



## Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 10:08 pm BST

PDB ID : 8R6F / pdb\_00008r6f  
EMDB ID : EMD-18951  
Title : CryoEM structure of wheat 40S ribosomal subunit, body domain  
Authors : Kravchenko, O.V.; Baymukhametov, T.N.; Afonina, Z.A.; Vasilenko, K.S.  
Deposited on : 2023-11-22  
Resolution : 2.34 Å(reported)  
Based on initial model : 7qix

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

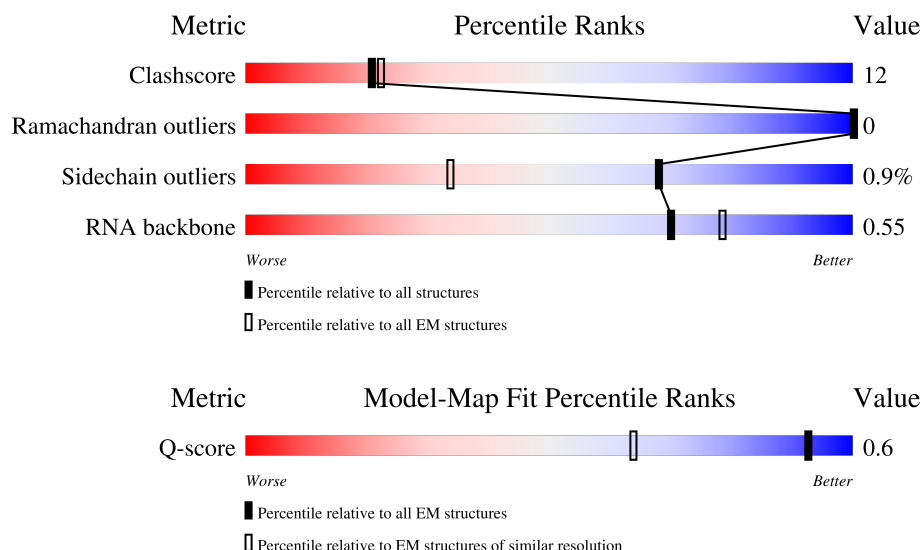
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.34 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.



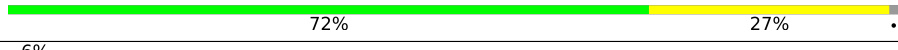
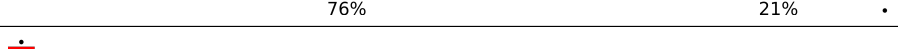
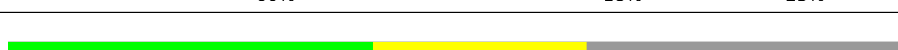
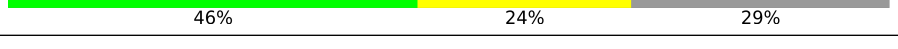
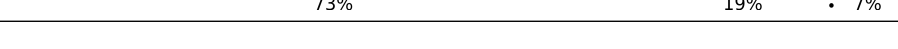
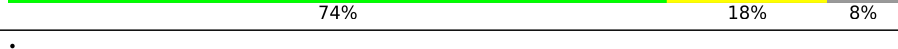
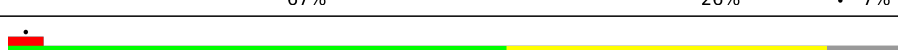
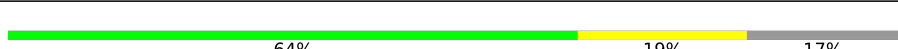
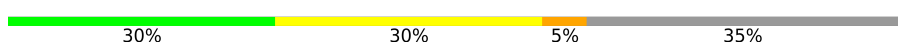
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 4520 ( 1.84 - 2.84 )                                     |

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   | Y     | 137    |                  |
| 2   | X     | 142    |                  |
| 3   | E     | 265    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | O     | 151    |    |
| 5   | W     | 130    |    |
| 6   | b     | 86     |    |
| 7   | e     | 62     |    |
| 8   | k     | 308    |    |
| 9   | B     | 263    |    |
| 10  | V     | 81     |    |
| 11  | a     | 139    |    |
| 12  | J     | 195    |    |
| 13  | C     | 275    |   |
| 14  | G     | 250    |  |
| 15  | H     | 192    |  |
| 16  | h     | 143    |  |
| 17  | L     | 159    |  |
| 18  | N     | 151    |  |
| 19  | n     | 25     |  |
| 20  | I     | 224    |  |
| 21  | A     | 1810   |  |

## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 49016 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 protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | Y     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1014  | 648 | 196 | 168 | 2 |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | X     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1088  | 690 | 212 | 183 | 3 |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | E     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2077  | 1322 | 387 | 361 | 7 |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S11, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | O     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 984   | 603 | 195 | 182 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| O     | 138     | IAS      | ASP    | conflict | UNP A0A3B6SS17 |

- Molecule 5 is a protein called Small ribosomal subunit protein uS8c.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | W     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 659 | 188 | 180 | 5 |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | b     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 645   | 405 | 117 | 116 | 7 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | e     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 383   | 232 | 87 | 64 |   |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | k     | 199      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1586  | 1004 | 285 | 286 | 11 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein eS1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | B     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1716  | 1094 | 310 | 303 | 9 |         |       |

- Molecule 10 is a protein called Genome assembly, chromosome: II.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | V     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 630   | 389 | 116 | 122 | 3 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | a     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 794   | 487 | 172 | 128 | 7 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S4, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | J     | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1494  | 947 | 298 | 245 | 4 |         |       |

- Molecule 13 is a protein called S5 DRBM domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | C     | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 1070 | 294 | 287 | 9 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | G     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1856  | 1157 | 366 | 325 | 8 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | H     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 962 | 278 | 266 | 2 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | h     | 27       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 208   | 129 | 34 | 42 | 3 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS17 N-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | L     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1167  | 745 | 224 | 193 | 5 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein uS15 N-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | N     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 731 | 215 | 190 | 2 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein eL41z/eL41y/eL41x/eL41w/eL41v.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | n     | 23       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 222   | 136 | 59 | 24 | 3 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | I     | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1510  | 936 | 302 | 268 | 4 |         |       |

- Molecule 21 is a RNA chain called RNA (1177-MER).

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 21  | A     | 1177     | Total | C     | N    | O    | P    | 0       | 0     |
|     |       |          | 25190 | 11273 | 4545 | 8196 | 1176 |         |       |

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 22  | a     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 23  | G     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 23  | A     | 31       | Total | Mg | 0       |
|     |       |          | 31    | 31 |         |

- Molecule 24 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | A     | 14       | Total | K  | 0       |
|     |       |          | 14    | 14 |         |

- Molecule 25 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 25  | Y     | 6        | Total | O  | 0       |
|     |       |          | 6     | 6  |         |
| 25  | X     | 14       | Total | O  | 0       |
|     |       |          | 14    | 14 |         |
| 25  | E     | 24       | Total | O  | 0       |
|     |       |          | 24    | 24 |         |
| 25  | O     | 3        | Total | O  | 0       |
|     |       |          | 3     | 3  |         |

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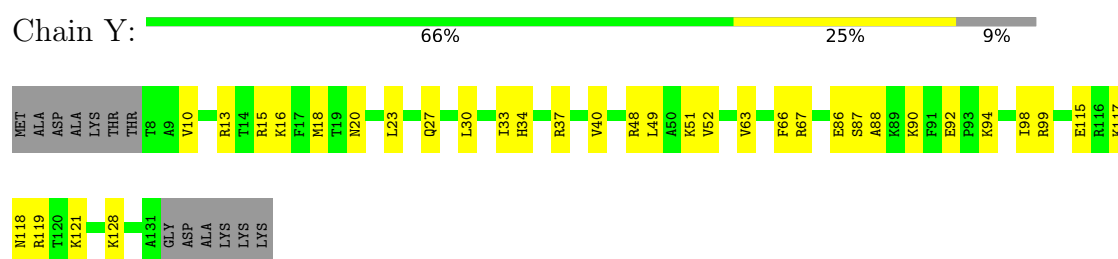
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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 25  | W     | 6        | Total<br>6   | O<br>6   | 0       |
| 25  | e     | 3        | Total<br>3   | O<br>3   | 0       |
| 25  | B     | 2        | Total<br>2   | O<br>2   | 0       |
| 25  | a     | 8        | Total<br>8   | O<br>8   | 0       |
| 25  | J     | 14       | Total<br>14  | O<br>14  | 0       |
| 25  | C     | 10       | Total<br>10  | O<br>10  | 0       |
| 25  | G     | 7        | Total<br>7   | O<br>7   | 0       |
| 25  | L     | 24       | Total<br>24  | O<br>24  | 0       |
| 25  | N     | 3        | Total<br>3   | O<br>3   | 0       |
| 25  | I     | 18       | Total<br>18  | O<br>18  | 0       |
| 25  | A     | 925      | Total<br>925 | O<br>925 | 0       |

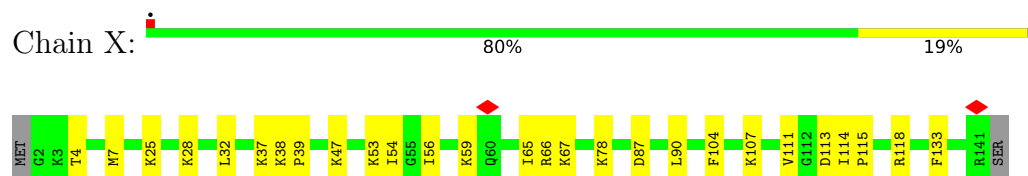
### 3 Residue-property plots

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

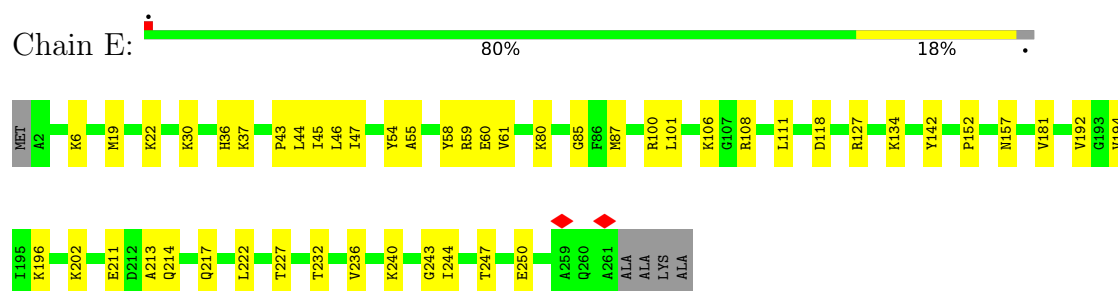
- Molecule 1: 40S ribosomal protein S24



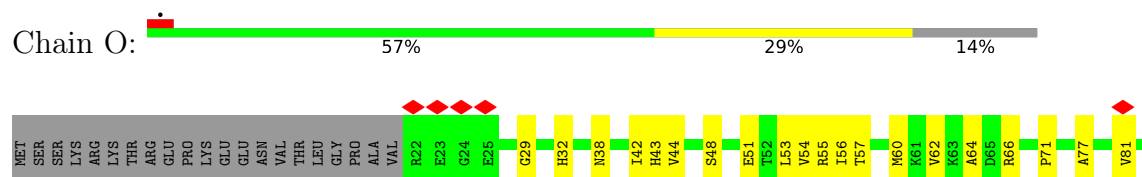
- Molecule 2: 40S ribosomal protein S23



- Molecule 3: 40S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S11, chloroplastic





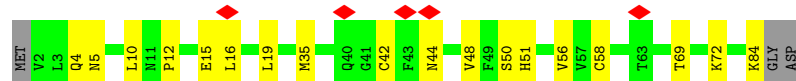
- Molecule 5: Small ribosomal subunit protein uS8c

Chain W: 72% 27%



- Molecule 6: 40S ribosomal protein S27

Chain b: 6% 76% 21%



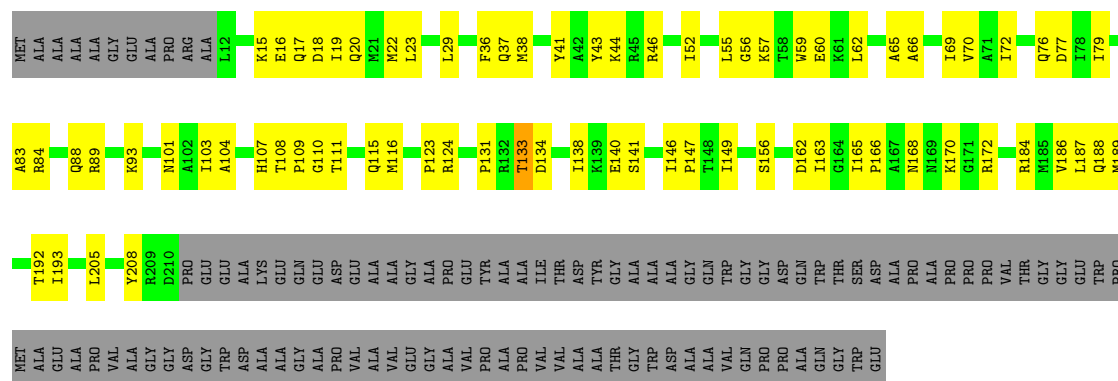
- Molecule 7: 40S ribosomal protein S30

Chain e: 60% 18% 23%



- Molecule 8: Small ribosomal subunit protein uS2

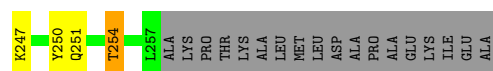
Chain k: 41% 24% 35%



- Molecule 9: Small ribosomal subunit protein eS1

Chain B: 5% 49% 29% 20%

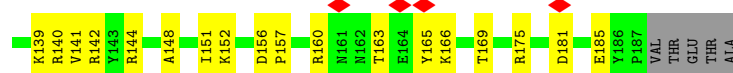
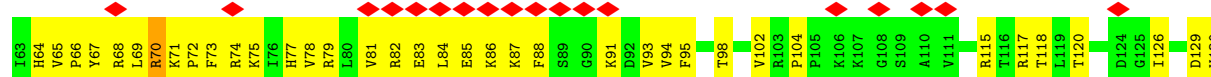
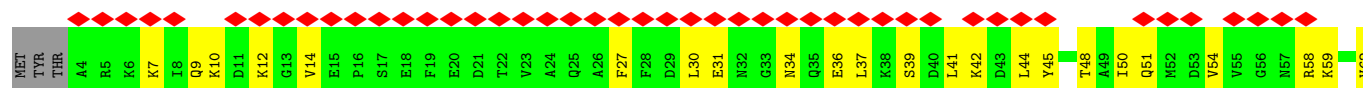




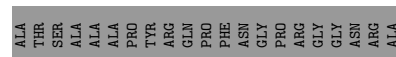
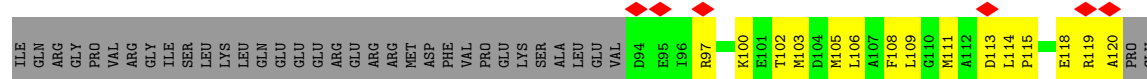
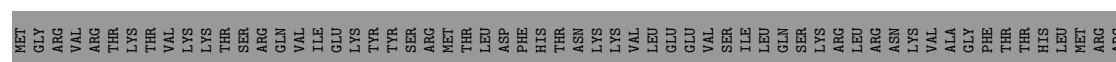
- Molecule 14: 40S ribosomal protein S6



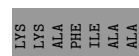
- Molecule 15: 40S ribosomal protein S7

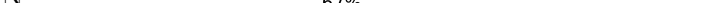


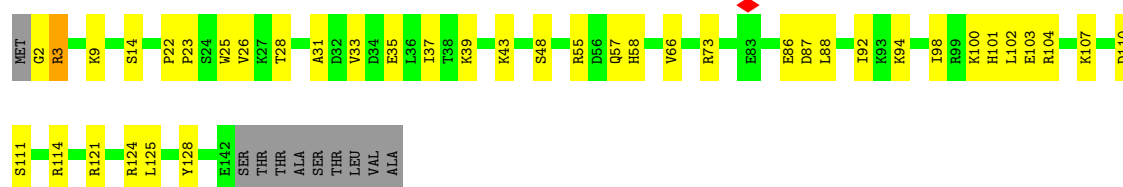
- Molecule 16: 40S ribosomal protein S17

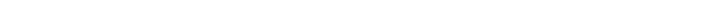


- Molecule 17: Small ribosomal subunit protein uS17 N-terminal domain-containing protein



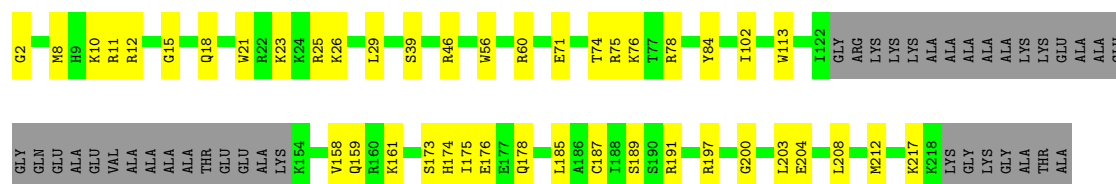
- Chain N:  67% 26% 7%



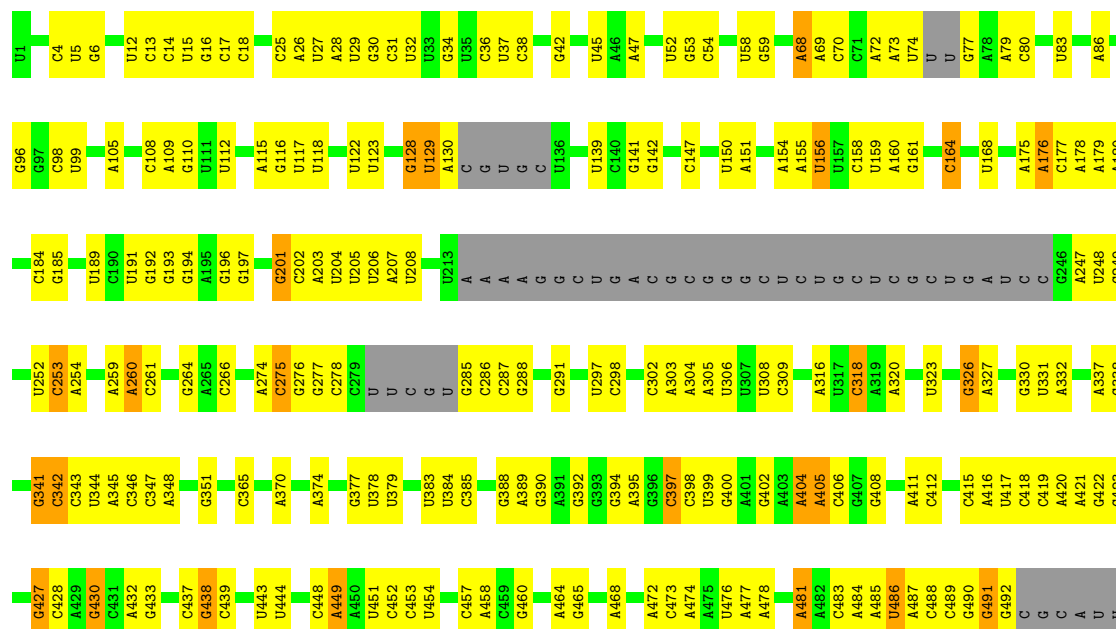
- Chain n: 



- Chain I:  64% 19% 17%



- Chain A: 







## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 256000                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 84                              | Depositor |
| Minimum defocus (nm)                 | 600                             | Depositor |
| Maximum defocus (nm)                 | 1800                            | Depositor |
| Magnification                        | 75000                           | Depositor |
| Image detector                       | FEI FALCON II (4k x 4k)         | Depositor |
| Maximum map value                    | 9.900                           | Depositor |
| Minimum map value                    | -6.521                          | Depositor |
| Average map value                    | 0.007                           | Depositor |
| Map value standard deviation         | 0.134                           | Depositor |
| Recommended contour level            | 0.4                             | Depositor |
| Map size ( $\text{\AA}$ )            | 412.80002, 412.80002, 412.80002 | wwPDB     |
| Map dimensions                       | 480, 480, 480                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.86, 0.86, 0.86                | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MG, 4AC, ZN, IAS, OMC, AME, MA6, OMG, K, OMU, A2M, UY1, 6MZ

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   | Y     | 0.30         | 0/1029         | 0.47        | 0/1366         |
| 2   | X     | 0.32         | 0/1107         | 0.49        | 0/1474         |
| 3   | E     | 0.22         | 0/2118         | 0.41        | 0/2846         |
| 4   | O     | 0.37         | 0/988          | 0.58        | 1/1322 (0.1%)  |
| 5   | W     | 0.47         | 0/1050         | 0.64        | 0/1405         |
| 6   | b     | 0.20         | 0/656          | 0.41        | 0/883          |
| 7   | e     | 0.33         | 0/387          | 0.56        | 0/510          |
| 8   | k     | 0.34         | 0/1620         | 0.55        | 2/2193 (0.1%)  |
| 9   | B     | 0.35         | 0/1745         | 0.59        | 0/2344         |
| 10  | V     | 0.49         | 0/628          | 0.77        | 2/847 (0.2%)   |
| 11  | a     | 0.38         | 0/809          | 0.55        | 0/1083         |
| 12  | J     | 0.25         | 0/1522         | 0.46        | 1/2037 (0.0%)  |
| 13  | C     | 0.34         | 0/1696         | 0.56        | 1/2292 (0.0%)  |
| 14  | G     | 0.18         | 0/1876         | 0.41        | 0/2492         |
| 15  | H     | 0.38         | 0/1535         | 0.64        | 1/2065 (0.0%)  |
| 16  | h     | 0.59         | 0/209          | 0.91        | 0/279          |
| 17  | L     | 0.28         | 0/1193         | 0.42        | 0/1599         |
| 18  | N     | 0.21         | 0/1162         | 0.39        | 0/1560         |
| 19  | n     | 0.57         | 0/223          | 0.93        | 0/283          |
| 20  | I     | 0.23         | 0/1532         | 0.49        | 0/2046         |
| 21  | A     | 0.20         | 2/26873 (0.0%) | 0.30        | 1/41868 (0.0%) |
| All | All   | 0.26         | 2/49958 (0.0%) | 0.41        | 9/72794 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 21  | A     | 468 | A2M  | O3'-P | 5.19 | 1.61        | 1.56     |
| 21  | A     | 802 | A2M  | O3'-P | 5.12 | 1.61        | 1.56     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | C     | 232 | TYR  | N-CA-C      | -5.87 | 105.69      | 112.92   |
| 10  | V     | 76  | ARG  | N-CA-C      | -5.80 | 104.87      | 111.14   |
| 21  | A     | 614 | G    | C4'-C3'-O3' | -5.60 | 104.60      | 113.00   |
| 8   | k     | 133 | THR  | N-CA-C      | -5.29 | 106.99      | 113.50   |
| 15  | H     | 70  | ARG  | CA-C-O      | -5.28 | 115.25      | 120.90   |
| 12  | J     | 64  | LEU  | CA-C-O      | -5.25 | 115.81      | 121.38   |
| 10  | V     | 11  | LEU  | N-CA-C      | -5.16 | 105.55      | 111.07   |
| 4   | O     | 145 | GLY  | CA-C-O      | -5.04 | 118.21      | 122.29   |
| 8   | k     | 83  | ALA  | N-CA-C      | -5.03 | 107.10      | 113.18   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Y     | 1014  | 0        | 1099     | 31      | 0            |
| 2   | X     | 1088  | 0        | 1153     | 24      | 0            |
| 3   | E     | 2077  | 0        | 2166     | 37      | 0            |
| 4   | O     | 984   | 0        | 1011     | 43      | 0            |
| 5   | W     | 1032  | 0        | 1068     | 27      | 0            |
| 6   | b     | 645   | 0        | 664      | 15      | 0            |
| 7   | e     | 383   | 0        | 406      | 9       | 0            |
| 8   | k     | 1586  | 0        | 1590     | 61      | 0            |
| 9   | B     | 1716  | 0        | 1790     | 71      | 0            |
| 10  | V     | 630   | 0        | 614      | 18      | 0            |
| 11  | a     | 794   | 0        | 812      | 33      | 0            |
| 12  | J     | 1494  | 0        | 1563     | 32      | 0            |
| 13  | C     | 1660  | 0        | 1743     | 37      | 0            |
| 14  | G     | 1856  | 0        | 1995     | 46      | 0            |
| 15  | H     | 1508  | 0        | 1573     | 74      | 0            |
| 16  | h     | 208   | 0        | 205      | 15      | 0            |
| 17  | L     | 1167  | 0        | 1228     | 22      | 0            |
| 18  | N     | 1138  | 0        | 1228     | 32      | 0            |
| 19  | n     | 222   | 0        | 271      | 8       | 0            |
| 20  | I     | 1510  | 0        | 1555     | 32      | 0            |
| 21  | A     | 25190 | 0        | 12722    | 490     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | a     | 1     | 0        | 0        | 1       | 0            |
| 23  | A     | 31    | 0        | 0        | 0       | 0            |
| 23  | G     | 1     | 0        | 0        | 0       | 0            |
| 24  | A     | 14    | 0        | 0        | 0       | 0            |
| 25  | A     | 925   | 0        | 0        | 22      | 0            |
| 25  | B     | 2     | 0        | 0        | 0       | 0            |
| 25  | C     | 10    | 0        | 0        | 0       | 0            |
| 25  | E     | 24    | 0        | 0        | 0       | 0            |
| 25  | G     | 7     | 0        | 0        | 0       | 0            |
| 25  | I     | 18    | 0        | 0        | 1       | 0            |
| 25  | J     | 14    | 0        | 0        | 0       | 0            |
| 25  | L     | 24    | 0        | 0        | 2       | 0            |
| 25  | N     | 3     | 0        | 0        | 0       | 0            |
| 25  | O     | 3     | 0        | 0        | 0       | 0            |
| 25  | W     | 6     | 0        | 0        | 0       | 0            |
| 25  | X     | 14    | 0        | 0        | 0       | 0            |
| 25  | Y     | 6     | 0        | 0        | 1       | 0            |
| 25  | a     | 8     | 0        | 0        | 0       | 0            |
| 25  | e     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 49016 | 0        | 36456    | 999     | 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 12.

All (999) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 21:A:1672:G:H1   | 21:A:1749:U:H3    | 1.13                     | 0.94              |
| 8:k:172:ARG:HD3  | 8:k:208:TYR:HD2   | 1.34                     | 0.91              |
| 19:n:10:MET:HE1  | 21:A:1118:A:H5'   | 1.51                     | 0.90              |
| 16:h:105:MET:HE3 | 16:h:109:LEU:HD12 | 1.56                     | 0.87              |
| 20:I:2:GLY:N     | 21:A:1740:U:HO2'  | 1.72                     | 0.87              |
| 15:H:88:PHE:HB2  | 15:H:91:LYS:HD2   | 1.58                     | 0.85              |
| 9:B:34:ALA:O     | 9:B:41:ARG:HD2    | 1.76                     | 0.84              |
| 8:k:172:ARG:CD   | 8:k:208:TYR:HD2   | 1.91                     | 0.83              |
| 9:B:67:GLU:OE1   | 9:B:85:ARG:HG3    | 1.78                     | 0.83              |
| 8:k:84:ARG:HH22  | 8:k:170:LYS:HG2   | 1.44                     | 0.83              |
| 16:h:118:GLU:HG3 | 16:h:120:ALA:H    | 1.44                     | 0.83              |
| 2:X:87:ASP:HB2   | 21:A:572:G:H4'    | 1.60                     | 0.82              |
| 9:B:27:LYS:HD3   | 9:B:47:LEU:HD13   | 1.61                     | 0.82              |
| 15:H:66:PRO:HD2  | 15:H:69:LEU:HD21  | 1.62                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:N:87:ASP:CG    | 18:N:125:LEU:HD21 | 2.04                     | 0.81              |
| 15:H:31:GLU:HA    | 15:H:41:LEU:HD13  | 1.62                     | 0.81              |
| 15:H:117:ARG:HH12 | 21:A:863:G:H5'    | 1.47                     | 0.80              |
| 14:G:43:GLU:OE2   | 14:G:46:LYS:HE3   | 1.81                     | 0.79              |
| 9:B:162:ARG:HB3   | 9:B:166:ARG:HH21  | 1.45                     | 0.79              |
| 11:a:44:ILE:HD12  | 11:a:65:PRO:HG2   | 1.63                     | 0.79              |
| 8:k:172:ARG:HD3   | 8:k:208:TYR:CD2   | 2.19                     | 0.78              |
| 21:A:823:A:H2'    | 21:A:824:U:C6     | 2.20                     | 0.76              |
| 21:A:784:C:H4'    | 21:A:785:A:H5'    | 1.68                     | 0.75              |
| 9:B:179:CYS:SG    | 9:B:187:LYS:NZ    | 2.60                     | 0.74              |
| 12:J:135:HIS:ND1  | 12:J:164:SER:OG   | 2.20                     | 0.74              |
| 15:H:30:LEU:HB3   | 15:H:87:LYS:HE3   | 1.69                     | 0.74              |
| 15:H:37:LEU:HD11  | 15:H:83:GLU:HG3   | 1.67                     | 0.74              |
| 9:B:180:ASP:OD1   | 9:B:181:LEU:N     | 2.22                     | 0.73              |
| 9:B:229:MET:HE3   | 9:B:229:MET:HA    | 1.71                     | 0.73              |
| 21:A:691:A:H2'    | 21:A:692:C:C6     | 2.24                     | 0.72              |
| 4:O:150:ARG:NH1   | 21:A:1796:U:OP1   | 2.22                     | 0.72              |
| 21:A:876:A:H2'    | 21:A:877:G:C8     | 2.24                     | 0.72              |
| 9:B:224:ASP:OD2   | 9:B:227:LYS:HG3   | 1.89                     | 0.72              |
| 21:A:692:C:H2'    | 21:A:693:C:C6     | 2.24                     | 0.72              |
| 10:V:54:LEU:HD21  | 10:V:68:LEU:HD13  | 1.71                     | 0.72              |
| 10:V:61:GLN:NE2   | 21:A:1087:U:O4'   | 2.23                     | 0.72              |
| 10:V:73:GLN:O     | 10:V:76:ARG:HG2   | 1.90                     | 0.71              |
| 8:k:43:TYR:HE2    | 8:k:44:LYS:HE3    | 1.55                     | 0.71              |
| 21:A:818:A:H2'    | 21:A:864:A:C2     | 2.26                     | 0.71              |
| 8:k:141:SER:HA    | 8:k:146:ILE:HD12  | 1.73                     | 0.70              |
| 12:J:175:LYS:NZ   | 21:A:515:A:OP1    | 2.23                     | 0.70              |
| 13:C:150:ARG:HB3  | 13:C:231:THR:HG22 | 1.71                     | 0.70              |
| 21:A:690:G:H2'    | 21:A:691:A:C8     | 2.27                     | 0.70              |
| 11:a:46:GLU:HG3   | 11:a:49:ALA:H     | 1.56                     | 0.70              |
| 2:X:65:ILE:O      | 2:X:67:LYS:NZ     | 2.25                     | 0.69              |
| 14:G:4:ASN:ND2    | 21:A:150:U:O2     | 2.24                     | 0.69              |
| 21:A:873:G:H1     | 21:A:965:U:H3     | 1.38                     | 0.69              |
| 21:A:444:U:H5'    | 25:A:2311:HOH:O   | 1.91                     | 0.69              |
| 15:H:72:PRO:HA    | 15:H:75:LYS:HD2   | 1.74                     | 0.68              |
| 21:A:893:U:H2'    | 21:A:894:U:C6     | 2.28                     | 0.68              |
| 8:k:15:LYS:O      | 8:k:19:ILE:HG13   | 1.93                     | 0.68              |
| 21:A:141:G:H2'    | 21:A:142:G:C8     | 2.29                     | 0.68              |
| 11:a:2:THR:N      | 21:A:1147:A:OP1   | 2.26                     | 0.68              |
| 18:N:121:ARG:NH1  | 21:A:873:G:OP1    | 2.24                     | 0.68              |
| 6:b:51:HIS:CE1    | 6:b:72:LYS:HG2    | 2.28                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:C:57:GLU:O    | 13:C:59:ARG:NH2   | 2.27                     | 0.68              |
| 15:H:65:VAL:HG12 | 15:H:67:TYR:H     | 1.60                     | 0.67              |
| 9:B:97:LEU:HB3   | 9:B:232:HIS:CD2   | 2.29                     | 0.67              |
| 14:G:53:MET:HG3  | 14:G:114:VAL:HG23 | 1.77                     | 0.67              |
| 14:G:25:ARG:NE   | 14:G:25:ARG:O     | 2.28                     | 0.67              |
| 3:E:58:TYR:OH    | 3:E:80:LYS:HE3    | 1.94                     | 0.67              |
| 20:I:78:ARG:HH11 | 20:I:78:ARG:HB2   | 1.60                     | 0.67              |
| 5:W:14:MET:HG2   | 5:W:25:VAL:HG11   | 1.77                     | 0.67              |
| 21:A:1046:G:H2'  | 21:A:1047:G:C8    | 2.29                     | 0.67              |
| 21:A:691:A:H2'   | 21:A:692:C:H6     | 1.58                     | 0.66              |
| 21:A:856:G:H2'   | 21:A:857:A:C8     | 2.31                     | 0.66              |
| 4:O:121:ARG:HG3  | 11:a:52:ASP:OD2   | 1.94                     | 0.66              |
| 21:A:890:G:H2'   | 21:A:891:U:C6     | 2.31                     | 0.66              |
| 1:Y:48:ARG:O     | 1:Y:52:VAL:HG23   | 1.95                     | 0.66              |
| 8:k:76:GLN:O     | 8:k:101:ASN:ND2   | 2.29                     | 0.66              |
| 20:I:197:ARG:NH1 | 21:A:261:C:O2     | 2.29                     | 0.65              |
| 11:a:4:LYS:NZ    | 21:A:1805:A:OP2   | 2.29                     | 0.65              |
| 9:B:168:MET:HG2  | 9:B:197:ILE:HG21  | 1.77                     | 0.65              |
| 12:J:2:VAL:N     | 21:A:465:G:OP1    | 2.30                     | 0.65              |
| 9:B:67:GLU:OE1   | 9:B:85:ARG:CG     | 2.44                     | 0.65              |
| 11:a:26:CYS:SG   | 22:a:201:ZN:ZN    | 1.86                     | 0.65              |
| 18:N:14:SER:HB2  | 21:A:964:U:H5''   | 1.79                     | 0.65              |
| 13:C:59:ARG:HE   | 13:C:59:ARG:N     | 1.93                     | 0.65              |
| 9:B:27:LYS:HD3   | 9:B:47:LEU:CD1    | 2.26                     | 0.65              |
| 20:I:78:ARG:HB2  | 20:I:78:ARG:NH1   | 2.11                     | 0.64              |
| 21:A:1648:OMC:H5 | 21:A:1774:6MZ:H6  | 1.44                     | 0.64              |
| 10:V:52:PHE:HZ   | 10:V:75:LYS:HG3   | 1.62                     | 0.64              |
| 1:Y:88:ALA:O     | 1:Y:92:GLU:HB2    | 1.96                     | 0.64              |
| 2:X:7:MET:HE2    | 5:W:77:PRO:HB2    | 1.80                     | 0.64              |
| 14:G:8:PRO:HD3   | 14:G:114:VAL:HG13 | 1.78                     | 0.64              |
| 15:H:58:ARG:NH2  | 15:H:165:TYR:O    | 2.26                     | 0.64              |
| 18:N:110:ASP:O   | 18:N:114:ARG:HG2  | 1.98                     | 0.64              |
| 21:A:784:C:H4'   | 21:A:785:A:C5'    | 2.28                     | 0.64              |
| 11:a:93:ARG:HH11 | 11:a:93:ARG:HG2   | 1.63                     | 0.63              |
| 21:A:1151:G:H2'  | 21:A:1152:A:C8    | 2.33                     | 0.63              |
| 21:A:690:G:H2'   | 21:A:691:A:H8     | 1.61                     | 0.63              |
| 8:k:110:GLY:N    | 8:k:140:GLU:OE2   | 2.26                     | 0.63              |
| 12:J:137:ARG:HA  | 12:J:142:ILE:HA   | 1.80                     | 0.63              |
| 14:G:193:ARG:NH2 | 21:A:288:G:N7     | 2.40                     | 0.63              |
| 2:X:59:LYS:HD2   | 2:X:113:ASP:HA    | 1.79                     | 0.63              |
| 4:O:147:ARG:HH22 | 21:A:1796:U:P     | 2.22                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:H:70:ARG:O    | 15:H:74:ARG:HG2   | 1.98                     | 0.63              |
| 21:A:517:U:H2'   | 21:A:518:G:C8     | 2.33                     | 0.63              |
| 21:A:820:A:H2    | 21:A:821:G:H1'    | 1.64                     | 0.63              |
| 9:B:175:GLN:N    | 9:B:175:GLN:OE1   | 2.32                     | 0.63              |
| 14:G:172:LYS:HD2 | 21:A:73:A:H62     | 1.64                     | 0.63              |
| 15:H:69:LEU:H    | 15:H:69:LEU:HD23  | 1.63                     | 0.63              |
| 20:I:2:GLY:N     | 21:A:1740:U:O2'   | 2.31                     | 0.63              |
| 21:A:5:U:H2'     | 21:A:6:G:H8       | 1.64                     | 0.63              |
| 21:A:944:A:H2'   | 21:A:945:A:C8     | 2.33                     | 0.63              |
| 15:H:84:LEU:HB3  | 15:H:88:PHE:CZ    | 2.33                     | 0.63              |
| 2:X:104:PHE:HB2  | 2:X:118:ARG:C     | 2.24                     | 0.62              |
| 8:k:36:PHE:CD1   | 21:A:1045:G:H4'   | 2.34                     | 0.62              |
| 3:E:214:GLN:HG3  | 3:E:244:ILE:HD12  | 1.82                     | 0.62              |
| 21:A:856:G:H2'   | 21:A:857:A:H8     | 1.61                     | 0.62              |
| 15:H:83:GLU:HA   | 15:H:86:LYS:HD2   | 1.80                     | 0.62              |
| 21:A:117:U:H2'   | 21:A:118:U:C6     | 2.34                     | 0.62              |
| 21:A:109:A:H2'   | 21:A:110:G:C8     | 2.33                     | 0.62              |
| 14:G:213:TYR:O   | 14:G:217:LEU:HD13 | 2.00                     | 0.62              |
| 21:A:1743:A:N7   | 25:A:2008:HOH:O   | 2.31                     | 0.62              |
| 17:L:70:ARG:NH1  | 21:A:803:G:O2'    | 2.30                     | 0.62              |
| 21:A:411:A:H2'   | 21:A:412:C:C6     | 2.35                     | 0.62              |
| 21:A:1697:C:H2'  | 21:A:1698:G:C8    | 2.35                     | 0.61              |
| 4:O:90:ILE:O     | 4:O:124:MET:HE1   | 1.99                     | 0.61              |
| 21:A:824:U:H3    | 21:A:858:G:H1     | 1.47                     | 0.61              |
| 3:E:106:LYS:NZ   | 21:A:794:G:OP1    | 2.34                     | 0.61              |
| 8:k:43:TYR:CE2   | 8:k:44:LYS:HE3    | 2.35                     | 0.61              |
| 21:A:893:U:H2'   | 21:A:894:U:H6     | 1.64                     | 0.61              |
| 12:J:129:VAL:O   | 12:J:133:GLN:HG2  | 2.00                     | 0.61              |
| 21:A:627:A:N6    | 21:A:975:A:OP1    | 2.27                     | 0.61              |
| 21:A:929:A:H2'   | 21:A:930:G:C8     | 2.35                     | 0.61              |
| 6:b:35:MET:CE    | 6:b:50:SER:HA     | 2.30                     | 0.61              |
| 5:W:71:LYS:NZ    | 21:A:1101:C:OP2   | 2.30                     | 0.61              |
| 20:I:76:LYS:HD3  | 21:A:261:C:H5''   | 1.80                     | 0.61              |
| 9:B:62:LYS:HG2   | 9:B:63:HIS:CD2    | 2.36                     | 0.61              |
| 18:N:9:LYS:NZ    | 21:A:1040:G:OP2   | 2.34                     | 0.61              |
| 20:I:174:HIS:O   | 20:I:178:GLN:HG2  | 2.01                     | 0.61              |
| 21:A:17:C:O2'    | 21:A:1142:A:N1    | 2.33                     | 0.61              |
| 4:O:143:LYS:HG3  | 21:A:996:G:P      | 2.41                     | 0.61              |
| 15:H:88:PHE:HE1  | 15:H:93:VAL:HB    | 1.66                     | 0.61              |
| 21:A:1650:C:H2'  | 21:A:1651:G:C8    | 2.36                     | 0.61              |
| 9:B:128:LYS:HE2  | 9:B:134:MET:HE2   | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:J:59:ARG:HD3   | 13:C:183:PRO:HG2  | 1.83                     | 0.60              |
| 13:C:114:VAL:HG23 | 13:C:146:ILE:HD11 | 1.84                     | 0.60              |
| 21:A:829:G:H1     | 21:A:853:U:H3     | 1.49                     | 0.60              |
| 9:B:61:LEU:HA     | 9:B:64:ARG:HD2    | 1.83                     | 0.60              |
| 8:k:88:GLN:HG3    | 8:k:104:ALA:HB1   | 1.84                     | 0.60              |
| 21:A:595:A:H2'    | 21:A:596:A:C8     | 2.36                     | 0.60              |
| 12:J:23:LYS:HE2   | 21:A:559:A:H4'    | 1.83                     | 0.59              |
| 14:G:213:TYR:CZ   | 14:G:217:LEU:HD11 | 2.36                     | 0.59              |
| 15:H:74:ARG:HH22  | 15:H:129:ASP:HA   | 1.67                     | 0.59              |
| 21:A:785:A:H5''   | 21:A:786:U:C5     | 2.37                     | 0.59              |
| 21:A:785:A:H5''   | 21:A:786:U:C6     | 2.38                     | 0.59              |
| 3:E:152:PRO:HD2   | 14:G:220:ARG:HH12 | 1.68                     | 0.59              |
| 18:N:101:HIS:HA   | 18:N:104:ARG:HE   | 1.67                     | 0.59              |
| 12:J:175:LYS:O    | 12:J:179:GLN:HG3  | 2.02                     | 0.59              |
| 14:G:31:ARG:NH2   | 21:A:1690:A:O3'   | 2.36                     | 0.59              |
| 18:N:87:ASP:OD1   | 18:N:88:LEU:N     | 2.35                     | 0.59              |
| 14:G:19:ASP:OD1   | 14:G:19:ASP:N     | 2.35                     | 0.59              |
| 17:L:113:SER:OG   | 17:L:115:CYS:SG   | 2.59                     | 0.59              |
| 9:B:131:ASP:OD1   | 9:B:131:ASP:N     | 2.35                     | 0.59              |
| 3:E:181:VAL:HG12  | 3:E:227:THR:HA    | 1.84                     | 0.59              |
| 16:h:102:THR:O    | 16:h:106:LEU:HG   | 2.03                     | 0.59              |
| 8:k:84:ARG:HH11   | 8:k:133:THR:HG21  | 1.68                     | 0.59              |
| 20:I:185:LEU:HB3  | 20:I:203:LEU:HD12 | 1.83                     | 0.59              |
| 21:A:477:A:H1'    | 25:A:2631:HOH:O   | 2.02                     | 0.59              |
| 5:W:87:GLU:OE1    | 5:W:117:ARG:NH2   | 2.35                     | 0.58              |
| 21:A:96:G:N7      | 25:A:2012:HOH:O   | 2.31                     | 0.58              |
| 3:E:55:ALA:HB1    | 3:E:60:GLU:HB3    | 1.83                     | 0.58              |
| 15:H:59:LYS:O     | 15:H:91:LYS:HA    | 2.03                     | 0.58              |
| 15:H:27:PHE:CZ    | 15:H:84:LEU:HD21  | 2.38                     | 0.58              |
| 21:A:5:U:H2'      | 21:A:6:G:C8       | 2.38                     | 0.58              |
| 4:O:53:LEU:HA     | 9:B:24:PHE:CE2    | 2.38                     | 0.58              |
| 11:a:22:ARG:NH1   | 11:a:27:ALA:O     | 2.36                     | 0.58              |
| 20:I:208:LEU:HG   | 20:I:212:MET:HE2  | 1.85                     | 0.58              |
| 21:A:1063:U:H3    | 21:A:1067:A:H61   | 1.50                     | 0.58              |
| 13:C:67:TYR:OH    | 13:C:146:ILE:HG22 | 2.03                     | 0.58              |
| 14:G:182:ARG:NH2  | 21:A:141:G:O6     | 2.34                     | 0.58              |
| 21:A:485:A:H2'    | 21:A:486:U:C6     | 2.39                     | 0.58              |
| 15:H:115:ARG:HA   | 15:H:118:THR:HG23 | 1.86                     | 0.58              |
| 18:N:87:ASP:OD2   | 18:N:125:LEU:HD21 | 2.04                     | 0.58              |
| 21:A:1740:U:H2'   | 21:A:1741:G:O4'   | 2.04                     | 0.58              |
| 9:B:111:ARG:HB3   | 11:a:68:TYR:HB2   | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 21:A:1696:G:H2'  | 21:A:1697:C:C6   | 2.38                     | 0.57              |
| 12:J:50:ALA:HA   | 12:J:53:ARG:NH1  | 2.19                     | 0.57              |
| 18:N:55:ARG:HD3  | 21:A:965:U:H5'   | 1.85                     | 0.57              |
| 21:A:454:U:H5    | 25:A:2416:HOH:O  | 1.87                     | 0.57              |
| 21:A:823:A:H2'   | 21:A:824:U:H6    | 1.69                     | 0.57              |
| 21:A:1743:A:H2'  | 21:A:1744:C:H6   | 1.69                     | 0.57              |
| 4:O:137:THR:HG23 | 21:A:891:U:H1'   | 1.84                     | 0.57              |
| 15:H:163:THR:HA  | 15:H:166:LYS:HD3 | 1.86                     | 0.57              |
| 21:A:693:C:H2'   | 21:A:694:C:C6    | 2.40                     | 0.57              |
| 1:Y:48:ARG:HA    | 1:Y:51:LYS:HE2   | 1.86                     | 0.57              |
| 7:e:30:PRO:HG2   | 7:e:38:ILE:HD11  | 1.86                     | 0.57              |
| 21:A:1147:A:N7   | 25:A:2018:HOH:O  | 2.32                     | 0.57              |
| 15:H:71:LYS:HB2  | 15:H:72:PRO:HD3  | 1.86                     | 0.57              |
| 13:C:55:VAL:HG21 | 13:C:78:ILE:HG23 | 1.86                     | 0.57              |
| 4:O:117:ARG:HD3  | 11:a:49:ALA:HB2  | 1.87                     | 0.57              |
| 14:G:85:ARG:HD2  | 21:A:159:U:H3'   | 1.87                     | 0.57              |
| 5:W:35:ILE:O     | 5:W:39:ILE:HD12  | 2.05                     | 0.57              |
| 15:H:44:LEU:HG   | 15:H:73:PHE:CZ   | 2.40                     | 0.57              |
| 5:W:107:SER:HA   | 21:A:810:A:C8    | 2.39                     | 0.56              |
| 8:k:205:LEU:HD12 | 8:k:205:LEU:H    | 1.70                     | 0.56              |
| 21:A:625:A:HO2'  | 21:A:1111:C:HO2' | 1.51                     | 0.56              |
| 18:N:39:LYS:C    | 18:N:43:LYS:HZ2  | 2.13                     | 0.56              |
| 21:A:74:U:O2'    | 21:A:77:G:N2     | 2.38                     | 0.56              |
| 21:A:464:A:H3'   | 21:A:465:G:H8    | 1.70                     | 0.56              |
| 21:A:543:G:OP2   | 21:A:543:G:N2    | 2.31                     | 0.56              |
| 21:A:812:A:H2'   | 21:A:813:A:H8    | 1.70                     | 0.56              |
| 21:A:1696:G:H2'  | 21:A:1697:C:H6   | 1.69                     | 0.56              |
| 21:A:451:U:H2'   | 21:A:452:C:O4'   | 2.05                     | 0.56              |
| 17:L:88:ARG:HD2  | 25:L:201:HOH:O   | 2.05                     | 0.56              |
| 15:H:81:VAL:O    | 15:H:85:GLU:HB2  | 2.05                     | 0.56              |
| 21:A:1659:U:H2'  | 21:A:1660:A:C8   | 2.41                     | 0.56              |
| 15:H:88:PHE:CE1  | 15:H:93:VAL:HB   | 2.40                     | 0.56              |
| 18:N:28:THR:HG22 | 18:N:33:VAL:HG23 | 1.88                     | 0.56              |
| 21:A:323:U:H4'   | 21:A:327:A:C8    | 2.41                     | 0.56              |
| 15:H:7:LYS:HE2   | 15:H:7:LYS:HA    | 1.87                     | 0.56              |
| 21:A:430:G:N7    | 25:A:2024:HOH:O  | 2.33                     | 0.56              |
| 4:O:60:MET:HG3   | 21:A:904:G:H4'   | 1.88                     | 0.56              |
| 21:A:862:U:H2'   | 21:A:863:G:H8    | 1.70                     | 0.56              |
| 21:A:1723:C:H2'  | 21:A:1724:G:H8   | 1.71                     | 0.56              |
| 4:O:29:GLY:O     | 4:O:94:HIS:N     | 2.36                     | 0.56              |
| 4:O:101:GLY:HA3  | 4:O:134:PRO:HG2  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:b:48:VAL:HG13   | 6:b:56:VAL:HG21   | 1.88                     | 0.56              |
| 14:G:221:LEU:HD12 | 14:G:224:GLN:OE1  | 2.05                     | 0.55              |
| 14:G:50:PHE:HB3   | 14:G:113:LEU:HD22 | 1.88                     | 0.55              |
| 14:G:179:LYS:HG3  | 21:A:80:C:H1'     | 1.88                     | 0.55              |
| 21:A:1787:A:H2'   | 21:A:1788:G:C8    | 2.41                     | 0.55              |
| 14:G:168:ASN:OD1  | 14:G:169:LYS:N    | 2.39                     | 0.55              |
| 15:H:84:LEU:HD22  | 15:H:95:PHE:HZ    | 1.71                     | 0.55              |
| 8:k:162:ASP:OD1   | 10:V:59:ARG:NH2   | 2.35                     | 0.55              |
| 3:E:134:LYS:NZ    | 21:A:202:C:OP1    | 2.31                     | 0.55              |
| 5:W:23:ARG:NH1    | 6:b:5:ASN:O       | 2.34                     | 0.55              |
| 6:b:69:THR:OG1    | 6:b:72:LYS:O      | 2.25                     | 0.55              |
| 17:L:6:GLU:CG     | 17:L:10:LEU:HD11  | 2.36                     | 0.55              |
| 21:A:646:G:N2     | 21:A:694:C:C2     | 2.74                     | 0.55              |
| 9:B:34:ALA:O      | 9:B:41:ARG:CD     | 2.52                     | 0.55              |
| 9:B:183:GLU:HA    | 9:B:186:ASN:HB2   | 1.87                     | 0.55              |
| 1:Y:15:ARG:HD2    | 21:A:783:C:N4     | 2.21                     | 0.55              |
| 17:L:47:ARG:HH21  | 17:L:51:ASP:CG    | 2.15                     | 0.55              |
| 21:A:818:A:H2'    | 21:A:864:A:N1     | 2.22                     | 0.55              |
| 11:a:6:ARG:NH2    | 21:A:1096:A:OP2   | 2.39                     | 0.55              |
| 21:A:865:U:H2'    | 21:A:866:U:C6     | 2.42                     | 0.55              |
| 8:k:18:ASP:OD2    | 8:k:184:ARG:NH2   | 2.40                     | 0.55              |
| 9:B:60:GLY:O      | 9:B:64:ARG:NE     | 2.40                     | 0.55              |
| 15:H:141:VAL:HG22 | 15:H:151:ILE:HG12 | 1.89                     | 0.55              |
| 21:A:16:G:H2'     | 21:A:17:C:C6      | 2.42                     | 0.55              |
| 21:A:758:A:H2     | 21:A:803:G:H22    | 1.55                     | 0.55              |
| 10:V:9:VAL:HG13   | 13:C:161:PRO:HG3  | 1.90                     | 0.54              |
| 14:G:156:ARG:HH21 | 14:G:183:LEU:HD21 | 1.72                     | 0.54              |
| 16:h:105:MET:HE2  | 16:h:106:LEU:HD23 | 1.87                     | 0.54              |
| 21:A:820:A:P      | 21:A:863:G:H22    | 2.30                     | 0.54              |
| 6:b:42:CYS:HB2    | 6:b:44:ASN:ND2    | 2.23                     | 0.54              |
| 6:b:44:ASN:ND2    | 6:b:58:CYS:SG     | 2.80                     | 0.54              |
| 21:A:411:A:H2'    | 21:A:412:C:H6     | 1.72                     | 0.54              |
| 4:O:32:HIS:HB2    | 4:O:43:HIS:HB3    | 1.89                     | 0.54              |
| 21:A:12:U:H2'     | 21:A:13:C:C6      | 2.43                     | 0.54              |
| 21:A:452:C:H2'    | 21:A:453:C:C6     | 2.43                     | 0.54              |
| 21:A:1092:A:H2'   | 21:A:1093:A:C8    | 2.43                     | 0.54              |
| 7:e:39:GLN:HG2    | 7:e:42:ARG:HH21   | 1.72                     | 0.54              |
| 21:A:1069:G:C2'   | 21:A:1070:A:H5'   | 2.38                     | 0.54              |
| 21:A:1669:A:C2    | 21:A:1753:U:C2    | 2.95                     | 0.54              |
| 8:k:16:GLU:HA     | 16:h:111:MET:HE1  | 1.88                     | 0.54              |
| 8:k:23:LEU:HD21   | 16:h:106:LEU:HD21 | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:J:112:GLN:HE21 | 12:J:124:ILE:HG13 | 1.71                     | 0.54              |
| 12:J:146:PRO:HD2  | 21:A:478:A:H5''   | 1.90                     | 0.54              |
| 21:A:385:C:O2'    | 21:A:761:A:N1     | 2.36                     | 0.54              |
| 21:A:554:A:N3     | 25:A:2020:HOH:O   | 2.32                     | 0.54              |
| 1:Y:87:SER:HA     | 1:Y:90:LYS:HZ1    | 1.73                     | 0.54              |
| 4:O:100:THR:HG21  | 4:O:104:LYS:HD2   | 1.89                     | 0.54              |
| 21:A:1739:U:H2'   | 21:A:1740:U:C6    | 2.43                     | 0.54              |
| 21:A:1787:A:H2'   | 21:A:1788:G:H8    | 1.73                     | 0.54              |
| 15:H:84:LEU:HD22  | 15:H:95:PHE:CZ    | 2.42                     | 0.54              |
| 15:H:104:PRO:HD3  | 21:A:643:U:C2     | 2.43                     | 0.54              |
| 21:A:38:OMC:O2    | 21:A:474:A:N1     | 2.41                     | 0.54              |
| 21:A:860:A:N1     | 21:A:862:U:H1'    | 2.23                     | 0.54              |
| 9:B:28:GLN:NE2    | 9:B:50:ARG:HG3    | 2.23                     | 0.53              |
| 21:A:629:C:H2'    | 21:A:630:U:C6     | 2.43                     | 0.53              |
| 4:O:107:THR:HG23  | 11:a:42:ARG:HH22  | 1.74                     | 0.53              |
| 21:A:15:U:H2'     | 21:A:16:G:O4'     | 2.08                     | 0.53              |
| 21:A:1119:G:O2'   | 21:A:1135:G:O6    | 2.24                     | 0.53              |
| 13:C:175:VAL:HG11 | 13:C:220:PHE:HA   | 1.91                     | 0.53              |
| 14:G:193:ARG:HD2  | 21:A:287:C:OP2    | 2.08                     | 0.53              |
| 15:H:12:LYS:O     | 15:H:14:VAL:N     | 2.40                     | 0.53              |
| 21:A:276:G:H2'    | 21:A:277:G:H8     | 1.72                     | 0.53              |
| 4:O:38:ASN:ND2    | 21:A:908:U:OP2    | 2.36                     | 0.53              |
| 8:k:107:HIS:NE2   | 8:k:111:THR:HB    | 2.23                     | 0.53              |
| 15:H:152:LYS:HD3  | 15:H:185:GLU:HG3  | 1.90                     | 0.53              |
| 21:A:108:C:H2'    | 21:A:109:A:H8     | 1.74                     | 0.53              |
| 9:B:52:GLN:HG2    | 9:B:53:GLY:H      | 1.74                     | 0.53              |
| 9:B:108:ASP:O     | 9:B:112:SER:OG    | 2.23                     | 0.53              |
| 11:a:6:ARG:HH22   | 21:A:1096:A:P     | 2.30                     | 0.53              |
| 12:J:50:ALA:HA    | 12:J:53:ARG:HH12  | 1.73                     | 0.53              |
| 20:I:187:CYS:HB2  | 20:I:203:LEU:HD21 | 1.91                     | 0.53              |
| 11:a:93:ARG:HG2   | 11:a:93:ARG:NH1   | 2.24                     | 0.53              |
| 12:J:66:GLU:HG2   | 12:J:71:ARG:CZ    | 2.39                     | 0.53              |
| 15:H:88:PHE:HD1   | 15:H:91:LYS:HB2   | 1.74                     | 0.53              |
| 21:A:122:U:H2'    | 21:A:123:OMU:H6   | 1.90                     | 0.53              |
| 21:A:862:U:H2'    | 21:A:863:G:C8     | 2.43                     | 0.53              |
| 3:E:211:GLU:HG3   | 3:E:217:GLN:HG3   | 1.90                     | 0.53              |
| 14:G:2:LYS:HD3    | 14:G:15:LYS:HD2   | 1.89                     | 0.53              |
| 14:G:178:PRO:O    | 21:A:79:A:O2'     | 2.26                     | 0.53              |
| 10:V:59:ARG:HA    | 10:V:64:ALA:HB2   | 1.91                     | 0.53              |
| 19:n:1:MET:HB2    | 21:A:1651:G:H5'   | 1.91                     | 0.53              |
| 1:Y:23:LEU:HD11   | 3:E:60:GLU:HG2    | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Y:118:ASN:HA    | 1:Y:121:LYS:HE3   | 1.90                     | 0.53              |
| 21:A:1069:G:H2'   | 21:A:1070:A:H5'   | 1.91                     | 0.53              |
| 3:E:47:ILE:HG23   | 3:E:111:LEU:HD11  | 1.91                     | 0.52              |
| 4:O:53:LEU:HD11   | 9:B:47:LEU:HD21   | 1.90                     | 0.52              |
| 15:H:120:THR:HG23 | 21:A:643:U:OP2    | 2.09                     | 0.52              |
| 18:N:31:ALA:O     | 18:N:35:GLU:HG3   | 2.10                     | 0.52              |
| 9:B:104:ASP:OD1   | 9:B:105:PHE:N     | 2.41                     | 0.52              |
| 15:H:54:VAL:HG21  | 15:H:169:THR:HG22 | 1.91                     | 0.52              |
| 15:H:166:LYS:H    | 15:H:166:LYS:HD2  | 1.74                     | 0.52              |
| 21:A:274:A:H2'    | 21:A:275:C:O4'    | 2.09                     | 0.52              |
| 2:X:53:LYS:HE3    | 2:X:90:LEU:HG     | 1.91                     | 0.52              |
| 4:O:42:ILE:HB     | 4:O:56:ILE:HG22   | 1.92                     | 0.52              |
| 4:O:66:ARG:HB3    | 21:A:910:A:H5''   | 1.91                     | 0.52              |
| 18:N:28:THR:CG2   | 18:N:33:VAL:HG23  | 2.39                     | 0.52              |
| 21:A:344:U:H2'    | 21:A:345:A:C8     | 2.45                     | 0.52              |
| 21:A:785:A:H2'    | 21:A:785:A:N3     | 2.24                     | 0.52              |
| 21:A:985:G:H4'    | 21:A:1787:A:H4'   | 1.92                     | 0.52              |
| 10:V:52:PHE:CZ    | 10:V:75:LYS:HG3   | 2.43                     | 0.52              |
| 13:C:226:ASP:OD2  | 13:C:230:LYS:HE3  | 2.10                     | 0.52              |
| 12:J:150:VAL:HG11 | 12:J:158:ILE:HD11 | 1.91                     | 0.52              |
| 10:V:74:GLN:O     | 10:V:78:GLU:HG3   | 2.10                     | 0.52              |
| 18:N:22:PRO:HG3   | 18:N:66:VAL:HA    | 1.91                     | 0.52              |
| 19:n:17:ARG:NH1   | 21:A:1121:A:OP1   | 2.43                     | 0.52              |
| 8:k:134:ASP:O     | 8:k:138:ILE:HG13  | 2.10                     | 0.52              |
| 9:B:47:LEU:HD12   | 9:B:47:LEU:C      | 2.35                     | 0.52              |
| 18:N:107:LYS:NZ   | 21:A:1024:A:OP2   | 2.43                     | 0.52              |
| 11:a:37:LYS:HE3   | 21:A:938:A:OP2    | 2.09                     | 0.52              |
| 21:A:1122:PSU:H2' | 21:A:1123:G:C8    | 2.44                     | 0.52              |
| 21:A:1769:U:H2'   | 21:A:1770:C:C6    | 2.44                     | 0.52              |
| 1:Y:20:ASN:ND2    | 3:E:54:TYR:O      | 2.42                     | 0.52              |
| 13:C:180:VAL:HB   | 13:C:207:PHE:HB2  | 1.92                     | 0.52              |
| 21:A:178:A:H2'    | 21:A:179:A:C8     | 2.45                     | 0.52              |
| 21:A:820:A:H3'    | 21:A:821:G:H4'    | 1.91                     | 0.52              |
| 21:A:958:G:H2'    | 21:A:959:G:H8     | 1.74                     | 0.52              |
| 15:H:41:LEU:O     | 15:H:41:LEU:HD23  | 2.10                     | 0.51              |
| 15:H:88:PHE:CD1   | 15:H:91:LYS:HB2   | 2.46                     | 0.51              |
| 21:A:1149:U:H2'   | 21:A:1150:U:C6    | 2.44                     | 0.51              |
| 2:X:28:LYS:O      | 2:X:32:LEU:HB2    | 2.09                     | 0.51              |
| 2:X:66:ARG:HG3    | 2:X:114:ILE:HG12  | 1.91                     | 0.51              |
| 21:A:30:G:H2'     | 21:A:31:C:C6      | 2.45                     | 0.51              |
| 21:A:207:A:H2'    | 21:A:208:PSU:H6   | 1.74                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:O:56:ILE:HG23   | 4:O:77:ALA:HB1   | 1.93                     | 0.51              |
| 17:L:73:ALA:HB1   | 17:L:123:HIS:HE1 | 1.76                     | 0.51              |
| 20:I:8:MET:HE2    | 20:I:21:TRP:CD1  | 2.46                     | 0.51              |
| 21:A:813:A:H2'    | 21:A:814:C:H6    | 1.75                     | 0.51              |
| 8:k:187:LEU:HB3   | 8:k:192:THR:HB   | 1.91                     | 0.51              |
| 13:C:151:ARG:HB3  | 13:C:161:PRO:HB2 | 1.92                     | 0.51              |
| 21:A:1122:PSU:H2' | 21:A:1123:G:H8   | 1.76                     | 0.51              |
| 21:A:1743:A:H2'   | 21:A:1744:C:C6   | 2.46                     | 0.51              |
| 4:O:53:LEU:HD23   | 4:O:90:ILE:HD11  | 1.90                     | 0.51              |
| 12:J:113:THR:O    | 12:J:117:LYS:HG2 | 2.10                     | 0.51              |
| 21:A:820:A:C2     | 21:A:821:G:H1'   | 2.46                     | 0.51              |
| 21:A:1763:G:H2'   | 21:A:1764:A:C8   | 2.46                     | 0.51              |
| 3:E:37:LYS:NZ     | 21:A:302:C:OP2   | 2.43                     | 0.51              |
| 8:k:107:HIS:NE2   | 8:k:140:GLU:OE1  | 2.44                     | 0.51              |
| 17:L:103:LYS:HD2  | 21:A:636:PSU:OP1 | 2.11                     | 0.51              |
| 21:A:1637:PSU:H2' | 21:A:1638:G:C8   | 2.46                     | 0.51              |
| 9:B:66:PHE:HE2    | 9:B:88:ALA:HB2   | 1.76                     | 0.51              |
| 10:V:32:VAL:HG22  | 10:V:59:ARG:HD2  | 1.92                     | 0.51              |
| 13:C:179:MET:HG3  | 13:C:227:CYS:SG  | 2.51                     | 0.51              |
| 21:A:1015:C:H2'   | 21:A:1016:C:O4'  | 2.11                     | 0.51              |
| 1:Y:20:ASN:ND2    | 1:Y:23:LEU:HD12  | 2.26                     | 0.51              |
| 12:J:137:ARG:NH2  | 12:J:159:ASP:OD2 | 2.44                     | 0.51              |
| 20:I:12:ARG:HG3   | 20:I:18:GLN:HG2  | 1.92                     | 0.51              |
| 3:E:87:MET:HE1    | 3:E:236:VAL:HG21 | 1.91                     | 0.50              |
| 14:G:172:LYS:NZ   | 21:A:72:A:N7     | 2.59                     | 0.50              |
| 15:H:117:ARG:NH1  | 21:A:863:G:H5''  | 2.22                     | 0.50              |
| 21:A:484:A:H2'    | 21:A:485:A:C8    | 2.46                     | 0.50              |
| 21:A:569:C:O2'    | 21:A:581:G:N2    | 2.42                     | 0.50              |
| 3:E:100:ARG:NH2   | 3:E:118:ASP:O    | 2.44                     | 0.50              |
| 8:k:60:GLU:OE2    | 8:k:60:GLU:HA    | 2.11                     | 0.50              |
| 9:B:185:VAL:O     | 9:B:189:ILE:HG12 | 2.11                     | 0.50              |
| 21:A:399:U:H2'    | 21:A:400:G:O4'   | 2.11                     | 0.50              |
| 21:A:452:C:H2'    | 21:A:453:C:H6    | 1.76                     | 0.50              |
| 21:A:1750:C:H2'   | 21:A:1751:A:C8   | 2.45                     | 0.50              |
| 3:E:6:LYS:O       | 3:E:30:LYS:NZ    | 2.25                     | 0.50              |
| 4:O:38:ASN:OD1    | 21:A:908:U:H5    | 1.94                     | 0.50              |
| 1:Y:18:MET:HE1    | 3:E:54:TYR:CE1   | 2.46                     | 0.50              |
| 4:O:62:VAL:HG12   | 4:O:64:ALA:H     | 1.76                     | 0.50              |
| 8:k:70:VAL:HG11   | 8:k:189:MET:HB2  | 1.94                     | 0.50              |
| 9:B:198:GLU:HB3   | 21:A:1061:G:N7   | 2.26                     | 0.50              |
| 11:a:17:HIS:NE2   | 21:A:1800:G:OP1  | 2.39                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:A:484:A:H2'   | 21:A:485:A:H8     | 1.77                     | 0.50              |
| 21:A:900:G:H1    | 21:A:922:U:H3     | 1.57                     | 0.50              |
| 21:A:1699:A:H2'  | 21:A:1700:C:H6    | 1.76                     | 0.50              |
| 21:A:1736:C:H2'  | 21:A:1737:C:C6    | 2.45                     | 0.50              |
| 21:A:1796:U:H2'  | 21:A:1797:G:H8    | 1.76                     | 0.50              |
| 3:E:43:PRO:HD2   | 3:E:46:LEU:HD22   | 1.93                     | 0.50              |
| 3:E:202:LYS:HE3  | 25:A:2134:HOH:O   | 2.12                     | 0.50              |
| 9:B:43:VAL:HG13  | 9:B:68:VAL:HG11   | 1.94                     | 0.50              |
| 15:H:31:GLU:HG2  | 15:H:41:LEU:HD21  | 1.93                     | 0.50              |
| 20:I:173:SER:HA  | 20:I:176:GLU:HB3  | 1.94                     | 0.50              |
| 8:k:36:PHE:CE2   | 8:k:37:GLN:HG3    | 2.47                     | 0.50              |
| 8:k:184:ARG:O    | 8:k:188:GLN:HG3   | 2.12                     | 0.50              |
| 17:L:58:LYS:HG2  | 17:L:132:LEU:HD22 | 1.93                     | 0.50              |
| 21:A:52:U:H2'    | 21:A:53:G:C8      | 2.47                     | 0.50              |
| 21:A:154:A:H2'   | 21:A:155:A:O4'    | 2.11                     | 0.50              |
| 21:A:791:C:OP1   | 21:A:792:U:H4'    | 2.12                     | 0.50              |
| 1:Y:90:LYS:NZ    | 1:Y:90:LYS:HB3    | 2.25                     | 0.50              |
| 21:A:488:C:H2'   | 21:A:489:C:C6     | 2.46                     | 0.50              |
| 21:A:1152:A:H2   | 25:A:2618:HOH:O   | 1.94                     | 0.50              |
| 1:Y:86:GLU:CD    | 1:Y:86:GLU:H      | 2.19                     | 0.50              |
| 21:A:206:U:H2'   | 21:A:207:A:H8     | 1.77                     | 0.50              |
| 21:A:626:A:O2'   | 21:A:1037:G:H5'   | 2.11                     | 0.50              |
| 8:k:147:PRO:HG3  | 10:V:32:VAL:HB    | 1.94                     | 0.49              |
| 9:B:168:MET:HG2  | 9:B:197:ILE:CG2   | 2.40                     | 0.49              |
| 13:C:55:VAL:HG11 | 13:C:78:ILE:HA    | 1.94                     | 0.49              |
| 21:A:524:A:H2'   | 21:A:525:A:C8     | 2.46                     | 0.49              |
| 21:A:606:PSU:H2' | 21:A:607:PSU:H6   | 1.77                     | 0.49              |
| 21:A:1723:C:H2'  | 21:A:1724:G:C8    | 2.47                     | 0.49              |
| 7:e:40:TYR:CG    | 12:J:34:GLY:HA3   | 2.47                     | 0.49              |
| 17:L:134:LYS:HB2 | 21:A:341:G:H3'    | 1.94                     | 0.49              |
| 18:N:110:ASP:OD2 | 21:A:882:G:N2     | 2.37                     | 0.49              |
| 20:I:71:GLU:HB3  | 20:I:113:TRP:CH2  | 2.47                     | 0.49              |
| 21:A:1753:U:H2'  | 21:A:1754:U:C6    | 2.48                     | 0.49              |
| 15:H:34:ASN:H    | 15:H:37:LEU:HB2   | 1.77                     | 0.49              |
| 20:I:39:SER:HB3  | 20:I:60:ARG:HG2   | 1.93                     | 0.49              |
| 2:X:67:LYS:HB3   | 2:X:90:LEU:HD22   | 1.94                     | 0.49              |
| 15:H:27:PHE:HA   | 15:H:30:LEU:HG    | 1.95                     | 0.49              |
| 18:N:94:LYS:O    | 18:N:98:ILE:HG13  | 2.12                     | 0.49              |
| 21:A:589:A:H2'   | 21:A:590:G:C8     | 2.48                     | 0.49              |
| 21:A:862:U:O2'   | 21:A:863:G:H5'    | 2.11                     | 0.49              |
| 21:A:867:A:H8    | 21:A:867:A:OP2    | 1.96                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:A:1651:G:HO2'  | 21:A:1792:MA6:HO2' | 1.56                     | 0.49              |
| 3:E:59:ARG:NH2    | 21:A:449:A:OP2     | 2.42                     | 0.49              |
| 5:W:32:LYS:HG2    | 21:A:641:C:OP1     | 2.12                     | 0.49              |
| 15:H:9:GLN:OE1    | 15:H:45:TYR:HB3    | 2.13                     | 0.49              |
| 17:L:6:GLU:HG2    | 17:L:10:LEU:HD11   | 1.93                     | 0.49              |
| 20:I:10:LYS:NZ    | 21:A:326:G:O2'     | 2.45                     | 0.49              |
| 21:A:308:PSU:H2'  | 21:A:309:C:C6      | 2.48                     | 0.49              |
| 21:A:437:C:H2'    | 21:A:438:G:O4'     | 2.13                     | 0.49              |
| 21:A:1793:MA6:H8  | 21:A:1793:MA6:H5'' | 1.93                     | 0.49              |
| 2:X:39:PRO:HA     | 2:X:78:LYS:HD2     | 1.93                     | 0.49              |
| 9:B:29:TRP:HE3    | 9:B:45:LYS:O       | 1.95                     | 0.49              |
| 15:H:82:ARG:O     | 15:H:86:LYS:HG3    | 2.12                     | 0.49              |
| 21:A:611:G:N2     | 21:A:618:C:H5''    | 2.27                     | 0.49              |
| 1:Y:18:MET:HG2    | 1:Y:27:GLN:HG3     | 1.95                     | 0.49              |
| 8:k:29:LEU:O      | 8:k:168:ASN:ND2    | 2.46                     | 0.49              |
| 21:A:304:A:H2'    | 21:A:305:A:C8      | 2.47                     | 0.49              |
| 21:A:486:U:O4     | 21:A:487:A:N6      | 2.46                     | 0.49              |
| 21:A:1152:A:H2'   | 21:A:1153:C:C6     | 2.48                     | 0.49              |
| 1:Y:20:ASN:HD21   | 1:Y:23:LEU:HD12    | 1.78                     | 0.49              |
| 8:k:43:TYR:CD2    | 8:k:44:LYS:HG3     | 2.48                     | 0.49              |
| 13:C:198:LEU:HD13 | 13:C:206:VAL:HG11  | 1.95                     | 0.49              |
| 15:H:144:ARG:HE   | 15:H:148:ALA:HB3   | 1.77                     | 0.49              |
| 21:A:206:U:H2'    | 21:A:207:A:C8      | 2.47                     | 0.49              |
| 21:A:530:A:H2'    | 21:A:531:A:O4'     | 2.13                     | 0.49              |
| 18:N:33:VAL:O     | 18:N:37:ILE:HG13   | 2.12                     | 0.49              |
| 21:A:611:G:H5'    | 21:A:617:G:N2      | 2.28                     | 0.49              |
| 1:Y:13:ARG:HH21   | 1:Y:33:ILE:HD13    | 1.78                     | 0.48              |
| 3:E:59:ARG:HH12   | 21:A:449:A:H5''    | 1.78                     | 0.48              |
| 3:E:240:LYS:HB2   | 21:A:791:C:C5      | 2.48                     | 0.48              |
| 14:G:70:SER:O     | 14:G:100:ARG:NH1   | 2.45                     | 0.48              |
| 15:H:48:THR:O     | 15:H:64:HIS:ND1    | 2.31                     | 0.48              |
| 21:A:397:C:H2'    | 21:A:398:C:C6      | 2.47                     | 0.48              |
| 21:A:1696:G:O2'   | 21:A:1697:C:H5'    | 2.12                     | 0.48              |
| 14:G:67:VAL:HG12  | 14:G:69:THR:HG22   | 1.95                     | 0.48              |
| 4:O:55:ARG:NH1    | 21:A:901:U:O2      | 2.46                     | 0.48              |
| 12:J:175:LYS:HB2  | 21:A:515:A:H5'     | 1.95                     | 0.48              |
| 20:I:197:ARG:NH2  | 21:A:204:U:O2      | 2.44                     | 0.48              |
| 21:A:606:PSU:H2'  | 21:A:607:PSU:C6    | 2.48                     | 0.48              |
| 21:A:966:U:H2'    | 21:A:967:C:H6      | 1.79                     | 0.48              |
| 5:W:20:ARG:HG3    | 5:W:20:ARG:HH11    | 1.77                     | 0.48              |
| 8:k:131:PRO:HG2   | 8:k:156:SER:HB3    | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:N:73:ARG:NH1  | 21:A:864:A:C4     | 2.80                     | 0.48              |
| 21:A:184:C:H2'   | 21:A:185:G:O4'    | 2.13                     | 0.48              |
| 21:A:207:A:H2'   | 21:A:208:PSU:C6   | 2.48                     | 0.48              |
| 21:A:859:U:H2'   | 21:A:860:A:C8     | 2.48                     | 0.48              |
| 21:A:939:C:C4    | 21:A:1082:C:H4'   | 2.49                     | 0.48              |
| 21:A:1112:G:O2'  | 21:A:1113:G:H5'   | 2.13                     | 0.48              |
| 15:H:51:GLN:OE1  | 15:H:59:LYS:HB3   | 2.13                     | 0.48              |
| 21:A:863:G:O2'   | 21:A:864:A:H5'    | 2.13                     | 0.48              |
| 12:J:80:ARG:HH22 | 21:A:770:U:P      | 2.37                     | 0.48              |
| 13:C:191:ALA:HB2 | 21:A:4:C:H4'      | 1.96                     | 0.48              |
| 15:H:78:VAL:O    | 15:H:82:ARG:HG3   | 2.14                     | 0.48              |
| 21:A:958:G:H2'   | 21:A:959:G:C8     | 2.48                     | 0.48              |
| 21:A:1798:C:H2'  | 21:A:1799:G:C8    | 2.47                     | 0.48              |
| 4:O:129:ILE:O    | 11:a:65:PRO:HG3   | 2.14                     | 0.48              |
| 5:W:106:THR:OG1  | 5:W:109:GLY:O     | 2.32                     | 0.48              |
| 9:B:193:ILE:O    | 9:B:197:ILE:HG13  | 2.13                     | 0.48              |
| 17:L:6:GLU:HG3   | 17:L:10:LEU:HD11  | 1.95                     | 0.48              |
| 19:n:17:ARG:O    | 19:n:21:ARG:HG2   | 2.13                     | 0.48              |
| 21:A:550:U:H2'   | 21:A:551:U:C6     | 2.49                     | 0.48              |
| 21:A:927:A:H2'   | 21:A:928:A:C8     | 2.49                     | 0.48              |
| 4:O:150:ARG:HD2  | 21:A:1780:U:O2    | 2.14                     | 0.48              |
| 15:H:64:HIS:HB3  | 15:H:98:THR:CG2   | 2.44                     | 0.48              |
| 16:h:114:LEU:HB2 | 16:h:115:PRO:HD3  | 1.96                     | 0.48              |
| 21:A:1746:U:H2'  | 21:A:1747:U:C6    | 2.48                     | 0.48              |
| 1:Y:90:LYS:HZ1   | 1:Y:90:LYS:HB3    | 1.78                     | 0.48              |
| 21:A:755:U:H2'   | 21:A:756:U:C6     | 2.48                     | 0.48              |
| 21:A:1096:A:H4'  | 21:A:1097:A:O4'   | 2.14                     | 0.48              |
| 21:A:1730:A:H2'  | 21:A:1731:G:O4'   | 2.13                     | 0.48              |
| 1:Y:128:LYS:HE2  | 21:A:86:A:H5''    | 1.95                     | 0.47              |
| 14:G:156:ARG:NH2 | 14:G:183:LEU:HD21 | 2.29                     | 0.47              |
| 17:L:44:LYS:HD2  | 17:L:44:LYS:N     | 2.29                     | 0.47              |
| 21:A:860:A:C2    | 21:A:862:U:H1'    | 2.49                     | 0.47              |
| 8:k:46:ARG:HD3   | 8:k:52:ILE:HD11   | 1.96                     | 0.47              |
| 17:L:20:LYS:NZ   | 20:I:71:GLU:OE2   | 2.48                     | 0.47              |
| 21:A:32:U:O2'    | 21:A:598:A:N1     | 2.44                     | 0.47              |
| 8:k:79:ILE:HG13  | 8:k:123:PRO:HB3   | 1.95                     | 0.47              |
| 13:C:211:ARG:HD2 | 21:A:1102:U:O4    | 2.14                     | 0.47              |
| 21:A:819:U:H1'   | 21:A:821:G:C5     | 2.48                     | 0.47              |
| 21:A:1674:C:H2'  | 21:A:1675:C:C6    | 2.50                     | 0.47              |
| 2:X:7:MET:HE2    | 5:W:77:PRO:CB     | 2.43                     | 0.47              |
| 8:k:131:PRO:CG   | 8:k:156:SER:HB3   | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:22:GLN:OE1   | 14:G:22:GLN:HA    | 2.13                     | 0.47              |
| 21:A:141:G:H2'    | 21:A:142:G:H8     | 1.78                     | 0.47              |
| 21:A:488:C:H2'    | 21:A:489:C:H6     | 1.80                     | 0.47              |
| 21:A:615:OMU:HM23 | 21:A:615:OMU:H1'  | 1.57                     | 0.47              |
| 21:A:1763:G:H2'   | 21:A:1764:A:H8    | 1.78                     | 0.47              |
| 8:k:84:ARG:HH22   | 8:k:170:LYS:CG    | 2.21                     | 0.47              |
| 9:B:222:LYS:NZ    | 9:B:223:PHE:O     | 2.46                     | 0.47              |
| 21:A:1770:C:H2'   | 21:A:1771:G:O4'   | 2.15                     | 0.47              |
| 21:A:253:C:H2'    | 21:A:254:A:H8     | 1.79                     | 0.47              |
| 21:A:417:U:H2'    | 21:A:418:OMC:C6   | 2.49                     | 0.47              |
| 21:A:608:U:H2'    | 21:A:609:A:O4'    | 2.15                     | 0.47              |
| 21:A:825:U:H2'    | 21:A:826:C:C6     | 2.50                     | 0.47              |
| 3:E:157:ASN:OD1   | 3:E:222:LEU:HD21  | 2.14                     | 0.47              |
| 10:V:57:PHE:O     | 10:V:61:GLN:HG2   | 2.15                     | 0.47              |
| 12:J:19:ARG:O     | 12:J:25:ARG:NH1   | 2.46                     | 0.47              |
| 15:H:79:ARG:HD3   | 15:H:82:ARG:NH1   | 2.29                     | 0.47              |
| 17:L:86:ILE:HD11  | 21:A:351:G:H5''   | 1.96                     | 0.47              |
| 21:A:346:C:H3'    | 25:A:2206:HOH:O   | 2.14                     | 0.47              |
| 21:A:900:G:H2'    | 21:A:901:U:C6     | 2.50                     | 0.47              |
| 21:A:926:G:H2'    | 21:A:927:A:H8     | 1.80                     | 0.47              |
| 21:A:1810:U:H4'   | 21:A:1811:G:C8    | 2.50                     | 0.47              |
| 9:B:149:GLN:HG3   | 21:A:1071:C:H4'   | 1.97                     | 0.47              |
| 1:Y:34:HIS:HB2    | 1:Y:37:ARG:HB2    | 1.96                     | 0.47              |
| 11:a:23:CYS:HB3   | 11:a:28:LYS:H     | 1.79                     | 0.47              |
| 14:G:221:LEU:HD12 | 14:G:221:LEU:HA   | 1.79                     | 0.47              |
| 21:A:1648:OMC:O2  | 21:A:1648:OMC:O5' | 2.33                     | 0.47              |
| 4:O:120:ALA:HB3   | 11:a:52:ASP:OD2   | 2.15                     | 0.47              |
| 18:N:57:GLN:O     | 18:N:58:HIS:ND1   | 2.48                     | 0.47              |
| 18:N:88:LEU:O     | 18:N:92:ILE:HG13  | 2.15                     | 0.47              |
| 21:A:751:U:H2'    | 21:A:752:A:H8     | 1.80                     | 0.47              |
| 21:A:1042:C:H2'   | 21:A:1043:C:C6    | 2.50                     | 0.47              |
| 4:O:126:ILE:N     | 11:a:56:ALA:O     | 2.35                     | 0.46              |
| 9:B:109:LYS:HE3   | 9:B:113:LEU:HD21  | 1.97                     | 0.46              |
| 14:G:176:LYS:NZ   | 21:A:68:A:OP1     | 2.44                     | 0.46              |
| 17:L:60:PRO:HG3   | 17:L:139:ASN:HB3  | 1.97                     | 0.46              |
| 20:I:189:SER:OG   | 20:I:200:GLY:HA2  | 2.15                     | 0.46              |
| 21:A:259:A:H2'    | 21:A:260:A:O4'    | 2.15                     | 0.46              |
| 3:E:19:MET:SD     | 3:E:108:ARG:HD2   | 2.56                     | 0.46              |
| 21:A:36:C:H2'     | 21:A:37:U:C6      | 2.51                     | 0.46              |
| 21:A:276:G:H2'    | 21:A:277:G:C8     | 2.49                     | 0.46              |
| 4:O:146:ARG:HG2   | 21:A:1798:C:OP2   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:N:3:ARG:HD3    | 18:N:3:ARG:HA     | 1.68                     | 0.46              |
| 21:A:108:C:H2'    | 21:A:109:A:C8     | 2.50                     | 0.46              |
| 15:H:166:LYS:HD2  | 15:H:166:LYS:N    | 2.31                     | 0.46              |
| 20:I:25:ARG:HA    | 21:A:404:A:H5''   | 1.97                     | 0.46              |
| 21:A:331:U:H2'    | 21:A:332:A:C8     | 2.50                     | 0.46              |
| 21:A:347:C:H2'    | 21:A:348:A:H8     | 1.80                     | 0.46              |
| 8:k:66:ALA:O      | 8:k:70:VAL:HG13   | 2.15                     | 0.46              |
| 13:C:250:TYR:O    | 13:C:254:THR:HG23 | 2.15                     | 0.46              |
| 21:A:205:U:H2'    | 21:A:206:U:C6     | 2.51                     | 0.46              |
| 21:A:1057:U:N3    | 21:A:1058:G:O6    | 2.49                     | 0.46              |
| 5:W:49:GLU:OE2    | 15:H:144:ARG:HA   | 2.16                     | 0.46              |
| 9:B:67:GLU:OE2    | 9:B:83:LYS:HB3    | 2.16                     | 0.46              |
| 13:C:62:LYS:HB2   | 13:C:64:GLU:OE1   | 2.15                     | 0.46              |
| 13:C:175:VAL:HG13 | 13:C:214:THR:HG22 | 1.98                     | 0.46              |
| 21:A:1059:U:C4    | 21:A:1060:U:C4    | 3.04                     | 0.46              |
| 21:A:1648:OMC:O2  | 21:A:1648:OMC:O4' | 2.34                     | 0.46              |
| 21:A:1648:OMC:H2' | 21:A:1649:C:O4'   | 2.15                     | 0.46              |
| 21:A:1695:G:C2    | 21:A:1696:G:C8    | 3.04                     | 0.46              |
| 2:X:28:LYS:NZ     | 21:A:1137:A:OP1   | 2.38                     | 0.46              |
| 4:O:51:GLU:HG2    | 9:B:64:ARG:HH22   | 1.79                     | 0.46              |
| 13:C:184:ARG:HA   | 13:C:205:ASP:OD2  | 2.16                     | 0.46              |
| 21:A:813:A:H2'    | 21:A:814:C:C6     | 2.51                     | 0.46              |
| 21:A:983:A:H2'    | 21:A:984:A:O4'    | 2.16                     | 0.46              |
| 1:Y:10:VAL:HG11   | 1:Y:40:VAL:HG21   | 1.98                     | 0.46              |
| 12:J:122:LYS:HD2  | 21:A:483:C:H4'    | 1.97                     | 0.46              |
| 5:W:111:MET:HE1   | 5:W:119:LYS:HD2   | 1.98                     | 0.46              |
| 8:k:107:HIS:CD2   | 8:k:140:GLU:OE1   | 2.69                     | 0.46              |
| 14:G:156:ARG:HE   | 14:G:156:ARG:HB3  | 1.21                     | 0.46              |
| 21:A:337:A:H2'    | 21:A:338:G:C8     | 2.50                     | 0.46              |
| 21:A:969:U:H4'    | 21:A:970:U:O4'    | 2.16                     | 0.46              |
| 2:X:37:LYS:HE2    | 2:X:37:LYS:HA     | 1.98                     | 0.46              |
| 5:W:29:PRO:HB3    | 5:W:58:SER:HB3    | 1.97                     | 0.46              |
| 6:b:10:LEU:C      | 6:b:12:PRO:HD3    | 2.41                     | 0.46              |
| 9:B:58:SER:OG     | 9:B:59:GLU:OE1    | 2.33                     | 0.46              |
| 9:B:125:VAL:HG13  | 9:B:127:VAL:HG13  | 1.98                     | 0.46              |
| 18:N:2:GLY:N      | 21:A:871:G:OP1    | 2.48                     | 0.46              |
| 21:A:27:U:H2'     | 21:A:28:A2M:H8    | 1.97                     | 0.46              |
| 21:A:518:G:O2'    | 21:A:519:A:H8     | 1.98                     | 0.46              |
| 21:A:1674:C:H2'   | 21:A:1675:C:H6    | 1.81                     | 0.46              |
| 21:A:1746:U:H2'   | 21:A:1747:U:H6    | 1.81                     | 0.46              |
| 21:A:1751:A:C6    | 21:A:1752:U:C4    | 3.03                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:A:1761:A2M:H8  | 21:A:1761:A2M:H5'' | 1.97                     | 0.46              |
| 6:b:15:GLU:HG3    | 6:b:16:LEU:HD13    | 1.97                     | 0.45              |
| 18:N:48:SER:OG    | 18:N:86:GLU:OE2    | 2.22                     | 0.45              |
| 20:I:102:ILE:HD12 | 20:I:203:LEU:HD11  | 1.97                     | 0.45              |
| 21:A:98:C:H2'     | 21:A:99:U:C6       | 2.51                     | 0.45              |
| 21:A:405:A:H5''   | 25:A:2047:HOH:O    | 2.16                     | 0.45              |
| 21:A:760:G:N2     | 21:A:800:U:OP1     | 2.49                     | 0.45              |
| 21:A:1773:A:H2'   | 21:A:1774:6MZ:H8   | 1.98                     | 0.45              |
| 7:e:34:ALA:O      | 7:e:38:ILE:HG13    | 2.15                     | 0.45              |
| 8:k:172:ARG:HD2   | 8:k:208:TYR:HD2    | 1.75                     | 0.45              |
| 20:I:8:MET:CE     | 20:I:21:TRP:CD1    | 2.99                     | 0.45              |
| 21:A:1681:A:H2'   | 21:A:1682:G:C8     | 2.51                     | 0.45              |
| 1:Y:16:LYS:HE3    | 21:A:781:A:H62     | 1.80                     | 0.45              |
| 1:Y:115:GLU:O     | 1:Y:119:ARG:HG3    | 2.16                     | 0.45              |
| 2:X:56:ILE:CD1    | 2:X:115:PRO:HD2    | 2.46                     | 0.45              |
| 9:B:146:ARG:HH21  | 21:A:1070:A:H1'    | 1.81                     | 0.45              |
| 9:B:224:ASP:OD2   | 9:B:227:LYS:HE3    | 2.16                     | 0.45              |
| 9:B:224:ASP:HB3   | 9:B:227:LYS:HD2    | 1.98                     | 0.45              |
| 15:H:94:VAL:HG11  | 15:H:130:VAL:HG23  | 1.99                     | 0.45              |
| 21:A:952:U:H2'    | 21:A:953:G:H8      | 1.81                     | 0.45              |
| 5:W:80:ASP:OD1    | 5:W:124:LYS:NZ     | 2.49                     | 0.45              |
| 5:W:99:PHE:CD1    | 13:C:237:PRO:HG2   | 2.51                     | 0.45              |
| 8:k:15:LYS:HG3    | 8:k:59:TRP:CD2     | 2.51                     | 0.45              |
| 12:J:51:LEU:HD13  | 12:J:106:PHE:CE1   | 2.51                     | 0.45              |
| 21:A:966:U:H2'    | 21:A:967:C:C6      | 2.52                     | 0.45              |
| 21:A:1022:U:C2    | 21:A:1023:C:C5     | 3.04                     | 0.45              |
| 4:O:44:VAL:HB     | 4:O:54:VAL:HG12    | 1.97                     | 0.45              |
| 8:k:38:MET:HE3    | 8:k:38:MET:HB3     | 1.85                     | 0.45              |
| 8:k:72:ILE:HD13   | 8:k:124:ARG:NH2    | 2.32                     | 0.45              |
| 8:k:88:GLN:O      | 8:k:89:ARG:C       | 2.60                     | 0.45              |
| 21:A:850:G:H2'    | 21:A:851:G:H8      | 1.82                     | 0.45              |
| 21:A:1022:U:H2'   | 21:A:1023:C:H6     | 1.82                     | 0.45              |
| 8:k:115:GLN:HG2   | 8:k:116:MET:HE2    | 1.99                     | 0.45              |
| 14:G:57:ASP:HB3   | 14:G:100:ARG:HD2   | 1.98                     | 0.45              |
| 21:A:178:A:H2'    | 21:A:179:A:H8      | 1.82                     | 0.45              |
| 21:A:1058:G:C4    | 21:A:1059:U:C5     | 3.05                     | 0.45              |
| 21:A:1726:C:O2'   | 21:A:1727:G:O5'    | 2.33                     | 0.45              |
| 3:E:213:ALA:HB3   | 3:E:244:ILE:HD11   | 1.97                     | 0.45              |
| 4:O:98:ARG:NH2    | 4:O:100:THR:O      | 2.49                     | 0.45              |
| 8:k:172:ARG:CD    | 8:k:208:TYR:CD2    | 2.83                     | 0.45              |
| 11:a:21:ILE:HD13  | 11:a:72:HIS:HB3    | 1.98                     | 0.45              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 14:G:145:LYS:HE2   | 14:G:145:LYS:HB2 | 1.82                     | 0.45              |
| 15:H:50:ILE:HG22   | 15:H:62:VAL:HG22 | 1.99                     | 0.45              |
| 20:I:158:VAL:O     | 20:I:161:LYS:HG2 | 2.17                     | 0.45              |
| 21:A:522:A:C2'     | 21:A:523:C:H5''  | 2.47                     | 0.45              |
| 21:A:824:U:H2'     | 21:A:825:U:C6    | 2.52                     | 0.45              |
| 5:W:77:PRO:HD2     | 5:W:79:PHE:CE2   | 2.52                     | 0.45              |
| 10:V:49:PHE:HZ     | 13:C:247:LYS:HE2 | 1.82                     | 0.45              |
| 11:a:12:LYS:HD2    | 11:a:16:GLY:O    | 2.17                     | 0.45              |
| 21:A:453:C:H2'     | 21:A:454:U:C6    | 2.52                     | 0.45              |
| 3:E:196:LYS:HZ3    | 3:E:211:GLU:HB3  | 1.81                     | 0.45              |
| 4:O:149:ARG:NH2    | 21:A:909:G:OP1   | 2.50                     | 0.45              |
| 6:b:72:LYS:HG3     | 21:A:1054:G:H5'' | 1.97                     | 0.45              |
| 8:k:41:TYR:HA      | 8:k:57:LYS:HD3   | 1.98                     | 0.45              |
| 9:B:138:PHE:HE2    | 9:B:216:LYS:HD3  | 1.81                     | 0.45              |
| 16:h:113:ASP:O     | 16:h:114:LEU:C   | 2.59                     | 0.45              |
| 21:A:17:C:H2'      | 21:A:18:C:C6     | 2.51                     | 0.45              |
| 21:A:927:A:H2'     | 21:A:928:A:H8    | 1.81                     | 0.45              |
| 21:A:1645:C:H4'    | 21:A:1646:C:H3'  | 1.99                     | 0.45              |
| 5:W:51:GLU:OE1     | 15:H:142:ARG:HA  | 2.16                     | 0.45              |
| 9:B:162:ARG:HB3    | 9:B:166:ARG:NH2  | 2.24                     | 0.45              |
| 11:a:40:LEU:HD12   | 11:a:71:VAL:HG21 | 1.99                     | 0.45              |
| 15:H:175:ARG:CZ    | 15:H:181:ASP:HA  | 2.47                     | 0.45              |
| 16:h:113:ASP:OD1   | 16:h:115:PRO:HD2 | 2.17                     | 0.45              |
| 21:A:29:U:H2'      | 21:A:30:G:H8     | 1.82                     | 0.45              |
| 21:A:594:C:H2'     | 21:A:595:A:C8    | 2.52                     | 0.45              |
| 21:A:1659:U:H2'    | 21:A:1660:A:H8   | 1.82                     | 0.45              |
| 8:k:70:VAL:HG12    | 8:k:186:VAL:HG13 | 1.98                     | 0.44              |
| 9:B:125:VAL:CG2    | 9:B:169:VAL:HG13 | 2.47                     | 0.44              |
| 14:G:57:ASP:HA     | 14:G:108:LEU:HA  | 1.98                     | 0.44              |
| 15:H:102:VAL:HG22  | 15:H:117:ARG:HB3 | 1.99                     | 0.44              |
| 19:n:20:MET:SD     | 19:n:20:MET:C    | 3.00                     | 0.44              |
| 21:A:483:C:H2'     | 21:A:484:A:H8    | 1.82                     | 0.44              |
| 21:A:1049:U:H2'    | 21:A:1050:C:C6   | 2.52                     | 0.44              |
| 5:W:115:GLU:O      | 5:W:119:LYS:HG3  | 2.17                     | 0.44              |
| 13:C:91:MET:HE3    | 13:C:91:MET:HB3  | 1.81                     | 0.44              |
| 13:C:168:VAL:HG13  | 13:C:227:CYS:SG  | 2.57                     | 0.44              |
| 16:h:106:LEU:HB3   | 16:h:111:MET:HB2 | 1.98                     | 0.44              |
| 18:N:128:TYR:CE1   | 21:A:969:U:H5''  | 2.53                     | 0.44              |
| 21:A:1014:OMU:HM22 | 21:A:1015:C:O4'  | 2.17                     | 0.44              |
| 21:A:1140:U:H2'    | 21:A:1141:U:C6   | 2.52                     | 0.44              |
| 21:A:1656:U:H2'    | 21:A:1657:C:C6   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 21:A:1678:U:H2'   | 21:A:1679:G:O4'  | 2.17                     | 0.44              |
| 4:O:48:SER:HB3    | 9:B:66:PHE:CE1   | 2.52                     | 0.44              |
| 14:G:163:ARG:HH21 | 14:G:175:SER:HB3 | 1.81                     | 0.44              |
| 20:I:159:GLN:HA   | 20:I:159:GLN:OE1 | 2.17                     | 0.44              |
| 21:A:130:A:N6     | 21:A:175:A:O2'   | 2.50                     | 0.44              |
| 21:A:160:A:N6     | 25:A:2202:HOH:O  | 2.50                     | 0.44              |
| 21:A:416:A:H2'    | 21:A:417:U:C6    | 2.52                     | 0.44              |
| 4:O:56:ILE:HD12   | 4:O:60:MET:CE    | 2.47                     | 0.44              |
| 12:J:63:THR:O     | 12:J:63:THR:HG22 | 2.18                     | 0.44              |
| 13:C:172:CYS:SG   | 13:C:222:LYS:HE3 | 2.57                     | 0.44              |
| 17:L:130:ARG:NH2  | 25:L:203:HOH:O   | 2.49                     | 0.44              |
| 21:A:926:G:H2'    | 21:A:927:A:C8    | 2.52                     | 0.44              |
| 21:A:963:U:H5     | 25:A:2555:HOH:O  | 2.01                     | 0.44              |
| 21:A:1727:G:H2'   | 21:A:1728:C:C6   | 2.53                     | 0.44              |
| 3:E:192:VAL:HB    | 3:E:243:GLY:HA3  | 2.00                     | 0.44              |
| 5:W:8:ASN:HB2     | 5:W:74:VAL:HG21  | 1.99                     | 0.44              |
| 11:a:79:ILE:HD13  | 21:A:1805:A:H1'  | 1.99                     | 0.44              |
| 21:A:202:C:C2     | 21:A:203:A:C8    | 3.05                     | 0.44              |
| 21:A:1661:C:H2'   | 21:A:1662:C:H6   | 1.82                     | 0.44              |
| 21:A:1662:C:H2'   | 21:A:1663:G:O4'  | 2.17                     | 0.44              |
| 3:E:194:VAL:HG11  | 3:E:232:THR:HG22 | 1.99                     | 0.44              |
| 9:B:59:GLU:OE1    | 9:B:59:GLU:N     | 2.49                     | 0.44              |
| 9:B:97:LEU:HB3    | 9:B:232:HIS:NE2  | 2.32                     | 0.44              |
| 12:J:33:VAL:HG13  | 12:J:38:LEU:HB2  | 2.00                     | 0.44              |
| 14:G:53:MET:HG3   | 14:G:114:VAL:CG2 | 2.45                     | 0.44              |
| 20:I:26:LYS:HG2   | 20:I:29:LEU:HD23 | 2.00                     | 0.44              |
| 1:Y:63:VAL:HB     | 1:Y:66:PHE:CE2   | 2.53                     | 0.44              |
| 5:W:26:MET:HE3    | 5:W:26:MET:HB3   | 1.79                     | 0.44              |
| 5:W:49:GLU:HB2    | 5:W:64:GLU:HG2   | 2.00                     | 0.44              |
| 12:J:80:ARG:NH1   | 21:A:769:G:OP1   | 2.51                     | 0.44              |
| 18:N:23:PRO:HG2   | 18:N:26:VAL:HG23 | 2.00                     | 0.44              |
| 20:I:23:LYS:HE3   | 21:A:395:A:OP2   | 2.18                     | 0.44              |
| 21:A:638:G:N1     | 21:A:970:U:OP2   | 2.40                     | 0.44              |
| 21:A:994:U:H2'    | 21:A:995:C:O4'   | 2.17                     | 0.44              |
| 21:A:1753:U:H3'   | 21:A:1754:U:C5   | 2.52                     | 0.44              |
| 21:A:1776:A:N6    | 25:A:2077:HOH:O  | 2.39                     | 0.44              |
| 1:Y:51:LYS:HE2    | 1:Y:51:LYS:HB2   | 1.72                     | 0.44              |
| 21:A:786:U:O2     | 21:A:786:U:C2'   | 2.66                     | 0.44              |
| 21:A:823:A:C2     | 21:A:824:U:C2    | 3.06                     | 0.44              |
| 21:A:1654:G:N3    | 21:A:1654:G:H2'  | 2.33                     | 0.44              |
| 21:A:1749:U:H2'   | 21:A:1750:C:C6   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:k:56:GLY:H      | 16:h:109:LEU:HD11  | 1.83                     | 0.44              |
| 14:G:135:ARG:HD2  | 21:A:164:C:O2      | 2.18                     | 0.44              |
| 16:h:103:MET:HE2  | 16:h:103:MET:HB3   | 1.83                     | 0.44              |
| 17:L:124:VAL:HG12 | 17:L:143:VAL:HG22  | 2.00                     | 0.44              |
| 21:A:1635:U:H2'   | 21:A:1636:U:C6     | 2.53                     | 0.44              |
| 3:E:202:LYS:NZ    | 21:A:249:G:H4'     | 2.33                     | 0.43              |
| 5:W:54:ASP:HB3    | 15:H:139:LYS:HB3   | 1.99                     | 0.43              |
| 9:B:36:LEU:HA     | 9:B:41:ARG:HH11    | 1.81                     | 0.43              |
| 9:B:125:VAL:HG21  | 9:B:169:VAL:HG13   | 2.00                     | 0.43              |
| 9:B:133:TYR:CD1   | 9:B:181:LEU:HD11   | 2.53                     | 0.43              |
| 13:C:89:GLU:HA    | 13:C:89:GLU:OE1    | 2.18                     | 0.43              |
| 21:A:247:A:H2'    | 21:A:248:U:C6      | 2.53                     | 0.43              |
| 21:A:338:G:H4'    | 25:A:2051:HOH:O    | 2.17                     | 0.43              |
| 21:A:342:C:H2'    | 21:A:343:C:C6      | 2.52                     | 0.43              |
| 21:A:344:U:H2'    | 21:A:345:A:H8      | 1.83                     | 0.43              |
| 21:A:952:U:H2'    | 21:A:953:G:C8      | 2.53                     | 0.43              |
| 21:A:1755:A:H2'   | 21:A:1756:G:O4'    | 2.18                     | 0.43              |
| 6:b:4:GLN:O       | 6:b:4:GLN:HG2      | 2.17                     | 0.43              |
| 11:a:51:ARG:O     | 11:a:55:GLU:HG3    | 2.17                     | 0.43              |
| 21:A:492:G:H1     | 21:A:503:U:H3      | 1.66                     | 0.43              |
| 2:X:7:MET:HA      | 17:L:100:ARG:HD2   | 2.00                     | 0.43              |
| 2:X:38:LYS:HA     | 2:X:38:LYS:HD3     | 1.84                     | 0.43              |
| 9:B:136:ARG:HD2   | 9:B:138:PHE:CZ     | 2.52                     | 0.43              |
| 21:A:204:U:H2'    | 21:A:205:U:C6      | 2.53                     | 0.43              |
| 21:A:647:G:H2'    | 21:A:648:C:H6      | 1.84                     | 0.43              |
| 21:A:820:A:H2'    | 21:A:822:G:O4'     | 2.19                     | 0.43              |
| 21:A:1304:G:H2'   | 21:A:1305:A:C8     | 2.53                     | 0.43              |
| 21:A:1650:C:H2'   | 21:A:1651:G:H8     | 1.82                     | 0.43              |
| 9:B:109:LYS:O     | 9:B:113:LEU:HG     | 2.18                     | 0.43              |
| 14:G:59:GLN:OE1   | 14:G:72:ARG:NH1    | 2.47                     | 0.43              |
| 17:L:56:ASP:HB3   | 17:L:59:CYS:HB2    | 2.01                     | 0.43              |
| 21:A:196:G:H2'    | 21:A:197:G:H8      | 1.84                     | 0.43              |
| 21:A:388:G:H2'    | 21:A:389:A:C8      | 2.54                     | 0.43              |
| 21:A:437:C:H1'    | 25:A:2256:HOH:O    | 2.18                     | 0.43              |
| 21:A:825:U:C2     | 21:A:858:G:C2      | 3.07                     | 0.43              |
| 4:O:121:ARG:HG3   | 11:a:52:ASP:CG     | 2.43                     | 0.43              |
| 7:e:40:TYR:O      | 7:e:44:PHE:HB2     | 2.19                     | 0.43              |
| 13:C:98:LYS:HD2   | 21:A:1306:PSU:H5'' | 1.99                     | 0.43              |
| 21:A:69:A:H2'     | 21:A:70:C:C6       | 2.53                     | 0.43              |
| 21:A:285:G:H2'    | 21:A:286:C:C6      | 2.53                     | 0.43              |
| 21:A:297:U:H2'    | 21:A:298:C:C6      | 2.53                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 21:A:967:C:H2'    | 21:A:968:A:O4'   | 2.18                     | 0.43              |
| 21:A:1634:C:H2'   | 21:A:1635:U:H6   | 1.83                     | 0.43              |
| 21:A:1781:U:H2'   | 21:A:1782:U:C6   | 2.54                     | 0.43              |
| 4:O:122:SER:O     | 4:O:122:SER:OG   | 2.36                     | 0.43              |
| 20:I:11:ARG:NH1   | 20:I:15:GLY:O    | 2.51                     | 0.43              |
| 21:A:991:G:H2'    | 21:A:992:G:O4'   | 2.19                     | 0.43              |
| 21:A:1008:A:H1'   | 21:A:1010:A:N7   | 2.33                     | 0.43              |
| 18:N:124:ARG:HH21 | 21:A:632:G:P     | 2.41                     | 0.43              |
| 19:n:14:LYS:O     | 19:n:15:ARG:C    | 2.62                     | 0.43              |
| 21:A:647:G:N2     | 21:A:693:C:C2    | 2.87                     | 0.43              |
| 21:A:820:A:O4'    | 21:A:863:G:N2    | 2.51                     | 0.43              |
| 21:A:826:C:H2'    | 21:A:827:C:H6    | 1.84                     | 0.43              |
| 21:A:880:G:O2'    | 21:A:882:G:OP2   | 2.34                     | 0.43              |
| 3:E:45:ILE:HG13   | 3:E:61:VAL:HG21  | 2.00                     | 0.43              |
| 4:O:43:HIS:HE1    | 21:A:900:G:N2    | 2.16                     | 0.43              |
| 14:G:172:LYS:NZ   | 21:A:72:A:H62    | 2.17                     | 0.43              |
| 15:H:51:GLN:OE1   | 15:H:59:LYS:HE2  | 2.18                     | 0.43              |
| 21:A:901:U:H2'    | 21:A:902:C:C6    | 2.54                     | 0.43              |
| 2:X:87:ASP:OD1    | 7:e:12:GLY:HA2   | 2.19                     | 0.43              |
| 15:H:12:LYS:O     | 15:H:14:VAL:HG23 | 2.19                     | 0.43              |
| 21:A:589:A:H2'    | 21:A:590:G:H8    | 1.83                     | 0.43              |
| 21:A:855:G:N1     | 21:A:856:G:C5    | 2.87                     | 0.43              |
| 21:A:898:U:O4     | 21:A:899:A:N6    | 2.52                     | 0.43              |
| 2:X:25:LYS:HD2    | 21:A:1114:G:OP2  | 2.18                     | 0.43              |
| 5:W:55:ASP:OD1    | 5:W:55:ASP:N     | 2.52                     | 0.43              |
| 8:k:184:ARG:HG2   | 8:k:184:ARG:HH11 | 1.82                     | 0.43              |
| 14:G:94:ARG:NH1   | 21:A:1683:U:OP1  | 2.52                     | 0.43              |
| 20:I:46:ARG:HG3   | 20:I:56:TRP:CH2  | 2.53                     | 0.43              |
| 21:A:492:G:N2     | 21:A:503:U:H3    | 2.16                     | 0.43              |
| 21:A:1048:A:H2    | 25:A:2293:HOH:O  | 2.01                     | 0.43              |
| 1:Y:15:ARG:HE     | 21:A:786:U:H3    | 1.67                     | 0.42              |
| 15:H:31:GLU:HA    | 15:H:41:LEU:CD1  | 2.41                     | 0.42              |
| 15:H:36:GLU:HG3   | 15:H:79:ARG:HH11 | 1.84                     | 0.42              |
| 21:A:58:U:OP1     | 21:A:460:G:O2'   | 2.35                     | 0.42              |
| 21:A:1087:U:O2'   | 21:A:1088:G:H5'  | 2.18                     | 0.42              |
| 21:A:1634:C:H2'   | 21:A:1635:U:C6   | 2.54                     | 0.42              |
| 1:Y:94:LYS:HE3    | 1:Y:98:ILE:HD11  | 2.01                     | 0.42              |
| 3:E:247:THR:OG1   | 3:E:250:GLU:HG3  | 2.19                     | 0.42              |
| 5:W:51:GLU:OE2    | 15:H:140:ARG:HB3 | 2.19                     | 0.42              |
| 8:k:188:GLN:HG2   | 8:k:193:ILE:HB   | 2.01                     | 0.42              |
| 13:C:123:LEU:HD21 | 13:C:222:LYS:HG3 | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:A:419:C:O2'    | 21:A:422:G:O6     | 2.29                     | 0.42              |
| 21:A:855:G:C2     | 21:A:856:G:C5     | 3.07                     | 0.42              |
| 21:A:1027:C:O2'   | 21:A:1130:A:N1    | 2.43                     | 0.42              |
| 21:A:1108:PSU:H2' | 21:A:1109:U:C6    | 2.54                     | 0.42              |
| 4:O:127:GLY:HA2   | 11:a:58:VAL:HG22  | 2.00                     | 0.42              |
| 10:V:50:THR:HG21  | 10:V:72:TRP:HZ3   | 1.85                     | 0.42              |
| 11:a:46:GLU:O     | 11:a:50:VAL:HG23  | 2.19                     | 0.42              |
| 15:H:68:ARG:O     | 15:H:68:ARG:HG2   | 2.18                     | 0.42              |
| 21:A:53:G:H2'     | 21:A:54:C:C6      | 2.55                     | 0.42              |
| 21:A:347:C:H2'    | 21:A:348:A:C8     | 2.54                     | 0.42              |
| 21:A:389:A:H2'    | 21:A:390:G:C8     | 2.54                     | 0.42              |
| 21:A:647:G:H2'    | 21:A:648:C:C6     | 2.54                     | 0.42              |
| 21:A:793:G:H2'    | 21:A:794:G:O4'    | 2.19                     | 0.42              |
| 21:A:1651:G:H2'   | 21:A:1652:U:H6    | 1.84                     | 0.42              |
| 8:k:93:LYS:HB2    | 8:k:93:LYS:HE2    | 1.64                     | 0.42              |
| 13:C:179:MET:SD   | 13:C:198:LEU:HD21 | 2.59                     | 0.42              |
| 19:n:15:ARG:HG3   | 19:n:18:ARG:NH2   | 2.34                     | 0.42              |
| 21:A:824:U:O2     | 21:A:858:G:N2     | 2.48                     | 0.42              |
| 21:A:1791:G:H2'   | 21:A:1792:MA6:H8  | 2.02                     | 0.42              |
| 9:B:198:GLU:HG3   | 9:B:210:VAL:HG21  | 2.01                     | 0.42              |
| 12:J:145:VAL:HG11 | 21:A:774:C:H1'    | 2.00                     | 0.42              |
| 15:H:69:LEU:H     | 15:H:69:LEU:CD2   | 2.31                     | 0.42              |
| 17:L:23:ASP:OD1   | 17:L:25:ALA:N     | 2.52                     | 0.42              |
| 21:A:383:U:H5''   | 25:A:2307:HOH:O   | 2.19                     | 0.42              |
| 7:e:28:LYS:NZ     | 21:A:481:A:OP1    | 2.52                     | 0.42              |
| 12:J:133:GLN:HB2  | 12:J:135:HIS:CD2  | 2.54                     | 0.42              |
| 14:G:58:LYS:HA    | 14:G:109:SER:OG   | 2.19                     | 0.42              |
| 21:A:155:A:O2'    | 21:A:156:U:H5'    | 2.20                     | 0.42              |
| 21:A:400:G:N2     | 21:A:402:G:H3'    | 2.35                     | 0.42              |
| 21:A:1681:A:H2'   | 21:A:1682:G:H8    | 1.85                     | 0.42              |
| 1:Y:67:ARG:NH1    | 21:A:534:C:O2     | 2.43                     | 0.42              |
| 3:E:101:LEU:HD23  | 3:E:101:LEU:HA    | 1.86                     | 0.42              |
| 5:W:100:GLY:HA2   | 5:W:130:TYR:HB3   | 2.02                     | 0.42              |
| 15:H:77:HIS:O     | 15:H:81:VAL:HG23  | 2.20                     | 0.42              |
| 16:h:97:ARG:C     | 16:h:119:ARG:HE   | 2.28                     | 0.42              |
| 21:A:464:A:H3'    | 21:A:465:G:C8     | 2.52                     | 0.42              |
| 21:A:955:C:H2'    | 21:A:956:A:C8     | 2.55                     | 0.42              |
| 21:A:1013:G:H2'   | 21:A:1014:OMU:H6  | 2.01                     | 0.42              |
| 21:A:1738:A:N7    | 25:A:2045:HOH:O   | 2.36                     | 0.42              |
| 6:b:35:MET:HE1    | 6:b:50:SER:HA     | 2.00                     | 0.42              |
| 8:k:65:ALA:O      | 8:k:69:ILE:HG13   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:B:231:VAL:HG12  | 9:B:231:VAL:O     | 2.19                     | 0.42              |
| 12:J:126:HIS:HA   | 12:J:129:VAL:HG22 | 2.01                     | 0.42              |
| 14:G:33:SER:O     | 14:G:51:LYS:NZ    | 2.47                     | 0.42              |
| 14:G:135:ARG:HH22 | 21:A:147:C:H1'    | 1.85                     | 0.42              |
| 15:H:156:ASP:OD1  | 15:H:157:PRO:HD2  | 2.20                     | 0.42              |
| 21:A:1675:C:H2'   | 21:A:1676:G:C8    | 2.54                     | 0.42              |
| 3:E:44:LEU:HD23   | 3:E:44:LEU:HA     | 1.92                     | 0.42              |
| 3:E:127:ARG:NH2   | 3:E:142:TYR:HA    | 2.35                     | 0.42              |
| 6:b:84:LYS:HE3    | 18:N:25:TRP:CD2   | 2.54                     | 0.42              |
| 9:B:111:ARG:HD3   | 11:a:68:TYR:O     | 2.20                     | 0.42              |
| 9:B:163:GLN:HB3   | 9:B:204:ILE:HD13  | 2.01                     | 0.42              |
| 10:V:15:ARG:NE    | 13:C:68:LEU:O     | 2.53                     | 0.42              |
| 21:A:853:U:H2'    | 21:A:854:C:C6     | 2.55                     | 0.42              |
| 21:A:981:G:N1     | 21:A:1028:A:O2'   | 2.42                     | 0.42              |
| 1:Y:15:ARG:NE     | 21:A:786:U:H3     | 2.17                     | 0.42              |
| 3:E:108:ARG:HE    | 3:E:108:ARG:HB2   | 1.60                     | 0.42              |
| 10:V:17:CYS:HB2   | 10:V:55:SER:HB2   | 2.01                     | 0.42              |
| 20:I:74:THR:O     | 20:I:75:ARG:HD3   | 2.20                     | 0.42              |
| 21:A:594:C:H2'    | 21:A:595:A:H8     | 1.85                     | 0.42              |
| 21:A:648:C:H2'    | 21:A:649:C:C6     | 2.54                     | 0.42              |
| 21:A:1137:A:H2'   | 21:A:1138:A:C8    | 2.54                     | 0.42              |
| 21:A:1754:U:O3'   | 21:A:1755:A:H8    | 2.03                     | 0.42              |
| 4:O:66:ARG:NH2    | 21:A:910:A:H4'    | 2.35                     | 0.41              |
| 7:e:14:VAL:HG21   | 21:A:571:A:N3     | 2.35                     | 0.41              |
| 9:B:39:THR:OG1    | 9:B:40:SER:N      | 2.52                     | 0.41              |
| 12:J:112:GLN:OE1  | 12:J:128:ARG:HD2  | 2.20                     | 0.41              |
| 17:L:70:ARG:HG3   | 21:A:308:PSU:O2'  | 2.20                     | 0.41              |
| 21:A:509:A:H2'    | 21:A:511:U:C5     | 2.55                     | 0.41              |
| 21:A:855:G:C2     | 21:A:856:G:C8     | 3.08                     | 0.41              |
| 21:A:1147:A:H2'   | 21:A:1148:A:C8    | 2.55                     | 0.41              |
| 21:A:1733:A:H2'   | 21:A:1734:G:O4'   | 2.20                     | 0.41              |
| 21:A:1797:G:H2'   | 21:A:1798:C:C6    | 2.55                     | 0.41              |
| 6:b:51:HIS:CE1    | 25:A:2713:HOH:O   | 2.74                     | 0.41              |
| 9:B:82:ARG:NH1    | 9:B:212:VAL:O     | 2.51                     | 0.41              |
| 13:C:236:THR:OG1  | 13:C:238:ASP:OD1  | 2.38                     | 0.41              |
| 21:A:52:U:H2'     | 21:A:53:G:H8      | 1.81                     | 0.41              |
| 21:A:316:A:C2     | 21:A:318:C:H2'    | 2.55                     | 0.41              |
| 21:A:822:G:N1     | 21:A:860:A:C6     | 2.88                     | 0.41              |
| 21:A:912:A:H2'    | 21:A:913:U:H6     | 1.85                     | 0.41              |
| 21:A:1683:U:H2'   | 21:A:1684:G:C8    | 2.56                     | 0.41              |
| 4:O:32:HIS:CD2    | 21:A:923:U:H4'    | 2.55                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:O:147:ARG:O     | 11:a:28:LYS:HG3  | 2.21                     | 0.41              |
| 8:k:62:LEU:HD23   | 8:k:165:ILE:HD13 | 2.02                     | 0.41              |
| 9:B:59:GLU:H      | 9:B:59:GLU:CD    | 2.28                     | 0.41              |
| 10:V:50:THR:HG21  | 10:V:72:TRP:CZ3  | 2.56                     | 0.41              |
| 11:a:88:SER:O     | 11:a:92:ARG:HG3  | 2.20                     | 0.41              |
| 12:J:80:ARG:NH2   | 21:A:770:U:OP1   | 2.51                     | 0.41              |
| 13:C:68:LEU:HD12  | 13:C:68:LEU:HA   | 1.90                     | 0.41              |
| 14:G:205:LYS:O    | 14:G:209:GLU:HG3 | 2.21                     | 0.41              |
| 15:H:165:TYR:CZ   | 15:H:166:LYS:HE3 | 2.55                     | 0.41              |
| 21:A:31:C:O2'     | 21:A:551:U:OP1   | 2.36                     | 0.41              |
| 21:A:392:OMG:OP2  | 21:A:427:G:O2'   | 2.37                     | 0.41              |
| 21:A:491:G:N2     | 21:A:505:U:O2    | 2.53                     | 0.41              |
| 21:A:570:C:H2'    | 21:A:571:A:O4'   | 2.20                     | 0.41              |
| 21:A:775:A:H2'    | 21:A:776:A:C8    | 2.56                     | 0.41              |
| 21:A:818:A:N6     | 21:A:864:A:OP2   | 2.54                     | 0.41              |
| 8:k:22:MET:HB3    | 8:k:55:LEU:HD21  | 2.02                     | 0.41              |
| 20:I:191:ARG:HD3  | 25:I:301:HOH:O   | 2.19                     | 0.41              |
| 21:A:30:G:H2'     | 21:A:31:C:H6     | 1.86                     | 0.41              |
| 21:A:432:A:H2'    | 21:A:433:G:O4'   | 2.20                     | 0.41              |
| 21:A:894:U:H2'    | 21:A:895:U:C6    | 2.55                     | 0.41              |
| 21:A:999:G:H2'    | 21:A:1000:A:C8   | 2.55                     | 0.41              |
| 4:O:71:PRO:HB3    | 4:O:114:SER:HB2  | 2.03                     | 0.41              |
| 15:H:10:LYS:HZ3   | 15:H:48:THR:HA   | 1.85                     | 0.41              |
| 20:I:217:LYS:HB2  | 20:I:217:LYS:HE3 | 1.85                     | 0.41              |
| 21:A:415:C:H2'    | 21:A:416:A:O4'   | 2.21                     | 0.41              |
| 21:A:417:U:H2'    | 21:A:418:OMC:H6  | 1.86                     | 0.41              |
| 21:A:973:U:H2'    | 21:A:974:C:O4'   | 2.21                     | 0.41              |
| 1:Y:99:ARG:NH1    | 25:Y:204:HOH:O   | 2.54                     | 0.41              |
| 8:k:124:ARG:CZ    | 13:C:251:GLN:HB3 | 2.50                     | 0.41              |
| 9:B:61:LEU:HG     | 9:B:96:VAL:HG21  | 2.02                     | 0.41              |
| 15:H:160:ARG:HE   | 15:H:160:ARG:HB2 | 1.77                     | 0.41              |
| 18:N:102:LEU:HD21 | 18:N:111:SER:HB2 | 2.03                     | 0.41              |
| 21:A:819:U:H1'    | 21:A:821:G:C4    | 2.55                     | 0.41              |
| 21:A:1657:C:H2'   | 21:A:1658:C:C6   | 2.56                     | 0.41              |
| 3:E:80:LYS:H      | 3:E:80:LYS:HG2   | 1.70                     | 0.41              |
| 4:O:57:THR:HB     | 4:O:60:MET:HB2   | 2.03                     | 0.41              |
| 12:J:13:THR:HG23  | 21:A:476:U:H5''  | 2.01                     | 0.41              |
| 13:C:151:ARG:HE   | 13:C:151:ARG:HB2 | 1.69                     | 0.41              |
| 21:A:1138:A:H2'   | 21:A:1139:C:O4'  | 2.21                     | 0.41              |
| 2:X:107:LYS:HD2   | 2:X:107:LYS:N    | 2.35                     | 0.41              |
| 5:W:28:ARG:HD3    | 5:W:60:LYS:HZ2   | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:B:27:LYS:HA    | 9:B:49:SER:HA    | 2.03                     | 0.41              |
| 11:a:11:ASN:OD1  | 21:A:939:C:H1'   | 2.21                     | 0.41              |
| 15:H:79:ARG:HA   | 15:H:82:ARG:HD2  | 2.03                     | 0.41              |
| 20:I:84:TYR:HB3  | 20:I:102:ILE:HB  | 2.03                     | 0.41              |
| 21:A:179:A:H2'   | 21:A:180:A:O4'   | 2.20                     | 0.41              |
| 21:A:614:G:N3    | 21:A:614:G:H2'   | 2.35                     | 0.41              |
| 21:A:850:G:H2'   | 21:A:851:G:C8    | 2.56                     | 0.41              |
| 21:A:1076:C:H2'  | 21:A:1077:C:C6   | 2.55                     | 0.41              |
| 21:A:1663:G:N2   | 21:A:1756:G:H2'  | 2.35                     | 0.41              |
| 1:Y:30:LEU:HD22  | 1:Y:49:LEU:HD11  | 2.03                     | 0.41              |
| 1:Y:86:GLU:CD    | 1:Y:86:GLU:N     | 2.78                     | 0.41              |
| 1:Y:117:LYS:HE3  | 1:Y:117:LYS:HB3  | 1.90                     | 0.41              |
| 3:E:22:LYS:NZ    | 12:J:7:TYR:O     | 2.52                     | 0.41              |
| 8:k:107:HIS:O    | 8:k:109:PRO:HD3  | 2.21                     | 0.41              |
| 9:B:28:GLN:HB2   | 9:B:30:TYR:HE1   | 1.85                     | 0.41              |
| 9:B:48:VAL:HG21  | 9:B:61:LEU:HD22  | 2.03                     | 0.41              |
| 14:G:26:ASN:ND2  | 14:G:40:LEU:HB3  | 2.36                     | 0.41              |
| 14:G:30:LYS:HE3  | 14:G:36:VAL:HG22 | 2.03                     | 0.41              |
| 14:G:199:LYS:HB3 | 21:A:176:A:N6    | 2.35                     | 0.41              |
| 15:H:31:GLU:HG2  | 15:H:41:LEU:CD2  | 2.50                     | 0.41              |
| 15:H:84:LEU:O    | 15:H:87:LYS:HB2  | 2.21                     | 0.41              |
| 21:A:128:G:OP1   | 21:A:201:G:O2'   | 2.36                     | 0.41              |
| 21:A:129:U:H5    | 21:A:201:G:H5'   | 1.86                     | 0.41              |
| 21:A:492:G:H22   | 21:A:503:U:H3    | 1.69                     | 0.41              |
| 21:A:635:G:H2'   | 21:A:636:PSU:H6  | 1.86                     | 0.41              |
| 21:A:830:U:H2'   | 21:A:831:C:C6    | 2.56                     | 0.41              |
| 21:A:1752:U:H2'  | 21:A:1753:U:C6   | 2.56                     | 0.41              |
| 6:b:10:LEU:HD22  | 15:H:140:ARG:HD3 | 2.03                     | 0.41              |
| 8:k:17:GLN:O     | 8:k:20:GLN:HB3   | 2.21                     | 0.41              |
| 8:k:108:THR:O    | 8:k:109:PRO:C    | 2.64                     | 0.41              |
| 16:h:114:LEU:H   | 16:h:114:LEU:CD1 | 2.34                     | 0.41              |
| 21:A:305:A:H2'   | 21:A:306:PSU:O4' | 2.21                     | 0.41              |
| 2:X:87:ASP:OD1   | 2:X:87:ASP:C     | 2.63                     | 0.40              |
| 9:B:222:LYS:HA   | 9:B:222:LYS:HD2  | 1.90                     | 0.40              |
| 13:C:63:MET:HG2  | 13:C:82:LEU:HB2  | 2.02                     | 0.40              |
| 17:L:57:LYS:HG3  | 17:L:58:LYS:HG3  | 2.04                     | 0.40              |
| 21:A:45:U:O2     | 21:A:438:G:H1'   | 2.21                     | 0.40              |
| 21:A:824:U:H2'   | 21:A:825:U:H6    | 1.85                     | 0.40              |
| 21:A:825:U:H2'   | 21:A:826:C:H6    | 1.86                     | 0.40              |
| 21:A:1656:U:H2'  | 21:A:1657:C:H6   | 1.85                     | 0.40              |
| 21:A:1722:A:H2'  | 21:A:1723:C:C6   | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:k:149:ILE:HG12 | 8:k:163:ILE:HB   | 2.03                     | 0.40              |
| 18:N:128:TYR:HE1 | 21:A:969:U:H5''  | 1.86                     | 0.40              |
| 21:A:37:U:O2'    | 21:A:776:A:N1    | 2.51                     | 0.40              |
| 21:A:193:G:H2'   | 21:A:194:G:O4'   | 2.20                     | 0.40              |
| 21:A:417:U:C2    | 21:A:418:OMC:C5  | 3.10                     | 0.40              |
| 21:A:644:U:N3    | 21:A:645:G:N7    | 2.69                     | 0.40              |
| 21:A:692:C:H2'   | 21:A:693:C:H6    | 1.75                     | 0.40              |
| 21:A:958:G:H1'   | 25:A:2511:HOH:O  | 2.20                     | 0.40              |
| 2:X:56:ILE:HD11  | 2:X:114:ILE:HG23 | 2.03                     | 0.40              |
| 9:B:145:ARG:NH2  | 9:B:151:LYS:O    | 2.47                     | 0.40              |
| 9:B:224:ASP:CG   | 9:B:227:LYS:HG3  | 2.45                     | 0.40              |
| 10:V:33:GLN:HG3  | 10:V:53:ALA:HB2  | 2.02                     | 0.40              |
| 11:a:37:LYS:HG2  | 11:a:72:HIS:ND1  | 2.36                     | 0.40              |
| 15:H:39:SER:HA   | 15:H:42:LYS:HE3  | 2.03                     | 0.40              |
| 16:h:100:LYS:HA  | 16:h:103:MET:SD  | 2.61                     | 0.40              |
| 21:A:330:G:H2'   | 21:A:331:U:C6    | 2.57                     | 0.40              |
| 21:A:378:U:H2'   | 21:A:379:U:C6    | 2.57                     | 0.40              |
| 21:A:812:A:H2'   | 21:A:813:A:C8    | 2.52                     | 0.40              |
| 21:A:824:U:C2    | 21:A:825:U:C5    | 3.09                     | 0.40              |
| 2:X:47:LYS:HG3   | 21:A:439:C:H5''  | 2.04                     | 0.40              |
| 2:X:104:PHE:O    | 2:X:111:VAL:HG21 | 2.21                     | 0.40              |
| 2:X:133:PHE:O    | 7:e:15:ARG:NH2   | 2.53                     | 0.40              |
| 8:k:29:LEU:HD23  | 8:k:29:LEU:HA    | 1.84                     | 0.40              |
| 8:k:41:TYR:CD1   | 8:k:166:PRO:HG3  | 2.57                     | 0.40              |
| 8:k:77:ASP:OD1   | 13:C:50:LYS:NZ   | 2.50                     | 0.40              |
| 15:H:45:TYR:H    | 15:H:69:LEU:HD11 | 1.86                     | 0.40              |
| 18:N:43:LYS:HD2  | 18:N:43:LYS:H    | 1.87                     | 0.40              |
| 19:n:15:ARG:HG2  | 19:n:19:LYS:HE3  | 2.03                     | 0.40              |
| 21:A:862:U:C2'   | 21:A:863:G:H5'   | 2.52                     | 0.40              |
| 21:A:999:G:H2'   | 21:A:1000:A:H8   | 1.86                     | 0.40              |
| 21:A:1068:G:C2   | 21:A:1069:G:C8   | 3.09                     | 0.40              |
| 21:A:1661:C:H2'  | 21:A:1662:C:C6   | 2.56                     | 0.40              |
| 21:A:1669:A:N1   | 21:A:1753:U:C2   | 2.90                     | 0.40              |
| 3:E:36:HIS:CG    | 3:E:85:GLY:HA3   | 2.56                     | 0.40              |
| 8:k:19:ILE:HG23  | 8:k:55:LEU:HB3   | 2.03                     | 0.40              |
| 9:B:179:CYS:HB3  | 9:B:183:GLU:CG   | 2.51                     | 0.40              |
| 18:N:100:LYS:O   | 18:N:104:ARG:HG3 | 2.21                     | 0.40              |
| 21:A:161:G:OP2   | 21:A:161:G:N2    | 2.43                     | 0.40              |
| 21:A:928:A:H2'   | 21:A:929:A:C8    | 2.56                     | 0.40              |
| 21:A:1094:U:O2'  | 21:A:1098:A:N1   | 2.52                     | 0.40              |
| 21:A:1695:G:C6   | 21:A:1696:G:N7   | 2.90                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 21:A:1766:A:H3' | 21:A:1767:A:H5'' | 2.03                     | 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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | Y     | 122/137 (89%) | 121 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 2   | X     | 138/142 (97%) | 132 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 3   | E     | 258/265 (97%) | 253 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 4   | O     | 126/151 (83%) | 123 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 5   | W     | 127/130 (98%) | 126 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 6   | b     | 81/86 (94%)   | 72 (89%)  | 9 (11%) | 0        | 100         | 100 |
| 7   | e     | 44/62 (71%)   | 42 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 8   | k     | 197/308 (64%) | 192 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 9   | B     | 208/263 (79%) | 203 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 10  | V     | 79/81 (98%)   | 77 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 11  | a     | 96/139 (69%)  | 94 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 12  | J     | 179/195 (92%) | 177 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 13  | C     | 212/275 (77%) | 206 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 14  | G     | 228/250 (91%) | 225 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 15  | H     | 182/192 (95%) | 170 (93%) | 12 (7%) | 0        | 100         | 100 |
| 16  | h     | 25/143 (18%)  | 23 (92%)  | 2 (8%)  | 0        | 100         | 100 |
| 17  | L     | 144/159 (91%) | 143 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 18  | N     | 139/151 (92%) | 136 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 19  | n     | 21/25 (84%)   | 21 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 20  | I     | 182/224 (81%)   | 176 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| All | All   | 2788/3378 (82%) | 2712 (97%) | 76 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | Y     | 108/117 (92%) | 108 (100%) | 0        | 100         | 100 |
| 2   | X     | 111/113 (98%) | 109 (98%)  | 2 (2%)   | 51          | 64  |
| 3   | E     | 222/224 (99%) | 222 (100%) | 0        | 100         | 100 |
| 4   | O     | 101/120 (84%) | 100 (99%)  | 1 (1%)   | 68          | 79  |
| 5   | W     | 111/112 (99%) | 111 (100%) | 0        | 100         | 100 |
| 6   | b     | 76/78 (97%)   | 75 (99%)   | 1 (1%)   | 61          | 73  |
| 7   | e     | 39/49 (80%)   | 39 (100%)  | 0        | 100         | 100 |
| 8   | k     | 170/233 (73%) | 169 (99%)  | 1 (1%)   | 78          | 86  |
| 9   | B     | 189/228 (83%) | 184 (97%)  | 5 (3%)   | 40          | 53  |
| 10  | V     | 65/65 (100%)  | 64 (98%)   | 1 (2%)   | 57          | 69  |
| 11  | a     | 85/108 (79%)  | 84 (99%)   | 1 (1%)   | 63          | 75  |
| 12  | J     | 154/162 (95%) | 152 (99%)  | 2 (1%)   | 61          | 73  |
| 13  | C     | 181/219 (83%) | 179 (99%)  | 2 (1%)   | 65          | 77  |
| 14  | G     | 202/215 (94%) | 201 (100%) | 1 (0%)   | 81          | 88  |
| 15  | H     | 164/171 (96%) | 163 (99%)  | 1 (1%)   | 78          | 86  |
| 16  | h     | 22/124 (18%)  | 21 (96%)   | 1 (4%)   | 24          | 32  |
| 17  | L     | 125/132 (95%) | 125 (100%) | 0        | 100         | 100 |
| 18  | N     | 123/131 (94%) | 121 (98%)  | 2 (2%)   | 55          | 67  |
| 19  | n     | 22/24 (92%)   | 22 (100%)  | 0        | 100         | 100 |
| 20  | I     | 160/179 (89%) | 158 (99%)  | 2 (1%)   | 61          | 73  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All   | 2430/2804 (87%) | 2407 (99%) | 23 (1%)  | 68 80       |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | X     | 4   | THR  |
| 2   | X     | 54  | ILE  |
| 4   | O     | 81  | VAL  |
| 6   | b     | 19  | LEU  |
| 8   | k     | 103 | ILE  |
| 9   | B     | 48  | VAL  |
| 9   | B     | 112 | SER  |
| 9   | B     | 131 | ASP  |
| 9   | B     | 175 | GLN  |
| 9   | B     | 232 | HIS  |
| 10  | V     | 9   | VAL  |
| 11  | a     | 95  | ARG  |
| 12  | J     | 59  | ARG  |
| 12  | J     | 142 | ILE  |
| 13  | C     | 232 | TYR  |
| 13  | C     | 254 | THR  |
| 14  | G     | 200 | LYS  |
| 15  | H     | 126 | ILE  |
| 16  | h     | 108 | PHE  |
| 18  | N     | 3   | ARG  |
| 18  | N     | 103 | GLU  |
| 20  | I     | 175 | ILE  |
| 20  | I     | 204 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 20  | ASN  |
| 2   | X     | 91  | ASN  |
| 3   | E     | 62  | GLN  |
| 6   | b     | 51  | HIS  |
| 9   | B     | 79  | GLN  |
| 9   | B     | 209 | ASN  |
| 11  | a     | 25  | ASN  |
| 13  | C     | 97  | GLN  |
| 13  | C     | 120 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | N     | 123 | HIS  |
| 20  | I     | 85  | ASN  |
| 20  | I     | 174 | HIS  |
| 20  | I     | 194 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 21  | A     | 1164/1810 (64%) | 207 (17%)         | 0               |

All (207) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | A     | 14  | C    |
| 21  | A     | 25  | C    |
| 21  | A     | 26  | A    |
| 21  | A     | 34  | G    |
| 21  | A     | 42  | G    |
| 21  | A     | 47  | A    |
| 21  | A     | 59  | G    |
| 21  | A     | 68  | A    |
| 21  | A     | 83  | U    |
| 21  | A     | 105 | A    |
| 21  | A     | 112 | U    |
| 21  | A     | 115 | A    |
| 21  | A     | 116 | G    |
| 21  | A     | 128 | G    |
| 21  | A     | 129 | U    |
| 21  | A     | 139 | U    |
| 21  | A     | 151 | A    |
| 21  | A     | 156 | U    |
| 21  | A     | 158 | C    |
| 21  | A     | 164 | C    |
| 21  | A     | 176 | A    |
| 21  | A     | 177 | C    |
| 21  | A     | 189 | U    |
| 21  | A     | 191 | U    |
| 21  | A     | 192 | G    |
| 21  | A     | 201 | G    |
| 21  | A     | 252 | U    |
| 21  | A     | 253 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | A     | 260 | A    |
| 21  | A     | 264 | G    |
| 21  | A     | 266 | C    |
| 21  | A     | 275 | C    |
| 21  | A     | 278 | C    |
| 21  | A     | 291 | G    |
| 21  | A     | 303 | A    |
| 21  | A     | 318 | C    |
| 21  | A     | 320 | A    |
| 21  | A     | 326 | G    |
| 21  | A     | 341 | G    |
| 21  | A     | 342 | C    |
| 21  | A     | 365 | C    |
| 21  | A     | 370 | A    |
| 21  | A     | 374 | A    |
| 21  | A     | 377 | G    |
| 21  | A     | 384 | U    |
| 21  | A     | 394 | G    |
| 21  | A     | 397 | C    |
| 21  | A     | 404 | A    |
| 21  | A     | 405 | A    |
| 21  | A     | 406 | C    |
| 21  | A     | 408 | G    |
| 21  | A     | 420 | A    |
| 21  | A     | 421 | A    |
| 21  | A     | 423 | G    |
| 21  | A     | 427 | G    |
| 21  | A     | 428 | C    |
| 21  | A     | 430 | G    |
| 21  | A     | 438 | G    |
| 21  | A     | 443 | U    |
| 21  | A     | 448 | C    |
| 21  | A     | 449 | A    |
| 21  | A     | 457 | C    |
| 21  | A     | 458 | A    |
| 21  | A     | 472 | A    |
| 21  | A     | 473 | C    |
| 21  | A     | 481 | A    |
| 21  | A     | 486 | U    |
| 21  | A     | 490 | G    |
| 21  | A     | 491 | G    |
| 21  | A     | 504 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | A     | 505 | U    |
| 21  | A     | 509 | A    |
| 21  | A     | 510 | A    |
| 21  | A     | 511 | U    |
| 21  | A     | 512 | U    |
| 21  | A     | 514 | G    |
| 21  | A     | 515 | A    |
| 21  | A     | 523 | C    |
| 21  | A     | 531 | A    |
| 21  | A     | 538 | A    |
| 21  | A     | 542 | A    |
| 21  | A     | 546 | U    |
| 21  | A     | 553 | G    |
| 21  | A     | 559 | A    |
| 21  | A     | 572 | G    |
| 21  | A     | 575 | G    |
| 21  | A     | 582 | U    |
| 21  | A     | 583 | A    |
| 21  | A     | 586 | U    |
| 21  | A     | 598 | A    |
| 21  | A     | 610 | A    |
| 21  | A     | 623 | A2M  |
| 21  | A     | 624 | A    |
| 21  | A     | 626 | A    |
| 21  | A     | 627 | A    |
| 21  | A     | 628 | G    |
| 21  | A     | 642 | C    |
| 21  | A     | 643 | U    |
| 21  | A     | 645 | G    |
| 21  | A     | 749 | G    |
| 21  | A     | 772 | C    |
| 21  | A     | 777 | A    |
| 21  | A     | 784 | C    |
| 21  | A     | 785 | A    |
| 21  | A     | 786 | U    |
| 21  | A     | 787 | C    |
| 21  | A     | 788 | G    |
| 21  | A     | 791 | C    |
| 21  | A     | 792 | U    |
| 21  | A     | 795 | A    |
| 21  | A     | 816 | U    |
| 21  | A     | 818 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | A     | 819  | U    |
| 21  | A     | 820  | A    |
| 21  | A     | 821  | G    |
| 21  | A     | 822  | G    |
| 21  | A     | 823  | A    |
| 21  | A     | 825  | U    |
| 21  | A     | 828  | G    |
| 21  | A     | 861  | A    |
| 21  | A     | 862  | U    |
| 21  | A     | 863  | G    |
| 21  | A     | 865  | U    |
| 21  | A     | 867  | A    |
| 21  | A     | 868  | A    |
| 21  | A     | 881  | G    |
| 21  | A     | 911  | A    |
| 21  | A     | 919  | G    |
| 21  | A     | 931  | A    |
| 21  | A     | 938  | A    |
| 21  | A     | 940  | U    |
| 21  | A     | 947  | G    |
| 21  | A     | 950  | U    |
| 21  | A     | 965  | U    |
| 21  | A     | 971  | A    |
| 21  | A     | 975  | A    |
| 21  | A     | 976  | A    |
| 21  | A     | 978  | A    |
| 21  | A     | 1003 | A    |
| 21  | A     | 1006 | A    |
| 21  | A     | 1008 | A    |
| 21  | A     | 1009 | U    |
| 21  | A     | 1010 | A    |
| 21  | A     | 1016 | C    |
| 21  | A     | 1031 | A    |
| 21  | A     | 1033 | C    |
| 21  | A     | 1035 | A    |
| 21  | A     | 1043 | C    |
| 21  | A     | 1058 | G    |
| 21  | A     | 1061 | G    |
| 21  | A     | 1062 | C    |
| 21  | A     | 1063 | U    |
| 21  | A     | 1070 | A    |
| 21  | A     | 1072 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | A     | 1075 | G    |
| 21  | A     | 1081 | A    |
| 21  | A     | 1087 | U    |
| 21  | A     | 1094 | U    |
| 21  | A     | 1097 | A    |
| 21  | A     | 1099 | G    |
| 21  | A     | 1102 | U    |
| 21  | A     | 1103 | U    |
| 21  | A     | 1118 | A    |
| 21  | A     | 1131 | OMG  |
| 21  | A     | 1143 | A    |
| 21  | A     | 1155 | G    |
| 21  | A     | 1156 | A    |
| 21  | A     | 1640 | A    |
| 21  | A     | 1643 | C    |
| 21  | A     | 1644 | A    |
| 21  | A     | 1645 | C    |
| 21  | A     | 1646 | C    |
| 21  | A     | 1647 | G    |
| 21  | A     | 1655 | C    |
| 21  | A     | 1656 | U    |
| 21  | A     | 1664 | A    |
| 21  | A     | 1666 | U    |
| 21  | A     | 1667 | G    |
| 21  | A     | 1671 | G    |
| 21  | A     | 1673 | U    |
| 21  | A     | 1674 | C    |
| 21  | A     | 1676 | G    |
| 21  | A     | 1677 | G    |
| 21  | A     | 1689 | G    |
| 21  | A     | 1695 | G    |
| 21  | A     | 1697 | C    |
| 21  | A     | 1726 | C    |
| 21  | A     | 1727 | G    |
| 21  | A     | 1753 | U    |
| 21  | A     | 1754 | U    |
| 21  | A     | 1761 | A2M  |
| 21  | A     | 1766 | A    |
| 21  | A     | 1767 | A    |
| 21  | A     | 1771 | G    |
| 21  | A     | 1773 | A    |
| 21  | A     | 1777 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | A     | 1780 | U    |
| 21  | A     | 1791 | G    |
| 21  | A     | 1793 | MA6  |
| 21  | A     | 1794 | C    |
| 21  | A     | 1803 | G    |
| 21  | A     | 1804 | G    |
| 21  | A     | 1805 | A    |
| 21  | A     | 1806 | U    |
| 21  | A     | 1807 | C    |
| 21  | A     | 1809 | U    |
| 21  | A     | 1810 | U    |

There are no RNA pucker outliers to report.

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

57 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 | $\# Z  > 2$ |
| 21  | A2M  | A     | 623  | 21,23    | 22,25,26     | 0.31 | 0           | 31,36,39    | 0.57 | 0           |
| 21  | PSU  | A     | 811  | 21       | 18,21,22     | 0.51 | 0           | 22,30,33    | 0.59 | 0           |
| 21  | PSU  | A     | 607  | 21       | 18,21,22     | 0.53 | 0           | 22,30,33    | 0.56 | 0           |
| 21  | 6MZ  | A     | 1774 | 21,24,23 | 22,25,26     | 0.38 | 0           | 30,36,39    | 0.81 | 1 (3%)      |
| 21  | A2M  | A     | 440  | 21       | 22,25,26     | 0.17 | 0           | 31,36,39    | 0.37 | 0           |
| 21  | OMU  | A     | 168  | 21       | 19,22,23     | 0.41 | 0           | 26,31,34    | 0.88 | 1 (3%)      |
| 21  | OMU  | A     | 1014 | 21       | 19,22,23     | 0.34 | 0           | 26,31,34    | 0.50 | 0           |
| 21  | PSU  | A     | 258  | 21       | 18,21,22     | 0.50 | 0           | 22,30,33    | 0.59 | 0           |
| 21  | PSU  | A     | 300  | 21       | 18,21,22     | 0.50 | 0           | 22,30,33    | 0.56 | 0           |
| 21  | PSU  | A     | 111  | 21,24    | 18,21,22     | 0.52 | 0           | 22,30,33    | 0.59 | 0           |
| 21  | PSU  | A     | 1637 | 21       | 18,21,22     | 0.52 | 0           | 22,30,33    | 0.57 | 0           |
| 21  | A2M  | A     | 545  | 21       | 22,25,26     | 0.20 | 0           | 31,36,39    | 0.56 | 0           |
| 21  | OMU  | A     | 123  | 21       | 19,22,23     | 0.36 | 0           | 26,31,34    | 0.46 | 0           |
| 21  | PSU  | A     | 208  | 21       | 18,21,22     | 0.50 | 0           | 22,30,33    | 0.59 | 0           |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | OMC  | A     | 38   | 21    | 19,22,23     | 0.33 | 0        | 26,31,34    | 0.51 | 0        |
| 21  | A2M  | A     | 468  | 21    | 22,25,26     | 0.24 | 0        | 31,36,39    | 0.65 | 0        |
| 21  | OMG  | A     | 599  | 21    | 23,26,27     | 0.36 | 0        | 33,38,41    | 0.42 | 0        |
| 21  | OMC  | A     | 418  | 21    | 19,22,23     | 0.30 | 0        | 26,31,34    | 0.47 | 0        |
| 21  | A2M  | A     | 1761 | 21    | 22,25,26     | 0.16 | 0        | 31,36,39    | 0.39 | 0        |
| 21  | OMU  | A     | 615  | 21    | 19,22,23     | 1.70 | 4 (21%)  | 26,31,34    | 1.83 | 6 (23%)  |
| 21  | 4AC  | A     | 1784 | 21    | 21,24,25     | 0.43 | 0        | 29,34,37    | 0.60 | 0        |
| 21  | A2M  | A     | 28   | 21    | 22,25,26     | 0.24 | 0        | 31,36,39    | 0.38 | 0        |
| 21  | MA6  | A     | 1792 | 21    | 23,26,27     | 0.36 | 0        | 34,38,41    | 0.71 | 2 (5%)   |
| 21  | PSU  | A     | 1108 | 21    | 18,21,22     | 0.53 | 0        | 22,30,33    | 0.57 | 0        |
| 21  | PSU  | A     | 1310 | 21    | 18,21,22     | 0.53 | 0        | 22,30,33    | 0.40 | 0        |
| 21  | UY1  | A     | 604  | 21    | 19,22,23     | 0.50 | 0        | 22,31,34    | 0.61 | 0        |
| 21  | PSU  | A     | 121  | 21    | 18,21,22     | 0.50 | 0        | 22,30,33    | 0.76 | 0        |
| 21  | PSU  | A     | 1306 | 21    | 18,21,22     | 0.57 | 0        | 22,30,33    | 0.55 | 0        |
| 21  | PSU  | A     | 362  | 21    | 18,21,22     | 0.50 | 0        | 22,30,33    | 0.63 | 0        |
| 10  | AME  | V     | 1    | 10    | 9,10,11      | 1.37 | 1 (11%)  | 9,11,13     | 1.62 | 2 (22%)  |
| 21  | PSU  | A     | 1084 | 21    | 18,21,22     | 0.48 | 0        | 22,30,33    | 0.63 | 0        |
| 21  | PSU  | A     | 806  | 21    | 18,21,22     | 0.48 | 0        | 22,30,33    | 0.61 | 0        |
| 21  | PSU  | A     | 1004 | 21    | 18,21,22     | 0.49 | 0        | 22,30,33    | 0.59 | 0        |
| 21  | PSU  | A     | 636  | 21    | 18,21,22     | 0.55 | 0        | 22,30,33    | 0.58 | 0        |
| 21  | PSU  | A     | 1122 | 21    | 18,21,22     | 0.50 | 0        | 22,30,33    | 0.61 | 0        |
| 21  | OMG  | A     | 1131 | 21    | 23,26,27     | 0.36 | 0        | 33,38,41    | 0.46 | 0        |
| 21  | PSU  | A     | 308  | 21    | 18,21,22     | 0.56 | 0        | 22,30,33    | 0.57 | 0        |
| 21  | MA6  | A     | 1793 | 21    | 23,26,27     | 0.35 | 0        | 34,38,41    | 0.89 | 2 (5%)   |
| 21  | A2M  | A     | 802  | 21    | 22,25,26     | 0.22 | 0        | 31,36,39    | 0.70 | 1 (3%)   |
| 21  | A2M  | A     | 424  | 21    | 22,25,26     | 0.22 | 0        | 31,36,39    | 0.55 | 0        |
| 21  | OMC  | A     | 1648 | 21    | 19,22,23     | 0.33 | 0        | 26,31,34    | 0.50 | 0        |
| 21  | OMG  | A     | 434  | 21    | 23,26,27     | 0.34 | 0        | 33,38,41    | 0.39 | 0        |
| 21  | PSU  | A     | 103  | 21    | 18,21,22     | 0.52 | 0        | 22,30,33    | 0.56 | 0        |
| 21  | PSU  | A     | 35   | 21    | 18,21,22     | 0.52 | 0        | 22,30,33    | 0.58 | 0        |
| 21  | A2M  | A     | 162  | 21    | 22,25,26     | 0.18 | 0        | 31,36,39    | 0.55 | 0        |
| 21  | PSU  | A     | 606  | 21    | 18,21,22     | 0.53 | 0        | 22,30,33    | 0.59 | 0        |
| 21  | PSU  | A     | 764  | 21    | 18,21,22     | 0.50 | 0        | 22,30,33    | 0.66 | 0        |
| 21  | PSU  | A     | 306  | 21    | 18,21,22     | 0.54 | 0        | 22,30,33    | 0.57 | 0        |
| 21  | PSU  | A     | 765  | 21    | 18,21,22     | 0.48 | 0        | 22,30,33    | 0.59 | 0        |
| 21  | OMG  | A     | 392  | 21    | 23,26,27     | 0.35 | 0        | 33,38,41    | 0.44 | 0        |
| 21  | A2M  | A     | 979  | 21    | 22,25,26     | 0.25 | 0        | 31,36,39    | 0.55 | 0        |
| 4   | IAS  | O     | 138  | 4     | 6,7,8        | 0.82 | 0        | 6,8,10      | 1.06 | 0        |
| 21  | OMG  | A     | 246  | 21    | 23,26,27     | 0.33 | 0        | 33,38,41    | 0.44 | 0        |
| 21  | PSU  | A     | 255  | 21,23 | 18,21,22     | 0.50 | 0        | 22,30,33    | 0.60 | 0        |
| 21  | PSU  | A     | 1295 | 21    | 18,21,22     | 0.46 | 0        | 22,30,33    | 0.60 | 0        |
| 21  | OMG  | A     | 1300 | 21    | 23,26,27     | 0.35 | 0        | 33,38,41    | 0.49 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | PSU  | A     | 1100 | 21   | 18,21,22     | 0.54 | 0        | 22,30,33    | 0.55 | 0        |

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   |
|-----|------|-------|------|----------|---------|------------|---------|
| 21  | A2M  | A     | 623  | 21,23    | -       | 3/9/27/28  | 0/3/3/3 |
| 21  | PSU  | A     | 811  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 607  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | 6MZ  | A     | 1774 | 21,24,23 | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | A2M  | A     | 440  | 21       | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | OMU  | A     | 168  | 21       | -       | 0/9/27/28  | 0/2/2/2 |
| 21  | OMU  | A     | 1014 | 21       | -       | 0/9/27/28  | 0/2/2/2 |
| 21  | PSU  | A     | 258  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 300  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 111  | 21,24    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 1637 | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | A2M  | A     | 545  | 21       | -       | 1/9/27/28  | 0/3/3/3 |
| 21  | OMU  | A     | 123  | 21       | -       | 1/9/27/28  | 0/2/2/2 |
| 21  | PSU  | A     | 208  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | OMC  | A     | 38   | 21       | -       | 0/9/27/28  | 0/2/2/2 |
| 21  | A2M  | A     | 468  | 21       | -       | 2/9/27/28  | 0/3/3/3 |
| 21  | OMG  | A     | 599  | 21       | -       | 1/9/27/28  | 0/3/3/3 |
| 21  | OMC  | A     | 418  | 21       | -       | 0/9/27/28  | 0/2/2/2 |
| 21  | A2M  | A     | 1761 | 21       | -       | 2/9/27/28  | 0/3/3/3 |
| 21  | OMU  | A     | 615  | 21       | -       | 1/9/27/28  | 0/2/2/2 |
| 21  | 4AC  | A     | 1784 | 21       | -       | 0/11/29/30 | 0/2/2/2 |
| 21  | A2M  | A     | 28   | 21       | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | MA6  | A     | 1792 | 21       | -       | 0/11/29/30 | 0/3/3/3 |
| 21  | PSU  | A     | 1108 | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 1310 | 21       | -       | 2/7/25/26  | 0/2/2/2 |
| 21  | UY1  | A     | 604  | 21       | -       | 0/9/27/28  | 0/2/2/2 |
| 21  | PSU  | A     | 121  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 1306 | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 362  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 10  | AME  | V     | 1    | 10       | -       | 2/9/10/12  | -       |
| 21  | PSU  | A     | 1084 | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 806  | 21       | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 1004 | 21       | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 21  | PSU  | A     | 636  | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 1122 | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | OMG  | A     | 1131 | 21    | -       | 1/9/27/28  | 0/3/3/3 |
| 21  | PSU  | A     | 308  | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | MA6  | A     | 1793 | 21    | -       | 2/11/29/30 | 0/3/3/3 |
| 21  | A2M  | A     | 802  | 21    | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | A2M  | A     | 424  | 21    | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | OMC  | A     | 1648 | 21    | -       | 2/9/27/28  | 0/2/2/2 |
| 21  | OMG  | A     | 434  | 21    | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | PSU  | A     | 103  | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 35   | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | A2M  | A     | 162  | 21    | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | PSU  | A     | 606  | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 764  | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 306  | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 765  | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | OMG  | A     | 392  | 21    | -       | 2/9/27/28  | 0/3/3/3 |
| 21  | A2M  | A     | 979  | 21    | -       | 0/9/27/28  | 0/3/3/3 |
| 4   | IAS  | O     | 138  | 4     | -       | 1/7/7/8    | -       |
| 21  | OMG  | A     | 246  | 21    | -       | 2/9/27/28  | 0/3/3/3 |
| 21  | PSU  | A     | 255  | 21,23 | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | PSU  | A     | 1295 | 21    | -       | 0/7/25/26  | 0/2/2/2 |
| 21  | OMG  | A     | 1300 | 21    | -       | 0/9/27/28  | 0/3/3/3 |
| 21  | PSU  | A     | 1100 | 21    | -       | 0/7/25/26  | 0/2/2/2 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 21  | A     | 615 | OMU  | C4-N3 | -4.31 | 1.30        | 1.38     |
| 21  | A     | 615 | OMU  | C2-N3 | -4.04 | 1.30        | 1.38     |
| 10  | V     | 1   | AME  | CT1-N | 3.31  | 1.45        | 1.34     |
| 21  | A     | 615 | OMU  | C5-C4 | -2.53 | 1.38        | 1.43     |
| 21  | A     | 615 | OMU  | C6-N1 | -2.07 | 1.33        | 1.38     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 21  | A     | 615  | OMU  | N3-C2-N1 | 4.45  | 120.80      | 114.89   |
| 21  | A     | 615  | OMU  | C4-N3-C2 | -4.42 | 120.75      | 126.58   |
| 21  | A     | 615  | OMU  | C5-C4-N3 | 4.33  | 121.32      | 114.84   |
| 21  | A     | 1774 | 6MZ  | C9-N6-C6 | 3.27  | 125.69      | 122.87   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | A     | 1793 | MA6  | N1-C6-N6    | -3.22 | 113.56      | 117.08   |
| 21  | A     | 1793 | MA6  | C2-N1-C6    | 2.85  | 118.50      | 111.75   |
| 21  | A     | 615  | OMU  | O2-C2-N3    | -2.75 | 116.37      | 121.50   |
| 10  | V     | 1    | AME  | CT2-CT1-N   | 2.64  | 120.56      | 116.10   |
| 10  | V     | 1    | AME  | CE-SD-CG    | 2.63  | 109.43      | 100.40   |
| 21  | A     | 1792 | MA6  | C2-N1-C6    | 2.60  | 117.90      | 111.75   |
| 21  | A     | 802  | A2M  | C2'-C1'-N9  | -2.42 | 109.45      | 113.53   |
| 21  | A     | 1792 | MA6  | N1-C6-N6    | -2.20 | 114.68      | 117.08   |
| 21  | A     | 615  | OMU  | C2'-C1'-N1  | -2.14 | 110.07      | 114.22   |
| 21  | A     | 615  | OMU  | O4-C4-C5    | -2.13 | 121.41      | 125.16   |
| 21  | A     | 168  | OMU  | O2'-C2'-C1' | 2.13  | 113.23      | 109.08   |

There are no chirality outliers.

All (25) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | A     | 246  | OMG  | O4'-C4'-C5'-O5' |
| 21  | A     | 615  | OMU  | C1'-C2'-O2'-CM2 |
| 21  | A     | 623  | A2M  | O4'-C4'-C5'-O5' |
| 21  | A     | 1310 | PSU  | C2'-C1'-C5-C4   |
| 21  | A     | 1648 | OMC  | O4'-C1'-N1-C2   |
| 21  | A     | 1648 | OMC  | O4'-C1'-N1-C6   |
| 21  | A     | 1761 | A2M  | O4'-C4'-C5'-O5' |
| 21  | A     | 1761 | A2M  | C3'-C4'-C5'-O5' |
| 21  | A     | 246  | OMG  | C3'-C4'-C5'-O5' |
| 21  | A     | 623  | A2M  | C3'-C4'-C5'-O5' |
| 10  | V     | 1    | AME  | CT2-CT1-N-CA    |
| 10  | V     | 1    | AME  | OT-CT1-N-CA     |
| 21  | A     | 468  | A2M  | O4'-C4'-C5'-O5' |
| 21  | A     | 1793 | MA6  | C3'-C4'-C5'-O5' |
| 21  | A     | 392  | OMG  | O4'-C4'-C5'-O5' |
| 21  | A     | 392  | OMG  | C3'-C4'-C5'-O5' |
| 21  | A     | 1793 | MA6  | O4'-C4'-C5'-O5' |
| 21  | A     | 123  | OMU  | C1'-C2'-O2'-CM2 |
| 21  | A     | 599  | OMG  | C4'-C5'-O5'-P   |
| 21  | A     | 1131 | OMG  | C4'-C5'-O5'-P   |
| 21  | A     | 468  | A2M  | C3'-C4'-C5'-O5' |
| 4   | O     | 138  | IAS  | CA-CB-CG-OD1    |
| 21  | A     | 1310 | PSU  | O4'-C1'-C5-C4   |
| 21  | A     | 545  | A2M  | O4'-C1'-N9-C8   |
| 21  | A     | 623  | A2M  | C2'-C1'-N9-C8   |

There are no ring outliers.

22 monomers are involved in 33 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 21  | A     | 607  | PSU  | 2       | 0            |
| 21  | A     | 1774 | 6MZ  | 2       | 0            |
| 21  | A     | 1014 | OMU  | 2       | 0            |
| 21  | A     | 1637 | PSU  | 1       | 0            |
| 21  | A     | 123  | OMU  | 1       | 0            |
| 21  | A     | 208  | PSU  | 2       | 0            |
| 21  | A     | 38   | OMC  | 1       | 0            |
| 21  | A     | 418  | OMC  | 3       | 0            |
| 21  | A     | 1761 | A2M  | 1       | 0            |
| 21  | A     | 615  | OMU  | 1       | 0            |
| 21  | A     | 28   | A2M  | 1       | 0            |
| 21  | A     | 1792 | MA6  | 2       | 0            |
| 21  | A     | 1108 | PSU  | 1       | 0            |
| 21  | A     | 1306 | PSU  | 1       | 0            |
| 21  | A     | 636  | PSU  | 2       | 0            |
| 21  | A     | 1122 | PSU  | 2       | 0            |
| 21  | A     | 308  | PSU  | 2       | 0            |
| 21  | A     | 1793 | MA6  | 1       | 0            |
| 21  | A     | 1648 | OMC  | 4       | 0            |
| 21  | A     | 606  | PSU  | 2       | 0            |
| 21  | A     | 306  | PSU  | 1       | 0            |
| 21  | A     | 392  | OMG  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 47 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.

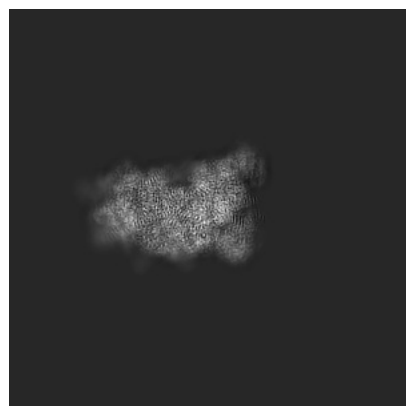
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18951. These allow visual inspection of the internal detail of the map and identification of artifacts.

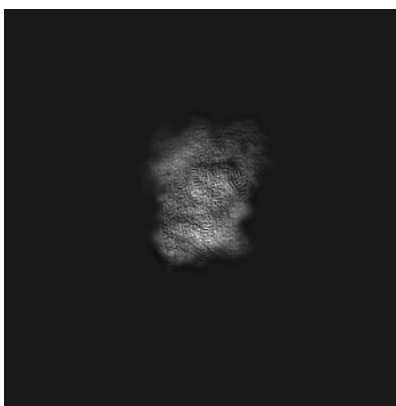
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

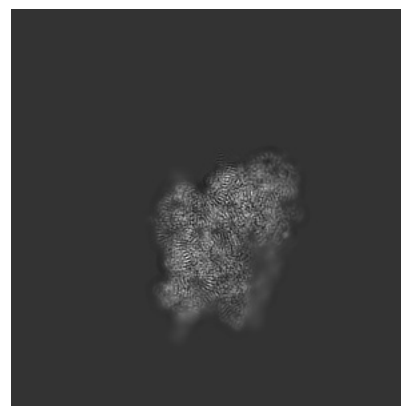
#### 6.1.1 Primary map



X

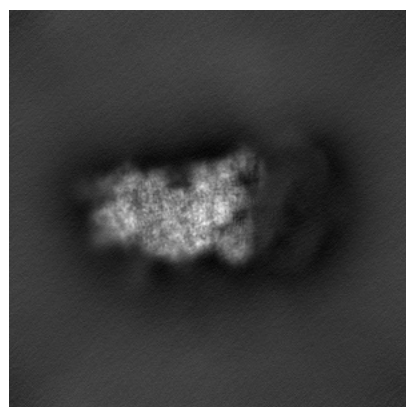


Y

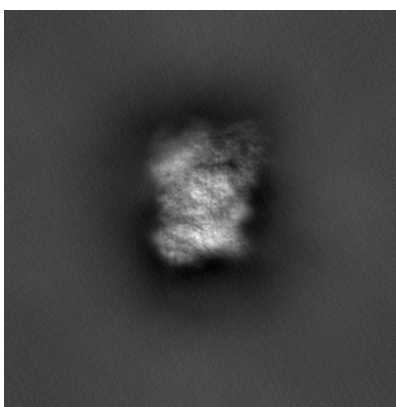


Z

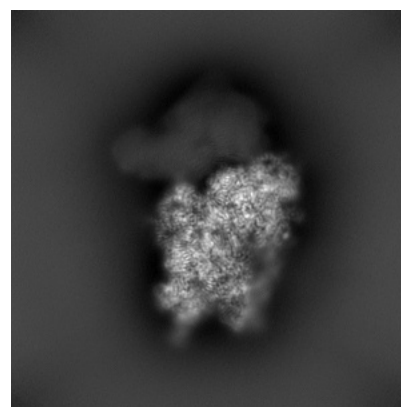
#### 6.1.2 Raw map



X



Y

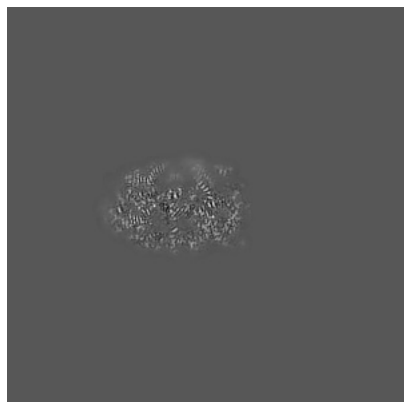


Z

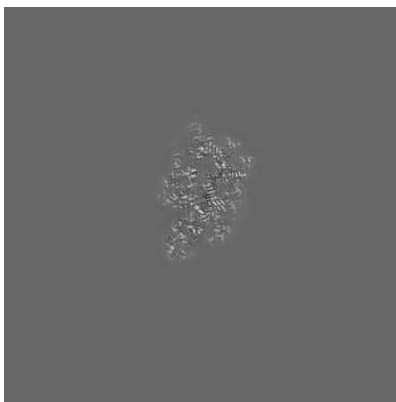
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

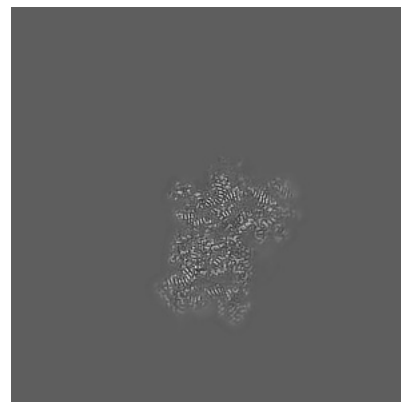
### 6.2.1 Primary map



X Index: 240

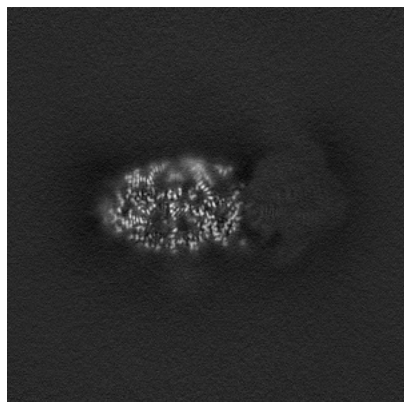


Y Index: 240

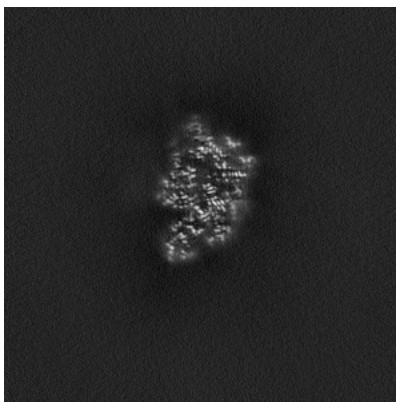


Z Index: 240

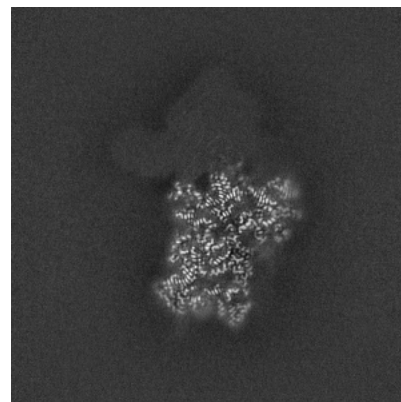
### 6.2.2 Raw map



X Index: 240



Y Index: 240

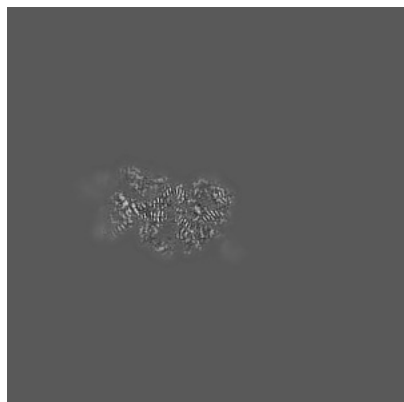


Z Index: 240

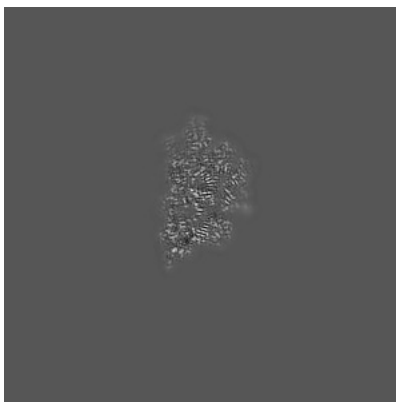
The images above show central slices of the map in three orthogonal directions.

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

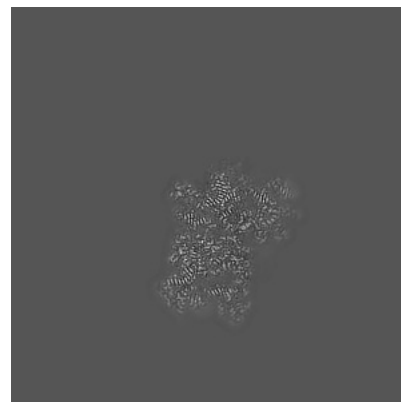
### 6.3.1 Primary map



X Index: 210

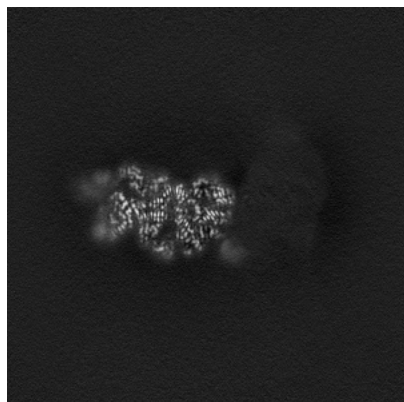


Y Index: 229

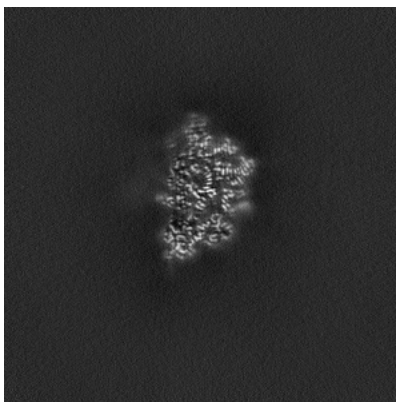


Z Index: 241

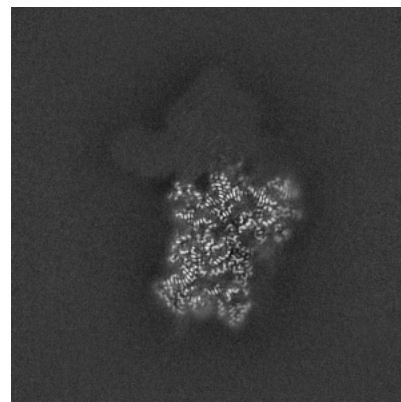
### 6.3.2 Raw map



X Index: 210



Y Index: 234

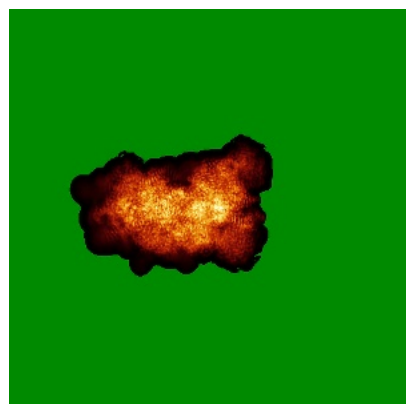


Z Index: 240

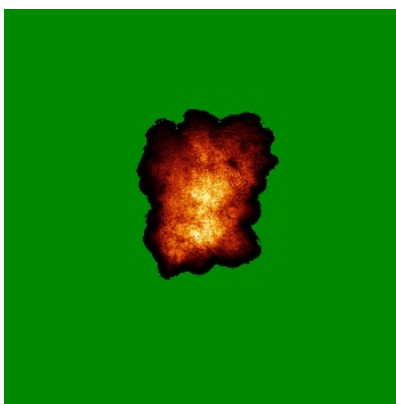
The images above show the largest variance slices of the map in three orthogonal directions.

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

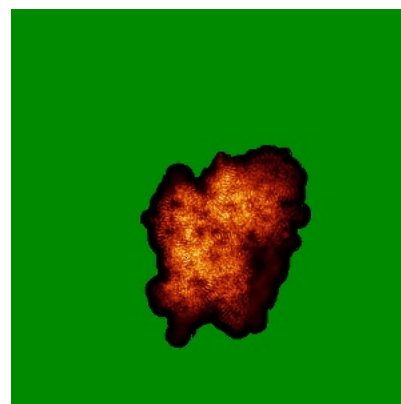
### 6.4.1 Primary map



X

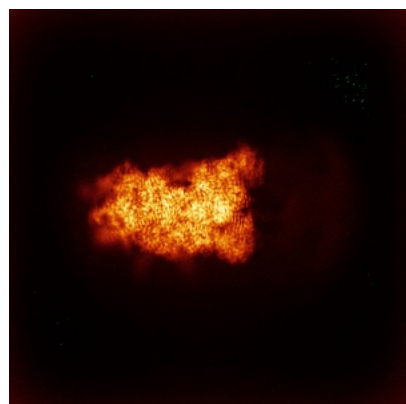


Y

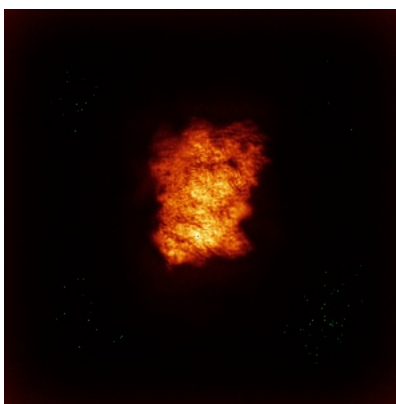


Z

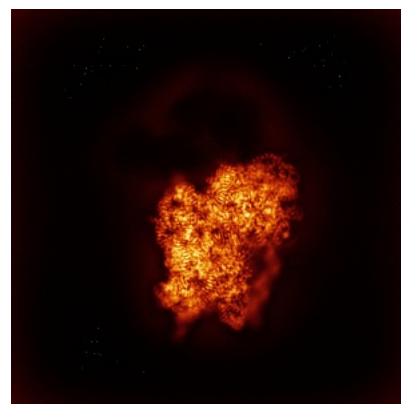
### 6.4.2 Raw map



X



Y



Z

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

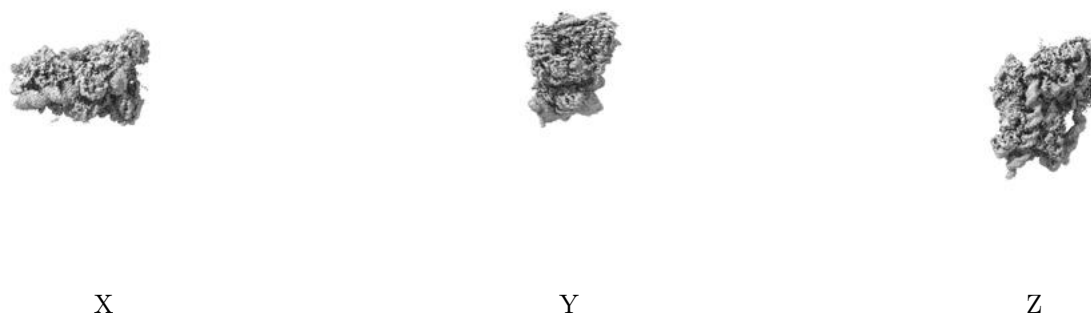
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

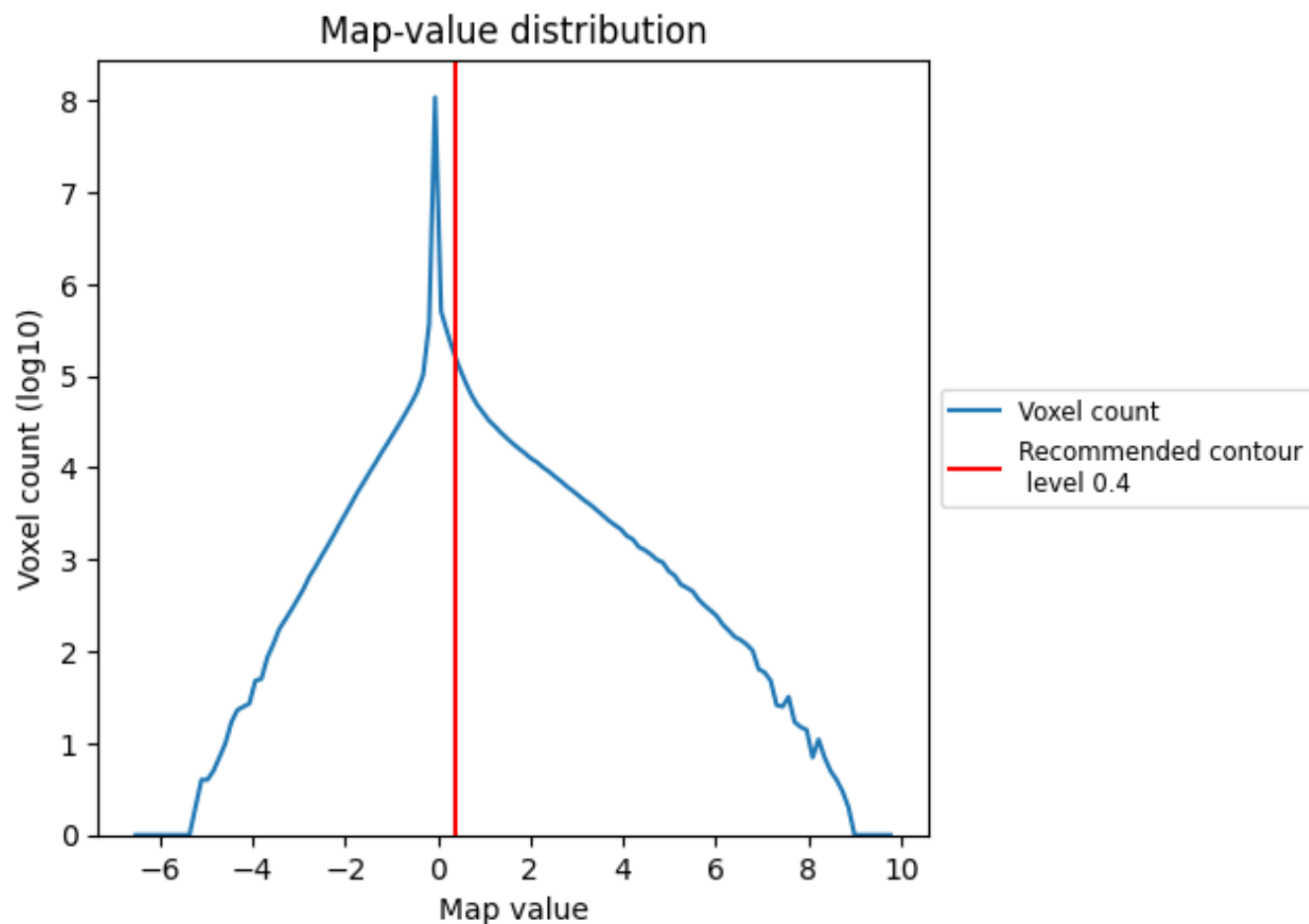
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

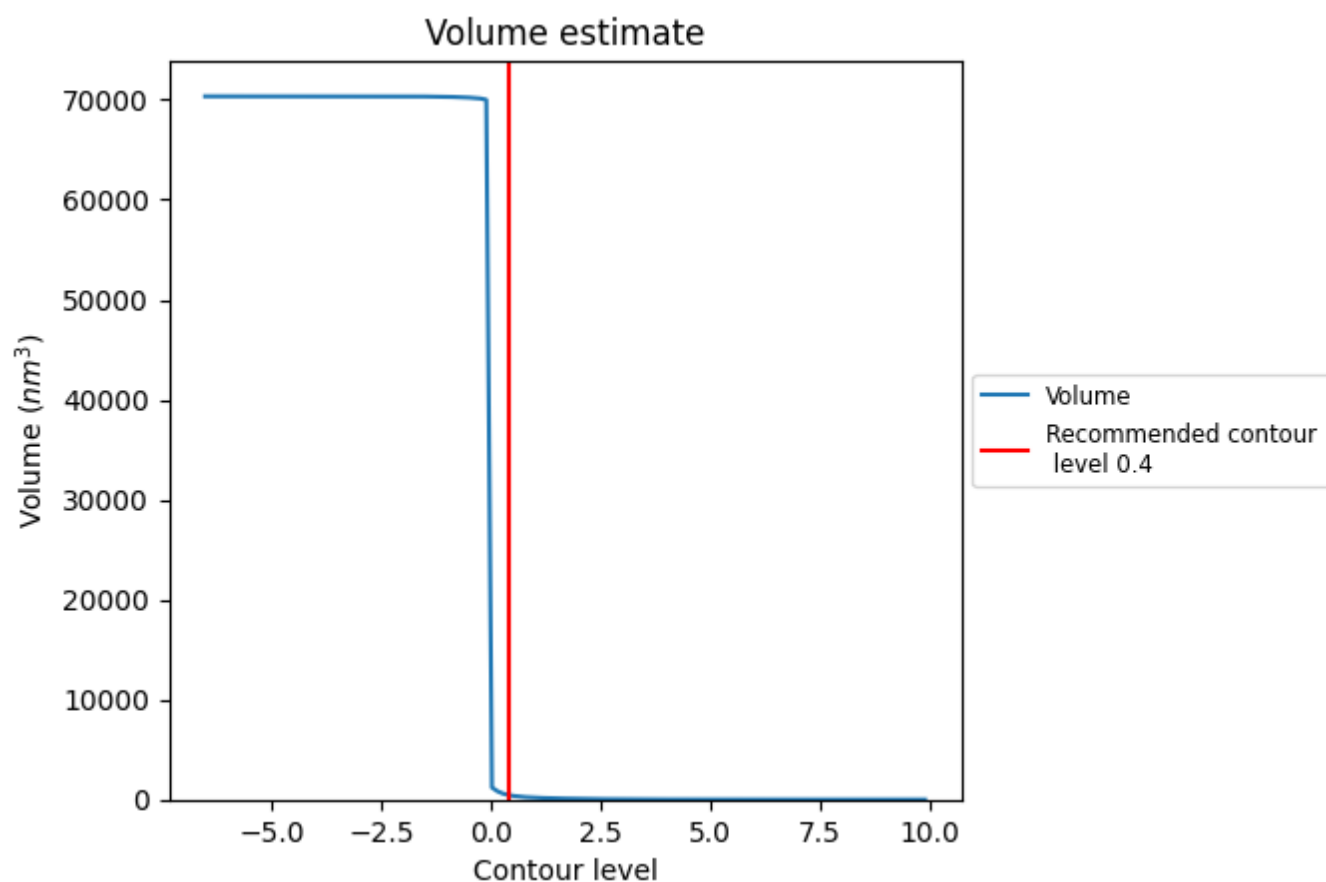
This section contains the results of statistical analysis of the map.

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



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

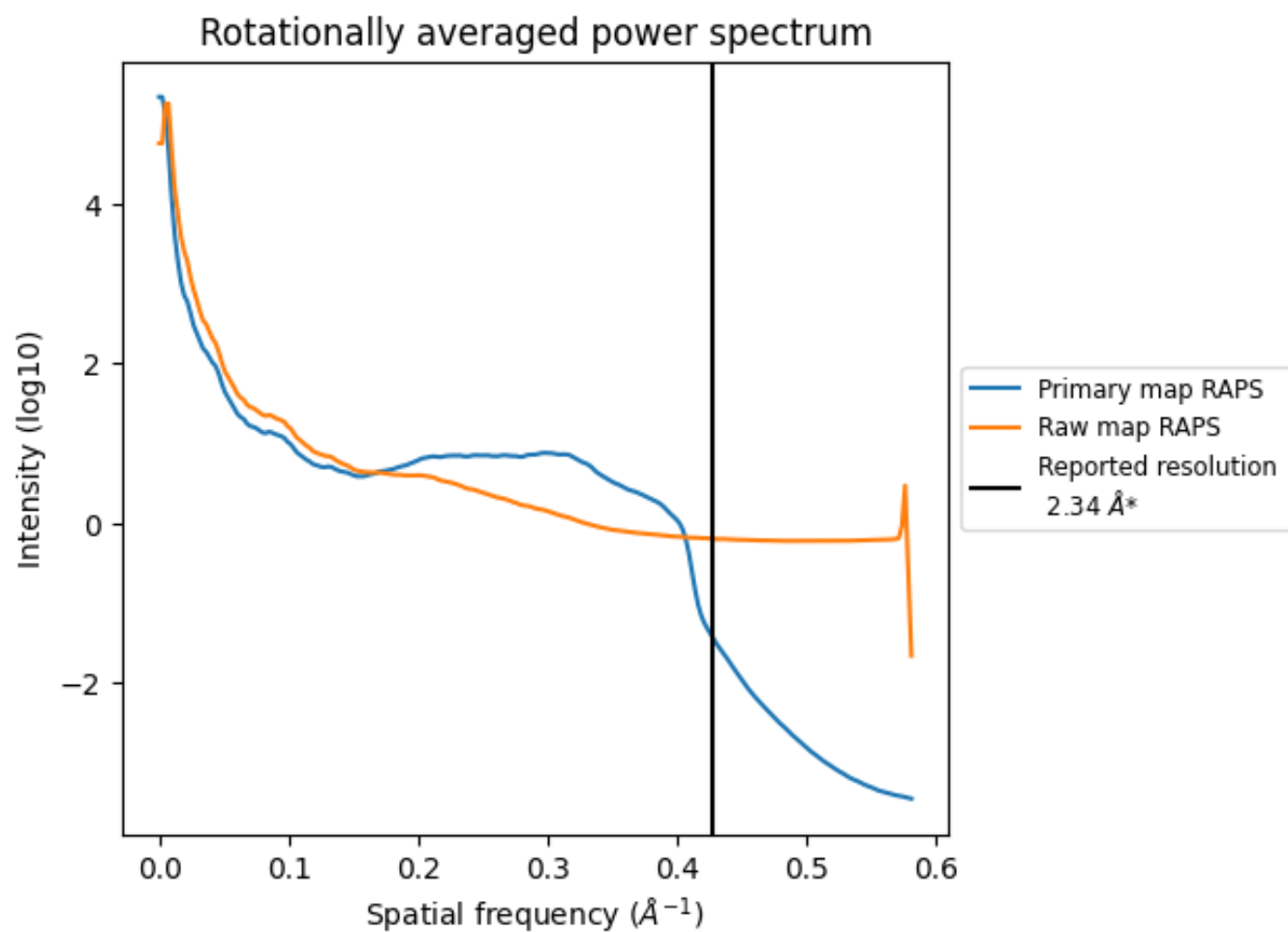
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 453  $\text{nm}^3$ ; this corresponds to an approximate mass of 409 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 ⓘ

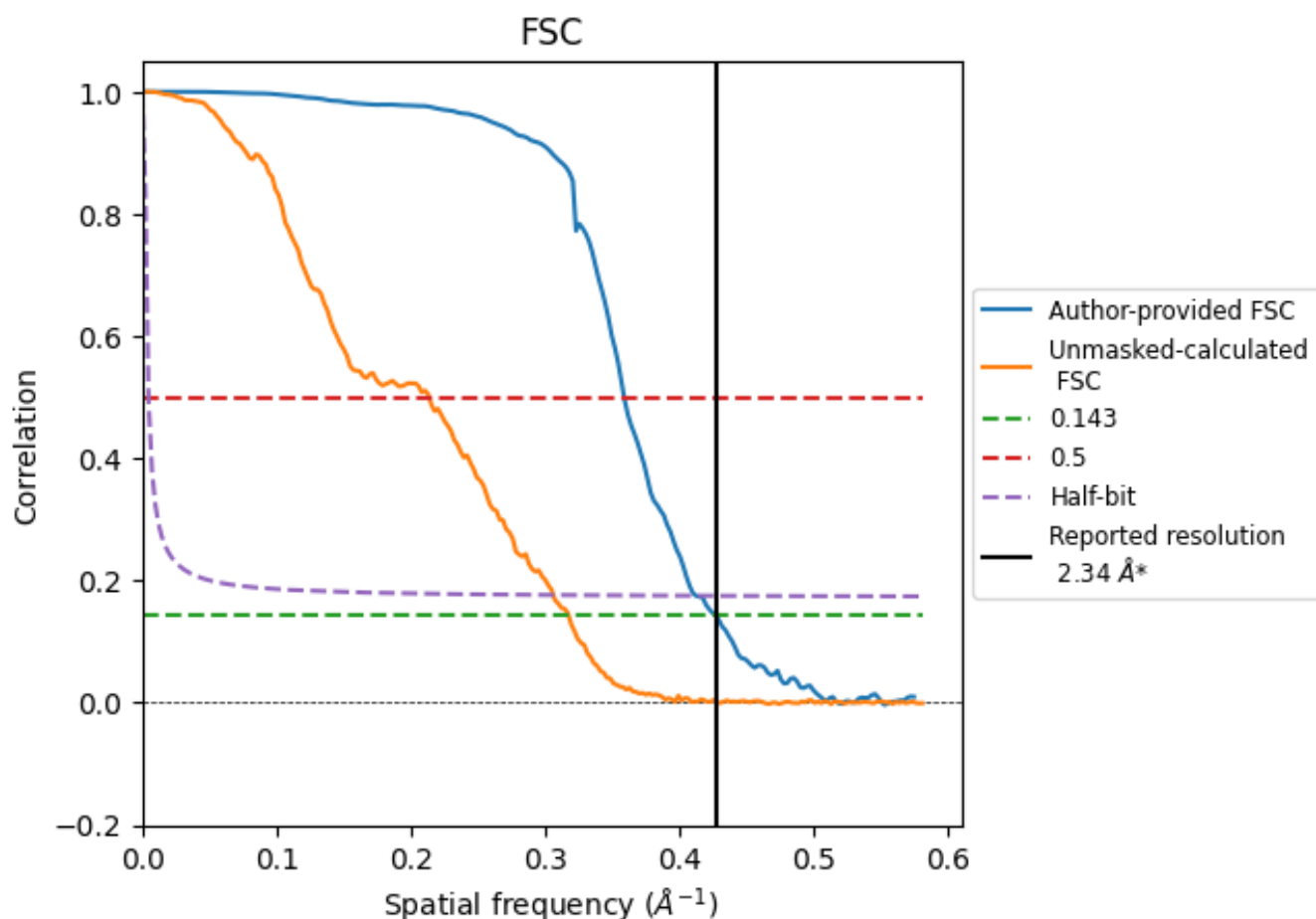


\*Reported resolution corresponds to spatial frequency of 0.427  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.427 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

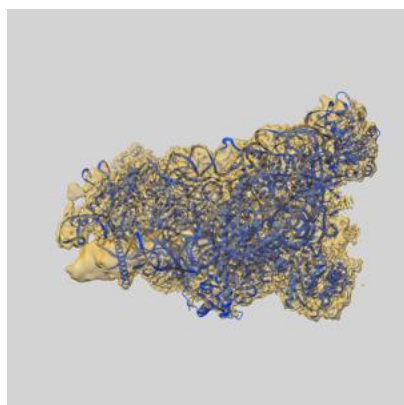
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.34                               | -    | -        |
| Author-provided FSC curve | 2.34                               | 2.78 | 2.42     |
| Unmasked-calculated*      | 3.15                               | 4.68 | 3.26     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.34 by more than 10 %

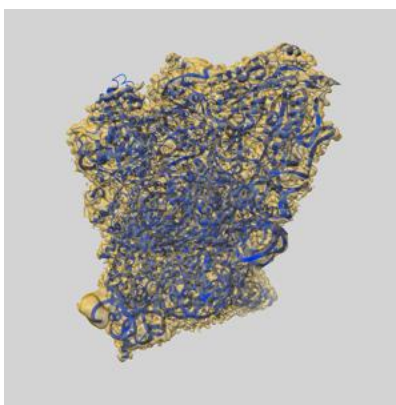
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18951 and PDB model 8R6F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

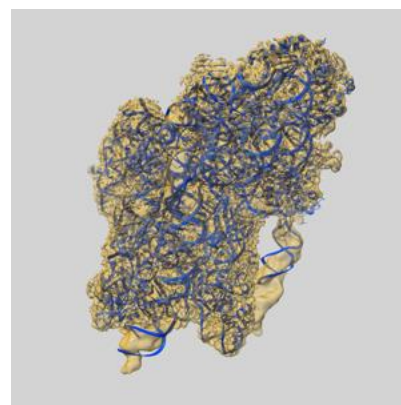
### 9.1 Map-model overlay [i](#)



X



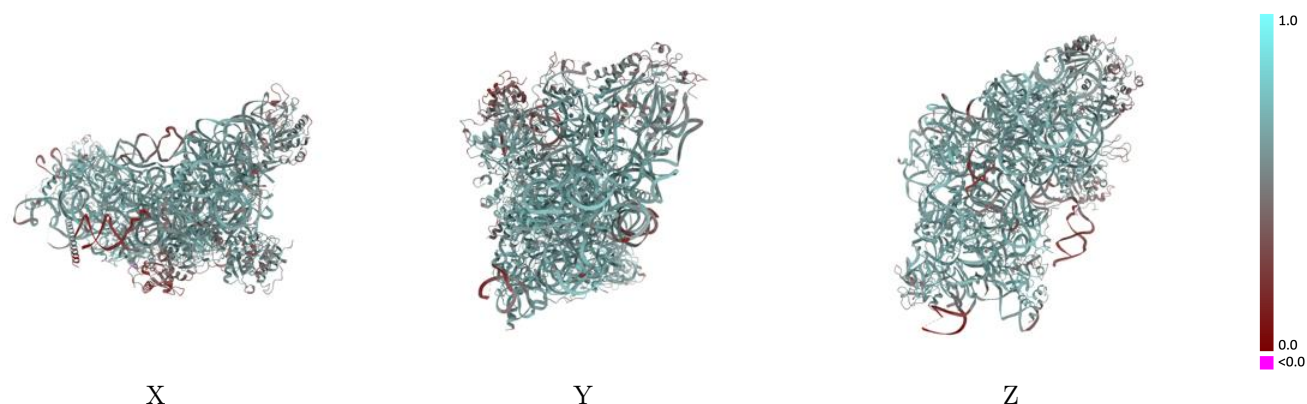
Y



Z

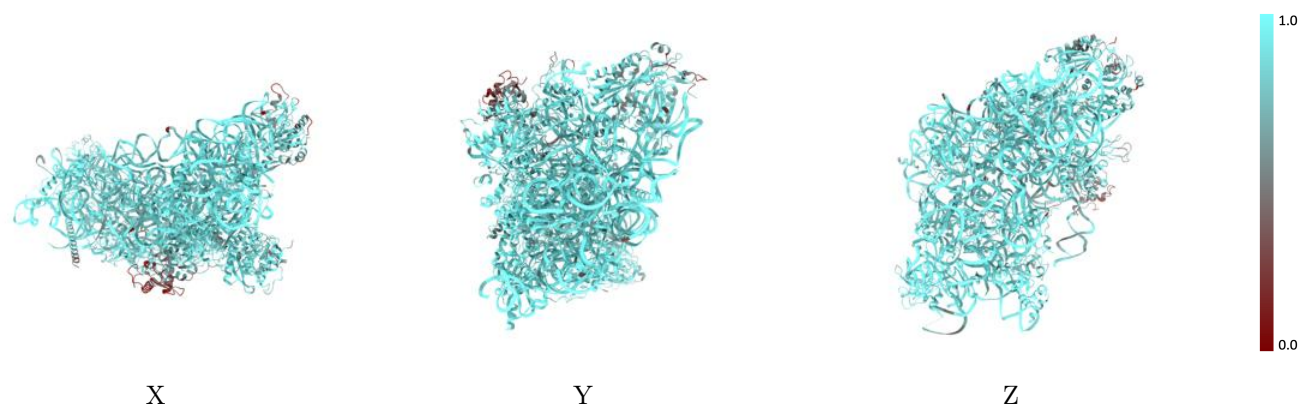
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



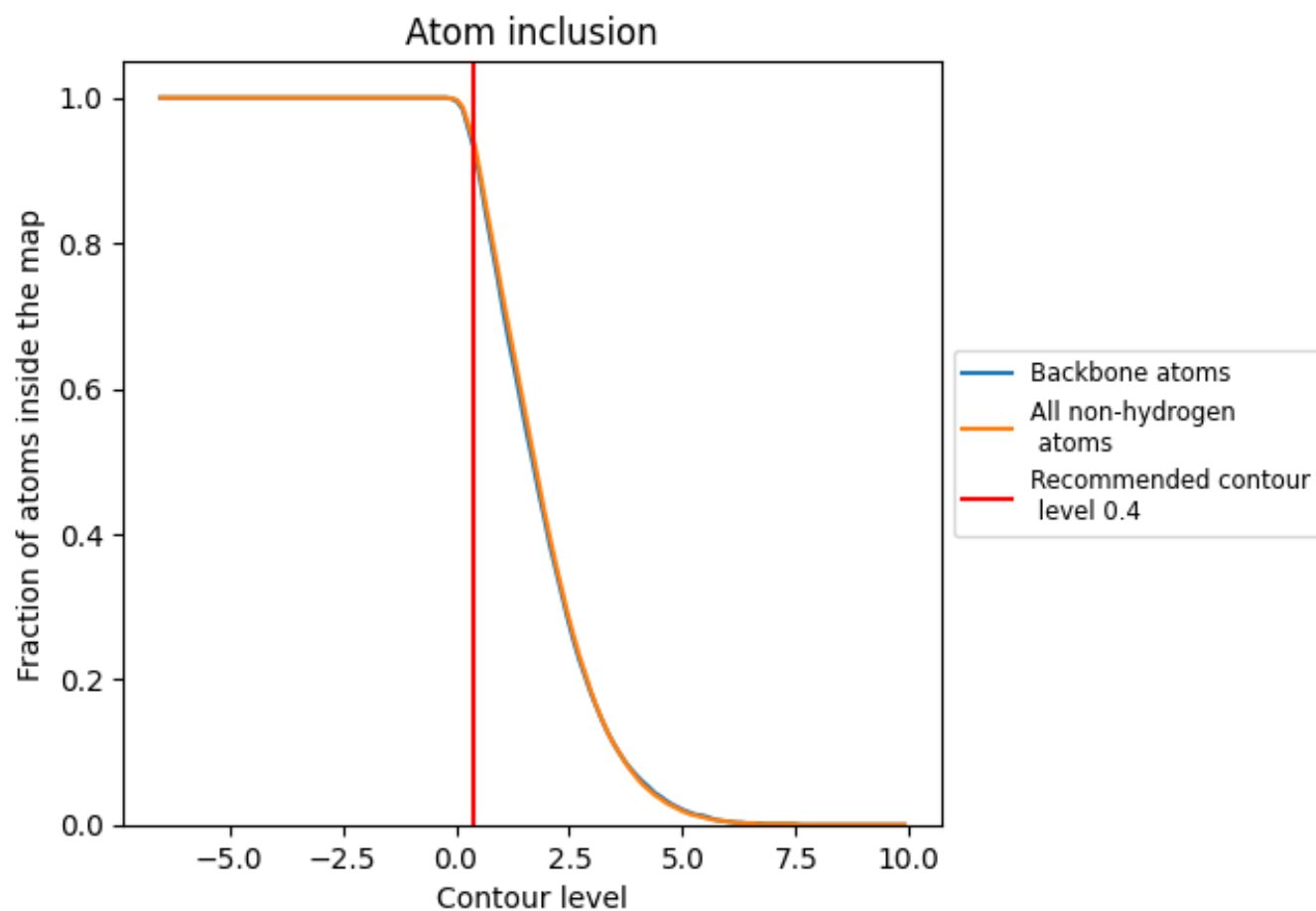
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9390   |  0.6000   |
| A     |  0.9700   |  0.6060   |
| B     |  0.8370   |  0.5260   |
| C     |  0.9620   |  0.6410   |
| E     |  0.9620   |  0.6430   |
| G     |  0.9280   |  0.5700   |
| H     |  0.5400   |  0.4000   |
| I     |  0.9670   |  0.6380   |
| J     |  0.9670   |  0.6490   |
| L     |  0.9750   |  0.6630   |
| N     |  0.9430   |  0.5980   |
| O     |  0.8410   |  0.5460   |
| V     |  0.9450   |  0.6060   |
| W     |  0.9820   |  0.6700   |
| X     |  0.9710  |  0.6460  |
| Y     |  0.9610 |  0.6320 |
| a     |  0.8850 |  0.6060 |
| b     |  0.8410 |  0.5120 |
| e     |  0.9180 |  0.6070 |
| h     |  0.6030 |  0.3810 |
| k     |  0.9410 |  0.5810 |
| n     |  0.9310 |  0.5990 |

