 5MC  | A     | 967  | 1    | 19,22,23     | 1.42 | 3 (15%)  | 26,32,35    | 1.58 | 6 (23%)  |
| 1   | MA6  | A     | 1518 | 1    | 23,26,27     | 1.50 | 5 (21%)  | 33,38,41    | 2.54 | 14 (42%) |
| 1   | 4OC  | A     | 1402 | 1    | 20,23,24     | 0.80 | 0        | 25,32,35    | 1.53 | 2 (8%)   |

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   | PSU  | A     | 516  | 1,24 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | A     | 1207 | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | 5MC  | A     | 1407 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 13  | D2T  | M     | 89   | 13   | -       | 1/7/12/14  | -       |
| 1   | G7M  | A     | 527  | 1    | -       | 3/7/25/26  | 0/3/3/3 |
| 1   | 2MG  | A     | 1516 | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | 2MG  | A     | 966  | 1    | -       | 5/9/27/28  | 0/3/3/3 |
| 1   | MA6  | A     | 1519 | 1    | -       | 6/11/29/30 | 0/3/3/3 |
| 1   | UR3  | A     | 1498 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 967  | 1    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | MA6  | A     | 1518 | 1    | -       | 1/11/29/30 | 0/3/3/3 |
| 1   | 4OC  | A     | 1402 | 1    | -       | 0/9/29/30  | 0/2/2/2 |

All (33) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1407 | 5MC  | C5-C4 | 6.13  | 1.48        | 1.44     |
| 13  | M     | 89   | D2T  | CB-CA | -6.06 | 1.52        | 1.54     |
| 1   | A     | 1519 | MA6  | C5-C4 | 4.59  | 1.47        | 1.39     |
| 1   | A     | 1518 | MA6  | C5-C4 | 4.50  | 1.47        | 1.39     |
| 1   | A     | 967  | 5MC  | C5-C4 | 3.87  | 1.47        | 1.44     |
| 1   | A     | 1207 | 2MG  | C6-N1 | -3.59 | 1.32        | 1.38     |
| 1   | A     | 516  | PSU  | C6-C5 | 3.54  | 1.39        | 1.35     |
| 1   | A     | 1407 | 5MC  | C6-N1 | -3.24 | 1.32        | 1.38     |
| 1   | A     | 1516 | 2MG  | C5-C4 | 3.14  | 1.47        | 1.38     |
| 1   | A     | 1207 | 2MG  | C4-N9 | -2.95 | 1.30        | 1.38     |
| 1   | A     | 1519 | MA6  | C5-C6 | 2.91  | 1.48        | 1.41     |
| 1   | A     | 1207 | 2MG  | C5-N7 | -2.89 | 1.33        | 1.39     |
| 1   | A     | 967  | 5MC  | C6-N1 | -2.79 | 1.33        | 1.38     |
| 1   | A     | 966  | 2MG  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 1   | A     | 966  | 2MG  | C5-N7 | -2.71 | 1.33        | 1.39     |
| 1   | A     | 1518 | MA6  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 1   | A     | 1516 | 2MG  | C2-N3 | 2.59  | 1.36        | 1.32     |
| 1   | A     | 1516 | 2MG  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 1   | A     | 527  | G7M  | C8-N7 | 2.51  | 1.37        | 1.33     |
| 1   | A     | 966  | 2MG  | C5-C4 | 2.45  | 1.45        | 1.38     |
| 1   | A     | 1207 | 2MG  | C2-N1 | -2.44 | 1.32        | 1.36     |
| 1   | A     | 967  | 5MC  | C6-C5 | 2.38  | 1.38        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1519 | MA6  | C8-N7 | 2.36  | 1.36        | 1.31     |
| 1   | A     | 1518 | MA6  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 1   | A     | 1498 | UR3  | C5-C4 | -2.31 | 1.38        | 1.43     |
| 1   | A     | 1207 | 2MG  | C5-C4 | 2.22  | 1.44        | 1.38     |
| 1   | A     | 966  | 2MG  | C4-N9 | -2.19 | 1.32        | 1.38     |
| 1   | A     | 1519 | MA6  | C5-N7 | -2.17 | 1.35        | 1.39     |
| 1   | A     | 1498 | UR3  | C6-N1 | -2.17 | 1.32        | 1.38     |
| 1   | A     | 1516 | 2MG  | C5-N7 | -2.10 | 1.34        | 1.39     |
| 1   | A     | 1518 | MA6  | C4-N9 | -2.09 | 1.33        | 1.37     |
| 1   | A     | 1518 | MA6  | C8-N7 | 2.09  | 1.35        | 1.31     |
| 1   | A     | 1519 | MA6  | C4-N9 | -2.07 | 1.33        | 1.37     |

All (82) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 1516 | 2MG  | C2-N3-C4   | 7.38  | 121.23      | 112.00   |
| 1   | A     | 966  | 2MG  | C2-N3-C4   | 7.08  | 120.85      | 112.00   |
| 1   | A     | 1498 | UR3  | C4-N3-C2   | -6.96 | 118.98      | 124.58   |
| 1   | A     | 1207 | 2MG  | C2-N3-C4   | 6.91  | 120.64      | 112.00   |
| 1   | A     | 1516 | 2MG  | C5-C4-N3   | -6.51 | 118.02      | 128.39   |
| 1   | A     | 1207 | 2MG  | C5-C4-N3   | -5.97 | 118.89      | 128.39   |
| 1   | A     | 1402 | 4OC  | C2'-C1'-N1 | -5.96 | 102.92      | 114.24   |
| 1   | A     | 966  | 2MG  | C5-C4-N3   | -5.83 | 119.12      | 128.39   |
| 1   | A     | 1518 | MA6  | C5-C4-N3   | -5.51 | 119.13      | 126.72   |
| 1   | A     | 1519 | MA6  | C5-C4-N3   | -5.43 | 119.23      | 126.72   |
| 1   | A     | 1518 | MA6  | N1-C6-N6   | 5.23  | 123.23      | 116.86   |
| 1   | A     | 1516 | 2MG  | N9-C4-N3   | 5.04  | 136.02      | 125.95   |
| 1   | A     | 1518 | MA6  | N3-C4-N9   | 4.70  | 135.16      | 127.17   |
| 1   | A     | 966  | 2MG  | N9-C4-N3   | 4.36  | 134.67      | 125.95   |
| 1   | A     | 1519 | MA6  | N3-C4-N9   | 4.24  | 134.38      | 127.17   |
| 1   | A     | 1519 | MA6  | C10-N6-C6  | -4.23 | 109.76      | 120.52   |
| 1   | A     | 967  | 5MC  | C5-C6-N1   | -4.17 | 118.78      | 123.31   |
| 1   | A     | 1407 | 5MC  | C5-C6-N1   | -4.17 | 118.79      | 123.31   |
| 1   | A     | 1519 | MA6  | C9-N6-C6   | -4.13 | 110.01      | 120.52   |
| 1   | A     | 1207 | 2MG  | N9-C4-N3   | 4.11  | 134.16      | 125.95   |
| 1   | A     | 1518 | MA6  | C2-N1-C6   | 4.09  | 121.82      | 111.83   |
| 1   | A     | 1519 | MA6  | C2-N1-C6   | 4.06  | 121.76      | 111.83   |
| 13  | M     | 89   | D2T  | CB1-SB-CB  | 3.99  | 109.54      | 102.36   |
| 1   | A     | 1518 | MA6  | C5-C6-N6   | -3.86 | 119.22      | 125.33   |
| 1   | A     | 1519 | MA6  | C2'-C1'-N9 | -3.73 | 104.04      | 113.30   |
| 1   | A     | 1518 | MA6  | C9-N6-C6   | -3.70 | 111.10      | 120.52   |
| 1   | A     | 1498 | UR3  | C5-C4-N3   | 3.60  | 119.78      | 115.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1207 | 2MG  | C6-C5-N7    | 3.59  | 136.83      | 130.29   |
| 1   | A     | 1498 | UR3  | O4'-C1'-C2' | -3.59 | 98.94       | 106.62   |
| 1   | A     | 1519 | MA6  | C2-N3-C4    | 3.58  | 120.57      | 111.83   |
| 1   | A     | 1519 | MA6  | C4-C5-N7    | -3.56 | 106.52      | 110.58   |
| 1   | A     | 1518 | MA6  | C2-N3-C4    | 3.53  | 120.46      | 111.83   |
| 1   | A     | 966  | 2MG  | C6-C5-N7    | 3.43  | 136.53      | 130.29   |
| 1   | A     | 1407 | 5MC  | C2'-C1'-N1  | -3.35 | 103.92      | 113.25   |
| 1   | A     | 1407 | 5MC  | CM5-C5-C6   | -3.29 | 118.39      | 122.85   |
| 1   | A     | 1518 | MA6  | C4-N9-C8    | 3.24  | 109.14      | 105.74   |
| 1   | A     | 1518 | MA6  | N1-C2-N3    | -3.24 | 123.69      | 128.58   |
| 1   | A     | 1519 | MA6  | N1-C2-N3    | -3.14 | 123.83      | 128.58   |
| 1   | A     | 1518 | MA6  | C2'-C1'-N9  | -3.11 | 105.58      | 113.30   |
| 1   | A     | 1518 | MA6  | C4-C5-N7    | -3.10 | 107.03      | 110.58   |
| 1   | A     | 967  | 5MC  | C2'-C1'-N1  | -3.03 | 104.82      | 113.25   |
| 1   | A     | 1516 | 2MG  | C6-C5-N7    | 3.00  | 135.76      | 130.29   |
| 1   | A     | 1518 | MA6  | C10-N6-C6   | -3.00 | 112.88      | 120.52   |
| 1   | A     | 966  | 2MG  | N1-C2-N2    | 2.98  | 119.61      | 116.56   |
| 13  | M     | 89   | D2T  | OD2-CG-CB   | 2.97  | 119.56      | 113.15   |
| 1   | A     | 1207 | 2MG  | C2-N1-C6    | -2.97 | 120.96      | 124.55   |
| 1   | A     | 1498 | UR3  | C3U-N3-C2   | 2.90  | 122.39      | 117.33   |
| 1   | A     | 1519 | MA6  | N1-C6-N6    | 2.89  | 120.38      | 116.86   |
| 1   | A     | 1519 | MA6  | C4-N9-C8    | 2.88  | 108.76      | 105.74   |
| 1   | A     | 527  | G7M  | C3'-C2'-C1' | -2.78 | 96.21       | 101.46   |
| 1   | A     | 1407 | 5MC  | O2-C2-N3    | -2.72 | 118.03      | 122.33   |
| 1   | A     | 1407 | 5MC  | C1'-N1-C6   | -2.72 | 116.68      | 121.15   |
| 1   | A     | 966  | 2MG  | C2-N1-C6    | -2.71 | 121.28      | 124.55   |
| 1   | A     | 1207 | 2MG  | CM2-N2-C2   | -2.70 | 117.84      | 123.65   |
| 1   | A     | 1207 | 2MG  | C4-C5-N7    | -2.67 | 106.43      | 110.67   |
| 1   | A     | 967  | 5MC  | C5-C4-N3    | -2.67 | 119.02      | 121.75   |
| 1   | A     | 966  | 2MG  | N2-C2-N3    | -2.65 | 117.14      | 120.51   |
| 1   | A     | 966  | 2MG  | O6-C6-C5    | -2.60 | 119.67      | 126.53   |
| 1   | A     | 1207 | 2MG  | N2-C2-N3    | -2.60 | 117.20      | 120.51   |
| 1   | A     | 1519 | MA6  | C5-N7-C8    | 2.56  | 107.47      | 103.45   |
| 1   | A     | 1498 | UR3  | C1'-N1-C2   | 2.53  | 121.19      | 117.04   |
| 1   | A     | 1516 | 2MG  | C4-C5-N7    | -2.47 | 106.75      | 110.67   |
| 1   | A     | 966  | 2MG  | C4-C5-N7    | -2.44 | 106.80      | 110.67   |
| 1   | A     | 1518 | MA6  | C5-N7-C8    | 2.41  | 107.24      | 103.45   |
| 1   | A     | 1516 | 2MG  | C2'-C1'-N9  | -2.37 | 106.66      | 113.25   |
| 1   | A     | 1207 | 2MG  | N1-C2-N2    | 2.34  | 118.95      | 116.56   |
| 1   | A     | 967  | 5MC  | O4'-C1'-N1  | 2.33  | 113.63      | 108.36   |
| 1   | A     | 1402 | 4OC  | C6-C5-C4    | 2.30  | 119.77      | 117.00   |
| 1   | A     | 967  | 5MC  | O2-C2-N3    | -2.29 | 118.72      | 122.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1498 | UR3  | O3'-C3'-C4' | -2.29 | 104.51      | 111.08   |
| 1   | A     | 1519 | MA6  | C5-C6-N6    | -2.27 | 121.74      | 125.33   |
| 1   | A     | 1498 | UR3  | C2'-C3'-C4' | -2.27 | 98.23       | 102.61   |
| 1   | A     | 1207 | 2MG  | C5-C6-N1    | 2.23  | 118.94      | 113.25   |
| 1   | A     | 966  | 2MG  | C5-C6-N1    | 2.19  | 118.82      | 113.25   |
| 1   | A     | 1519 | MA6  | N9-C8-N7    | -2.17 | 110.86      | 113.94   |
| 1   | A     | 1518 | MA6  | N9-C8-N7    | -2.16 | 110.87      | 113.94   |
| 1   | A     | 1516 | 2MG  | O6-C6-C5    | -2.15 | 120.86      | 126.53   |
| 1   | A     | 966  | 2MG  | CM2-N2-C2   | -2.10 | 119.14      | 123.65   |
| 1   | A     | 1519 | MA6  | C10-N6-C9   | -2.08 | 109.49      | 116.18   |
| 1   | A     | 1519 | MA6  | C6-C5-N7    | 2.08  | 136.75      | 133.43   |
| 1   | A     | 967  | 5MC  | N1-C2-N3    | 2.04  | 122.34      | 118.80   |
| 1   | A     | 1407 | 5MC  | C5-C4-N3    | -2.02 | 119.69      | 121.75   |

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A     | 966  | 2MG  | N1-C2-N2-CM2    |
| 1   | A     | 966  | 2MG  | N3-C2-N2-CM2    |
| 1   | A     | 1207 | 2MG  | O4'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 1   | A     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 1   | A     | 967  | 5MC  | O4'-C4'-C5'-O5' |
| 1   | A     | 967  | 5MC  | C3'-C4'-C5'-O5' |
| 1   | A     | 966  | 2MG  | C3'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | N1-C6-N6-C10    |
| 1   | A     | 1207 | 2MG  | C3'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | C4'-C5'-O5'-P   |
| 1   | A     | 966  | 2MG  | O4'-C4'-C5'-O5' |
| 1   | A     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 1   | A     | 1518 | MA6  | C5-C6-N6-C9     |
| 1   | A     | 527  | G7M  | C4'-C5'-O5'-P   |
| 1   | A     | 1519 | MA6  | C5-C6-N6-C9     |
| 1   | A     | 966  | 2MG  | C4'-C5'-O5'-P   |
| 13  | M     | 89   | D2T  | CG-CB-SB-CB1    |
| 1   | A     | 1516 | 2MG  | O4'-C4'-C5'-O5' |

There are no ring outliers.

9 monomers are involved in 23 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | A     | 1407 | 5MC  | 1       | 0            |
| 1   | A     | 527  | G7M  | 2       | 0            |
| 1   | A     | 1516 | 2MG  | 1       | 0            |
| 1   | A     | 966  | 2MG  | 4       | 0            |
| 1   | A     | 1519 | MA6  | 6       | 0            |
| 1   | A     | 1498 | UR3  | 4       | 0            |
| 1   | A     | 967  | 5MC  | 2       | 0            |
| 1   | A     | 1518 | MA6  | 6       | 0            |
| 1   | A     | 1402 | 4OC  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 86 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

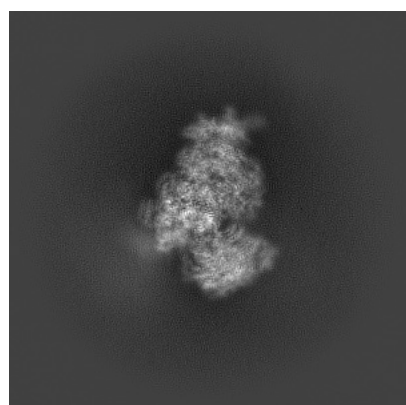
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51615. These allow visual inspection of the internal detail of the map and identification of artifacts.

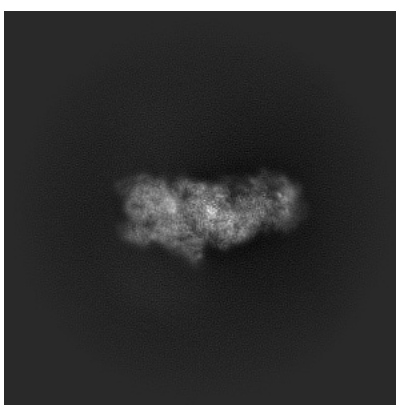
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

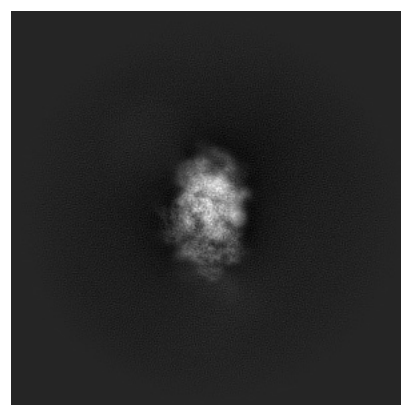
#### 6.1.1 Primary map



X



Y

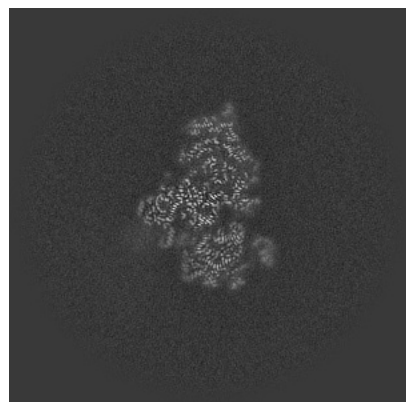


Z

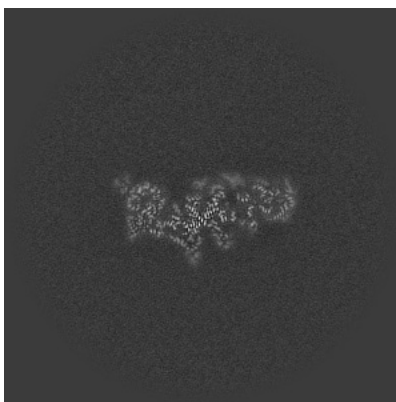
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

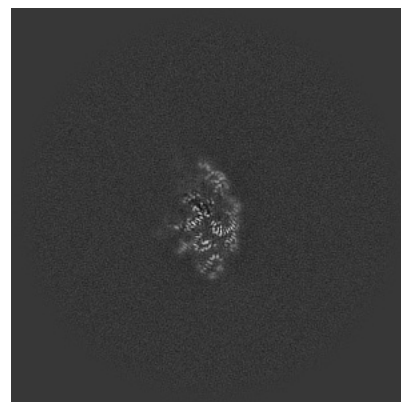
#### 6.2.1 Primary map



X Index: 300



Y Index: 300

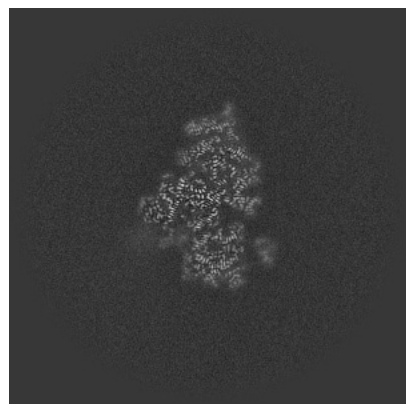


Z Index: 300

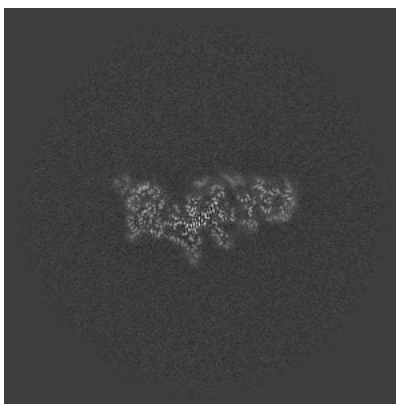
The images above show central slices of the map in three orthogonal directions.

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

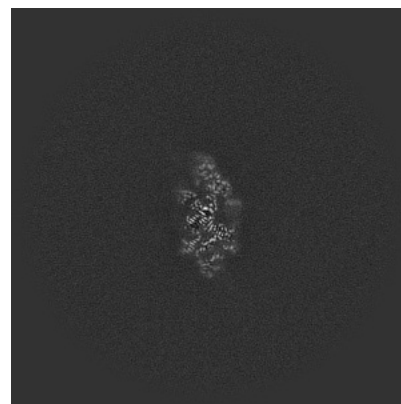
### 6.3.1 Primary map



X Index: 297



Y Index: 301

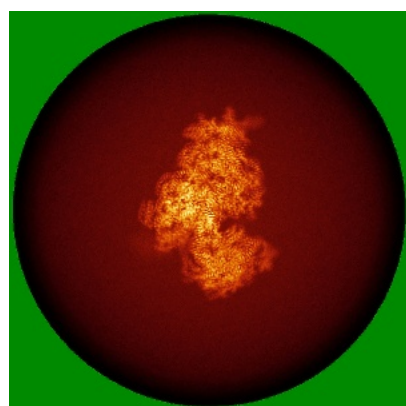


Z Index: 306

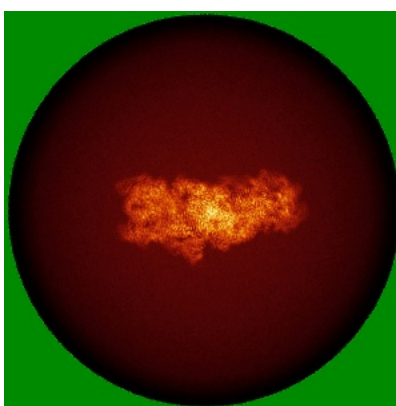
The images above show the largest variance slices of the map in three orthogonal directions.

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

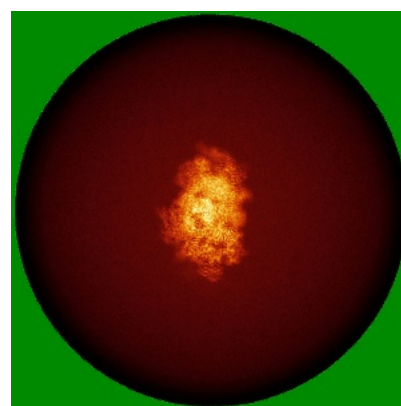
### 6.4.1 Primary map



X



Y



Z

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

This section was not generated.

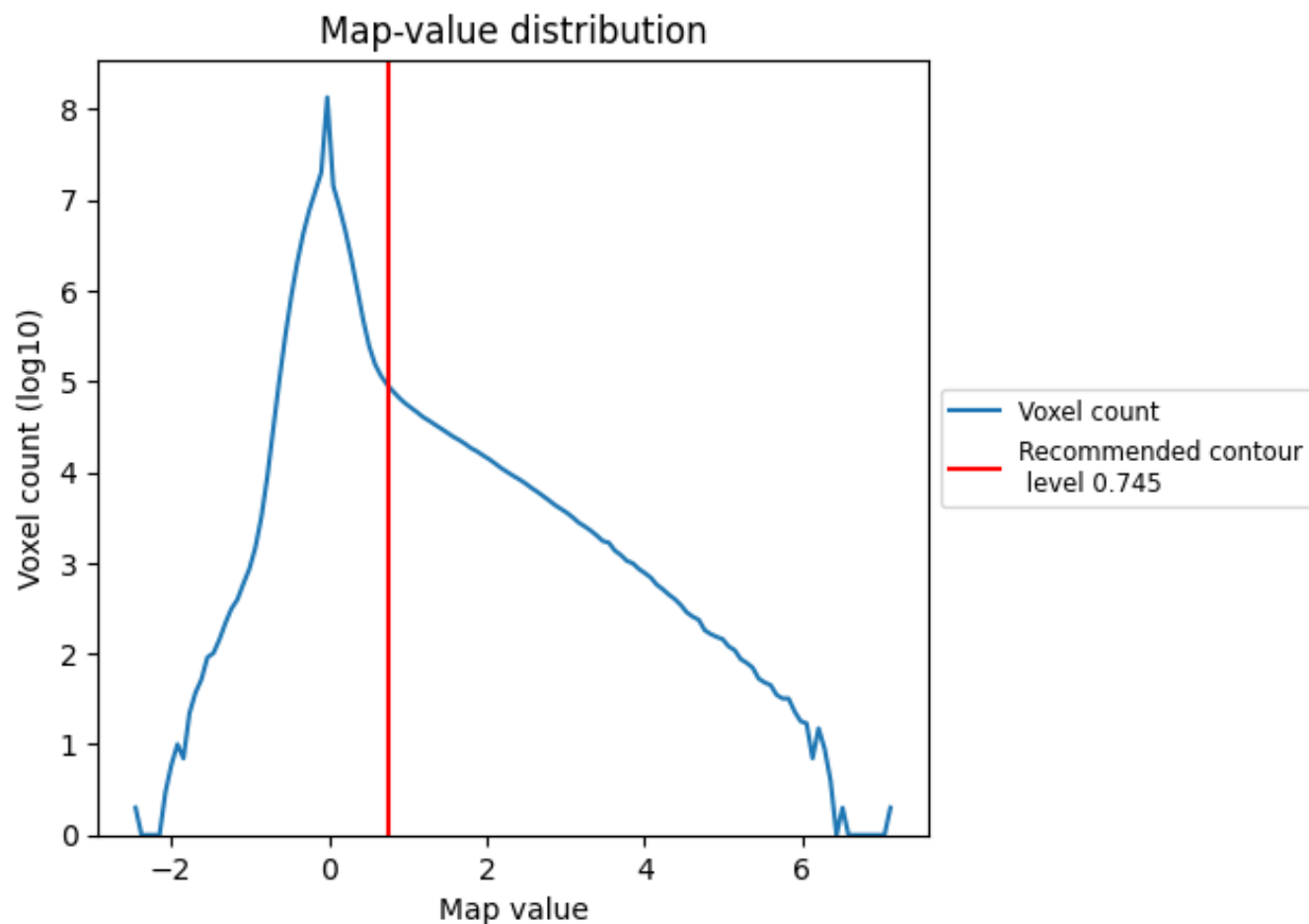
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

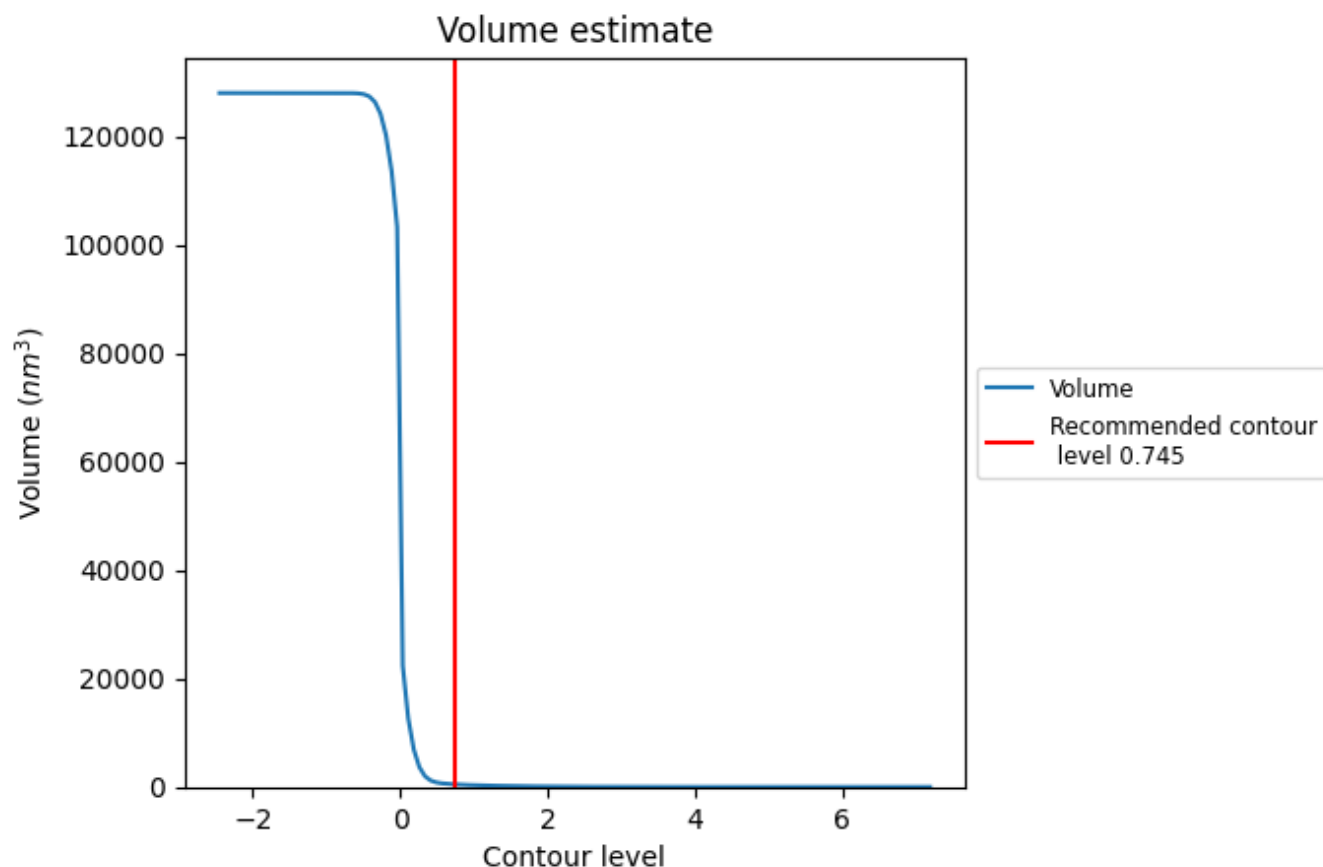
This section contains the results of statistical analysis of the map.

### 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.

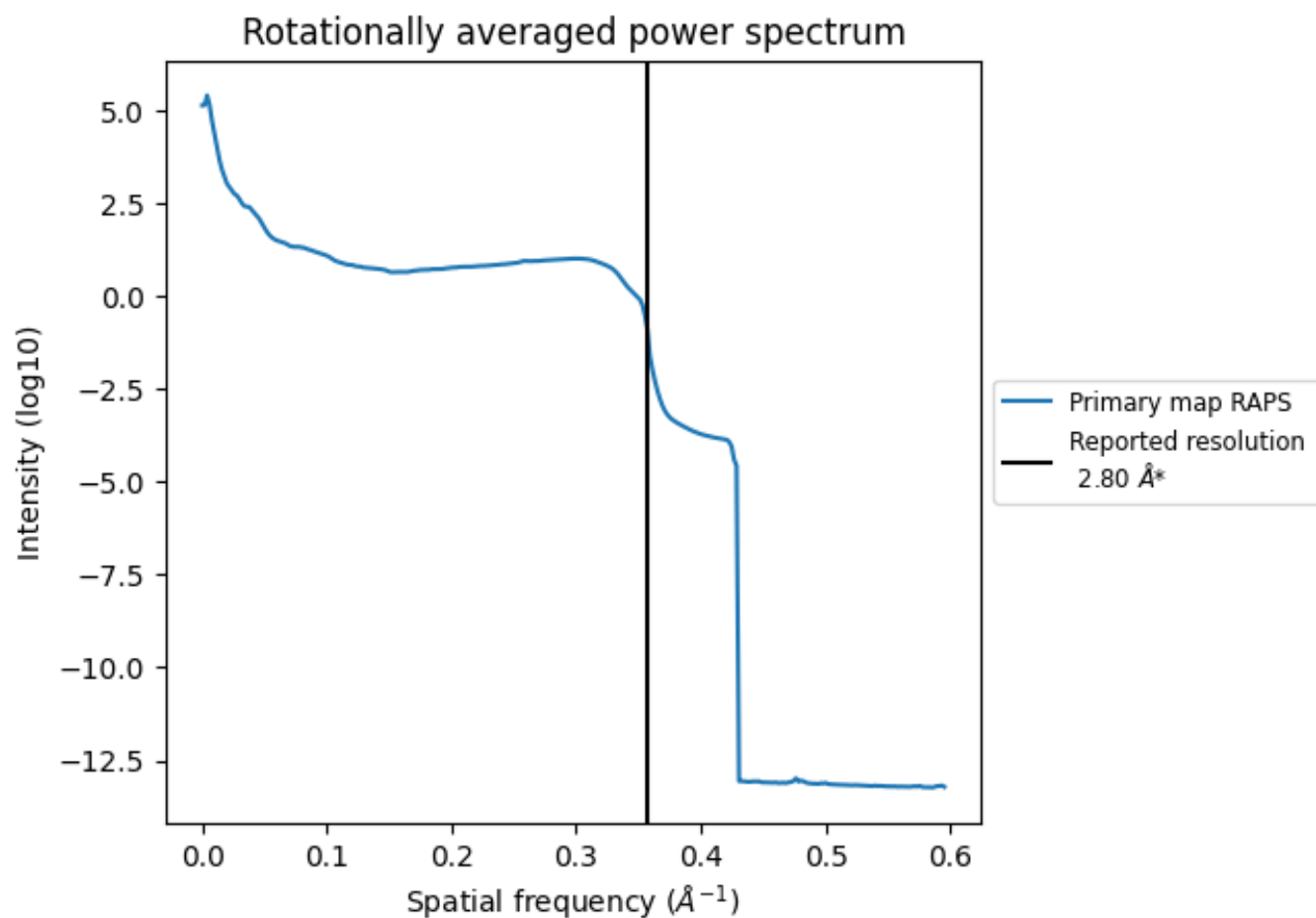
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 478  $\text{nm}^3$ ; this corresponds to an approximate mass of 432 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 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

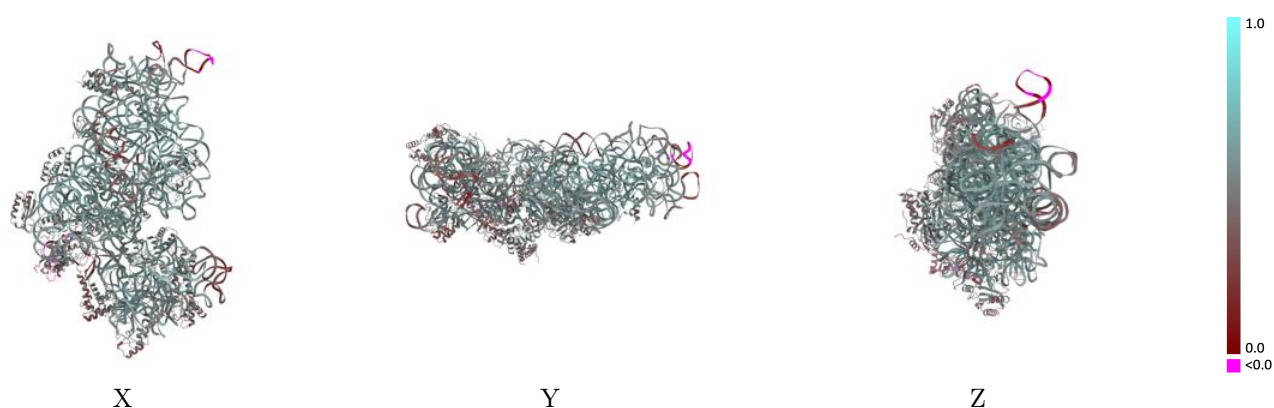
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51615 and PDB model 9GUP. Per-residue inclusion information can be found in section 3 on page 8.

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

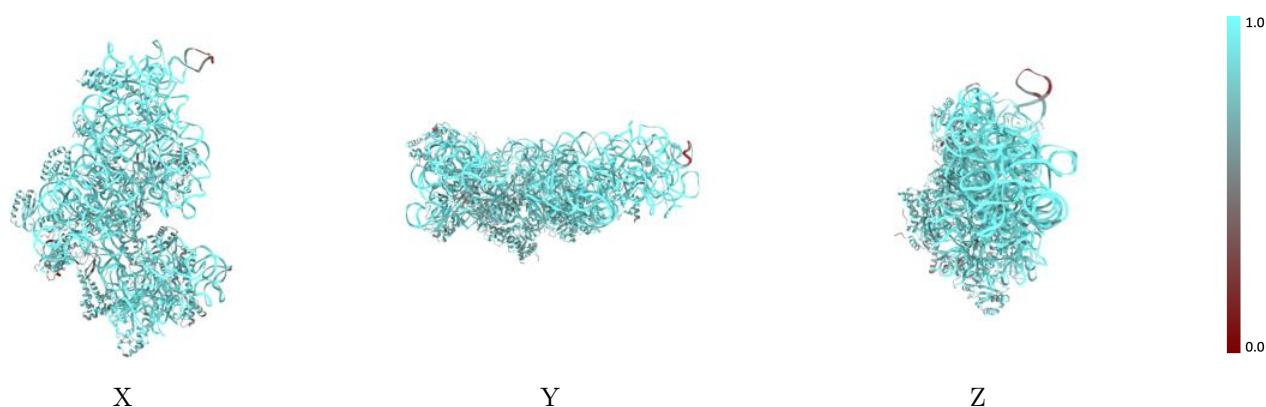
This section was not generated.

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



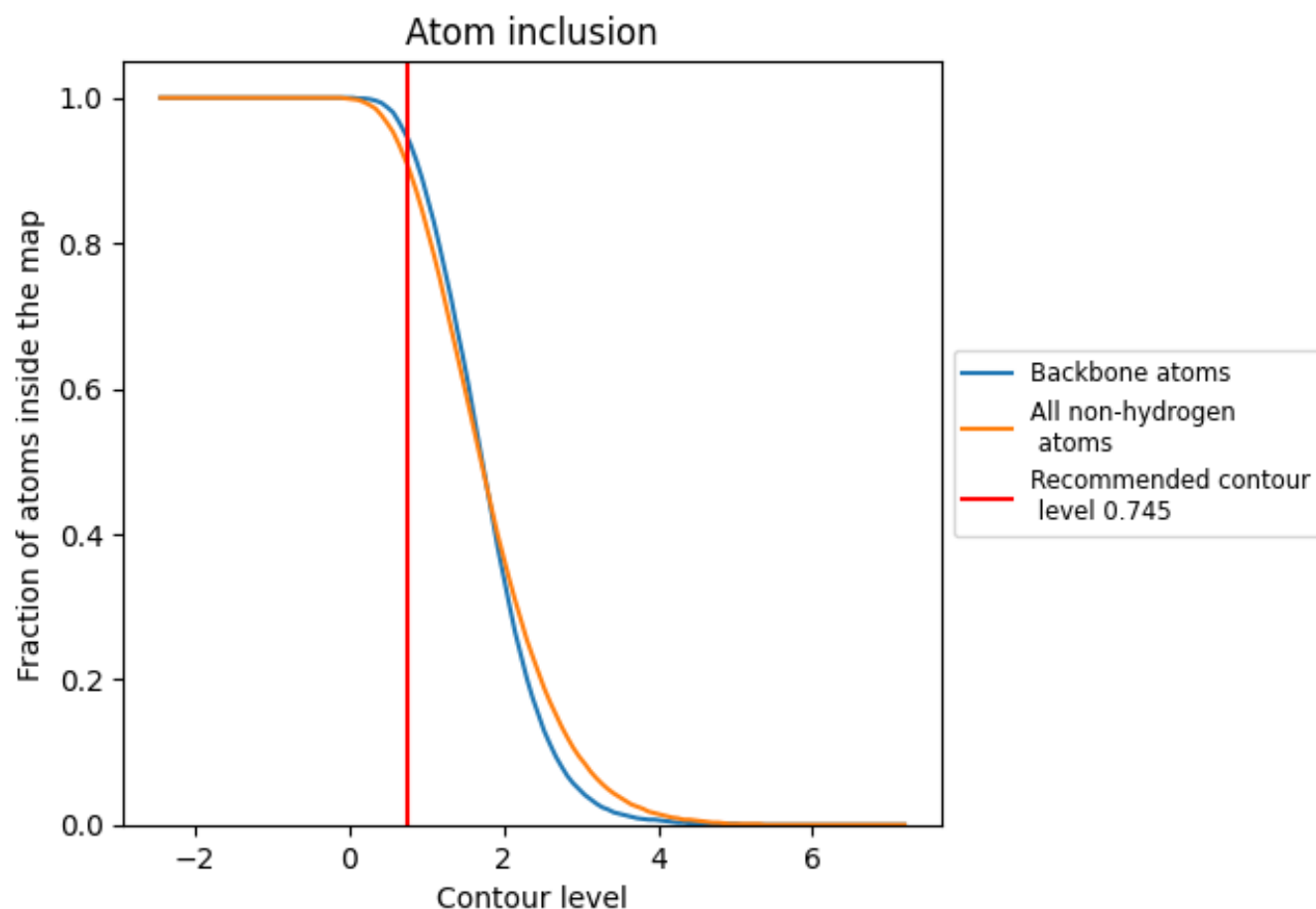
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.745).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.745) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9090   |  0.5160   |
| A     |  0.9700   |  0.5500   |
| B     |  0.5660   |  0.2830   |
| C     |  0.8360   |  0.4720   |
| D     |  0.7600   |  0.4610   |
| E     |  0.8550   |  0.4930   |
| F     |  0.8810   |  0.5280   |
| G     |  0.8170   |  0.4480   |
| H     |  0.7270   |  0.3700   |
| I     |  0.8800   |  0.5270   |
| J     |  0.8400   |  0.4910   |
| K     |  0.7610   |  0.4300   |
| L     |  0.8500   |  0.4660   |
| M     |  0.8810   |  0.5290   |
| N     |  0.8160  |  0.4630  |
| O     |  0.8100 |  0.4750 |
| P     |  0.8880 |  0.5010 |
| Q     |  0.8820 |  0.5410 |
| R     |  0.8560 |  0.5120 |
| S     |  0.8520 |  0.4920 |
| T     |  0.8550 |  0.4750 |
| U     |  0.8750 |  0.5180 |
| V     |  0.7660 |  0.4210 |
| X     |  0.4470 |  0.1050 |

