



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:32 AM UTC

PDB ID : 9HA6 / pdb\_00009ha6  
EMDB ID : EMD-51978  
Title : mature 50S subunit supplemented with Api137  
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.  
Deposited on : 2024-11-01  
Resolution : 3.08 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

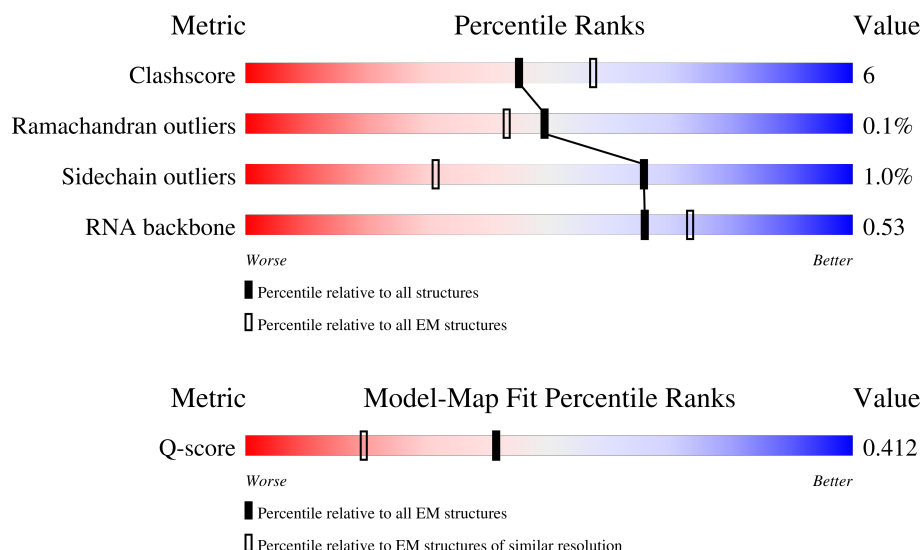
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.08 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.



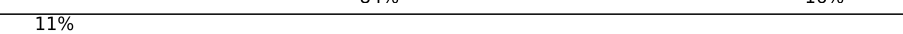
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14000 ( 2.58 - 3.58 )                                    |

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   | 0     | 56     | <br>14% 82% 16%  |
| 2   | 1     | 50     | <br>14% 92% 8%   |
| 3   | 2     | 46     | <br>14% 89% 9%   |

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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 4   | 3     | 64     |  80% 19% .      |
| 5   | 4     | 38     |  82% 18%        |
| 6   | B     | 120    |  70% 24% 6%     |
| 7   | C     | 271    |  85% 15%        |
| 8   | D     | 209    |  85% 15% .      |
| 9   | E     | 201    |  75% 24% .      |
| 10  | F     | 177    |  10% 77% 22% .  |
| 11  | G     | 176    |  7% 92% 7% .    |
| 12  | H     | 149    |  75% 89% 11%    |
| 13  | J     | 142    |  89% 10% .      |
| 14  | K     | 122    |  5% 89% 11%     |
| 15  | L     | 143    |  77% 23%        |
| 16  | M     | 136    |  87% 13%      |
| 17  | N     | 120    |  85% 14% .    |
| 18  | O     | 116    |  84% 16%      |
| 19  | P     | 114    |  11% 78% 22%  |
| 20  | Q     | 117    |  76% 23% .    |
| 21  | R     | 103    |  90% 10%      |
| 22  | S     | 110    |  82% 17% .    |
| 23  | T     | 93     |  83% 17%      |
| 24  | U     | 102    |  85% 15%      |
| 25  | V     | 94     |  79% 21%      |
| 26  | W     | 75     |  84% 16%      |
| 27  | X     | 77     |  88% 12%      |
| 28  | Y     | 63     |  6% 87% 11% . |

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| Mol | Chain | Length | Quality of chain                                                 |
|-----|-------|--------|------------------------------------------------------------------|
| 29  | Z     | 58     | <div><div></div><div>5%</div><div>81%</div><div>19%</div></div>  |
| 30  | A     | 2904   | <div><div></div><div>64%</div><div>31%</div><div>5%</div></div>  |
| 31  | y     | 17     | <div><div></div><div>47%</div><div>41%</div><div>12%</div></div> |
| 31  | z     | 17     | <div><div></div><div>53%</div><div>47%</div></div>               |

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 90242 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 Large ribosomal subunit protein bL32.

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

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 2   | 1     | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |       |

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 4   | 3     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 5 is a protein called Large ribosomal subunit protein bL36A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 6   | B     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2572  | 1145 | 471 | 836 | 120 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| B     | 120     | A        | U      | conflict | GB 1402434313 |

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | D     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | E     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | F     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | G     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | H     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | J     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | K     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |       |

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | L     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | M     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 17 is a protein called Large ribosomal subunit protein bL17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | N     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18  | O     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein bL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | P     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 20 is a protein called Large ribosomal subunit protein bL20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20  | Q     | 117      | Total | C   | N   | O   |         |       |
|     |       |          | 947   | 604 | 192 | 151 | 0       | 0     |

- Molecule 21 is a protein called Large ribosomal subunit protein bL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | R     | 103      | Total | C   | N   | O   | S |         |       |
|     |       |          | 816   | 516 | 153 | 145 | 2 | 0       | 0     |

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | S     | 110      | Total | C   | N   | O   | S |         |       |
|     |       |          | 868   | 538 | 170 | 157 | 3 | 1       | 0     |

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | T     | 93       | Total | C   | N   | O   | S |         |       |
|     |       |          | 738   | 466 | 139 | 131 | 2 | 0       | 0     |

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 24  | U     | 102      | Total | C   | N   | O   |         |       |
|     |       |          | 779   | 492 | 146 | 141 | 0       | 0     |

- Molecule 25 is a protein called Large ribosomal subunit protein bL25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | V     | 94       | Total | C   | N   | O   | S |         |       |
|     |       |          | 753   | 479 | 137 | 134 | 3 | 0       | 0     |

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | W     | 75       | Total | C   | N   | O   | S |         |       |
|     |       |          | 575   | 356 | 116 | 102 | 1 | 0       | 0     |

- Molecule 27 is a protein called Large ribosomal subunit protein bL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | X     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 28 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | Y     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | Z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 30 is a RNA chain called 23S ribosomal rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 30  | A     | 2900     | Total | C     | N     | O     | P    | 1       | 0     |
|     |       |          | 62281 | 27783 | 11461 | 20136 | 2901 |         |       |

- Molecule 31 is a protein called Apidaecins type 22.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 31  | z     | 17       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 148   | 94 | 33 | 21 |         |       |
| 31  | y     | 17       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 148   | 94 | 33 | 21 |         |       |

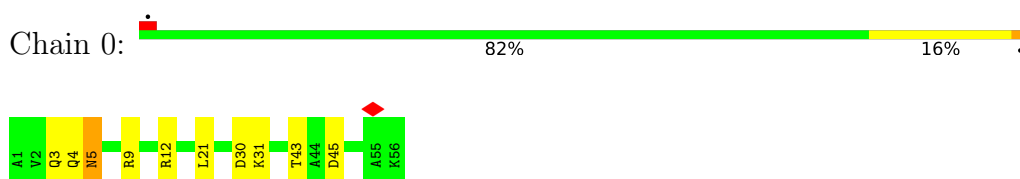
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| z     | 10      | ARG      | GLN    | conflict | UNP P35581 |
| y     | 10      | ARG      | GLN    | conflict | UNP P35581 |

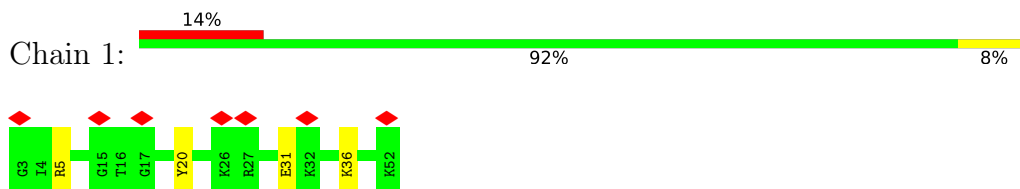
### 3 Residue-property plots [i](#)

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.

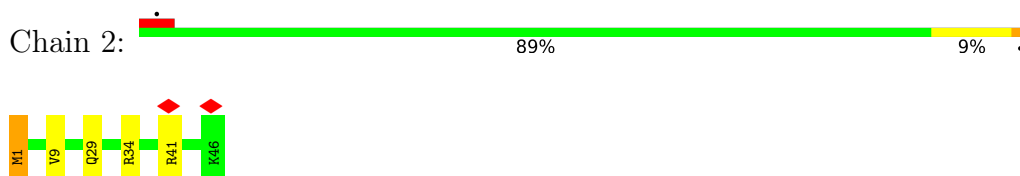
- Molecule 1: Large ribosomal subunit protein bL32



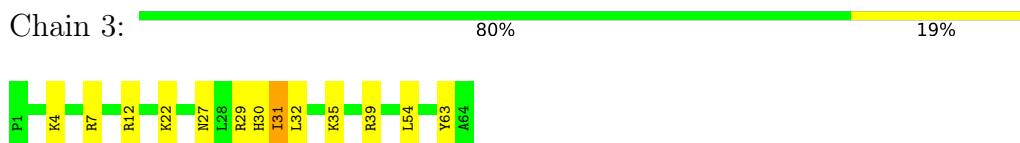
- Molecule 2: Large ribosomal subunit protein bL33



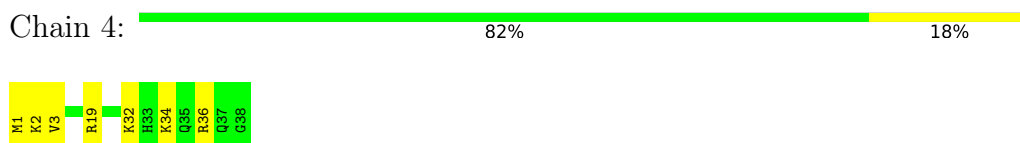
- Molecule 3: Large ribosomal subunit protein bL34



- Molecule 4: Large ribosomal subunit protein bL35

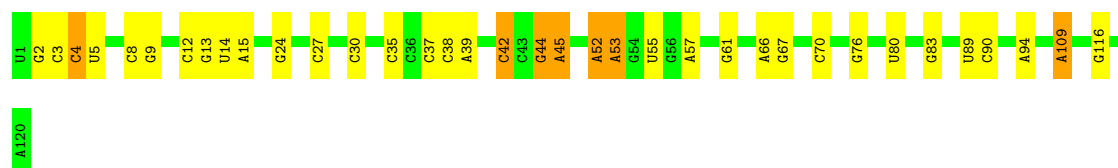


- Molecule 5: Large ribosomal subunit protein bL36A



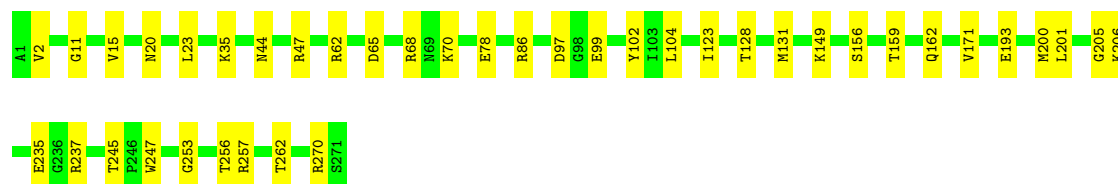
- Molecule 6: 5S ribosomal RNA

Chain B:  70% 24% 6%



- Molecule 7: Large ribosomal subunit protein uL2

Chain C:  85% 15%



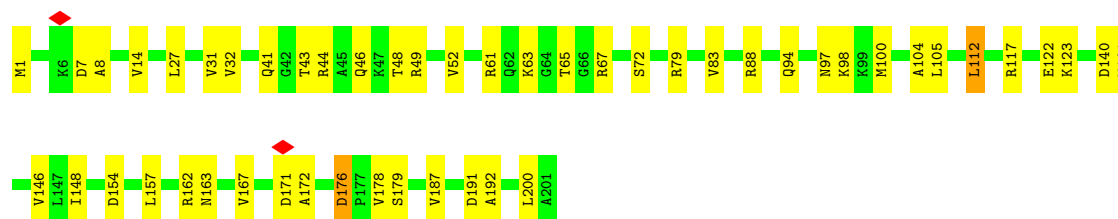
- Molecule 8: 50S ribosomal protein L3

Chain D:  85% 15%



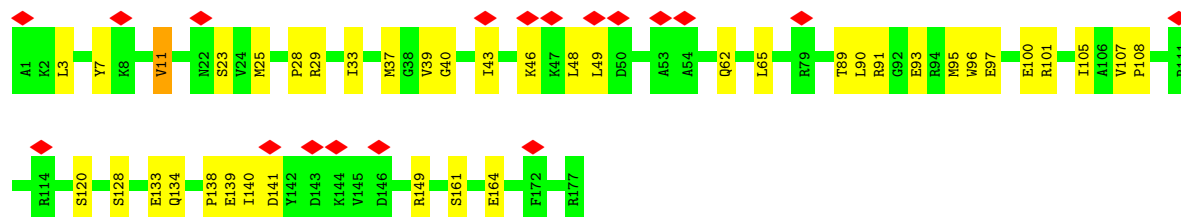
- Molecule 9: Large ribosomal subunit protein uL4

Chain E:  75% 24%

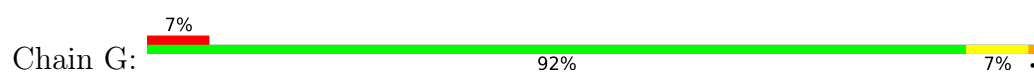


- Molecule 10: Large ribosomal subunit protein uL5

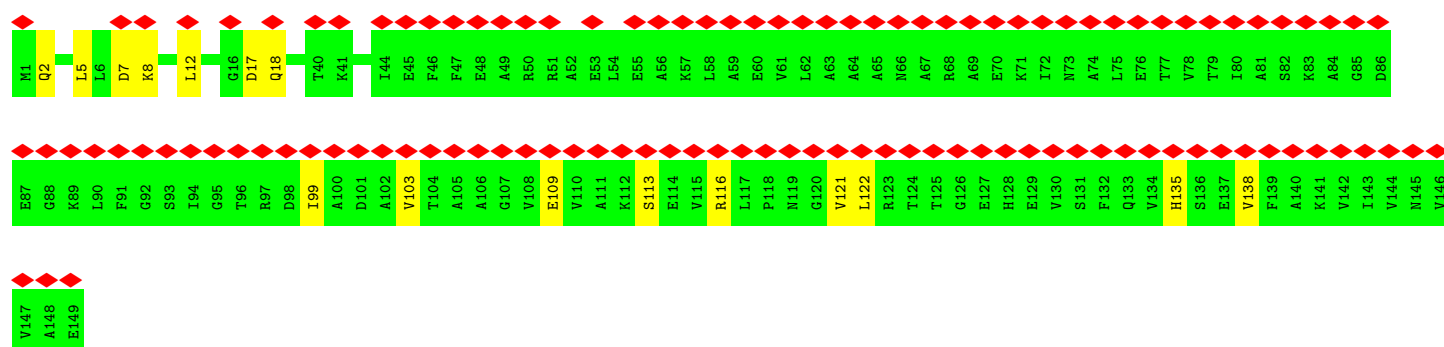
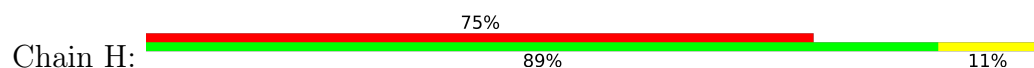
Chain F:  10% 77% 22%



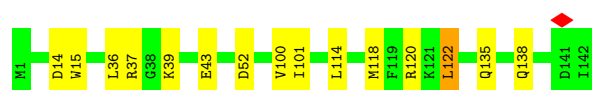
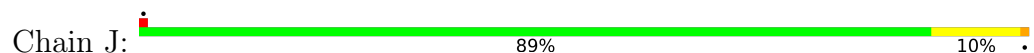
- Molecule 11: Large ribosomal subunit protein uL6



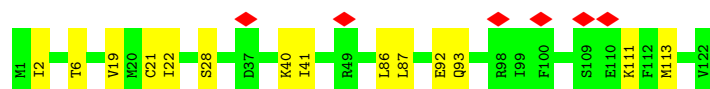
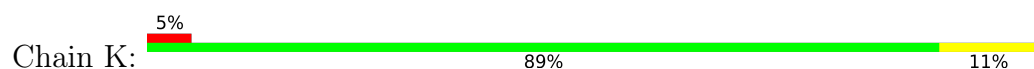
- Molecule 12: Large ribosomal subunit protein bL9



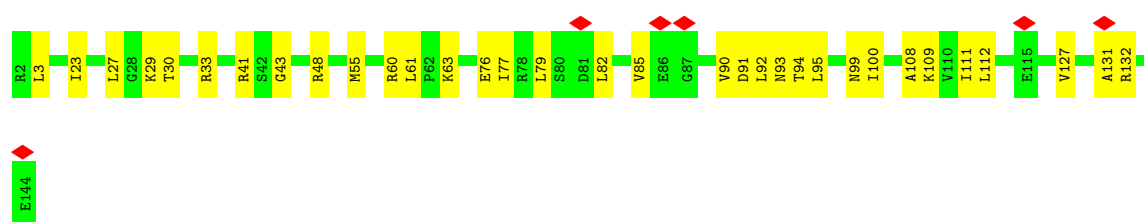
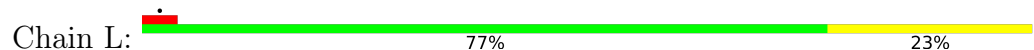
- Molecule 13: Large ribosomal subunit protein uL13



- Molecule 14: Large ribosomal subunit protein uL14

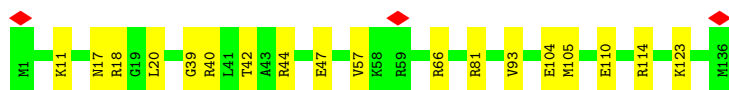


- Molecule 15: Large ribosomal subunit protein uL15

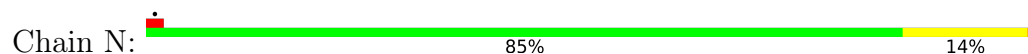


- Molecule 16: 50S ribosomal protein L16

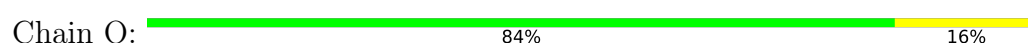




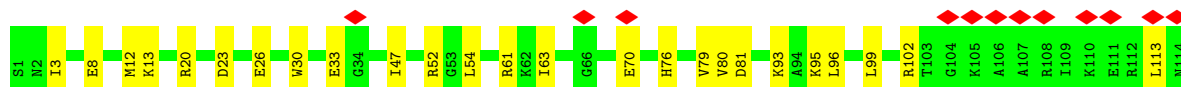
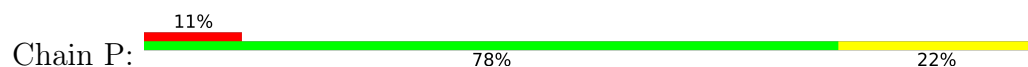
- Molecule 17: Large ribosomal subunit protein bL17



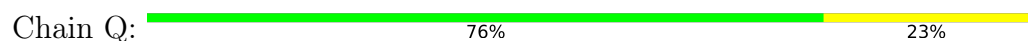
- Molecule 18: Large ribosomal subunit protein uL18



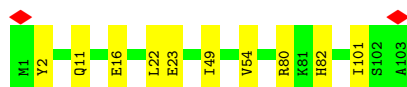
- Molecule 19: Large ribosomal subunit protein bL19



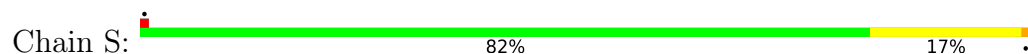
- Molecule 20: Large ribosomal subunit protein bL20



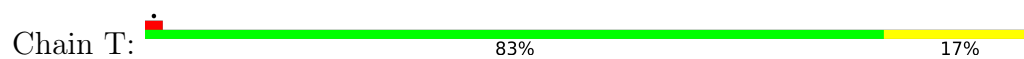
- Molecule 21: Large ribosomal subunit protein bL21



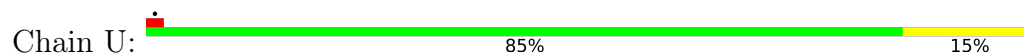
- Molecule 22: Large ribosomal subunit protein uL22



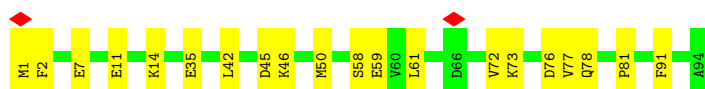
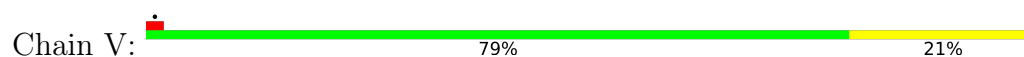
- Molecule 23: Large ribosomal subunit protein uL23



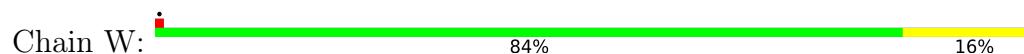
- Molecule 24: Large ribosomal subunit protein uL24



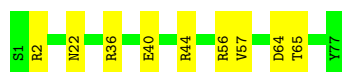
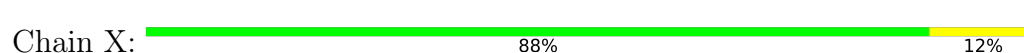
- Molecule 25: Large ribosomal subunit protein bL25



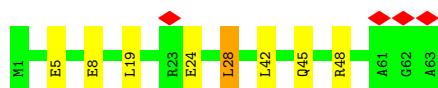
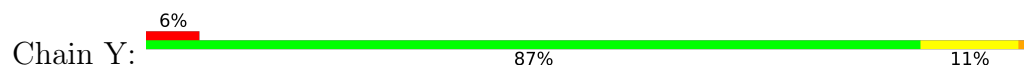
- Molecule 26: Large ribosomal subunit protein bL27



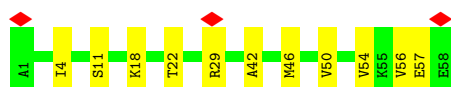
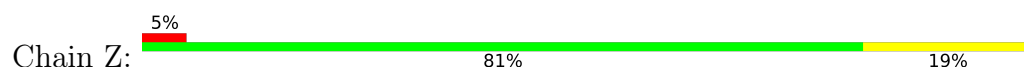
- Molecule 27: Large ribosomal subunit protein bL28



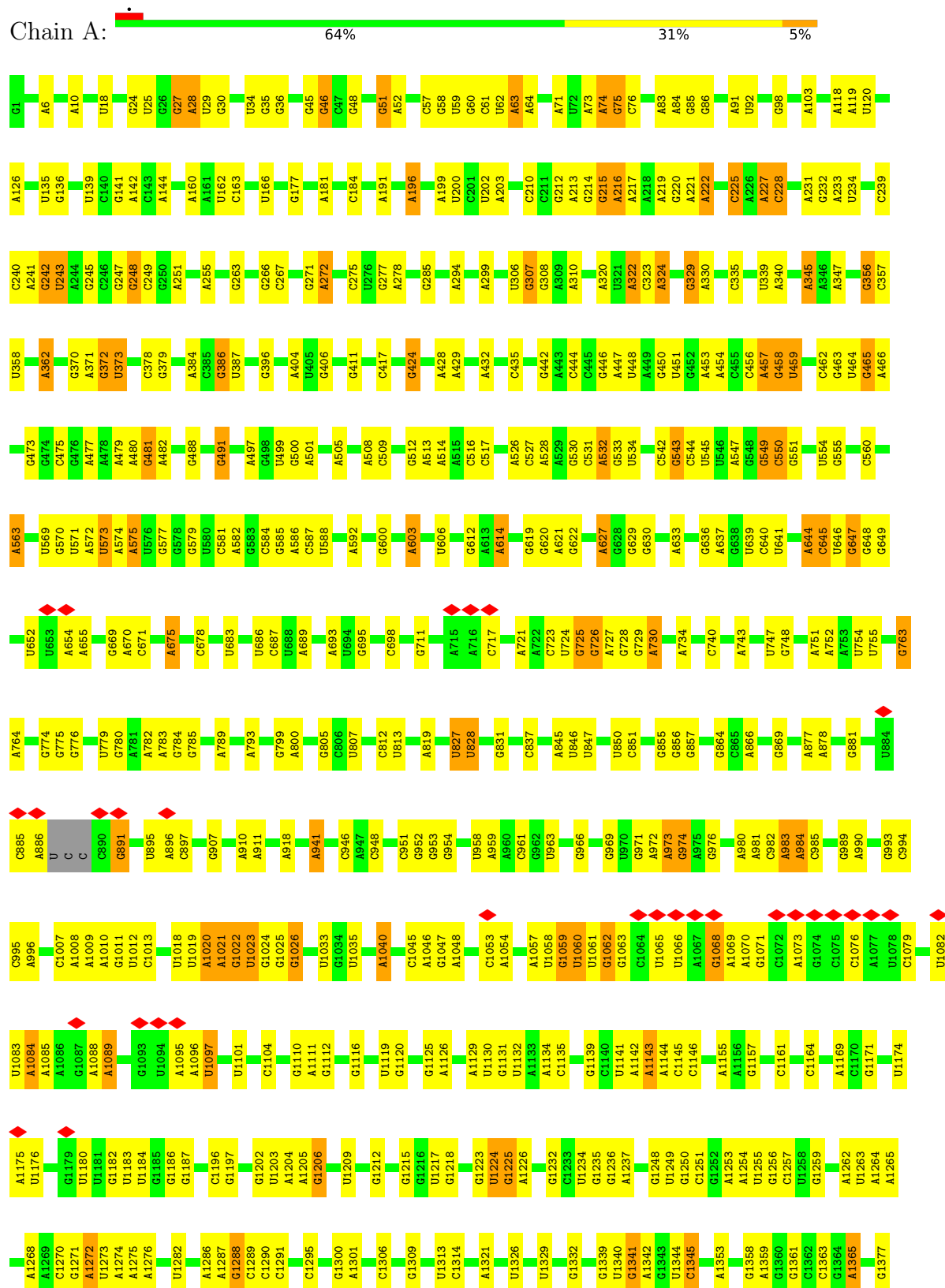
- Molecule 28: Large ribosomal subunit protein uL29



- Molecule 29: Large ribosomal subunit protein uL30



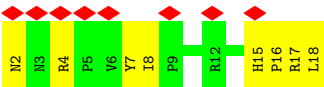
• Molecule 30: 23S ribosomal rRNA







● Molecule 31: Apidaecins type 22



● Molecule 31: Apidaecins type 22



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 41476                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 46.2                                    | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.850                                   | Depositor |
| Minimum map value                    | -0.385                                  | Depositor |
| Average map value                    | -0.002                                  | Depositor |
| Map value standard deviation         | 0.040                                   | Depositor |
| Recommended contour level            | 0.1                                     | Depositor |
| Map size (Å)                         | 399.6, 399.6, 399.6                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.332, 1.332, 1.332                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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   | 0     | 0.12         | 0/450       | 0.25        | 0/599           |
| 2   | 1     | 0.07         | 0/416       | 0.19        | 0/554           |
| 3   | 2     | 0.11         | 0/380       | 0.18        | 0/498           |
| 4   | 3     | 0.07         | 0/513       | 0.19        | 0/676           |
| 5   | 4     | 0.12         | 0/303       | 0.18        | 0/397           |
| 6   | B     | 0.07         | 0/2876      | 0.19        | 0/4483          |
| 7   | C     | 0.09         | 0/2121      | 0.24        | 0/2852          |
| 8   | D     | 0.09         | 0/1586      | 0.20        | 0/2134          |
| 9   | E     | 0.10         | 0/1571      | 0.21        | 0/2113          |
| 10  | F     | 0.10         | 0/1434      | 0.25        | 0/1926          |
| 11  | G     | 0.09         | 0/1343      | 0.20        | 0/1816          |
| 12  | H     | 0.10         | 0/1122      | 0.22        | 0/1515          |
| 13  | J     | 0.09         | 0/1152      | 0.19        | 0/1551          |
| 14  | K     | 0.09         | 0/947       | 0.22        | 0/1268          |
| 15  | L     | 0.09         | 0/1054      | 0.27        | 0/1403          |
| 16  | M     | 0.09         | 0/1093      | 0.20        | 0/1460          |
| 17  | N     | 0.12         | 0/973       | 0.29        | 0/1301          |
| 18  | O     | 0.07         | 0/902       | 0.20        | 0/1209          |
| 19  | P     | 0.09         | 0/929       | 0.19        | 0/1242          |
| 20  | Q     | 0.10         | 0/960       | 0.21        | 0/1278          |
| 21  | R     | 0.10         | 0/829       | 0.22        | 0/1107          |
| 22  | S     | 0.10         | 0/875       | 0.21        | 0/1170          |
| 23  | T     | 0.28         | 0/744       | 0.41        | 0/994           |
| 24  | U     | 0.10         | 0/787       | 0.24        | 0/1051          |
| 25  | V     | 0.10         | 0/766       | 0.20        | 0/1025          |
| 26  | W     | 0.07         | 0/582       | 0.20        | 0/769           |
| 27  | X     | 0.10         | 0/635       | 0.19        | 0/848           |
| 28  | Y     | 0.11         | 0/510       | 0.19        | 0/677           |
| 29  | Z     | 0.11         | 0/453       | 0.19        | 0/605           |
| 30  | A     | 0.07         | 0/69755     | 0.20        | 2/108820 (0.0%) |
| 31  | y     | 0.15         | 0/155       | 0.38        | 0/212           |
| 31  | z     | 0.09         | 0/155       | 0.26        | 0/212           |
| All | All   | 0.08         | 0/98371     | 0.21        | 2/147765 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 23  | T     | 0                   | 1                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 30  | A     | 1913 | A    | OP1-P-O3' | -8.77 | 81.70       | 108.00   |
| 30  | A     | 1913 | A    | OP2-P-O3' | -8.31 | 83.07       | 108.00   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 23  | T     | 73  | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 444   | 0        | 461      | 7       | 0            |
| 2   | 1     | 409   | 0        | 440      | 5       | 0            |
| 3   | 2     | 377   | 0        | 418      | 4       | 0            |
| 4   | 3     | 504   | 0        | 574      | 11      | 0            |
| 5   | 4     | 302   | 0        | 343      | 6       | 0            |
| 6   | B     | 2572  | 0        | 1302     | 22      | 0            |
| 7   | C     | 2082  | 0        | 2157     | 33      | 0            |
| 8   | D     | 1565  | 0        | 1616     | 22      | 0            |
| 9   | E     | 1552  | 0        | 1619     | 39      | 0            |
| 10  | F     | 1410  | 0        | 1447     | 31      | 0            |
| 11  | G     | 1323  | 0        | 1374     | 10      | 0            |
| 12  | H     | 1111  | 0        | 1148     | 12      | 0            |
| 13  | J     | 1129  | 0        | 1162     | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | K     | 938   | 0        | 1012     | 11      | 0            |
| 15  | L     | 1045  | 0        | 1117     | 28      | 0            |
| 16  | M     | 1074  | 0        | 1157     | 12      | 0            |
| 17  | N     | 960   | 0        | 1000     | 13      | 0            |
| 18  | O     | 892   | 0        | 923      | 14      | 0            |
| 19  | P     | 917   | 0        | 965      | 17      | 0            |
| 20  | Q     | 947   | 0        | 1022     | 24      | 0            |
| 21  | R     | 816   | 0        | 839      | 8       | 0            |
| 22  | S     | 868   | 0        | 934      | 15      | 0            |
| 23  | T     | 738   | 0        | 807      | 11      | 0            |
| 24  | U     | 779   | 0        | 834      | 12      | 0            |
| 25  | V     | 753   | 0        | 780      | 16      | 0            |
| 26  | W     | 575   | 0        | 592      | 10      | 0            |
| 27  | X     | 625   | 0        | 655      | 8       | 0            |
| 28  | Y     | 509   | 0        | 543      | 7       | 0            |
| 29  | Z     | 449   | 0        | 491      | 10      | 0            |
| 30  | A     | 62281 | 0        | 31323    | 620     | 0            |
| 31  | y     | 148   | 0        | 152      | 40      | 0            |
| 31  | z     | 148   | 0        | 150      | 57      | 0            |
| All | All   | 90242 | 0        | 59357    | 904     | 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 6.

All (904) 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) |
|-------------------|-----------------|--------------------------|-------------------|
| 30:A:2505:G:N1    | 31:z:15:HIS:CD2 | 2.15                     | 1.13              |
| 30:A:1321:A:H1'   | 31:y:15:HIS:O   | 1.49                     | 1.13              |
| 30:A:2505:G:C6    | 31:z:15:HIS:CE1 | 2.34                     | 1.12              |
| 30:A:508:A:C8     | 31:y:13:PRO:HB3 | 1.86                     | 1.09              |
| 30:A:1321:A:C8    | 31:y:16:PRO:HA  | 1.92                     | 1.04              |
| 30:A:2506[A]:U:H3 | 31:z:17:ARG:CD  | 1.74                     | 1.00              |
| 30:A:508:A:N7     | 31:y:13:PRO:HB3 | 1.78                     | 0.99              |
| 30:A:1321:A:H4'   | 31:y:17:ARG:HE  | 1.25                     | 0.98              |
| 30:A:2505:G:C2    | 31:z:15:HIS:HB3 | 1.98                     | 0.98              |
| 30:A:2505:G:N3    | 31:z:15:HIS:HB3 | 1.83                     | 0.94              |
| 30:A:2505:G:O6    | 31:z:15:HIS:CE1 | 2.22                     | 0.93              |
| 30:A:2506[A]:U:C4 | 31:z:17:ARG:NH1 | 2.35                     | 0.93              |
| 30:A:2506[A]:U:H3 | 31:z:17:ARG:HD2 | 1.32                     | 0.93              |
| 30:A:727:A:OP2    | 30:A:1431:A:O2' | 1.88                     | 0.91              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:A:1321:A:N9    | 31:y:16:PRO:HA   | 1.86                     | 0.91              |
| 30:A:2505:G:C6    | 31:z:15:HIS:NE2  | 2.39                     | 0.90              |
| 30:A:2505:G:C2    | 31:z:15:HIS:CG   | 2.61                     | 0.89              |
| 30:A:177:G:OP2    | 30:A:177:G:N2    | 2.05                     | 0.89              |
| 30:A:2505:G:C6    | 31:z:15:HIS:CD2  | 2.59                     | 0.89              |
| 30:A:1257:C:OP1   | 31:z:4:ARG:NH2   | 2.06                     | 0.88              |
| 15:L:93:ASN:O     | 15:L:94:THR:OG1  | 1.91                     | 0.88              |
| 30:A:1321:A:C4'   | 31:y:17:ARG:HE   | 1.87                     | 0.88              |
| 30:A:2506[A]:U:N3 | 31:z:17:ARG:HD2  | 1.89                     | 0.87              |
| 30:A:1837:C:O2'   | 30:A:1927:A:N3   | 2.05                     | 0.87              |
| 30:A:2343:U:HO2'  | 30:A:2373:G:HO2' | 1.12                     | 0.87              |
| 30:A:2505:G:N1    | 31:z:15:HIS:CG   | 2.43                     | 0.87              |
| 30:A:2258:C:O2'   | 30:A:2427:C:OP2  | 1.92                     | 0.87              |
| 30:A:2506[A]:U:H3 | 31:z:17:ARG:NE   | 1.72                     | 0.85              |
| 30:A:959:A:N3     | 30:A:2457:U:O2'  | 2.09                     | 0.85              |
| 30:A:1681:G:OP2   | 30:A:1757:A:N6   | 2.09                     | 0.85              |
| 30:A:2576:G:O2'   | 30:A:2579:C:OP2  | 1.93                     | 0.85              |
| 30:A:2505:G:C6    | 31:z:15:HIS:CG   | 2.65                     | 0.85              |
| 30:A:1798:U:O2'   | 30:A:1802:A:N3   | 2.10                     | 0.85              |
| 30:A:948:C:O2     | 30:A:984:A:O2'   | 1.96                     | 0.84              |
| 7:C:253:GLY:O     | 30:A:1843:C:O2'  | 1.96                     | 0.84              |
| 30:A:2522:U:O2'   | 30:A:2647:U:OP1  | 1.93                     | 0.84              |
| 30:A:2530:A:OP2   | 30:A:2535:G:N2   | 2.11                     | 0.83              |
| 18:O:117:PHE:O    | 30:A:2377:A:O2'  | 1.95                     | 0.83              |
| 30:A:1447:C:O2'   | 30:A:1544:A:N3   | 2.09                     | 0.83              |
| 6:B:5:U:OP1       | 6:B:61:G:O2'     | 1.96                     | 0.83              |
| 30:A:751:A:C2     | 31:z:7:TYR:CE1   | 2.65                     | 0.83              |
| 30:A:1826:G:O2'   | 30:A:1971:U:OP2  | 1.97                     | 0.83              |
| 30:A:275:C:O2     | 30:A:362:A:N6    | 2.12                     | 0.82              |
| 30:A:612:G:N2     | 30:A:614:A:O2'   | 2.12                     | 0.82              |
| 30:A:1962:C:O2'   | 30:A:1964:G:OP2  | 1.97                     | 0.82              |
| 30:A:1942:C:OP2   | 30:A:1943:U:O2'  | 1.96                     | 0.82              |
| 30:A:227:A:O2'    | 30:A:228:C:O5'   | 1.97                     | 0.82              |
| 30:A:1321:A:H4'   | 31:y:17:ARG:NE   | 1.95                     | 0.81              |
| 9:E:27:LEU:HD13   | 9:E:100:MET:HE3  | 1.62                     | 0.81              |
| 30:A:463:G:N2     | 30:A:466:A:OP2   | 2.14                     | 0.81              |
| 20:Q:52:ARG:NH2   | 30:A:994:C:OP1   | 2.13                     | 0.81              |
| 30:A:2505:G:C5    | 31:z:15:HIS:ND1  | 2.48                     | 0.81              |
| 2:1:5:ARG:NH1     | 30:A:2285:C:OP2  | 2.13                     | 0.81              |
| 30:A:2326:C:O2'   | 30:A:2327:A:OP1  | 1.98                     | 0.80              |
| 15:L:55:MET:O     | 15:L:60:ARG:NH1  | 2.14                     | 0.80              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:A:698:C:O2'    | 30:A:734:A:N6    | 2.14                     | 0.80              |
| 29:Z:29:ARG:NE    | 30:A:1184:U:OP1  | 2.14                     | 0.80              |
| 30:A:2506[A]:U:O4 | 31:z:17:ARG:NH1  | 2.14                     | 0.80              |
| 21:R:80:ARG:NH2   | 30:A:572:A:OP2   | 2.15                     | 0.80              |
| 30:A:2144:G:O2'   | 30:A:2147:A:N1   | 2.15                     | 0.80              |
| 30:A:234:U:O4     | 30:A:263:G:N2    | 2.15                     | 0.79              |
| 30:A:63:A:C5      | 31:y:6:VAL:HG13  | 2.17                     | 0.79              |
| 30:A:2645:G:OP2   | 30:A:2645:G:N2   | 2.13                     | 0.79              |
| 30:A:200:U:O2     | 30:A:386:G:N2    | 2.15                     | 0.79              |
| 30:A:1257:C:H5''  | 31:z:4:ARG:HH12  | 1.46                     | 0.79              |
| 30:A:2505:G:C6    | 31:z:15:HIS:ND1  | 2.49                     | 0.79              |
| 30:A:2857:G:N2    | 30:A:2860:A:OP2  | 2.14                     | 0.79              |
| 7:C:149:LYS:NZ    | 30:A:1801:A:OP2  | 2.15                     | 0.79              |
| 30:A:1779:U:OP2   | 30:A:1784:A:N6   | 2.16                     | 0.79              |
| 1:0:4:GLN:OE1     | 30:A:2056:G:O2'  | 2.00                     | 0.79              |
| 16:M:66:ARG:NH1   | 16:M:104:GLU:OE2 | 2.15                     | 0.79              |
| 30:A:2505:G:O6    | 31:z:15:HIS:NE2  | 2.16                     | 0.78              |
| 19:P:102:ARG:NH2  | 30:A:1754:A:O2'  | 2.17                     | 0.78              |
| 25:V:11:GLU:N     | 25:V:11:GLU:OE1  | 2.17                     | 0.78              |
| 30:A:1907:G:O6    | 30:A:1924:C:N4   | 2.16                     | 0.78              |
| 30:A:1953:A:O2'   | 30:A:2559:C:O2   | 2.00                     | 0.78              |
| 9:E:63:LYS:NZ     | 30:A:2061:G:OP2  | 2.16                     | 0.78              |
| 30:A:751:A:C2     | 31:z:7:TYR:CZ    | 2.72                     | 0.78              |
| 27:X:22:ASN:OD1   | 30:A:2079:U:O2'  | 2.01                     | 0.78              |
| 30:A:191:A:O2'    | 30:A:678:C:O2    | 2.00                     | 0.78              |
| 30:A:675:A:N3     | 30:A:2443:C:O2'  | 2.16                     | 0.78              |
| 17:N:86:ARG:NH2   | 17:N:117:ASP:OD2 | 2.16                     | 0.77              |
| 30:A:2505:G:C2    | 31:z:15:HIS:CB   | 2.66                     | 0.77              |
| 4:3:31:ILE:O      | 4:3:35:LYS:NZ    | 2.17                     | 0.77              |
| 11:G:29:ASN:ND2   | 11:G:77:GLY:O    | 2.18                     | 0.77              |
| 25:V:58:SER:OG    | 25:V:59:GLU:OE1  | 2.03                     | 0.77              |
| 29:Z:11:SER:OG    | 30:A:989:G:OP2   | 2.03                     | 0.76              |
| 15:L:41:ARG:NH2   | 30:A:807:U:OP2   | 2.18                     | 0.76              |
| 30:A:1321:A:C4'   | 31:y:17:ARG:NE   | 2.48                     | 0.76              |
| 9:E:163:ASN:ND2   | 30:A:320:A:N3    | 2.33                     | 0.76              |
| 23:T:36:LYS:NZ    | 30:A:57:C:O2'    | 2.19                     | 0.76              |
| 9:E:67:ARG:NE     | 30:A:1257:C:OP1  | 2.19                     | 0.76              |
| 26:W:37:ARG:NH2   | 30:A:2387:U:O2'  | 2.19                     | 0.76              |
| 30:A:1321:A:O4'   | 31:y:17:ARG:HG2  | 1.86                     | 0.76              |
| 30:A:2816:G:N3    | 30:A:2883:A:O2'  | 2.19                     | 0.75              |
| 30:A:570:G:O4'    | 30:A:983:A:N6    | 2.20                     | 0.75              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:B:14:U:OP2      | 6:B:70:C:O2'     | 2.04                     | 0.75              |
| 30:A:2006:C:O2'   | 30:A:2823:A:N3   | 2.18                     | 0.75              |
| 30:A:2595:G:O2'   | 30:A:2597:G:O6   | 2.03                     | 0.75              |
| 30:A:2115:G:N2    | 30:A:2118:U:OP2  | 2.19                     | 0.75              |
| 30:A:1668:A:N3    | 30:A:1670:C:N4   | 2.34                     | 0.74              |
| 20:Q:101:ASP:OD2  | 21:R:2:TYR:OH    | 2.04                     | 0.74              |
| 30:A:2063:C:N4    | 30:A:2501:C:O2   | 2.21                     | 0.74              |
| 28:Y:48:ARG:NH1   | 30:A:76:C:OP1    | 2.21                     | 0.74              |
| 30:A:2506[A]:U:N3 | 31:z:17:ARG:CZ   | 2.51                     | 0.74              |
| 30:A:248:G:O2'    | 30:A:2432:A:OP1  | 2.05                     | 0.74              |
| 30:A:725:G:O2'    | 30:A:726:G:O4'   | 2.04                     | 0.74              |
| 30:A:2469:A:N6    | 30:A:2481:G:O2'  | 2.21                     | 0.74              |
| 30:A:2646:C:OP2   | 30:A:2732:G:O2'  | 2.06                     | 0.73              |
| 30:A:647:G:N2     | 30:A:2350:C:O2'  | 2.21                     | 0.73              |
| 30:A:542:C:N4     | 30:A:543:G:O6    | 2.20                     | 0.73              |
| 3:2:34:ARG:NH2    | 3:2:41:ARG:O     | 2.21                     | 0.73              |
| 5:4:19:ARG:NE     | 30:A:2756:U:OP2  | 2.20                     | 0.73              |
| 30:A:2564:A:O2'   | 30:A:2565:A:O4'  | 2.01                     | 0.73              |
| 21:R:11:GLN:N     | 21:R:11:GLN:OE1  | 2.21                     | 0.73              |
| 10:F:25:MET:O     | 10:F:29:ARG:NH1  | 2.22                     | 0.72              |
| 15:L:77:ILE:HD11  | 15:L:108:ALA:HB1 | 1.71                     | 0.72              |
| 16:M:40:ARG:NH2   | 30:A:958:U:OP1   | 2.21                     | 0.72              |
| 30:A:1936:A:OP2   | 30:A:1962:C:N4   | 2.22                     | 0.72              |
| 30:A:240:C:OP2    | 30:A:241:A:O2'   | 2.03                     | 0.72              |
| 30:A:1209:U:O2'   | 30:A:1237:A:N1   | 2.20                     | 0.72              |
| 8:D:115:GLY:N     | 30:A:2821:A:OP2  | 2.22                     | 0.72              |
| 18:O:8:ILE:O      | 18:O:12:THR:HG23 | 1.89                     | 0.72              |
| 30:A:1724:G:O6    | 30:A:1737:G:N2   | 2.23                     | 0.72              |
| 2:1:20:TYR:HH     | 30:A:2347:C:HO2' | 1.38                     | 0.72              |
| 30:A:2865:U:OP2   | 30:A:2866:U:O2'  | 2.06                     | 0.71              |
| 30:A:1834:U:O2'   | 30:A:1970:A:OP2  | 2.08                     | 0.71              |
| 30:A:372:G:O2'    | 30:A:373:U:O5'   | 2.09                     | 0.71              |
| 30:A:603:A:N6     | 30:A:655:A:O4'   | 2.23                     | 0.71              |
| 30:A:1550:C:OP1   | 30:A:1720:U:O2'  | 2.08                     | 0.71              |
| 9:E:44:ARG:NH1    | 30:A:1248:G:OP1  | 2.24                     | 0.71              |
| 16:M:81:ARG:NH1   | 30:A:2251:G:OP1  | 2.23                     | 0.71              |
| 30:A:571:U:O2'    | 30:A:573:U:OP2   | 2.08                     | 0.70              |
| 30:A:807:U:O2'    | 30:A:2060:A:N1   | 2.22                     | 0.70              |
| 30:A:963:U:O4'    | 30:A:2250:G:N2   | 2.24                     | 0.70              |
| 30:A:1062:G:O2'   | 30:A:1063:G:O4'  | 2.06                     | 0.70              |
| 7:C:70:LYS:NZ     | 7:C:99:GLU:OE2   | 2.25                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:A:1048:A:OP2   | 30:A:1110:G:N2   | 2.24                     | 0.70              |
| 30:A:1638:C:O2    | 30:A:2698:U:O2'  | 2.09                     | 0.70              |
| 15:L:99:ASN:ND2   | 30:A:621:A:OP2   | 2.25                     | 0.70              |
| 4:3:39:ARG:NH2    | 30:A:2362:C:OP1  | 2.25                     | 0.70              |
| 15:L:93:ASN:C     | 15:L:94:THR:HG1  | 1.99                     | 0.70              |
| 25:V:45:ASP:OD1   | 25:V:46:LYS:N    | 2.24                     | 0.70              |
| 30:A:2505:G:H1    | 31:z:15:HIS:CD2  | 2.08                     | 0.70              |
| 30:A:227:A:HO2'   | 30:A:228:C:P     | 2.15                     | 0.70              |
| 30:A:584:C:N4     | 30:A:585:G:O6    | 2.25                     | 0.70              |
| 6:B:76:G:O2'      | 25:V:78:GLN:OE1  | 2.09                     | 0.69              |
| 30:A:18:U:O2'     | 30:A:554:U:OP1   | 2.10                     | 0.69              |
| 30:A:2504:U:N3    | 31:z:17:ARG:NH2  | 2.40                     | 0.69              |
| 30:A:2506[A]:U:H3 | 31:z:17:ARG:CZ   | 2.03                     | 0.69              |
| 30:A:219:A:N3     | 30:A:234:U:O2'   | 2.25                     | 0.69              |
| 30:A:249:C:OP2    | 30:A:2394:C:O2'  | 2.05                     | 0.69              |
| 1:0:5:ASN:ND2     | 30:A:2022:U:O4   | 2.24                     | 0.69              |
| 18:O:31:THR:OG1   | 18:O:33:ARG:O    | 2.10                     | 0.69              |
| 30:A:2705:A:O2'   | 30:A:2852:G:OP1  | 2.09                     | 0.69              |
| 10:F:134:GLN:NE2  | 10:F:149:ARG:O   | 2.25                     | 0.69              |
| 7:C:86:ARG:NH2    | 30:A:1817:G:OP1  | 2.26                     | 0.69              |
| 30:A:1125:G:OP2   | 30:A:1126:A:O2'  | 2.10                     | 0.69              |
| 30:A:1129:A:O2'   | 30:A:2515:C:O2   | 2.10                     | 0.69              |
| 30:A:1264:A:OP2   | 30:A:1265:A:O2'  | 2.08                     | 0.69              |
| 30:A:1426:G:OP2   | 30:A:1427:A:O2'  | 2.11                     | 0.69              |
| 30:A:2506[A]:U:C4 | 31:z:17:ARG:HD2  | 2.28                     | 0.69              |
| 19:P:30:TRP:NE1   | 19:P:81:ASP:OD2  | 2.26                     | 0.69              |
| 30:A:28:A:HO2'    | 30:A:582:A:HO2'  | 1.41                     | 0.69              |
| 30:A:1019:U:OP1   | 30:A:1035:U:O2'  | 2.07                     | 0.69              |
| 30:A:1682:G:OP2   | 30:A:1699:G:N2   | 2.26                     | 0.69              |
| 30:A:2505:G:C2    | 31:z:15:HIS:CD2  | 2.80                     | 0.69              |
| 30:A:1218:G:N1    | 30:A:1232:G:N7   | 2.41                     | 0.68              |
| 30:A:1869:G:N2    | 30:A:1872:A:OP2  | 2.26                     | 0.68              |
| 8:D:70:LYS:NZ     | 30:A:2786:U:OP1  | 2.26                     | 0.68              |
| 12:H:113:SER:O    | 12:H:116:ARG:NH1 | 2.25                     | 0.68              |
| 30:A:514:A:N3     | 30:A:581:C:O2'   | 2.26                     | 0.68              |
| 30:A:743:A:O2'    | 30:A:1659:G:OP1  | 2.09                     | 0.68              |
| 30:A:2788:C:O2'   | 30:A:2809:A:N3   | 2.24                     | 0.68              |
| 8:D:118:PHE:O     | 30:A:1654:A:O2'  | 2.11                     | 0.68              |
| 20:Q:57:ARG:HE    | 20:Q:61:ILE:HD11 | 1.59                     | 0.68              |
| 30:A:1696:G:N2    | 30:A:1977:A:O2'  | 2.22                     | 0.68              |
| 10:F:89:THR:OG1   | 10:F:91:ARG:NH2  | 2.27                     | 0.68              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 27:X:36:ARG:NH2   | 30:A:2199:A:OP1  | 2.27                     | 0.68              |
| 30:A:1528:A:OP2   | 30:A:1543:G:N2   | 2.27                     | 0.68              |
| 23:T:19:LYS:NZ    | 30:A:1340:U:OP1  | 2.27                     | 0.67              |
| 30:A:239:C:O2'    | 30:A:622:G:O2'   | 2.12                     | 0.67              |
| 4:3:4:LYS:O       | 15:L:48:ARG:NH1  | 2.27                     | 0.67              |
| 7:C:156:SER:HG    | 7:C:159:THR:HG1  | 1.29                     | 0.67              |
| 30:A:648:G:O2'    | 30:A:2351:G:OP1  | 2.13                     | 0.67              |
| 30:A:1712:U:OP2   | 30:A:1713:A:O2'  | 2.02                     | 0.67              |
| 30:A:1363:C:O2'   | 30:A:1809:A:N3   | 2.26                     | 0.67              |
| 7:C:62:ARG:NH2    | 30:A:1568:G:OP2  | 2.28                     | 0.67              |
| 30:A:2595:G:N2    | 30:A:2598:A:OP2  | 2.25                     | 0.67              |
| 3:2:29:GLN:NE2    | 30:A:210:C:OP1   | 2.28                     | 0.67              |
| 22:S:25:ARG:NH1   | 22:S:74:ILE:O    | 2.28                     | 0.66              |
| 30:A:1021:A:H61   | 30:A:1142:A:H61  | 1.43                     | 0.66              |
| 30:A:2528:U:O2'   | 30:A:2530:A:OP1  | 2.10                     | 0.66              |
| 30:A:2659:G:N2    | 30:A:2662:A:OP2  | 2.29                     | 0.66              |
| 30:A:1721:G:O2'   | 30:A:1739:A:N6   | 2.28                     | 0.66              |
| 17:N:42:LYS:NZ    | 30:A:2817:U:OP1  | 2.29                     | 0.66              |
| 22:S:49:LYS:NZ    | 30:A:488:G:O3'   | 2.28                     | 0.66              |
| 30:A:1536:C:O2'   | 30:A:1537:G:N2   | 2.29                     | 0.66              |
| 2:1:20:TYR:OH     | 30:A:2347:C:O2'  | 2.13                     | 0.66              |
| 13:J:37:ARG:NH1   | 30:A:1007:C:OP1  | 2.29                     | 0.66              |
| 29:Z:46:MET:O     | 29:Z:50:VAL:HG22 | 1.95                     | 0.66              |
| 30:A:508:A:C5     | 31:y:13:PRO:HB3  | 2.30                     | 0.66              |
| 30:A:693:A:O2'    | 30:A:1353:A:N3   | 2.26                     | 0.66              |
| 9:E:65:THR:HA     | 31:z:8:ILE:HD13  | 1.77                     | 0.66              |
| 9:E:97:ASN:OD1    | 9:E:98:LYS:N     | 2.29                     | 0.65              |
| 10:F:133:GLU:OE1  | 10:F:133:GLU:N   | 2.29                     | 0.65              |
| 30:A:1217:U:O2    | 30:A:1232:G:O6   | 2.14                     | 0.65              |
| 9:E:46:GLN:O      | 9:E:88:ARG:NH2   | 2.29                     | 0.65              |
| 30:A:482:A:O2'    | 30:A:497:A:N1    | 2.27                     | 0.65              |
| 30:A:969:G:N2     | 30:A:984:A:O2'   | 2.28                     | 0.65              |
| 30:A:1801:A:N6    | 30:A:2201:G:O2'  | 2.30                     | 0.65              |
| 30:A:2506[A]:U:N3 | 31:z:17:ARG:NH1  | 2.44                     | 0.65              |
| 22:S:18:ARG:NH1   | 22:S:76:VAL:O    | 2.30                     | 0.65              |
| 6:B:80:U:O4       | 25:V:14:LYS:NZ   | 2.30                     | 0.65              |
| 30:A:569:U:O2'    | 30:A:983:A:N1    | 2.26                     | 0.65              |
| 15:L:76:GLU:OE1   | 15:L:76:GLU:N    | 2.29                     | 0.64              |
| 6:B:27:C:OP1      | 18:O:34:HIS:NE2  | 2.31                     | 0.64              |
| 30:A:1929:G:OP2   | 30:A:1929:G:N2   | 2.31                     | 0.64              |
| 30:A:2505:G:C5    | 31:z:15:HIS:CE1  | 2.85                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:S:18:ARG:NH2  | 30:A:517:C:O2'   | 2.31                     | 0.64              |
| 28:Y:8:GLU:N     | 28:Y:8:GLU:OE1   | 2.31                     | 0.64              |
| 12:H:7:ASP:OD1   | 12:H:8:LYS:N     | 2.30                     | 0.64              |
| 22:S:77:ASP:OD2  | 30:A:24:G:O2'    | 2.11                     | 0.64              |
| 29:Z:18:LYS:O    | 29:Z:22:THR:HG23 | 1.97                     | 0.64              |
| 30:A:751:A:N3    | 31:z:7:TYR:CZ    | 2.65                     | 0.64              |
| 15:L:33:ARG:NH2  | 30:A:587:C:O2    | 2.31                     | 0.64              |
| 30:A:1321:A:O2'  | 31:y:17:ARG:CZ   | 2.45                     | 0.64              |
| 7:C:257:ARG:NH2  | 7:C:262:THR:OG1  | 2.31                     | 0.63              |
| 20:Q:36:GLN:NE2  | 30:A:563:A:N3    | 2.46                     | 0.63              |
| 30:A:577:G:O2'   | 30:A:1254:A:OP1  | 2.16                     | 0.63              |
| 30:A:881:G:O6    | 30:A:895:U:O2    | 2.16                     | 0.63              |
| 30:A:1361:G:HO2' | 30:A:2215:C:HO2' | 1.43                     | 0.63              |
| 10:F:7:TYR:OH    | 10:F:28:PRO:O    | 2.16                     | 0.63              |
| 9:E:148:ILE:HG21 | 9:E:157:LEU:HD21 | 1.81                     | 0.63              |
| 18:O:48:LEU:O    | 18:O:85:LYS:NZ   | 2.30                     | 0.63              |
| 25:V:76:ASP:OD1  | 25:V:77:VAL:N    | 2.31                     | 0.63              |
| 30:A:1223:G:N2   | 30:A:1226:A:OP2  | 2.28                     | 0.63              |
| 30:A:2594:C:N4   | 30:A:2595:G:O6   | 2.31                     | 0.63              |
| 30:A:475:C:O2    | 30:A:479:A:N6    | 2.31                     | 0.63              |
| 20:Q:48:ASP:OD2  | 30:A:534:U:O2'   | 2.05                     | 0.63              |
| 29:Z:22:THR:HG22 | 30:A:850:U:O2'   | 1.98                     | 0.63              |
| 30:A:2504:U:C2   | 31:z:17:ARG:NH2  | 2.67                     | 0.63              |
| 17:N:71:ARG:NH2  | 30:A:2707:U:O2   | 2.32                     | 0.63              |
| 30:A:271:G:O2'   | 30:A:272:A:OP2   | 2.13                     | 0.63              |
| 9:E:1:MET:N      | 9:E:14:VAL:O     | 2.32                     | 0.62              |
| 12:H:109:GLU:N   | 12:H:109:GLU:OE1 | 2.33                     | 0.62              |
| 30:A:1697:G:OP2  | 30:A:1698:A:O2'  | 2.13                     | 0.62              |
| 25:V:35:GLU:N    | 25:V:35:GLU:OE1  | 2.32                     | 0.62              |
| 6:B:80:U:O2'     | 30:A:918:A:N3    | 2.31                     | 0.62              |
| 30:A:2291:U:O2'  | 30:A:2374:C:O2   | 2.17                     | 0.62              |
| 30:A:972:A:OP2   | 30:A:973:A:O2'   | 2.17                     | 0.62              |
| 30:A:1060:U:O2'  | 30:A:1071:G:OP1  | 2.17                     | 0.62              |
| 30:A:2452:C:N3   | 31:z:17:ARG:NH2  | 2.38                     | 0.62              |
| 11:G:46:ASP:O    | 11:G:47:ASN:ND2  | 2.33                     | 0.62              |
| 30:A:83:A:O2'    | 30:A:103:A:N6    | 2.33                     | 0.62              |
| 1:O:9:ARG:NH2    | 30:A:516:C:OP1   | 2.33                     | 0.61              |
| 30:A:345:A:N3    | 30:A:347:A:N6    | 2.47                     | 0.61              |
| 8:D:16:THR:OG1   | 8:D:18:ASP:OD1   | 2.16                     | 0.61              |
| 30:A:966:G:H4'   | 30:A:2271:G:H22  | 1.64                     | 0.61              |
| 30:A:2047:C:O2'  | 30:A:2823:A:N1   | 2.33                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:F:161:SER:N   | 10:F:164:GLU:OE2  | 2.34                     | 0.61              |
| 17:N:73:ASN:OD1  | 30:A:1454:C:N4    | 2.33                     | 0.61              |
| 27:X:40:GLU:OE1  | 27:X:40:GLU:N     | 2.34                     | 0.61              |
| 30:A:1021:A:N6   | 30:A:1142:A:H61   | 1.98                     | 0.61              |
| 8:D:148:GLN:OE1  | 8:D:148:GLN:N     | 2.34                     | 0.61              |
| 6:B:42:C:C5      | 10:F:65:LEU:HD13  | 2.36                     | 0.60              |
| 30:A:36:G:N3     | 30:A:450:G:O2'    | 2.34                     | 0.60              |
| 30:A:2505:G:N3   | 31:z:15:HIS:CB    | 2.60                     | 0.60              |
| 30:A:2099:U:O2'  | 30:A:2100:G:O5'   | 2.20                     | 0.60              |
| 25:V:58:SER:O    | 25:V:73:LYS:NZ    | 2.35                     | 0.60              |
| 1:O:43:THR:OG1   | 1:O:45:ASP:OD1    | 2.18                     | 0.60              |
| 30:A:1864:U:OP1  | 30:A:2410:G:O2'   | 2.19                     | 0.60              |
| 20:Q:88:GLU:N    | 20:Q:88:GLU:OE1   | 2.35                     | 0.60              |
| 6:B:52:A:O2'     | 6:B:53:A:OP2      | 2.17                     | 0.60              |
| 23:T:13:ALA:O    | 23:T:33:LYS:N     | 2.35                     | 0.60              |
| 30:A:2439:A:O2'  | 30:A:2600:A:OP1   | 2.18                     | 0.60              |
| 8:D:131:ASP:O    | 8:D:136:ASN:ND2   | 2.34                     | 0.59              |
| 27:X:56:ARG:NH2  | 30:A:372:G:O6     | 2.34                     | 0.59              |
| 7:C:256:THR:OG1  | 30:A:1797:G:O2'   | 2.18                     | 0.59              |
| 30:A:754:U:O2'   | 30:A:1272:A:N1    | 2.35                     | 0.59              |
| 30:A:2032:G:OP2  | 30:A:2454:G:O2'   | 2.13                     | 0.59              |
| 30:A:160:A:N3    | 30:A:2208:C:O2'   | 2.33                     | 0.59              |
| 30:A:1771:C:O2'  | 30:A:1786:A:O4'   | 2.18                     | 0.59              |
| 30:A:2090:A:N6   | 30:A:2230:G:O6    | 2.35                     | 0.59              |
| 1:O:12:ARG:NH2   | 30:A:517:C:OP1    | 2.35                     | 0.59              |
| 17:N:29:VAL:HG21 | 17:N:79:LEU:HD11  | 1.82                     | 0.59              |
| 28:Y:5:GLU:OE1   | 28:Y:5:GLU:N      | 2.36                     | 0.59              |
| 12:H:135:HIS:HB3 | 12:H:138:VAL:HG12 | 1.85                     | 0.59              |
| 22:S:79:GLY:N    | 22:S:100:THR:O    | 2.35                     | 0.59              |
| 14:K:28:SER:OG   | 30:A:2566:A:N1    | 2.35                     | 0.59              |
| 30:A:1130:U:N3   | 30:A:2025:C:OP1   | 2.35                     | 0.59              |
| 9:E:97:ASN:ND2   | 30:A:606:U:OP1    | 2.36                     | 0.58              |
| 30:A:2505:G:C5   | 31:z:15:HIS:CG    | 2.91                     | 0.58              |
| 11:G:66:THR:HG22 | 30:A:2747:G:O2'   | 2.03                     | 0.58              |
| 30:A:1321:A:O4'  | 31:y:17:ARG:NE    | 2.36                     | 0.58              |
| 25:V:1:MET:SD    | 25:V:1:MET:N      | 2.77                     | 0.58              |
| 9:E:43:THR:O     | 30:A:442:G:N2     | 2.33                     | 0.58              |
| 10:F:120:SER:OG  | 10:F:128:SER:O    | 2.22                     | 0.58              |
| 22:S:2:GLU:OE1   | 22:S:2:GLU:N      | 2.36                     | 0.58              |
| 26:W:37:ARG:O    | 26:W:53:HIS:ND1   | 2.33                     | 0.58              |
| 30:A:2504:U:H3   | 31:z:17:ARG:NH2   | 2.02                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:S:78:GLU:OE1  | 22:S:78:GLU:N     | 2.37                     | 0.58              |
| 26:W:25:GLU:OE2  | 30:A:855:G:N2     | 2.37                     | 0.58              |
| 30:A:726:G:O5'   | 30:A:1432:G:O2'   | 2.21                     | 0.58              |
| 8:D:151:THR:OG1  | 30:A:2032:G:N2    | 2.37                     | 0.58              |
| 20:Q:101:ASP:N   | 20:Q:101:ASP:OD1  | 2.36                     | 0.58              |
| 30:A:644:A:O2'   | 30:A:645:C:O5'    | 2.14                     | 0.58              |
| 30:A:1068:G:N2   | 30:A:1095:A:O2'   | 2.36                     | 0.58              |
| 9:E:49:ARG:NH2   | 9:E:72:SER:OG     | 2.36                     | 0.58              |
| 9:E:122:GLU:OE1  | 9:E:123:LYS:N     | 2.37                     | 0.58              |
| 5:4:1:MET:SD     | 5:4:34:LYS:NZ     | 2.77                     | 0.57              |
| 22:S:77:ASP:O    | 22:S:102:HIS:N    | 2.35                     | 0.57              |
| 30:A:2580:U:O2'  | 30:A:2581:G:O4'   | 2.20                     | 0.57              |
| 10:F:37:MET:SD   | 10:F:37:MET:N     | 2.78                     | 0.57              |
| 30:A:1040:A:N6   | 30:A:1116:G:O6    | 2.37                     | 0.57              |
| 7:C:235:GLU:N    | 7:C:235:GLU:OE1   | 2.37                     | 0.57              |
| 10:F:97:GLU:OE1  | 10:F:101:ARG:NE   | 2.37                     | 0.57              |
| 30:A:324:A:N6    | 30:A:339:U:O4'    | 2.37                     | 0.57              |
| 30:A:2324:U:O2'  | 30:A:2337:G:OP1   | 2.21                     | 0.57              |
| 6:B:37:C:O2      | 18:O:100:HIS:NE2  | 2.37                     | 0.57              |
| 8:D:1:MET:HE1    | 8:D:100:LEU:HB3   | 1.85                     | 0.57              |
| 15:L:95:LEU:HD11 | 15:L:100:ILE:HD11 | 1.85                     | 0.57              |
| 30:A:629:G:N3    | 30:A:639:U:O2'    | 2.38                     | 0.57              |
| 30:A:1326:U:HO2' | 30:A:2010:G:HO2'  | 1.52                     | 0.57              |
| 30:A:2632:A:HO2' | 30:A:2811:G:HO2'  | 1.53                     | 0.57              |
| 7:C:99:GLU:N     | 7:C:99:GLU:OE1    | 2.37                     | 0.57              |
| 23:T:54:GLU:OE1  | 23:T:54:GLU:N     | 2.37                     | 0.57              |
| 24:U:3:LYS:O     | 24:U:93:ARG:NH1   | 2.37                     | 0.57              |
| 30:A:2061:G:N2   | 31:z:17:ARG:HB3   | 2.20                     | 0.57              |
| 30:A:2505:G:H21  | 31:z:16:PRO:HD2   | 1.68                     | 0.57              |
| 24:U:6:ARG:N     | 30:A:85:G:OP1     | 2.37                     | 0.57              |
| 10:F:93:GLU:OE1  | 10:F:93:GLU:N     | 2.37                     | 0.57              |
| 4:3:30:HIS:NE2   | 30:A:2392:A:OP2   | 2.37                     | 0.57              |
| 7:C:270:ARG:NH2  | 30:A:1798:U:OP2   | 2.33                     | 0.57              |
| 30:A:2692:G:N3   | 30:A:2847:U:O2'   | 2.38                     | 0.57              |
| 8:D:123:LYS:NZ   | 30:A:1999:C:OP1   | 2.38                     | 0.57              |
| 30:A:1257:C:H5'' | 31:z:4:ARG:NH1    | 2.16                     | 0.57              |
| 16:M:20:LEU:HD21 | 25:V:81:PRO:HG2   | 1.87                     | 0.56              |
| 29:Z:57:GLU:N    | 29:Z:57:GLU:OE1   | 2.38                     | 0.56              |
| 9:E:162:ARG:NH2  | 30:A:340:A:O2'    | 2.38                     | 0.56              |
| 9:E:154:ASP:OD1  | 9:E:154:ASP:N     | 2.38                     | 0.56              |
| 9:E:176:ASP:N    | 9:E:176:ASP:OD1   | 2.35                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 11:G:87:GLN:OE1   | 11:G:87:GLN:N    | 2.39                     | 0.56              |
| 30:A:586:A:OP2    | 30:A:1251:C:N4   | 2.38                     | 0.56              |
| 30:A:641:U:O2'    | 30:A:2350:C:OP1  | 2.17                     | 0.56              |
| 30:A:2505:G:N2    | 31:z:16:PRO:HD2  | 2.20                     | 0.56              |
| 10:F:62:GLN:OE1   | 10:F:62:GLN:N    | 2.39                     | 0.56              |
| 10:F:7:TYR:HA     | 10:F:11:VAL:HG12 | 1.88                     | 0.56              |
| 26:W:7:ARG:O      | 26:W:10:ARG:NH1  | 2.38                     | 0.56              |
| 30:A:527:C:OP2    | 30:A:2779:U:N3   | 2.35                     | 0.56              |
| 8:D:25:THR:OG1    | 8:D:191:GLY:O    | 2.14                     | 0.55              |
| 15:L:111:ILE:HD11 | 30:A:627:A:C5    | 2.40                     | 0.55              |
| 20:Q:47:ARG:NH2   | 30:A:560:C:O2    | 2.39                     | 0.55              |
| 25:V:61:LEU:N     | 25:V:72:VAL:O    | 2.39                     | 0.55              |
| 4:3:32:LEU:HD22   | 30:A:2419:U:OP2  | 2.06                     | 0.55              |
| 30:A:2637:U:O4    | 30:A:2776:A:N7   | 2.40                     | 0.55              |
| 16:M:11:LYS:O     | 30:A:911:A:N6    | 2.39                     | 0.55              |
| 30:A:1321:A:O4'   | 31:y:17:ARG:CG   | 2.55                     | 0.55              |
| 2:1:31:GLU:OE1    | 2:1:31:GLU:N     | 2.39                     | 0.55              |
| 24:U:16:LYS:N     | 30:A:329:G:O6    | 2.39                     | 0.55              |
| 27:X:57:VAL:HG12  | 30:A:372:G:H3'   | 1.89                     | 0.55              |
| 30:A:84:A:N1      | 30:A:98:G:O2'    | 2.31                     | 0.55              |
| 30:A:1353:A:OP2   | 30:A:1377:G:N1   | 2.36                     | 0.55              |
| 24:U:85:ARG:NE    | 24:U:87:GLU:OE2  | 2.40                     | 0.55              |
| 30:A:976:G:O2'    | 30:A:1155:A:O2'  | 2.14                     | 0.55              |
| 30:A:1205:A:O2'   | 30:A:1206:G:OP1  | 2.22                     | 0.55              |
| 30:A:2451:A:OP1   | 30:A:2497:A:N6   | 2.39                     | 0.55              |
| 18:O:116:GLN:OE1  | 18:O:116:GLN:N   | 2.39                     | 0.54              |
| 30:A:1007:C:OP2   | 30:A:1008:A:O2'  | 2.12                     | 0.54              |
| 7:C:78:GLU:N      | 7:C:78:GLU:OE1   | 2.40                     | 0.54              |
| 30:A:184:C:O2'    | 30:A:217:A:N3    | 2.41                     | 0.54              |
| 30:A:793:A:OP2    | 30:A:2071:A:O2'  | 2.25                     | 0.54              |
| 30:A:2349:G:O6    | 30:A:2369:A:N6   | 2.40                     | 0.54              |
| 30:A:2776:A:O2'   | 30:A:2782:G:N7   | 2.37                     | 0.54              |
| 19:P:13:LYS:NZ    | 19:P:76:HIS:O    | 2.41                     | 0.54              |
| 30:A:222:A:H61    | 30:A:232:G:H1'   | 1.71                     | 0.54              |
| 12:H:2:GLN:N      | 12:H:2:GLN:OE1   | 2.39                     | 0.54              |
| 13:J:138:GLN:OE1  | 13:J:138:GLN:N   | 2.37                     | 0.54              |
| 14:K:6:THR:HG23   | 30:A:1666:G:H4'  | 1.89                     | 0.54              |
| 30:A:2075:U:O2'   | 30:A:2077:A:OP2  | 2.15                     | 0.54              |
| 30:A:2509:G:N1    | 30:A:2580:U:O4   | 2.41                     | 0.54              |
| 4:3:12:ARG:NE     | 15:L:61:LEU:O    | 2.39                     | 0.54              |
| 30:A:1341:G:OP1   | 30:A:1397:U:N3   | 2.40                     | 0.54              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 30:A:1999:C:O2     | 30:A:2687:U:O2'  | 2.23                     | 0.54              |
| 30:A:1084:A:N6     | 30:A:1085:A:N1   | 2.56                     | 0.54              |
| 30:A:2133:G:N2     | 30:A:2157:G:O6   | 2.41                     | 0.54              |
| 30:A:2552:U:O2'    | 30:A:2553:G:N7   | 2.41                     | 0.54              |
| 8:D:155:VAL:HG21   | 30:A:2618:G:H21  | 1.73                     | 0.54              |
| 19:P:33:GLU:N      | 19:P:33:GLU:OE1  | 2.40                     | 0.54              |
| 30:A:48:G:H22      | 30:A:177:G:P     | 2.31                     | 0.54              |
| 30:A:63:A:C4       | 31:y:6:VAL:HG13  | 2.42                     | 0.54              |
| 30:A:462:C:N4      | 30:A:463:G:O6    | 2.41                     | 0.54              |
| 30:A:1018:U:O3'    | 30:A:1120:G:N2   | 2.41                     | 0.54              |
| 30:A:2751:G:OP1    | 30:A:2751:G:N2   | 2.37                     | 0.53              |
| 19:P:93:LYS:NZ     | 30:A:2848:G:OP1  | 2.40                     | 0.53              |
| 9:E:79:ARG:NE      | 30:A:448:U:O4'   | 2.41                     | 0.53              |
| 15:L:91:ASP:OD1    | 15:L:92:LEU:N    | 2.41                     | 0.53              |
| 30:A:245:G:O2'     | 30:A:384:A:N1    | 2.37                     | 0.53              |
| 8:D:3:GLY:C        | 8:D:4:LEU:HD12   | 2.34                     | 0.53              |
| 30:A:508:A:OP2     | 31:y:13:PRO:HG3  | 2.08                     | 0.53              |
| 30:A:1048:A:O2'    | 30:A:1112:G:N2   | 2.41                     | 0.53              |
| 30:A:1662:U:O2'    | 30:A:2687:U:OP1  | 2.24                     | 0.53              |
| 30:A:1779:U:O2     | 30:A:1783:A:N6   | 2.41                     | 0.53              |
| 13:J:135:GLN:NE2   | 30:A:6:A:N3      | 2.56                     | 0.53              |
| 30:A:1954:G:O2'    | 30:A:1956:U:O4   | 2.25                     | 0.53              |
| 30:A:575:A:OP2     | 30:A:2055:C:N4   | 2.42                     | 0.53              |
| 30:A:2077:A:N3     | 30:A:2434:A:O2'  | 2.40                     | 0.53              |
| 30:A:453:A:N3      | 30:A:457:A:O2'   | 2.42                     | 0.53              |
| 26:W:11:ASP:OD1    | 26:W:12:SER:N    | 2.40                     | 0.53              |
| 30:A:799:G:OP2     | 30:A:800:A:O2'   | 2.22                     | 0.53              |
| 30:A:1951:U:O2'    | 30:A:1953:A:N7   | 2.36                     | 0.53              |
| 4:3:7:ARG:NH1      | 30:A:243:U:OP1   | 2.42                     | 0.53              |
| 10:F:139:GLU:OE1   | 10:F:139:GLU:N   | 2.40                     | 0.53              |
| 19:P:12:MET:HB2    | 19:P:54:LEU:HD11 | 1.91                     | 0.53              |
| 26:W:25:GLU:N      | 26:W:25:GLU:OE1  | 2.42                     | 0.53              |
| 30:A:370:G:O2'     | 30:A:424:G:OP1   | 2.26                     | 0.53              |
| 30:A:2506[A]:U:OP2 | 30:A:2576:G:N1   | 2.39                     | 0.53              |
| 9:E:32:VAL:HG23    | 9:E:178:VAL:HG22 | 1.89                     | 0.52              |
| 17:N:1:MET:N       | 30:A:1654:A:OP2  | 2.42                     | 0.52              |
| 30:A:630:G:N2      | 30:A:633:A:OP2   | 2.41                     | 0.52              |
| 9:E:140:ASP:OD1    | 9:E:141:MET:N    | 2.42                     | 0.52              |
| 9:E:146:VAL:HG21   | 9:E:187:VAL:HG13 | 1.90                     | 0.52              |
| 25:V:72:VAL:HG21   | 25:V:91:PHE:HB3  | 1.91                     | 0.52              |
| 30:A:2250:G:O2'    | 30:A:2496:C:OP1  | 2.27                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:A:2468:A:O2'  | 30:A:2469:A:O4'  | 2.25                     | 0.52              |
| 30:A:212:G:H2'   | 30:A:213:A:C8    | 2.45                     | 0.52              |
| 30:A:477:A:N6    | 30:A:501:A:OP1   | 2.43                     | 0.52              |
| 30:A:1020:A:H1'  | 30:A:1021:A:OP2  | 2.09                     | 0.52              |
| 13:J:39:LYS:NZ   | 30:A:1009:A:OP2  | 2.35                     | 0.52              |
| 30:A:966:G:O4'   | 30:A:2267:A:N6   | 2.43                     | 0.52              |
| 30:A:2628:C:O2'  | 30:A:2782:G:OP1  | 2.22                     | 0.52              |
| 10:F:134:GLN:N   | 10:F:134:GLN:OE1 | 2.42                     | 0.52              |
| 19:P:26:GLU:N    | 19:P:26:GLU:OE1  | 2.42                     | 0.52              |
| 19:P:47:ILE:HG22 | 19:P:99:LEU:HD12 | 1.91                     | 0.52              |
| 20:Q:85:ALA:O    | 20:Q:86:SER:OG   | 2.21                     | 0.52              |
| 25:V:7:GLU:N     | 25:V:7:GLU:OE1   | 2.42                     | 0.52              |
| 30:A:981:A:OP2   | 30:A:982:C:N4    | 2.37                     | 0.52              |
| 30:A:2468:A:P    | 30:A:2476:A:H61  | 2.33                     | 0.52              |
| 28:Y:24:GLU:HA   | 28:Y:28:LEU:HD23 | 1.92                     | 0.52              |
| 30:A:974:G:O4'   | 30:A:990:A:N6    | 2.43                     | 0.52              |
| 13:J:14:ASP:OD1  | 13:J:15:TRP:N    | 2.43                     | 0.52              |
| 21:R:22:LEU:HD12 | 21:R:23:GLU:O    | 2.10                     | 0.52              |
| 9:E:171:ASP:OD1  | 9:E:172:ALA:N    | 2.41                     | 0.51              |
| 30:A:1321:A:O2'  | 31:y:17:ARG:NH2  | 2.43                     | 0.51              |
| 30:A:1321:A:C4   | 31:y:16:PRO:HA   | 2.45                     | 0.51              |
| 30:A:45:G:N7     | 30:A:215:G:O2'   | 2.43                     | 0.51              |
| 30:A:59:U:O2'    | 30:A:74:A:OP2    | 2.19                     | 0.51              |
| 30:A:372:G:HO2'  | 30:A:373:U:P     | 2.33                     | 0.51              |
| 30:A:1026:G:OP2  | 30:A:1134:A:O2'  | 2.27                     | 0.51              |
| 15:L:29:LYS:O    | 15:L:30:THR:OG1  | 2.17                     | 0.51              |
| 22:S:18:ARG:NH2  | 22:S:78:GLU:OE2  | 2.43                     | 0.51              |
| 30:A:28:A:O2'    | 30:A:582:A:O2'   | 2.17                     | 0.51              |
| 9:E:48:THR:O     | 9:E:52:VAL:HG23  | 2.11                     | 0.51              |
| 7:C:47:ARG:NH1   | 30:A:774:G:OP1   | 2.44                     | 0.51              |
| 30:A:574:A:N6    | 30:A:2034:U:OP1  | 2.41                     | 0.51              |
| 20:Q:8:ILE:HD12  | 20:Q:8:ILE:H     | 1.76                     | 0.51              |
| 22:S:109:ASP:OD1 | 22:S:110:ARG:N   | 2.43                     | 0.51              |
| 30:A:1688:U:O2'  | 30:A:1700:A:N7   | 2.39                     | 0.51              |
| 15:L:82:LEU:O    | 15:L:82:LEU:HD23 | 2.11                     | 0.51              |
| 30:A:1255:U:O4'  | 30:A:2502:G:N2   | 2.43                     | 0.51              |
| 30:A:2505:G:C4   | 31:z:15:HIS:CG   | 2.99                     | 0.51              |
| 19:P:79:VAL:HG13 | 19:P:80:VAL:HG13 | 1.93                     | 0.51              |
| 30:A:1447:C:N4   | 30:A:1448:G:O6   | 2.43                     | 0.51              |
| 30:A:2243:U:O2'  | 30:A:2434:A:N1   | 2.41                     | 0.51              |
| 30:A:2637:U:H3   | 30:A:2776:A:H62  | 1.57                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:L:79:LEU:HD21 | 15:L:131:ALA:HB1 | 1.93                     | 0.50              |
| 30:A:2076:U:OP2  | 30:A:2238:G:N2   | 2.41                     | 0.50              |
| 20:Q:54:ARG:NH2  | 30:A:1155:A:O3'  | 2.44                     | 0.50              |
| 30:A:378:C:N4    | 30:A:379:G:O6    | 2.44                     | 0.50              |
| 24:U:67:SER:O    | 30:A:335:C:O2'   | 2.25                     | 0.50              |
| 30:A:1141:U:O2   | 30:A:1142:A:N6   | 2.44                     | 0.50              |
| 7:C:62:ARG:NH2   | 30:A:1567:G:O2'  | 2.45                     | 0.50              |
| 30:A:1131:G:O2'  | 30:A:2025:C:O2'  | 2.22                     | 0.50              |
| 30:A:1733:G:C2   | 30:A:1734:G:N7   | 2.79                     | 0.50              |
| 30:A:1814:G:OP2  | 30:A:1815:A:O2'  | 2.26                     | 0.50              |
| 30:A:2638:G:O2'  | 30:A:2778:A:N6   | 2.44                     | 0.50              |
| 30:A:1275:A:N1   | 30:A:1295:C:O2'  | 2.37                     | 0.50              |
| 6:B:52:A:O2'     | 6:B:53:A:P       | 2.70                     | 0.50              |
| 30:A:308:G:O2'   | 30:A:329:G:N2    | 2.45                     | 0.50              |
| 30:A:951:C:N4    | 30:A:952:G:O6    | 2.44                     | 0.50              |
| 9:E:61:ARG:HH12  | 31:z:8:ILE:HG23  | 1.77                     | 0.50              |
| 18:O:61:GLN:OE1  | 18:O:61:GLN:N    | 2.44                     | 0.50              |
| 30:A:1018:U:O2'  | 30:A:1120:G:N2   | 2.36                     | 0.50              |
| 2:1:36:LYS:NZ    | 30:A:2372:U:O2'  | 2.43                     | 0.49              |
| 22:S:67:ASP:OD1  | 22:S:68:ASP:N    | 2.45                     | 0.49              |
| 30:A:447:A:N1    | 30:A:454:A:O2'   | 2.41                     | 0.49              |
| 6:B:8:C:OP1      | 18:O:15:ARG:NH2  | 2.45                     | 0.49              |
| 9:E:191:ASP:OD1  | 9:E:192:ALA:N    | 2.45                     | 0.49              |
| 24:U:44:HIS:N    | 30:A:481:G:OP2   | 2.39                     | 0.49              |
| 30:A:724:U:C2'   | 30:A:725:G:O5'   | 2.60                     | 0.49              |
| 30:A:837:C:N3    | 30:A:941:A:N6    | 2.61                     | 0.49              |
| 30:A:1022:G:H4'  | 30:A:1023:U:O5'  | 2.12                     | 0.49              |
| 30:A:2743:U:OP2  | 30:A:2755:C:N4   | 2.45                     | 0.49              |
| 7:C:123:ILE:O    | 7:C:123:ILE:HG22 | 2.11                     | 0.49              |
| 9:E:27:LEU:CD1   | 9:E:100:MET:HE3  | 2.37                     | 0.49              |
| 30:A:644:A:HO2'  | 30:A:645:C:P     | 2.33                     | 0.49              |
| 30:A:1664:A:H61  | 30:A:1996:C:N4   | 2.10                     | 0.49              |
| 30:A:2808:G:O2'  | 30:A:2809:A:N7   | 2.45                     | 0.49              |
| 30:A:2577:A:O4'  | 30:A:2612:C:N4   | 2.45                     | 0.49              |
| 7:C:245:THR:HG23 | 7:C:247:TRP:H    | 1.77                     | 0.49              |
| 22:S:80:PRO:O    | 22:S:100:THR:OG1 | 2.28                     | 0.49              |
| 30:A:63:A:C6     | 31:y:6:VAL:CG1   | 2.96                     | 0.49              |
| 30:A:220:G:N1    | 30:A:428:A:OP2   | 2.44                     | 0.49              |
| 30:A:1282:U:O4   | 30:A:1286:A:N7   | 2.45                     | 0.49              |
| 30:A:1321:A:O4'  | 31:y:17:ARG:CD   | 2.61                     | 0.49              |
| 20:Q:53:LYS:NZ   | 30:A:994:C:OP2   | 2.45                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:W:38:GLY:HA2  | 30:A:2330:G:H21   | 1.76                     | 0.49              |
| 29:Z:4:ILE:HD11  | 29:Z:56:VAL:CG2   | 2.42                     | 0.49              |
| 30:A:2063:C:O2'  | 31:z:18:LEU:HB2   | 2.12                     | 0.49              |
| 14:K:22:ILE:HD11 | 14:K:40:LYS:HG2   | 1.95                     | 0.49              |
| 30:A:451:U:O2    | 30:A:453:A:N6     | 2.46                     | 0.49              |
| 30:A:1288:G:OP2  | 30:A:1288:G:N2    | 2.33                     | 0.49              |
| 30:A:2474:U:H2'  | 30:A:2474:U:O2    | 2.12                     | 0.49              |
| 10:F:25:MET:SD   | 10:F:25:MET:N     | 2.84                     | 0.49              |
| 10:F:90:LEU:HD23 | 10:F:90:LEU:H     | 1.77                     | 0.49              |
| 7:C:237:ARG:NH2  | 30:A:1787:A:OP1   | 2.46                     | 0.49              |
| 30:A:1794:A:N6   | 30:A:1826:G:O6    | 2.45                     | 0.49              |
| 14:K:19:VAL:HG11 | 14:K:41:ILE:HD12  | 1.94                     | 0.48              |
| 20:Q:10:ARG:NH2  | 30:A:513:A:N3     | 2.59                     | 0.48              |
| 30:A:357:C:C2    | 30:A:358:U:C5     | 3.01                     | 0.48              |
| 30:A:864:G:H21   | 30:A:866:A:H62    | 1.61                     | 0.48              |
| 7:C:20:ASN:O     | 7:C:23:LEU:HD22   | 2.12                     | 0.48              |
| 9:E:7:ASP:OD1    | 9:E:8:ALA:N       | 2.46                     | 0.48              |
| 17:N:67:PHE:HA   | 17:N:76:VAL:HG11  | 1.94                     | 0.48              |
| 30:A:63:A:C2     | 31:y:6:VAL:HG12   | 2.48                     | 0.48              |
| 20:Q:65:ASN:OD1  | 20:Q:69:ARG:NE    | 2.45                     | 0.48              |
| 24:U:3:LYS:NZ    | 24:U:82:VAL:O     | 2.46                     | 0.48              |
| 30:A:1275:A:O2'  | 30:A:1645:G:N3    | 2.46                     | 0.48              |
| 16:M:110:GLU:OE2 | 16:M:114:ARG:NE   | 2.47                     | 0.48              |
| 30:A:549:G:HO2'  | 30:A:550:C:P      | 2.37                     | 0.48              |
| 4:3:22:LYS:NZ    | 30:A:630:G:OP1    | 2.41                     | 0.48              |
| 6:B:38:C:O4'     | 18:O:100:HIS:NE2  | 2.46                     | 0.48              |
| 30:A:549:G:O2'   | 30:A:550:C:P      | 2.72                     | 0.48              |
| 30:A:1270:C:N4   | 30:A:1648:U:O4    | 2.47                     | 0.48              |
| 12:H:12:LEU:H    | 12:H:12:LEU:HD23  | 1.79                     | 0.48              |
| 13:J:36:LEU:HD21 | 13:J:122:LEU:HD13 | 1.95                     | 0.48              |
| 30:A:225:C:N3    | 30:A:231:A:N6     | 2.61                     | 0.48              |
| 30:A:1276:A:N6   | 30:A:1645:G:O6    | 2.46                     | 0.48              |
| 30:A:1638:C:OP1  | 30:A:2710:C:O2'   | 2.32                     | 0.48              |
| 8:D:114:LYS:NZ   | 30:A:2723:C:OP1   | 2.39                     | 0.48              |
| 19:P:8:GLU:HB2   | 19:P:54:LEU:HD13  | 1.95                     | 0.48              |
| 15:L:82:LEU:HD23 | 15:L:90:VAL:HG21  | 1.96                     | 0.48              |
| 30:A:92:U:C1'    | 31:y:7:TYR:HE2    | 2.27                     | 0.48              |
| 30:A:27:G:O2'    | 30:A:28:A:OP2     | 2.24                     | 0.48              |
| 30:A:2720:U:C2   | 30:A:2721:A:C8    | 3.01                     | 0.48              |
| 6:B:83:G:O6      | 6:B:94:A:N6       | 2.47                     | 0.48              |
| 8:D:8:LYS:HA     | 8:D:27:ILE:HD12   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:A:1289:C:C2    | 30:A:1290:C:C5   | 3.02                     | 0.48              |
| 30:A:2581:G:N2    | 30:A:2581:G:OP2  | 2.47                     | 0.48              |
| 30:A:2699:C:N4    | 30:A:2700:A:H62  | 2.12                     | 0.48              |
| 7:C:193:GLU:N     | 7:C:193:GLU:OE1  | 2.46                     | 0.47              |
| 30:A:61:C:O2'     | 31:y:3:ASN:ND2   | 2.47                     | 0.47              |
| 8:D:129:THR:OG1   | 30:A:1997:C:O5'  | 2.26                     | 0.47              |
| 25:V:59:GLU:OE1   | 25:V:59:GLU:N    | 2.43                     | 0.47              |
| 6:B:15:A:N3       | 6:B:109:A:N6     | 2.61                     | 0.47              |
| 30:A:1754:A:N6    | 30:A:2717:C:O4'  | 2.46                     | 0.47              |
| 4:3:63:TYR:OH     | 30:A:592:A:O2'   | 2.19                     | 0.47              |
| 19:P:61:ARG:NH1   | 19:P:70:GLU:OE2  | 2.43                     | 0.47              |
| 24:U:98:ASN:O     | 24:U:98:ASN:CG   | 2.58                     | 0.47              |
| 30:A:1139:G:O2'   | 30:A:1143:A:N1   | 2.46                     | 0.47              |
| 30:A:1288:G:OP1   | 30:A:1289:C:N4   | 2.47                     | 0.47              |
| 15:L:82:LEU:CD2   | 15:L:90:VAL:HG21 | 2.44                     | 0.47              |
| 23:T:70:HIS:CE1   | 31:y:9:PRO:HD3   | 2.48                     | 0.47              |
| 30:A:2679:A:N6    | 30:A:2729:G:O6   | 2.48                     | 0.47              |
| 7:C:15:VAL:HG22   | 7:C:205:GLY:HA3  | 1.95                     | 0.47              |
| 30:A:63:A:C5      | 31:y:6:VAL:CG1   | 2.93                     | 0.47              |
| 30:A:63:A:N1      | 31:y:6:VAL:HG12  | 2.29                     | 0.47              |
| 23:T:37:ASP:OD1   | 23:T:38:ALA:N    | 2.47                     | 0.47              |
| 11:G:154:GLU:OE1  | 11:G:156:TYR:N   | 2.48                     | 0.47              |
| 12:H:17:ASP:OD1   | 12:H:18:GLN:N    | 2.48                     | 0.47              |
| 30:A:2504:U:H3    | 31:z:17:ARG:HH22 | 1.62                     | 0.47              |
| 6:B:45:A:O4'      | 10:F:91:ARG:NH1  | 2.48                     | 0.47              |
| 16:M:44:ARG:NH2   | 30:A:2484:G:OP2  | 2.47                     | 0.47              |
| 30:A:63:A:C4      | 31:y:6:VAL:CG1   | 2.98                     | 0.47              |
| 30:A:299:A:N6     | 30:A:322:A:O2'   | 2.45                     | 0.47              |
| 30:A:2286:G:N2    | 30:A:2344:U:O2   | 2.48                     | 0.47              |
| 30:A:2655:G:O2'   | 30:A:2656:U:O5'  | 2.33                     | 0.47              |
| 30:A:2506[A]:U:O4 | 31:z:17:ARG:HD2  | 2.13                     | 0.46              |
| 4:3:27:ASN:ND2    | 30:A:2361:G:O3'  | 2.48                     | 0.46              |
| 9:E:31:VAL:HG21   | 9:E:104:ALA:CB   | 2.45                     | 0.46              |
| 9:E:65:THR:HG22   | 31:z:8:ILE:HG21  | 1.97                     | 0.46              |
| 17:N:66:ALA:O     | 17:N:69:ARG:O    | 2.33                     | 0.46              |
| 23:T:70:HIS:HD2   | 30:A:64:A:C2     | 2.33                     | 0.46              |
| 26:W:17:LEU:HD21  | 26:W:37:ARG:HD3  | 1.98                     | 0.46              |
| 30:A:727:A:H2'    | 30:A:728:G:O4'   | 2.15                     | 0.46              |
| 30:A:780:G:O2'    | 30:A:783:A:N6    | 2.42                     | 0.46              |
| 31:z:18:LEU:H     | 31:z:18:LEU:HD23 | 1.81                     | 0.46              |
| 8:D:14:ILE:HD13   | 8:D:178:VAL:CG1  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:E:100:MET:HE1   | 30:A:600:G:O4'    | 2.15                     | 0.46              |
| 15:L:3:LEU:HD21   | 30:A:1202:G:O2'   | 2.14                     | 0.46              |
| 23:T:82:LYS:NZ    | 30:A:1339:G:OP1   | 2.49                     | 0.46              |
| 24:U:36:GLU:O     | 24:U:38:ILE:HD12  | 2.14                     | 0.46              |
| 30:A:2652:C:H2'   | 30:A:2653:U:O4'   | 2.16                     | 0.46              |
| 15:L:43:GLY:N     | 30:A:671:C:OP1    | 2.42                     | 0.46              |
| 20:Q:29:ARG:NH1   | 30:A:18:U:OP1     | 2.42                     | 0.46              |
| 5:4:3:VAL:HG12    | 5:4:3:VAL:O       | 2.14                     | 0.46              |
| 6:B:116:G:H4'     | 18:O:54:VAL:HG12  | 1.98                     | 0.46              |
| 8:D:124:ARG:NH1   | 30:A:2620:C:O2'   | 2.44                     | 0.46              |
| 20:Q:71:ASN:OD1   | 20:Q:109:VAL:HG11 | 2.16                     | 0.46              |
| 30:A:971:G:O2'    | 30:A:983:A:N3     | 2.32                     | 0.46              |
| 30:A:1432:G:H2'   | 30:A:1433:A:C8    | 2.50                     | 0.46              |
| 5:4:2:LYS:NZ      | 5:4:32:LYS:O      | 2.49                     | 0.46              |
| 7:C:65:ASP:N      | 7:C:102:TYR:O     | 2.45                     | 0.46              |
| 10:F:3:LEU:HD21   | 10:F:96:TRP:HB3   | 1.96                     | 0.46              |
| 10:F:33:ILE:CD1   | 10:F:95:MET:HE2   | 2.46                     | 0.46              |
| 14:K:92:GLU:OE1   | 14:K:92:GLU:N     | 2.45                     | 0.46              |
| 16:M:123:LYS:O    | 30:A:2484:G:O2'   | 2.34                     | 0.46              |
| 30:A:1857:G:HO2'  | 30:A:1858:A:H8    | 1.58                     | 0.46              |
| 7:C:44:ASN:N      | 30:A:1812:U:O2'   | 2.46                     | 0.46              |
| 17:N:28:LEU:C     | 17:N:28:LEU:HD23  | 2.41                     | 0.46              |
| 30:A:969:G:H22    | 30:A:984:A:HO2'   | 1.61                     | 0.46              |
| 30:A:1290:C:C2    | 30:A:1291:C:C5    | 3.04                     | 0.46              |
| 7:C:104:LEU:H     | 7:C:104:LEU:HD12  | 1.81                     | 0.46              |
| 14:K:2:ILE:HG23   | 14:K:6:THR:HG21   | 1.98                     | 0.46              |
| 16:M:17:ASN:ND2   | 16:M:39:GLY:O     | 2.48                     | 0.46              |
| 20:Q:89:ILE:HD12  | 20:Q:94:LEU:HD21  | 1.98                     | 0.46              |
| 30:A:1497:U:OP2   | 30:A:1498:C:N4    | 2.42                     | 0.46              |
| 10:F:105:ILE:HD12 | 10:F:138:PRO:HG2  | 1.98                     | 0.46              |
| 19:P:95:LYS:NZ    | 30:A:2847:U:OP1   | 2.47                     | 0.46              |
| 30:A:24:G:C2      | 30:A:25:U:C5      | 3.04                     | 0.46              |
| 30:A:63:A:C6      | 31:y:6:VAL:HG13   | 2.50                     | 0.46              |
| 30:A:92:U:H1'     | 31:y:7:TYR:HE2    | 1.80                     | 0.46              |
| 30:A:1734:G:C2    | 30:A:1735:A:N7    | 2.84                     | 0.46              |
| 5:4:1:MET:N       | 30:A:2526:G:N3    | 2.64                     | 0.46              |
| 30:A:723:C:C2     | 30:A:724:U:C5     | 3.03                     | 0.46              |
| 30:A:1342:A:O2'   | 30:A:1344:U:OP1   | 2.29                     | 0.46              |
| 23:T:7:LEU:O      | 23:T:10:VAL:HG12  | 2.16                     | 0.45              |
| 30:A:954:G:O2'    | 30:A:2274:A:N1    | 2.38                     | 0.45              |
| 30:A:2564:A:C2    | 30:A:2647:U:H4'   | 2.51                     | 0.45              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 9:E:105:LEU:HD23   | 9:E:200:LEU:HD21 | 1.97                     | 0.45              |
| 30:A:728:G:O2'     | 30:A:730:A:O4'   | 2.31                     | 0.45              |
| 30:A:1022:G:H1'    | 30:A:1023:U:OP2  | 2.16                     | 0.45              |
| 30:A:1344:U:H3'    | 30:A:1345:C:H5'  | 1.98                     | 0.45              |
| 30:A:2777:G:OP2    | 30:A:2781:A:O2'  | 2.24                     | 0.45              |
| 1:0:3:GLN:NE2      | 30:A:1263:U:O2'  | 2.42                     | 0.45              |
| 30:A:51:G:O2'      | 30:A:52:A:OP2    | 2.33                     | 0.45              |
| 30:A:1024:G:OP2    | 30:A:1025:G:O2'  | 2.31                     | 0.45              |
| 30:A:1205:A:HO2'   | 30:A:1206:G:P    | 2.39                     | 0.45              |
| 30:A:2061:G:C2     | 31:z:17:ARG:HB3  | 2.52                     | 0.45              |
| 30:A:2506[B]:U:OP2 | 30:A:2576:G:N2   | 2.43                     | 0.45              |
| 30:A:2848:G:O2'    | 30:A:2868:A:N6   | 2.47                     | 0.45              |
| 24:U:35:VAL:HB     | 24:U:38:ILE:HD13 | 1.99                     | 0.45              |
| 30:A:729:G:O2'     | 30:A:763:G:H4'   | 2.17                     | 0.45              |
| 9:E:148:ILE:N      | 9:E:148:ILE:HD12 | 2.32                     | 0.45              |
| 14:K:21:CYS:HA     | 14:K:41:ILE:HG22 | 1.99                     | 0.45              |
| 15:L:127:VAL:HG23  | 15:L:131:ALA:HB3 | 1.97                     | 0.45              |
| 21:R:16:GLU:OE2    | 21:R:101:ILE:N   | 2.49                     | 0.45              |
| 27:X:44:ARG:NH1    | 30:A:166:U:O2'   | 2.50                     | 0.45              |
| 30:A:29:U:C2       | 30:A:30:G:C8     | 3.05                     | 0.45              |
| 30:A:1141:U:H4'    | 30:A:1142:A:O4'  | 2.16                     | 0.45              |
| 30:A:1259:G:OP1    | 31:z:2:ASN:HB3   | 2.17                     | 0.45              |
| 30:A:1378:A:C4'    | 30:A:1379:U:OP1  | 2.65                     | 0.45              |
| 10:F:3:LEU:HD22    | 10:F:100:GLU:HG2 | 1.98                     | 0.45              |
| 17:N:70:THR:O      | 17:N:71:ARG:C    | 2.60                     | 0.45              |
| 30:A:639:U:C2      | 30:A:640:C:C5    | 3.05                     | 0.45              |
| 30:A:2120:G:N1     | 30:A:2121:G:O6   | 2.50                     | 0.45              |
| 14:K:113:MET:SD    | 14:K:113:MET:N   | 2.90                     | 0.45              |
| 30:A:526:A:O2'     | 30:A:2043:C:O2   | 2.27                     | 0.45              |
| 30:A:725:G:HO2'    | 30:A:726:G:C4'   | 2.27                     | 0.45              |
| 30:A:1203:U:OP2    | 30:A:1204:A:O2'  | 2.13                     | 0.45              |
| 30:A:1272:A:O2'    | 30:A:1274:A:OP1  | 2.35                     | 0.45              |
| 15:L:77:ILE:HD12   | 15:L:109:LYS:O   | 2.17                     | 0.45              |
| 30:A:1378:A:O2'    | 30:A:1380:G:OP2  | 2.29                     | 0.45              |
| 30:A:1702:G:C6     | 30:A:1703:G:N7   | 2.85                     | 0.45              |
| 20:Q:78:PHE:CE2    | 20:Q:82:LEU:HD11 | 2.52                     | 0.45              |
| 30:A:532:A:N7      | 30:A:2021:C:O2'  | 2.40                     | 0.45              |
| 30:A:554:U:H2'     | 30:A:555:G:O4'   | 2.17                     | 0.45              |
| 30:A:1224:U:H4'    | 30:A:1225:G:OP1  | 2.18                     | 0.45              |
| 30:A:1827:U:OP1    | 30:A:1971:U:O2'  | 2.35                     | 0.45              |
| 19:P:20:ARG:NH1    | 30:A:2849:U:O4   | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:A:48:G:N2      | 30:A:177:G:OP2    | 2.50                     | 0.44              |
| 30:A:58:G:O2'     | 30:A:73:A:N1      | 2.45                     | 0.44              |
| 30:A:1058:U:H2'   | 30:A:1059:G:C4    | 2.52                     | 0.44              |
| 30:A:2552:U:H3'   | 30:A:2552:U:O2    | 2.17                     | 0.44              |
| 6:B:39:A:C2       | 6:B:44:G:C2       | 3.05                     | 0.44              |
| 23:T:2:ILE:HD11   | 30:A:144:A:H4'    | 1.99                     | 0.44              |
| 30:A:724:U:H2'    | 30:A:725:G:O5'    | 2.16                     | 0.44              |
| 30:A:1425:G:H2'   | 30:A:1426:G:O4'   | 2.17                     | 0.44              |
| 30:A:2756:U:H4'   | 30:A:2757:A:OP1   | 2.17                     | 0.44              |
| 11:G:36:LEU:HD23  | 11:G:37:ASN:H     | 1.83                     | 0.44              |
| 21:R:23:GLU:OE2   | 30:A:1161:C:O2'   | 2.31                     | 0.44              |
| 30:A:508:A:P      | 31:y:13:PRO:HG3   | 2.57                     | 0.44              |
| 30:A:1663:G:O2'   | 30:A:1664:A:O5'   | 2.32                     | 0.44              |
| 30:A:1769:U:O2    | 30:A:1983:G:O6    | 2.35                     | 0.44              |
| 9:E:31:VAL:HG21   | 9:E:104:ALA:HB2   | 1.99                     | 0.44              |
| 21:R:82:HIS:ND1   | 21:R:82:HIS:O     | 2.50                     | 0.44              |
| 30:A:247:G:N2     | 30:A:251:A:OP2    | 2.49                     | 0.44              |
| 30:A:508:A:C8     | 31:y:13:PRO:CB    | 2.79                     | 0.44              |
| 30:A:1477:A:N6    | 30:A:1514:G:O2'   | 2.49                     | 0.44              |
| 7:C:35:LYS:NZ     | 30:A:1353:A:O3'   | 2.50                     | 0.44              |
| 9:E:41:GLN:NE2    | 30:A:442:G:O4'    | 2.51                     | 0.44              |
| 15:L:111:ILE:HD12 | 30:A:636:G:N2     | 2.33                     | 0.44              |
| 30:A:2050:C:H2'   | 30:A:2051:A:O4'   | 2.17                     | 0.44              |
| 7:C:11:GLY:O      | 7:C:15:VAL:HG23   | 2.18                     | 0.44              |
| 9:E:176:ASP:OD1   | 9:E:179:SER:OG    | 2.12                     | 0.44              |
| 11:G:36:LEU:HD23  | 11:G:37:ASN:N     | 2.32                     | 0.44              |
| 24:U:29:SER:OG    | 30:A:86:G:OP1     | 2.30                     | 0.44              |
| 30:A:725:G:H2'    | 30:A:726:G:C4     | 2.52                     | 0.44              |
| 3:2:1:MET:SD      | 3:2:1:MET:N       | 2.66                     | 0.44              |
| 5:4:1:MET:HE2     | 5:4:36:ARG:HB2    | 2.00                     | 0.44              |
| 12:H:122:LEU:O    | 12:H:122:LEU:HD12 | 2.18                     | 0.44              |
| 18:O:46:GLU:OE1   | 18:O:46:GLU:N     | 2.51                     | 0.44              |
| 22:S:13:SER:O     | 22:S:17:VAL:HG23  | 2.18                     | 0.44              |
| 30:A:372:G:O2'    | 30:A:373:U:P      | 2.74                     | 0.44              |
| 30:A:1129:A:N6    | 30:A:2491:U:OP1   | 2.50                     | 0.44              |
| 30:A:1142:A:C4    | 30:A:1144:A:N7    | 2.86                     | 0.44              |
| 30:A:1145:C:C2    | 30:A:1146:C:C5    | 3.05                     | 0.44              |
| 30:A:1313:U:O2'   | 30:A:1332:G:O4'   | 2.34                     | 0.44              |
| 30:A:1737:G:O3'   | 30:A:1738:G:O4'   | 2.35                     | 0.44              |
| 30:A:1790:C:H2'   | 30:A:1791:A:C8    | 2.53                     | 0.44              |
| 30:A:2822:G:O2'   | 30:A:2824:C:OP2   | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:C:2:VAL:HG21    | 7:C:201:LEU:HG    | 1.99                     | 0.44              |
| 8:D:162:ALA:O     | 30:A:2620:C:O2'   | 2.28                     | 0.44              |
| 9:E:112:LEU:HD13  | 9:E:117:ARG:HB2   | 1.98                     | 0.44              |
| 10:F:107:VAL:N    | 10:F:108:PRO:CD   | 2.81                     | 0.44              |
| 16:M:57:VAL:HG11  | 16:M:105:MET:HE1  | 2.00                     | 0.44              |
| 20:Q:89:ILE:CD1   | 20:Q:94:LEU:HD21  | 2.48                     | 0.44              |
| 29:Z:42:ALA:O     | 30:A:851:C:O2'    | 2.35                     | 0.44              |
| 30:A:213:A:H2'    | 30:A:214:G:C8     | 2.52                     | 0.44              |
| 30:A:754:U:C2     | 30:A:755:U:C5     | 3.06                     | 0.44              |
| 20:Q:111:LYS:NZ   | 21:R:49:ILE:O     | 2.39                     | 0.44              |
| 24:U:97:SER:O     | 24:U:98:ASN:OD1   | 2.36                     | 0.44              |
| 30:A:91:A:C2      | 31:y:7:TYR:HB3    | 2.53                     | 0.44              |
| 30:A:216:A:C8     | 30:A:432:A:N6     | 2.86                     | 0.44              |
| 30:A:549:G:C2'    | 30:A:550:C:O5'    | 2.66                     | 0.44              |
| 30:A:579:G:C6     | 30:A:1262:A:N6    | 2.86                     | 0.44              |
| 7:C:68:ARG:NH1    | 7:C:128:THR:OG1   | 2.51                     | 0.43              |
| 18:O:9:ARG:NH2    | 30:A:2296:U:OP2   | 2.51                     | 0.43              |
| 30:A:582:A:N6     | 30:A:1259:G:O6    | 2.51                     | 0.43              |
| 30:A:640:C:N4     | 30:A:649:G:O6     | 2.50                     | 0.43              |
| 10:F:23:SER:OG    | 10:F:25:MET:SD    | 2.76                     | 0.43              |
| 13:J:120:ARG:NE   | 30:A:2780:G:OP2   | 2.51                     | 0.43              |
| 30:A:508:A:C5     | 31:y:13:PRO:CB    | 3.00                     | 0.43              |
| 30:A:1071:G:N3    | 30:A:1089:A:O2'   | 2.47                     | 0.43              |
| 30:A:1164:C:O2'   | 30:A:1224:U:C4    | 2.72                     | 0.43              |
| 30:A:2375:G:N1    | 30:A:2379:G:O6    | 2.51                     | 0.43              |
| 26:W:16:ARG:NE    | 30:A:2357:G:OP1   | 2.44                     | 0.43              |
| 30:A:2700:A:N6    | 30:A:2708:G:O6    | 2.51                     | 0.43              |
| 7:C:131:MET:HE2   | 7:C:171:VAL:HB    | 2.01                     | 0.43              |
| 10:F:140:ILE:N    | 10:F:140:ILE:HD12 | 2.33                     | 0.43              |
| 12:H:121:VAL:HG12 | 12:H:121:VAL:O    | 2.18                     | 0.43              |
| 30:A:2058:A:H61   | 30:A:2611:C:N4    | 2.16                     | 0.43              |
| 30:A:2089:C:N4    | 30:A:2090:A:H62   | 2.17                     | 0.43              |
| 14:K:86:LEU:O     | 14:K:87:LEU:HD12  | 2.18                     | 0.43              |
| 30:A:723:C:N3     | 30:A:724:U:C5     | 2.86                     | 0.43              |
| 30:A:1264:A:O5'   | 30:A:1265:A:H2'   | 2.19                     | 0.43              |
| 30:A:2749:A:OP2   | 30:A:2750:A:O2'   | 2.20                     | 0.43              |
| 14:K:92:GLU:OE2   | 14:K:111:LYS:NZ   | 2.34                     | 0.43              |
| 15:L:112:LEU:HD21 | 30:A:627:A:N6     | 2.33                     | 0.43              |
| 16:M:42:THR:HG22  | 16:M:93:VAL:HG12  | 1.99                     | 0.43              |
| 19:P:52:ARG:NH1   | 30:A:2845:U:O3'   | 2.51                     | 0.43              |
| 27:X:64:ASP:OD1   | 27:X:65:THR:N     | 2.52                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:A:28:A:C5       | 30:A:29:U:C5      | 3.07                     | 0.43              |
| 7:C:97:ASP:OD1     | 7:C:97:ASP:N      | 2.51                     | 0.43              |
| 13:J:52:ASP:OD1    | 13:J:52:ASP:N     | 2.51                     | 0.43              |
| 30:A:645:C:H2'     | 30:A:647:G:C8     | 2.53                     | 0.43              |
| 30:A:711:G:C6      | 30:A:721:A:C6     | 3.07                     | 0.43              |
| 16:M:18:ARG:NH1    | 30:A:952:G:OP1    | 2.52                     | 0.43              |
| 17:N:4:ARG:NE      | 30:A:2874:C:OP1   | 2.50                     | 0.43              |
| 30:A:1287:A:C2'    | 30:A:1288:G:O5'   | 2.67                     | 0.43              |
| 6:B:55:U:O2'       | 10:F:25:MET:SD    | 2.73                     | 0.43              |
| 9:E:148:ILE:HD13   | 9:E:167:VAL:HG23  | 2.01                     | 0.43              |
| 28:Y:19:LEU:C      | 28:Y:19:LEU:HD23  | 2.44                     | 0.43              |
| 30:A:62:U:H4'      | 31:y:3:ASN:HB2    | 2.01                     | 0.43              |
| 30:A:92:U:H1'      | 31:y:7:TYR:CE2    | 2.54                     | 0.43              |
| 30:A:689:A:N3      | 30:A:779:U:O2'    | 2.49                     | 0.43              |
| 30:A:1068:G:H2'    | 30:A:1069:A:O4'   | 2.19                     | 0.43              |
| 30:A:2117:A:N1     | 30:A:2170:A:N6    | 2.64                     | 0.43              |
| 30:A:29:U:O2       | 30:A:1215:G:O2'   | 2.37                     | 0.43              |
| 30:A:543:G:O6      | 30:A:551:G:O6     | 2.36                     | 0.43              |
| 6:B:42:C:C4        | 10:F:65:LEU:HD22  | 2.54                     | 0.42              |
| 7:C:206:LYS:NZ     | 30:A:729:G:O5'    | 2.52                     | 0.42              |
| 26:W:33:ILE:HD11   | 26:W:78:ILE:HD11  | 2.00                     | 0.42              |
| 30:A:442:G:C6      | 30:A:444:C:N4     | 2.87                     | 0.42              |
| 30:A:458:G:O2'     | 30:A:459:U:P      | 2.77                     | 0.42              |
| 30:A:488:G:H22     | 30:A:491:G:H5''   | 1.84                     | 0.42              |
| 30:A:570:G:C1'     | 30:A:983:A:N6     | 2.82                     | 0.42              |
| 30:A:1287:A:N6     | 30:A:1649:G:O2'   | 2.52                     | 0.42              |
| 30:A:1995:U:OP2    | 30:A:1996:C:O2'   | 2.30                     | 0.42              |
| 30:A:2345:G:O2'    | 30:A:2381:A:N3    | 2.44                     | 0.42              |
| 30:A:2506[A]:U:OP2 | 30:A:2576:G:N2    | 2.51                     | 0.42              |
| 10:F:43:ILE:HD12   | 10:F:43:ILE:N     | 2.35                     | 0.42              |
| 10:F:48:LEU:HD12   | 10:F:48:LEU:C     | 2.44                     | 0.42              |
| 11:G:62:ALA:O      | 11:G:66:THR:HG23  | 2.19                     | 0.42              |
| 28:Y:19:LEU:HD23   | 28:Y:19:LEU:O     | 2.19                     | 0.42              |
| 30:A:2834:G:O2'    | 30:A:2835:A:O5'   | 2.34                     | 0.42              |
| 8:D:7:LYS:N        | 8:D:28:GLU:O      | 2.42                     | 0.42              |
| 30:A:512:G:OP1     | 30:A:1234:U:O2'   | 2.22                     | 0.42              |
| 30:A:1686:C:N4     | 30:A:1703:G:O6    | 2.53                     | 0.42              |
| 3:2:9:VAL:HG12     | 30:A:1309:G:OP1   | 2.19                     | 0.42              |
| 12:H:99:ILE:O      | 12:H:103:VAL:HG23 | 2.19                     | 0.42              |
| 13:J:114:LEU:HD21  | 13:J:118:MET:HE3  | 2.01                     | 0.42              |
| 22:S:36:LEU:HD22   | 22:S:47:VAL:CG1   | 2.49                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 25:V:2:PHE:HD1    | 25:V:50:MET:HE2  | 1.85                     | 0.42              |
| 30:A:1663:G:O6    | 30:A:1998:A:N6   | 2.52                     | 0.42              |
| 30:A:1684:G:C6    | 30:A:1705:A:N6   | 2.87                     | 0.42              |
| 30:A:1992:G:N2    | 30:A:1996:C:O2'  | 2.48                     | 0.42              |
| 9:E:97:ASN:HB3    | 9:E:100:MET:HG2  | 2.01                     | 0.42              |
| 28:Y:42:LEU:HD13  | 28:Y:45:GLN:OE1  | 2.20                     | 0.42              |
| 20:Q:60:TRP:O     | 20:Q:64:ILE:HG12 | 2.20                     | 0.42              |
| 30:A:2627:G:O2'   | 30:A:2781:A:N1   | 2.45                     | 0.42              |
| 12:H:5:LEU:HD12   | 12:H:5:LEU:N     | 2.34                     | 0.42              |
| 19:P:3:ILE:N      | 19:P:3:ILE:HD12  | 2.35                     | 0.42              |
| 30:A:827:U:OP2    | 30:A:828:U:N3    | 2.53                     | 0.42              |
| 30:A:1425:G:N2    | 30:A:1574:C:C4   | 2.88                     | 0.42              |
| 30:A:2487:G:C2    | 30:A:2488:G:C5   | 3.08                     | 0.42              |
| 29:Z:4:ILE:HD11   | 29:Z:56:VAL:HG21 | 2.01                     | 0.42              |
| 30:A:1268:A:H1'   | 30:A:2013:A:H61  | 1.84                     | 0.42              |
| 30:A:1466:U:O3'   | 30:A:1546:G:O2'  | 2.37                     | 0.42              |
| 30:A:1788:C:C2    | 30:A:1789:A:C8   | 3.07                     | 0.42              |
| 14:K:92:GLU:O     | 14:K:93:GLN:C    | 2.63                     | 0.42              |
| 29:Z:50:VAL:O     | 29:Z:54:VAL:HG22 | 2.19                     | 0.42              |
| 30:A:379:G:C6     | 30:A:396:G:O6    | 2.73                     | 0.42              |
| 30:A:2202:U:O2'   | 30:A:2204:G:OP1  | 2.32                     | 0.42              |
| 31:y:8:ILE:H      | 31:y:8:ILE:HG13  | 1.53                     | 0.42              |
| 6:B:2:G:H2'       | 6:B:3:C:C6       | 2.55                     | 0.42              |
| 6:B:30:C:H1'      | 6:B:57:A:H61     | 1.85                     | 0.42              |
| 30:A:63:A:C6      | 31:y:6:VAL:HG12  | 2.54                     | 0.42              |
| 30:A:2028:U:O4    | 30:A:2033:A:N7   | 2.53                     | 0.42              |
| 30:A:2506[A]:U:O4 | 31:z:17:ARG:O    | 2.38                     | 0.42              |
| 7:C:156:SER:OG    | 7:C:159:THR:OG1  | 2.06                     | 0.41              |
| 30:A:619:G:O5'    | 30:A:620:G:N2    | 2.53                     | 0.41              |
| 30:A:1386:C:H2'   | 30:A:1387:A:C8   | 2.55                     | 0.41              |
| 30:A:1604:C:O2'   | 30:A:1610:A:N1   | 2.42                     | 0.41              |
| 4:3:29:ARG:NH2    | 15:L:63:LYS:O    | 2.52                     | 0.41              |
| 8:D:81:GLU:OE1    | 30:A:2635:A:O2'  | 2.37                     | 0.41              |
| 23:T:11:LEU:HD23  | 23:T:12:ARG:N    | 2.35                     | 0.41              |
| 30:A:464:U:C2'    | 30:A:465:G:O5'   | 2.68                     | 0.41              |
| 30:A:1024:G:H1'   | 30:A:1144:A:O2'  | 2.19                     | 0.41              |
| 30:A:1186:G:H2'   | 30:A:1187:G:O4'  | 2.20                     | 0.41              |
| 30:A:1321:A:H4'   | 31:y:17:ARG:CZ   | 2.50                     | 0.41              |
| 6:B:3:C:H3'       | 6:B:4:C:H5''     | 2.02                     | 0.41              |
| 11:G:51:PHE:CZ    | 11:G:71:LEU:HD22 | 2.55                     | 0.41              |
| 30:A:619:G:H3'    | 30:A:620:G:H21   | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:A:619:G:OP2    | 30:A:620:G:N2     | 2.53                     | 0.41              |
| 30:A:2058:A:H61   | 30:A:2611:C:H42   | 1.67                     | 0.41              |
| 30:A:2074:U:O2'   | 30:A:2597:G:H1'   | 2.20                     | 0.41              |
| 30:A:2464:G:C6    | 30:A:2487:G:C6    | 3.07                     | 0.41              |
| 30:A:2506[A]:U:N3 | 31:z:17:ARG:NE    | 2.52                     | 0.41              |
| 8:D:33:ARG:HD2    | 8:D:73:VAL:HG13   | 2.01                     | 0.41              |
| 11:G:47:ASN:O     | 11:G:48:THR:HG23  | 2.20                     | 0.41              |
| 12:H:12:LEU:HD23  | 12:H:12:LEU:N     | 2.35                     | 0.41              |
| 13:J:43:GLU:N     | 13:J:43:GLU:OE1   | 2.53                     | 0.41              |
| 15:L:23:ILE:N     | 30:A:813:U:OP2    | 2.53                     | 0.41              |
| 20:Q:78:PHE:CZ    | 20:Q:82:LEU:HD11  | 2.56                     | 0.41              |
| 30:A:202:U:H2'    | 30:A:203:A:O4'    | 2.20                     | 0.41              |
| 30:A:633:A:O2'    | 30:A:2404:U:OP1   | 2.38                     | 0.41              |
| 30:A:2085:U:O2    | 30:A:2234:G:O6    | 2.38                     | 0.41              |
| 30:A:2447:G:H2'   | 30:A:2500:U:OP2   | 2.21                     | 0.41              |
| 30:A:2364:C:H2'   | 30:A:2365:G:O4'   | 2.21                     | 0.41              |
| 30:A:2489:U:H2'   | 30:A:2490:G:O4'   | 2.20                     | 0.41              |
| 19:P:96:LEU:HD12  | 19:P:96:LEU:N     | 2.35                     | 0.41              |
| 30:A:45:G:H5''    | 30:A:46:G:H5'     | 2.02                     | 0.41              |
| 30:A:458:G:O2'    | 30:A:459:U:O5'    | 2.38                     | 0.41              |
| 30:A:1164:C:O2'   | 30:A:1224:U:O4    | 2.37                     | 0.41              |
| 30:A:1425:G:N2    | 30:A:1574:C:N3    | 2.69                     | 0.41              |
| 30:A:1664:A:H61   | 30:A:1996:C:H42   | 1.69                     | 0.41              |
| 30:A:2125:G:N2    | 30:A:2170:A:O3'   | 2.50                     | 0.41              |
| 30:A:2357:G:N1    | 30:A:2360:G:OP2   | 2.48                     | 0.41              |
| 10:F:46:LYS:O     | 10:F:49:LEU:HD22  | 2.20                     | 0.41              |
| 30:A:242:G:H4'    | 30:A:243:U:O5'    | 2.20                     | 0.41              |
| 30:A:2028:U:H3    | 30:A:2033:A:H62   | 1.69                     | 0.41              |
| 30:A:2063:C:H1'   | 31:z:18:LEU:CB    | 2.51                     | 0.41              |
| 9:E:162:ARG:NE    | 30:A:322:A:OP1    | 2.41                     | 0.41              |
| 13:J:100:VAL:HG23 | 13:J:101:ILE:N    | 2.36                     | 0.41              |
| 17:N:28:LEU:HD23  | 17:N:28:LEU:O     | 2.21                     | 0.41              |
| 20:Q:116:LEU:C    | 20:Q:116:LEU:HD23 | 2.46                     | 0.41              |
| 30:A:725:G:O2'    | 30:A:726:G:C4'    | 2.67                     | 0.41              |
| 7:C:200:MET:HE2   | 7:C:200:MET:HA    | 2.02                     | 0.41              |
| 15:L:127:VAL:HG21 | 15:L:132:ARG:N    | 2.35                     | 0.41              |
| 17:N:31:HIS:O     | 17:N:32:GLU:HB2   | 2.20                     | 0.41              |
| 18:O:72:ALA:O     | 18:O:76:LYS:HG2   | 2.21                     | 0.41              |
| 19:P:63:ILE:O     | 19:P:63:ILE:HG23  | 2.20                     | 0.41              |
| 25:V:72:VAL:HG22  | 25:V:73:LYS:N     | 2.36                     | 0.41              |
| 30:A:196:A:H61    | 30:A:831:G:H21    | 1.69                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:A:499:U:H2'    | 30:A:500:G:O4'   | 2.21                     | 0.41              |
| 30:A:1096:A:H3'   | 30:A:1097:U:H5'' | 2.03                     | 0.41              |
| 30:A:1197:G:N2    | 30:A:1249:U:O2'  | 2.52                     | 0.41              |
| 30:A:1321:A:C1'   | 31:y:15:HIS:O    | 2.42                     | 0.41              |
| 30:A:2505:G:C4    | 31:z:15:HIS:CB   | 3.04                     | 0.41              |
| 30:A:2585:U:O2    | 30:A:2585:U:O4'  | 2.38                     | 0.41              |
| 10:F:39:VAL:HG13  | 10:F:40:GLY:N    | 2.36                     | 0.41              |
| 30:A:306:U:H2'    | 30:A:307:G:O4'   | 2.21                     | 0.41              |
| 30:A:1215:G:O6    | 30:A:1235:G:C2   | 2.74                     | 0.41              |
| 7:C:162:GLN:OE1   | 7:C:162:GLN:N    | 2.53                     | 0.40              |
| 30:A:1394:U:H2'   | 30:A:1395:A:C4   | 2.56                     | 0.40              |
| 30:A:2106:U:N3    | 30:A:2107:G:N7   | 2.69                     | 0.40              |
| 1:O:30:ASP:OD1    | 1:O:31:LYS:N     | 2.54                     | 0.40              |
| 20:Q:50:ARG:NH2   | 30:A:993:G:OP2   | 2.54                     | 0.40              |
| 30:A:75:G:N3      | 30:A:75:G:H2'    | 2.36                     | 0.40              |
| 30:A:285:G:C6     | 30:A:356:G:C5    | 3.09                     | 0.40              |
| 30:A:751:A:N3     | 31:z:7:TYR:OH    | 2.53                     | 0.40              |
| 30:A:1182:G:H2'   | 30:A:1183:U:O4'  | 2.22                     | 0.40              |
| 30:A:1264:A:H4'   | 30:A:2615:U:H5'  | 2.03                     | 0.40              |
| 30:A:1390:U:O4    | 30:A:1395:A:N7   | 2.54                     | 0.40              |
| 30:A:2655:G:O2'   | 30:A:2656:U:P    | 2.78                     | 0.40              |
| 8:D:130:GLN:NE2   | 30:A:2578:G:H21  | 2.19                     | 0.40              |
| 27:X:2:ARG:NH1    | 30:A:1365:A:OP1  | 2.51                     | 0.40              |
| 30:A:1196:C:C2    | 30:A:1197:G:C8   | 3.10                     | 0.40              |
| 30:A:2553:G:H1'   | 30:A:2582:G:H21  | 1.86                     | 0.40              |
| 15:L:111:ILE:HD12 | 30:A:636:G:C2    | 2.57                     | 0.40              |
| 30:A:1601:G:H2'   | 30:A:1602:U:O4'  | 2.21                     | 0.40              |
| 30:A:886:A:O4'    | 30:A:891:G:N1    | 2.55                     | 0.40              |
| 30:A:2687:U:H2'   | 30:A:2688:G:O4'  | 2.21                     | 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   | 0     | 54/56 (96%)     | 53 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 2   | 1     | 48/50 (96%)     | 47 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 3   | 2     | 44/46 (96%)     | 44 (100%)  | 0        | 0        | 100         | 100 |
| 4   | 3     | 62/64 (97%)     | 60 (97%)   | 1 (2%)   | 1 (2%)   | 7           | 28  |
| 5   | 4     | 36/38 (95%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 7   | C     | 269/271 (99%)   | 258 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 8   | D     | 207/209 (99%)   | 196 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 9   | E     | 199/201 (99%)   | 192 (96%)  | 6 (3%)   | 1 (0%)   | 24          | 54  |
| 10  | F     | 175/177 (99%)   | 168 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 11  | G     | 174/176 (99%)   | 170 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 12  | H     | 147/149 (99%)   | 140 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 13  | J     | 140/142 (99%)   | 137 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 14  | K     | 120/122 (98%)   | 116 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 15  | L     | 141/143 (99%)   | 132 (94%)  | 9 (6%)   | 0        | 100         | 100 |
| 16  | M     | 134/136 (98%)   | 130 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 17  | N     | 118/120 (98%)   | 109 (92%)  | 9 (8%)   | 0        | 100         | 100 |
| 18  | O     | 114/116 (98%)   | 113 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 19  | P     | 112/114 (98%)   | 109 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 20  | Q     | 115/117 (98%)   | 113 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 21  | R     | 101/103 (98%)   | 98 (97%)   | 2 (2%)   | 1 (1%)   | 12          | 39  |
| 22  | S     | 109/110 (99%)   | 105 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 23  | T     | 91/93 (98%)     | 88 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 24  | U     | 100/102 (98%)   | 89 (89%)   | 11 (11%) | 0        | 100         | 100 |
| 25  | V     | 92/94 (98%)     | 91 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 26  | W     | 73/75 (97%)     | 69 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 27  | X     | 75/77 (97%)     | 74 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 28  | Y     | 61/63 (97%)     | 58 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 29  | Z     | 56/58 (97%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 31  | y     | 15/17 (88%)     | 12 (80%)   | 3 (20%)  | 0        | 100         | 100 |
| 31  | z     | 15/17 (88%)     | 15 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 3197/3256 (98%) | 3076 (96%) | 118 (4%) | 3 (0%)   | 49          | 76  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | R     | 54  | VAL  |
| 9   | E     | 83  | VAL  |
| 4   | 3     | 31  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 0     | 47/47 (100%)   | 45 (96%)   | 2 (4%)   | 26          | 55  |
| 2   | 1     | 45/45 (100%)   | 45 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 38/38 (100%)   | 37 (97%)   | 1 (3%)   | 40          | 65  |
| 4   | 3     | 51/51 (100%)   | 50 (98%)   | 1 (2%)   | 48          | 69  |
| 5   | 4     | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 7   | C     | 216/216 (100%) | 216 (100%) | 0        | 100         | 100 |
| 8   | D     | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 9   | E     | 165/165 (100%) | 162 (98%)  | 3 (2%)   | 51          | 70  |
| 10  | F     | 148/148 (100%) | 146 (99%)  | 2 (1%)   | 59          | 73  |
| 11  | G     | 137/137 (100%) | 136 (99%)  | 1 (1%)   | 76          | 80  |
| 12  | H     | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 13  | J     | 116/116 (100%) | 115 (99%)  | 1 (1%)   | 70          | 78  |
| 14  | K     | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 15  | L     | 102/102 (100%) | 100 (98%)  | 2 (2%)   | 48          | 69  |
| 16  | M     | 109/109 (100%) | 108 (99%)  | 1 (1%)   | 70          | 78  |
| 17  | N     | 100/100 (100%) | 98 (98%)   | 2 (2%)   | 48          | 69  |
| 18  | O     | 86/86 (100%)   | 85 (99%)   | 1 (1%)   | 63          | 75  |
| 19  | P     | 99/99 (100%)   | 97 (98%)   | 2 (2%)   | 48          | 69  |
| 20  | Q     | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 76  |
| 21  | R     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 22  | S     | 94/93 (101%)   | 93 (99%)   | 1 (1%)   | 65          | 76  |
| 23  | T     | 80/80 (100%)   | 79 (99%)   | 1 (1%)   | 61          | 74  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 24  | U     | 83/83 (100%)     | 83 (100%)  | 0        | 100         | 100 |
| 25  | V     | 78/78 (100%)     | 77 (99%)   | 1 (1%)   | 61          | 74  |
| 26  | W     | 57/57 (100%)     | 57 (100%)  | 0        | 100         | 100 |
| 27  | X     | 67/67 (100%)     | 67 (100%)  | 0        | 100         | 100 |
| 28  | Y     | 55/55 (100%)     | 54 (98%)   | 1 (2%)   | 51          | 70  |
| 29  | Z     | 48/48 (100%)     | 48 (100%)  | 0        | 100         | 100 |
| 31  | y     | 17/17 (100%)     | 15 (88%)   | 2 (12%)  | 5           | 20  |
| 31  | z     | 17/17 (100%)     | 17 (100%)  | 0        | 100         | 100 |
| All | All   | 2643/2642 (100%) | 2617 (99%) | 26 (1%)  | 65          | 77  |

All (26) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 5   | ASN  |
| 1   | 0     | 21  | LEU  |
| 3   | 2     | 1   | MET  |
| 4   | 3     | 54  | LEU  |
| 9   | E     | 94  | GLN  |
| 9   | E     | 112 | LEU  |
| 9   | E     | 176 | ASP  |
| 10  | F     | 11  | VAL  |
| 10  | F     | 141 | ASP  |
| 11  | G     | 36  | LEU  |
| 13  | J     | 122 | LEU  |
| 15  | L     | 27  | LEU  |
| 15  | L     | 85  | VAL  |
| 16  | M     | 47  | GLU  |
| 17  | N     | 20  | MET  |
| 17  | N     | 73  | ASN  |
| 18  | O     | 35  | ILE  |
| 19  | P     | 23  | ASP  |
| 19  | P     | 113 | LEU  |
| 20  | Q     | 101 | ASP  |
| 22  | S     | 77  | ASP  |
| 23  | T     | 72  | GLN  |
| 25  | V     | 42  | LEU  |
| 28  | Y     | 28  | LEU  |
| 31  | y     | 6   | VAL  |
| 31  | y     | 8   | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 3   | GLN  |
| 7   | C     | 57  | HIS  |
| 8   | D     | 134 | HIS  |
| 8   | D     | 173 | GLN  |
| 9   | E     | 41  | GLN  |
| 12  | H     | 11  | ASN  |
| 13  | J     | 135 | GLN  |
| 14  | K     | 88  | ASN  |
| 14  | K     | 90  | ASN  |
| 14  | K     | 93  | GLN  |
| 15  | L     | 38  | GLN  |
| 17  | N     | 9   | GLN  |
| 22  | S     | 60  | HIS  |
| 23  | T     | 70  | HIS  |
| 23  | T     | 72  | GLN  |
| 24  | U     | 26  | ASN  |
| 24  | U     | 44  | HIS  |
| 24  | U     | 52  | ASN  |
| 27  | X     | 5   | GLN  |
| 31  | z     | 2   | ASN  |
| 31  | y     | 3   | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 30  | A     | 2897/2904 (99%) | 462 (15%)         | 18 (0%)         |
| 6   | B     | 119/120 (99%)   | 14 (11%)          | 2 (1%)          |
| All | All   | 3016/3024 (99%) | 476 (15%)         | 20 (0%)         |

All (476) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | B     | 4   | C    |
| 6   | B     | 9   | G    |
| 6   | B     | 12  | C    |
| 6   | B     | 13  | G    |
| 6   | B     | 24  | G    |
| 6   | B     | 35  | C    |
| 6   | B     | 42  | C    |
| 6   | B     | 44  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | B     | 45  | A    |
| 6   | B     | 53  | A    |
| 6   | B     | 67  | G    |
| 6   | B     | 89  | U    |
| 6   | B     | 90  | C    |
| 6   | B     | 109 | A    |
| 30  | A     | 10  | A    |
| 30  | A     | 27  | G    |
| 30  | A     | 28  | A    |
| 30  | A     | 34  | U    |
| 30  | A     | 35  | G    |
| 30  | A     | 46  | G    |
| 30  | A     | 51  | G    |
| 30  | A     | 60  | G    |
| 30  | A     | 63  | A    |
| 30  | A     | 71  | A    |
| 30  | A     | 74  | A    |
| 30  | A     | 75  | G    |
| 30  | A     | 118 | A    |
| 30  | A     | 119 | A    |
| 30  | A     | 120 | U    |
| 30  | A     | 126 | A    |
| 30  | A     | 135 | U    |
| 30  | A     | 136 | G    |
| 30  | A     | 139 | U    |
| 30  | A     | 141 | G    |
| 30  | A     | 142 | A    |
| 30  | A     | 162 | U    |
| 30  | A     | 163 | C    |
| 30  | A     | 181 | A    |
| 30  | A     | 196 | A    |
| 30  | A     | 199 | A    |
| 30  | A     | 215 | G    |
| 30  | A     | 216 | A    |
| 30  | A     | 221 | A    |
| 30  | A     | 222 | A    |
| 30  | A     | 225 | C    |
| 30  | A     | 228 | C    |
| 30  | A     | 233 | A    |
| 30  | A     | 242 | G    |
| 30  | A     | 243 | U    |
| 30  | A     | 248 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | A     | 255 | A    |
| 30  | A     | 266 | G    |
| 30  | A     | 267 | C    |
| 30  | A     | 272 | A    |
| 30  | A     | 277 | G    |
| 30  | A     | 278 | A    |
| 30  | A     | 294 | A    |
| 30  | A     | 307 | G    |
| 30  | A     | 310 | A    |
| 30  | A     | 322 | A    |
| 30  | A     | 323 | C    |
| 30  | A     | 324 | A    |
| 30  | A     | 329 | G    |
| 30  | A     | 330 | A    |
| 30  | A     | 345 | A    |
| 30  | A     | 356 | G    |
| 30  | A     | 362 | A    |
| 30  | A     | 371 | A    |
| 30  | A     | 372 | G    |
| 30  | A     | 373 | U    |
| 30  | A     | 386 | G    |
| 30  | A     | 387 | U    |
| 30  | A     | 404 | A    |
| 30  | A     | 406 | G    |
| 30  | A     | 411 | G    |
| 30  | A     | 417 | C    |
| 30  | A     | 424 | G    |
| 30  | A     | 429 | A    |
| 30  | A     | 435 | C    |
| 30  | A     | 446 | G    |
| 30  | A     | 456 | C    |
| 30  | A     | 457 | A    |
| 30  | A     | 458 | G    |
| 30  | A     | 459 | U    |
| 30  | A     | 465 | G    |
| 30  | A     | 473 | G    |
| 30  | A     | 480 | A    |
| 30  | A     | 481 | G    |
| 30  | A     | 491 | G    |
| 30  | A     | 505 | A    |
| 30  | A     | 509 | C    |
| 30  | A     | 528 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | A     | 530 | G    |
| 30  | A     | 531 | C    |
| 30  | A     | 532 | A    |
| 30  | A     | 533 | G    |
| 30  | A     | 543 | G    |
| 30  | A     | 544 | C    |
| 30  | A     | 545 | U    |
| 30  | A     | 547 | A    |
| 30  | A     | 550 | C    |
| 30  | A     | 563 | A    |
| 30  | A     | 573 | U    |
| 30  | A     | 575 | A    |
| 30  | A     | 588 | U    |
| 30  | A     | 603 | A    |
| 30  | A     | 614 | A    |
| 30  | A     | 627 | A    |
| 30  | A     | 637 | A    |
| 30  | A     | 645 | C    |
| 30  | A     | 646 | U    |
| 30  | A     | 647 | G    |
| 30  | A     | 652 | U    |
| 30  | A     | 654 | A    |
| 30  | A     | 669 | G    |
| 30  | A     | 670 | A    |
| 30  | A     | 675 | A    |
| 30  | A     | 683 | U    |
| 30  | A     | 686 | U    |
| 30  | A     | 687 | C    |
| 30  | A     | 695 | G    |
| 30  | A     | 717 | C    |
| 30  | A     | 725 | G    |
| 30  | A     | 726 | G    |
| 30  | A     | 730 | A    |
| 30  | A     | 740 | C    |
| 30  | A     | 747 | U    |
| 30  | A     | 748 | G    |
| 30  | A     | 752 | A    |
| 30  | A     | 763 | G    |
| 30  | A     | 764 | A    |
| 30  | A     | 775 | G    |
| 30  | A     | 776 | G    |
| 30  | A     | 782 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 784  | G    |
| 30  | A     | 785  | G    |
| 30  | A     | 789  | A    |
| 30  | A     | 805  | G    |
| 30  | A     | 812  | C    |
| 30  | A     | 819  | A    |
| 30  | A     | 827  | U    |
| 30  | A     | 828  | U    |
| 30  | A     | 845  | A    |
| 30  | A     | 846  | U    |
| 30  | A     | 847  | U    |
| 30  | A     | 856  | G    |
| 30  | A     | 857  | G    |
| 30  | A     | 869  | G    |
| 30  | A     | 877  | A    |
| 30  | A     | 878  | A    |
| 30  | A     | 885  | C    |
| 30  | A     | 891  | G    |
| 30  | A     | 896  | A    |
| 30  | A     | 897  | C    |
| 30  | A     | 907  | G    |
| 30  | A     | 910  | A    |
| 30  | A     | 941  | A    |
| 30  | A     | 946  | C    |
| 30  | A     | 953  | G    |
| 30  | A     | 961  | C    |
| 30  | A     | 973  | A    |
| 30  | A     | 974  | G    |
| 30  | A     | 980  | A    |
| 30  | A     | 983  | A    |
| 30  | A     | 984  | A    |
| 30  | A     | 985  | C    |
| 30  | A     | 995  | C    |
| 30  | A     | 996  | A    |
| 30  | A     | 1010 | A    |
| 30  | A     | 1011 | G    |
| 30  | A     | 1012 | U    |
| 30  | A     | 1013 | C    |
| 30  | A     | 1021 | A    |
| 30  | A     | 1022 | G    |
| 30  | A     | 1023 | U    |
| 30  | A     | 1026 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 1033 | U    |
| 30  | A     | 1040 | A    |
| 30  | A     | 1045 | C    |
| 30  | A     | 1046 | A    |
| 30  | A     | 1047 | G    |
| 30  | A     | 1053 | C    |
| 30  | A     | 1054 | A    |
| 30  | A     | 1057 | A    |
| 30  | A     | 1059 | G    |
| 30  | A     | 1060 | U    |
| 30  | A     | 1061 | U    |
| 30  | A     | 1062 | G    |
| 30  | A     | 1065 | U    |
| 30  | A     | 1066 | U    |
| 30  | A     | 1068 | G    |
| 30  | A     | 1070 | A    |
| 30  | A     | 1073 | A    |
| 30  | A     | 1076 | C    |
| 30  | A     | 1079 | C    |
| 30  | A     | 1082 | U    |
| 30  | A     | 1083 | U    |
| 30  | A     | 1084 | A    |
| 30  | A     | 1088 | A    |
| 30  | A     | 1089 | A    |
| 30  | A     | 1097 | U    |
| 30  | A     | 1101 | U    |
| 30  | A     | 1104 | C    |
| 30  | A     | 1111 | A    |
| 30  | A     | 1119 | U    |
| 30  | A     | 1132 | U    |
| 30  | A     | 1135 | C    |
| 30  | A     | 1143 | A    |
| 30  | A     | 1157 | G    |
| 30  | A     | 1169 | A    |
| 30  | A     | 1171 | G    |
| 30  | A     | 1174 | U    |
| 30  | A     | 1175 | A    |
| 30  | A     | 1176 | U    |
| 30  | A     | 1180 | U    |
| 30  | A     | 1206 | G    |
| 30  | A     | 1212 | G    |
| 30  | A     | 1225 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 1236 | G    |
| 30  | A     | 1250 | G    |
| 30  | A     | 1253 | A    |
| 30  | A     | 1256 | G    |
| 30  | A     | 1271 | G    |
| 30  | A     | 1272 | A    |
| 30  | A     | 1273 | U    |
| 30  | A     | 1288 | G    |
| 30  | A     | 1300 | G    |
| 30  | A     | 1301 | A    |
| 30  | A     | 1306 | C    |
| 30  | A     | 1314 | C    |
| 30  | A     | 1329 | U    |
| 30  | A     | 1341 | G    |
| 30  | A     | 1345 | C    |
| 30  | A     | 1359 | A    |
| 30  | A     | 1365 | A    |
| 30  | A     | 1378 | A    |
| 30  | A     | 1379 | U    |
| 30  | A     | 1383 | A    |
| 30  | A     | 1416 | G    |
| 30  | A     | 1419 | A    |
| 30  | A     | 1420 | A    |
| 30  | A     | 1421 | G    |
| 30  | A     | 1428 | C    |
| 30  | A     | 1437 | C    |
| 30  | A     | 1454 | C    |
| 30  | A     | 1458 | U    |
| 30  | A     | 1461 | C    |
| 30  | A     | 1475 | G    |
| 30  | A     | 1482 | G    |
| 30  | A     | 1490 | A    |
| 30  | A     | 1491 | G    |
| 30  | A     | 1508 | A    |
| 30  | A     | 1515 | A    |
| 30  | A     | 1524 | G    |
| 30  | A     | 1535 | A    |
| 30  | A     | 1536 | C    |
| 30  | A     | 1537 | G    |
| 30  | A     | 1559 | U    |
| 30  | A     | 1560 | G    |
| 30  | A     | 1563 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 1565 | C    |
| 30  | A     | 1566 | A    |
| 30  | A     | 1569 | A    |
| 30  | A     | 1578 | U    |
| 30  | A     | 1585 | C    |
| 30  | A     | 1608 | A    |
| 30  | A     | 1622 | G    |
| 30  | A     | 1634 | A    |
| 30  | A     | 1646 | C    |
| 30  | A     | 1647 | U    |
| 30  | A     | 1648 | U    |
| 30  | A     | 1654 | A    |
| 30  | A     | 1664 | A    |
| 30  | A     | 1674 | G    |
| 30  | A     | 1699 | G    |
| 30  | A     | 1715 | G    |
| 30  | A     | 1729 | U    |
| 30  | A     | 1730 | C    |
| 30  | A     | 1731 | G    |
| 30  | A     | 1732 | C    |
| 30  | A     | 1733 | G    |
| 30  | A     | 1735 | A    |
| 30  | A     | 1737 | G    |
| 30  | A     | 1738 | G    |
| 30  | A     | 1744 | A    |
| 30  | A     | 1756 | G    |
| 30  | A     | 1764 | C    |
| 30  | A     | 1773 | A    |
| 30  | A     | 1776 | G    |
| 30  | A     | 1781 | U    |
| 30  | A     | 1800 | C    |
| 30  | A     | 1801 | A    |
| 30  | A     | 1808 | A    |
| 30  | A     | 1816 | C    |
| 30  | A     | 1819 | A    |
| 30  | A     | 1820 | U    |
| 30  | A     | 1829 | A    |
| 30  | A     | 1833 | C    |
| 30  | A     | 1835 | G    |
| 30  | A     | 1866 | A    |
| 30  | A     | 1871 | A    |
| 30  | A     | 1901 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 1906 | G    |
| 30  | A     | 1913 | A    |
| 30  | A     | 1917 | U    |
| 30  | A     | 1927 | A    |
| 30  | A     | 1929 | G    |
| 30  | A     | 1930 | G    |
| 30  | A     | 1937 | A    |
| 30  | A     | 1940 | U    |
| 30  | A     | 1941 | C    |
| 30  | A     | 1955 | U    |
| 30  | A     | 1963 | U    |
| 30  | A     | 1967 | C    |
| 30  | A     | 1970 | A    |
| 30  | A     | 1971 | U    |
| 30  | A     | 1972 | G    |
| 30  | A     | 1991 | U    |
| 30  | A     | 1992 | G    |
| 30  | A     | 1997 | C    |
| 30  | A     | 2022 | U    |
| 30  | A     | 2023 | C    |
| 30  | A     | 2030 | A    |
| 30  | A     | 2031 | A    |
| 30  | A     | 2033 | A    |
| 30  | A     | 2043 | C    |
| 30  | A     | 2052 | A    |
| 30  | A     | 2055 | C    |
| 30  | A     | 2056 | G    |
| 30  | A     | 2059 | A    |
| 30  | A     | 2060 | A    |
| 30  | A     | 2061 | G    |
| 30  | A     | 2062 | A    |
| 30  | A     | 2069 | G    |
| 30  | A     | 2072 | C    |
| 30  | A     | 2093 | G    |
| 30  | A     | 2096 | C    |
| 30  | A     | 2100 | G    |
| 30  | A     | 2104 | C    |
| 30  | A     | 2110 | G    |
| 30  | A     | 2111 | U    |
| 30  | A     | 2112 | G    |
| 30  | A     | 2113 | U    |
| 30  | A     | 2118 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 2119 | A    |
| 30  | A     | 2120 | G    |
| 30  | A     | 2124 | G    |
| 30  | A     | 2125 | G    |
| 30  | A     | 2127 | G    |
| 30  | A     | 2131 | U    |
| 30  | A     | 2132 | U    |
| 30  | A     | 2133 | G    |
| 30  | A     | 2136 | G    |
| 30  | A     | 2137 | U    |
| 30  | A     | 2139 | U    |
| 30  | A     | 2145 | C    |
| 30  | A     | 2162 | G    |
| 30  | A     | 2164 | C    |
| 30  | A     | 2172 | U    |
| 30  | A     | 2173 | A    |
| 30  | A     | 2184 | A    |
| 30  | A     | 2189 | U    |
| 30  | A     | 2199 | A    |
| 30  | A     | 2204 | G    |
| 30  | A     | 2211 | A    |
| 30  | A     | 2213 | U    |
| 30  | A     | 2225 | A    |
| 30  | A     | 2226 | C    |
| 30  | A     | 2238 | G    |
| 30  | A     | 2239 | G    |
| 30  | A     | 2250 | G    |
| 30  | A     | 2251 | G    |
| 30  | A     | 2266 | A    |
| 30  | A     | 2279 | G    |
| 30  | A     | 2283 | C    |
| 30  | A     | 2286 | G    |
| 30  | A     | 2287 | A    |
| 30  | A     | 2297 | A    |
| 30  | A     | 2305 | U    |
| 30  | A     | 2309 | A    |
| 30  | A     | 2325 | G    |
| 30  | A     | 2327 | A    |
| 30  | A     | 2333 | A    |
| 30  | A     | 2334 | U    |
| 30  | A     | 2335 | A    |
| 30  | A     | 2336 | A    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 2345 | G    |
| 30  | A     | 2350 | C    |
| 30  | A     | 2357 | G    |
| 30  | A     | 2383 | G    |
| 30  | A     | 2385 | C    |
| 30  | A     | 2396 | G    |
| 30  | A     | 2402 | U    |
| 30  | A     | 2407 | A    |
| 30  | A     | 2422 | C    |
| 30  | A     | 2424 | C    |
| 30  | A     | 2425 | A    |
| 30  | A     | 2428 | G    |
| 30  | A     | 2429 | G    |
| 30  | A     | 2430 | A    |
| 30  | A     | 2434 | A    |
| 30  | A     | 2435 | A    |
| 30  | A     | 2441 | U    |
| 30  | A     | 2445 | G    |
| 30  | A     | 2447 | G    |
| 30  | A     | 2448 | A    |
| 30  | A     | 2475 | C    |
| 30  | A     | 2476 | A    |
| 30  | A     | 2491 | U    |
| 30  | A     | 2492 | U    |
| 30  | A     | 2494 | G    |
| 30  | A     | 2497 | A    |
| 30  | A     | 2498 | C    |
| 30  | A     | 2502 | G    |
| 30  | A     | 2503 | A    |
| 30  | A     | 2504 | U    |
| 30  | A     | 2505 | G    |
| 30  | A     | 2513 | A    |
| 30  | A     | 2518 | A    |
| 30  | A     | 2520 | C    |
| 30  | A     | 2529 | G    |
| 30  | A     | 2530 | A    |
| 30  | A     | 2535 | G    |
| 30  | A     | 2547 | A    |
| 30  | A     | 2554 | U    |
| 30  | A     | 2564 | A    |
| 30  | A     | 2566 | A    |
| 30  | A     | 2567 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 2573 | C    |
| 30  | A     | 2582 | G    |
| 30  | A     | 2597 | G    |
| 30  | A     | 2602 | A    |
| 30  | A     | 2609 | U    |
| 30  | A     | 2610 | C    |
| 30  | A     | 2613 | U    |
| 30  | A     | 2614 | A    |
| 30  | A     | 2629 | U    |
| 30  | A     | 2655 | G    |
| 30  | A     | 2656 | U    |
| 30  | A     | 2661 | G    |
| 30  | A     | 2682 | A    |
| 30  | A     | 2689 | U    |
| 30  | A     | 2690 | U    |
| 30  | A     | 2714 | G    |
| 30  | A     | 2718 | G    |
| 30  | A     | 2722 | G    |
| 30  | A     | 2726 | A    |
| 30  | A     | 2733 | A    |
| 30  | A     | 2739 | U    |
| 30  | A     | 2744 | G    |
| 30  | A     | 2748 | A    |
| 30  | A     | 2762 | C    |
| 30  | A     | 2764 | A    |
| 30  | A     | 2765 | A    |
| 30  | A     | 2778 | A    |
| 30  | A     | 2779 | U    |
| 30  | A     | 2780 | G    |
| 30  | A     | 2791 | G    |
| 30  | A     | 2799 | A    |
| 30  | A     | 2800 | A    |
| 30  | A     | 2809 | A    |
| 30  | A     | 2818 | U    |
| 30  | A     | 2820 | A    |
| 30  | A     | 2833 | U    |
| 30  | A     | 2849 | U    |
| 30  | A     | 2867 | G    |
| 30  | A     | 2868 | A    |
| 30  | A     | 2871 | U    |
| 30  | A     | 2872 | A    |
| 30  | A     | 2880 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | A     | 2883 | A    |
| 30  | A     | 2891 | U    |
| 30  | A     | 2894 | G    |
| 30  | A     | 2901 | C    |
| 30  | A     | 2902 | C    |
| 30  | A     | 2903 | U    |

All (20) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | B     | 52   | A    |
| 6   | B     | 66   | A    |
| 30  | A     | 227  | A    |
| 30  | A     | 242  | G    |
| 30  | A     | 372  | G    |
| 30  | A     | 458  | G    |
| 30  | A     | 549  | G    |
| 30  | A     | 644  | A    |
| 30  | A     | 784  | G    |
| 30  | A     | 1020 | A    |
| 30  | A     | 1022 | G    |
| 30  | A     | 1224 | U    |
| 30  | A     | 1358 | G    |
| 30  | A     | 1378 | A    |
| 30  | A     | 1663 | G    |
| 30  | A     | 1940 | U    |
| 30  | A     | 2058 | A    |
| 30  | A     | 2326 | C    |
| 30  | A     | 2655 | G    |
| 30  | A     | 2808 | G    |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

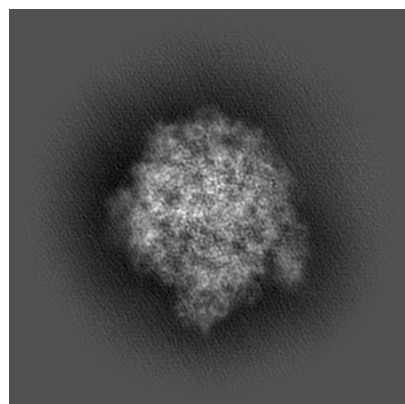
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51978. These allow visual inspection of the internal detail of the map and identification of artifacts.

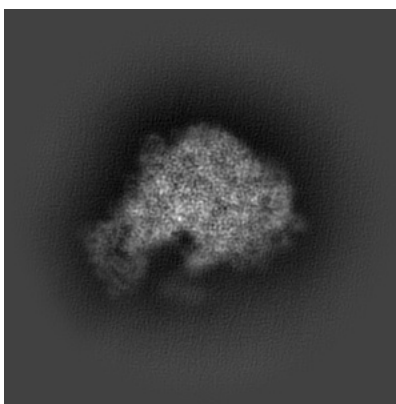
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

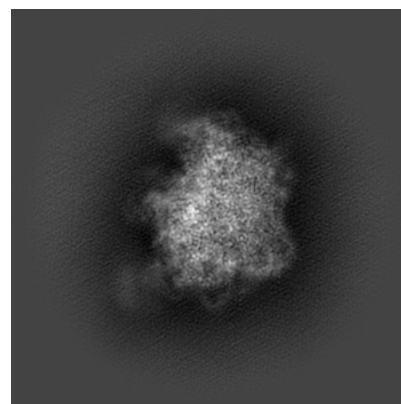
#### 6.1.1 Primary map



X

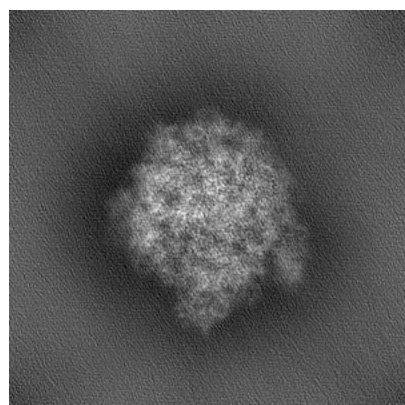


Y

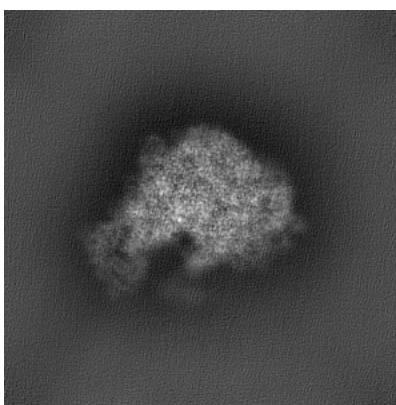


Z

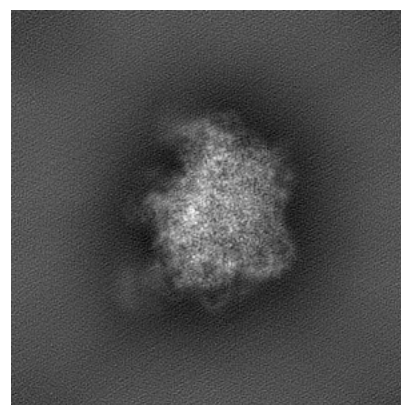
#### 6.1.2 Raw map



X



Y

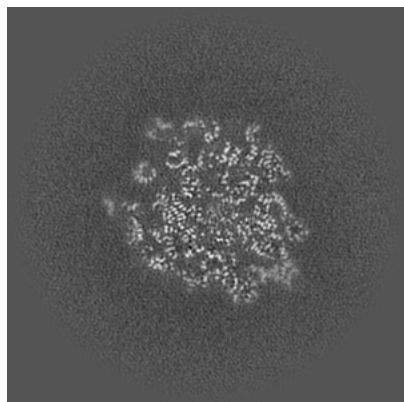


Z

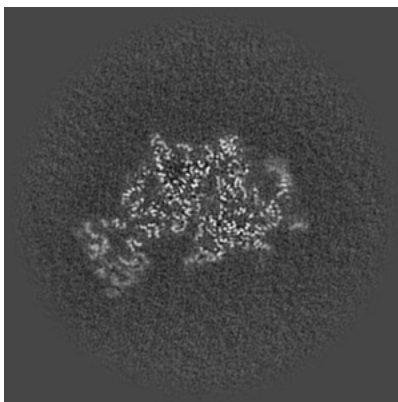
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

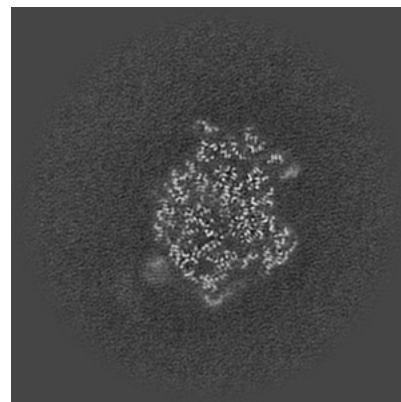
### 6.2.1 Primary map



X Index: 150

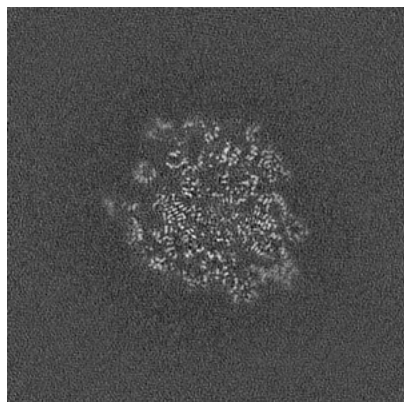


Y Index: 150

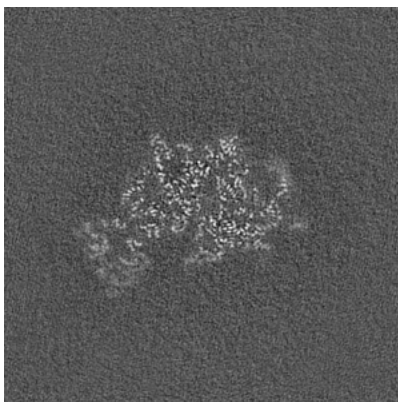


Z Index: 150

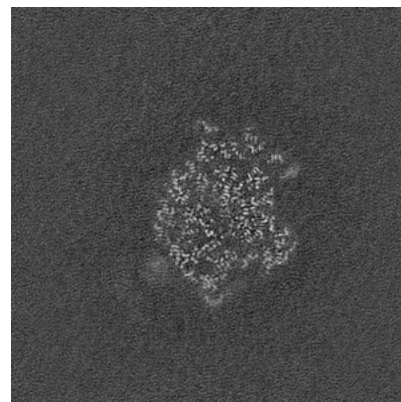
### 6.2.2 Raw map



X Index: 150



Y Index: 150

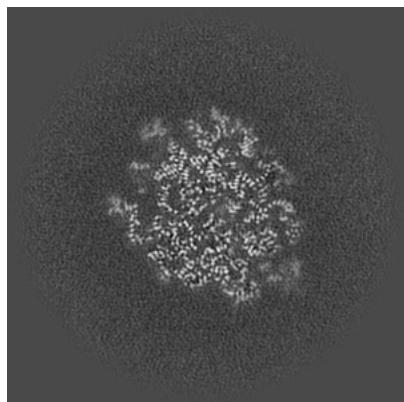


Z Index: 150

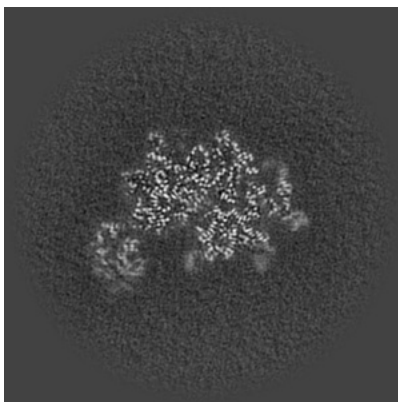
The images above show central slices of the map in three orthogonal directions.

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

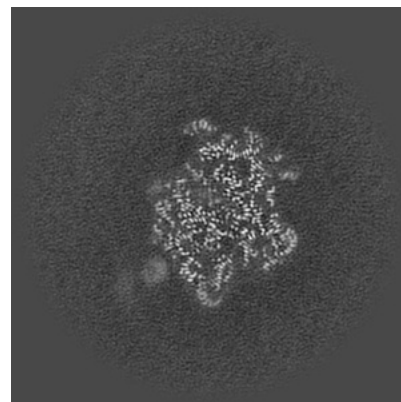
### 6.3.1 Primary map



X Index: 145

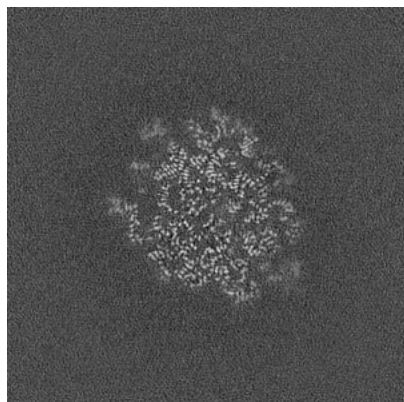


Y Index: 155

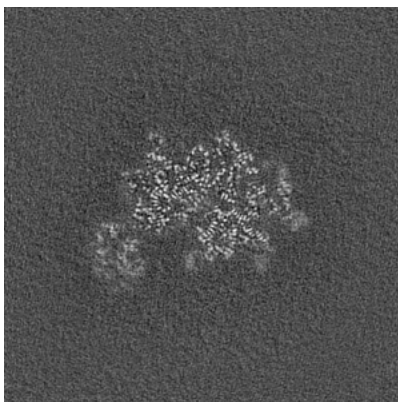


Z Index: 147

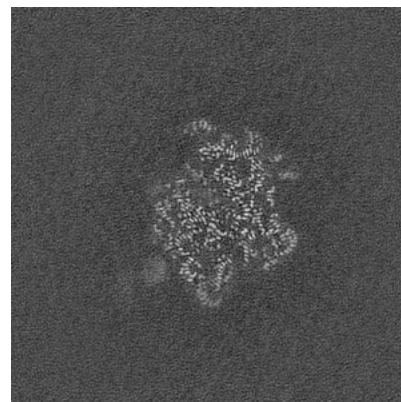
### 6.3.2 Raw map



X Index: 145



Y Index: 155

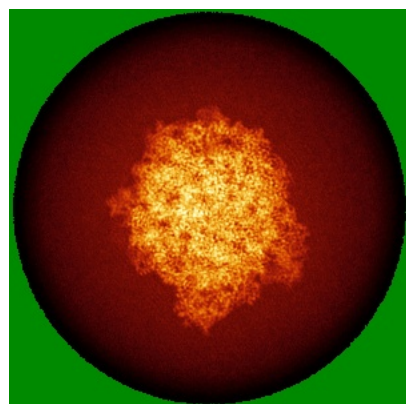


Z Index: 147

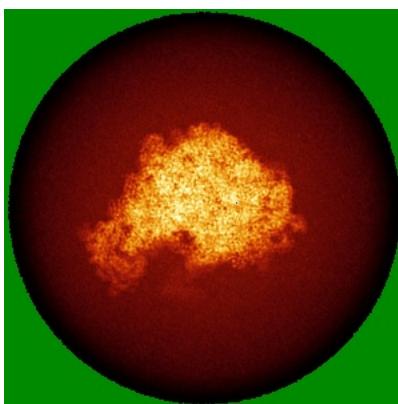
The images above show the largest variance slices of the map in three orthogonal directions.

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

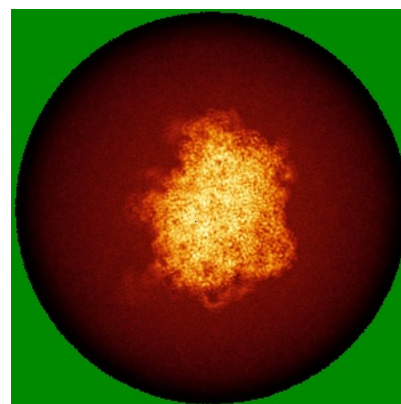
### 6.4.1 Primary map



X

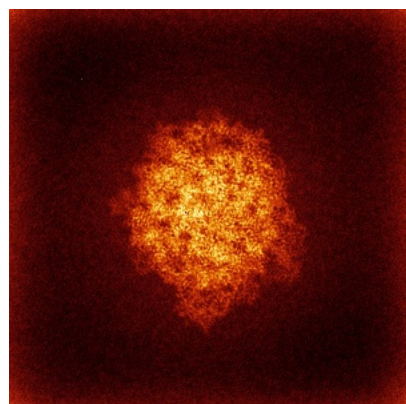


Y

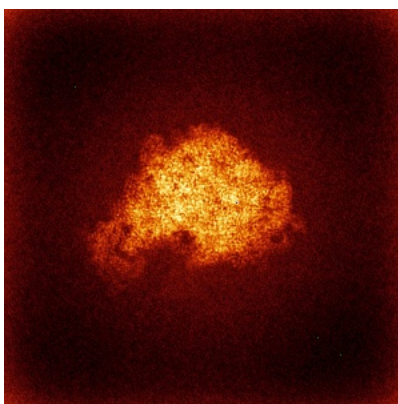


Z

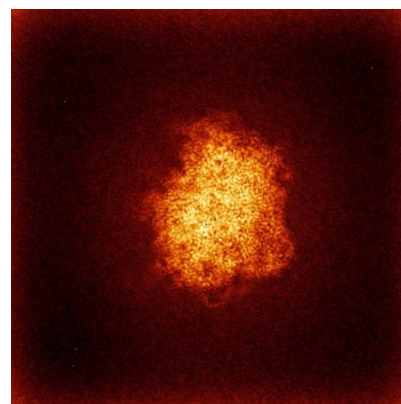
### 6.4.2 Raw map



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.

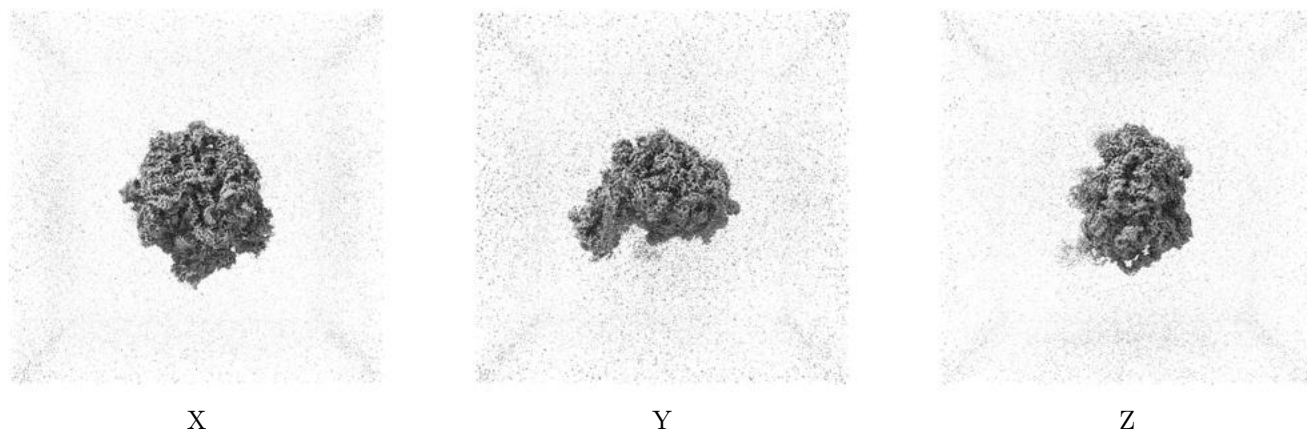
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

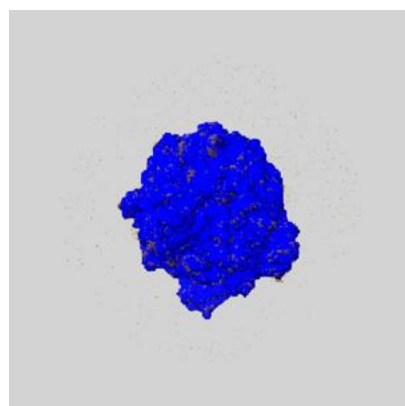
## 6.6 Mask visualisation [i](#)

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

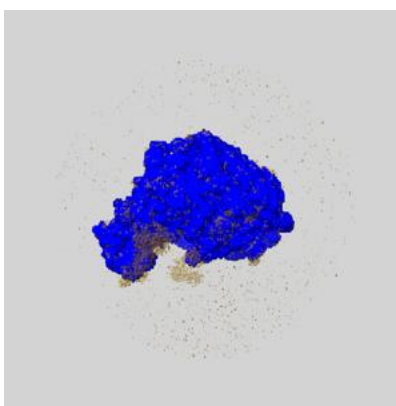
A mask typically either:

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

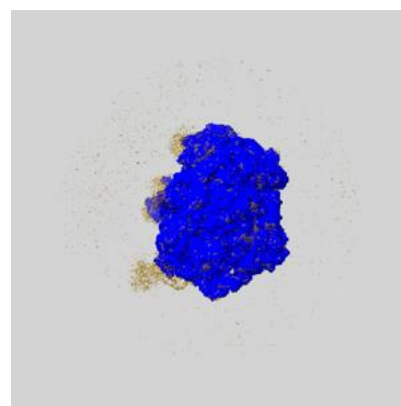
### 6.6.1 emd\_51978\_msk\_1.map [i](#)



X



Y

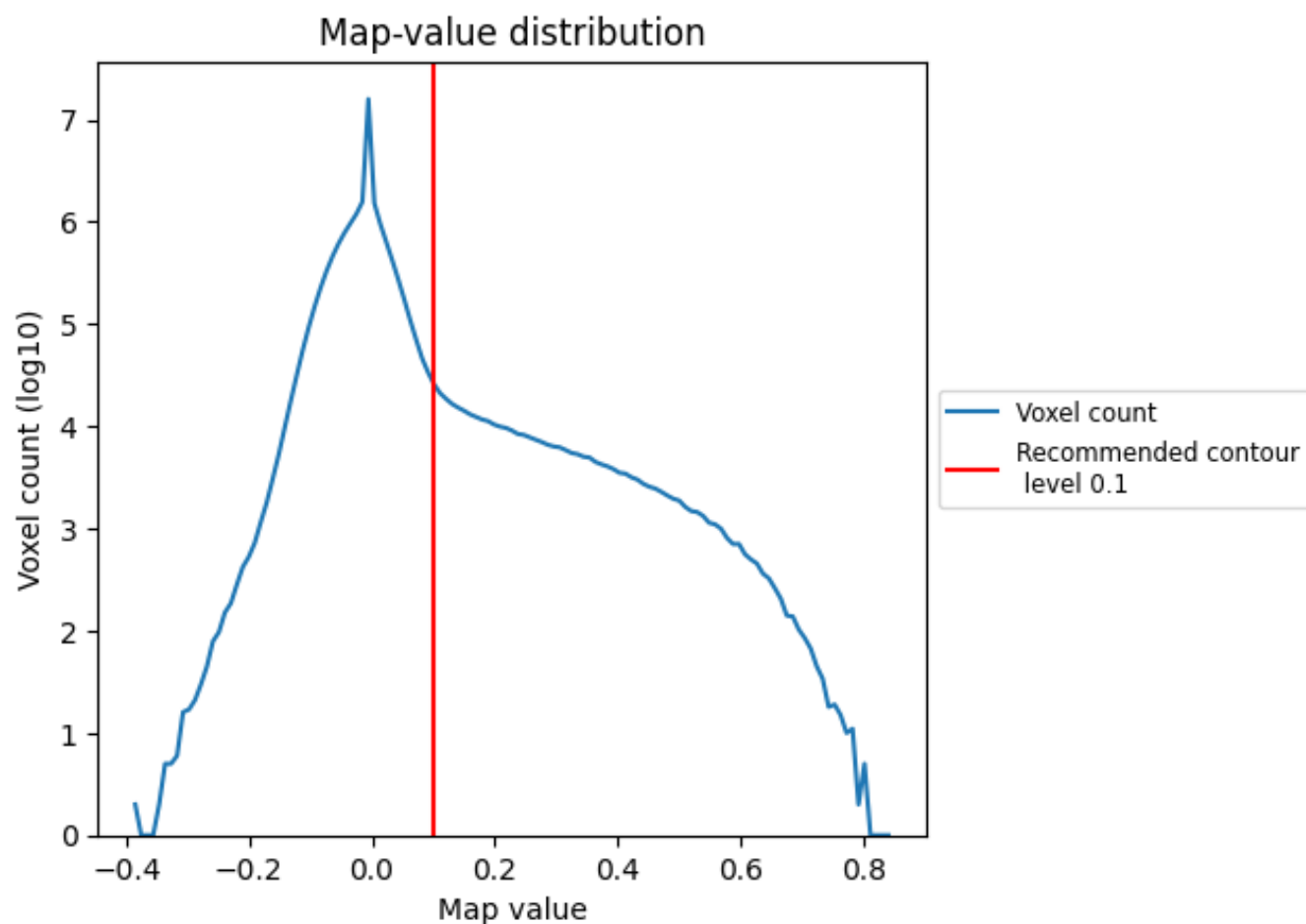


Z

## 7 Map analysis [i](#)

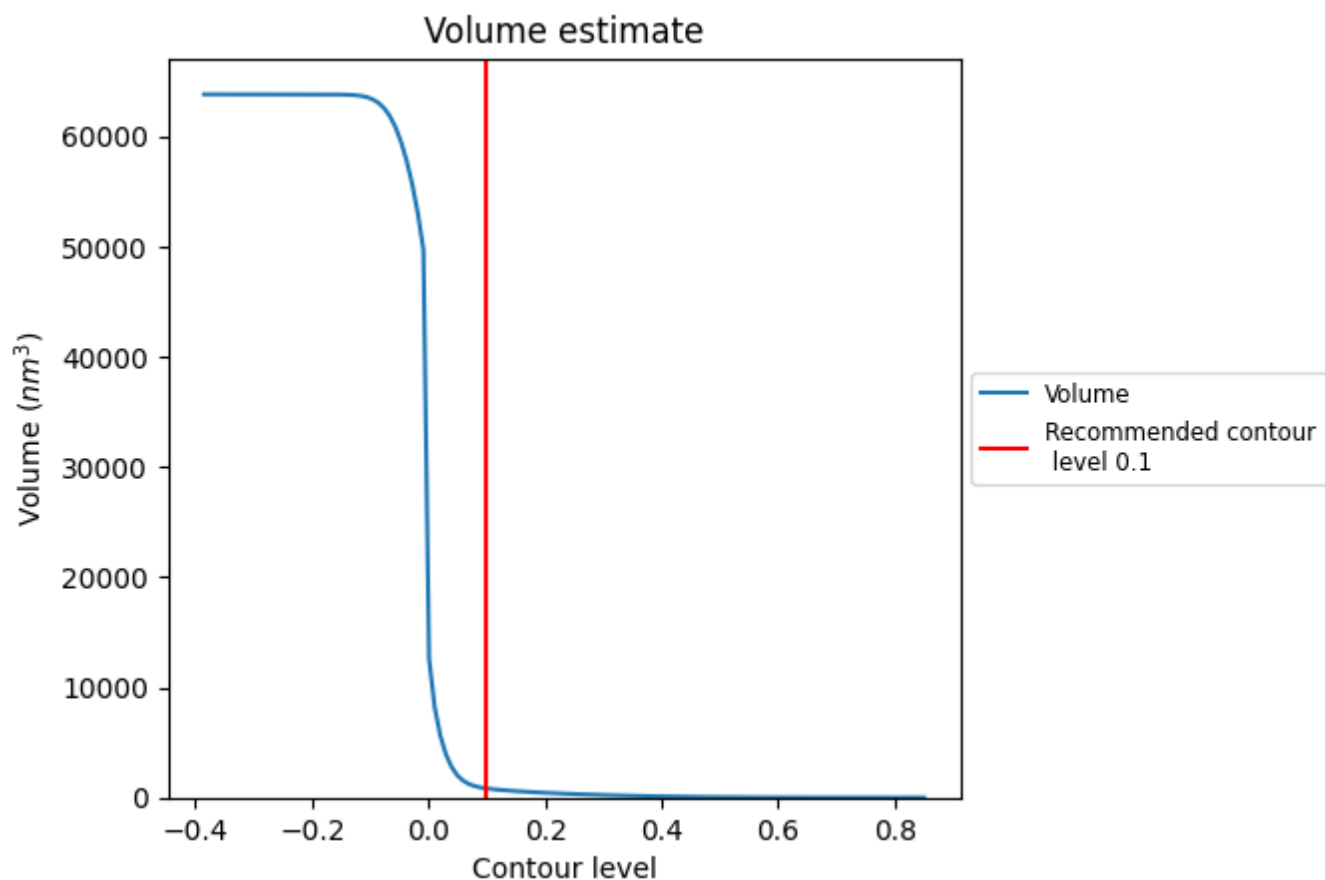
This section contains the results of statistical analysis of the map.

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



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

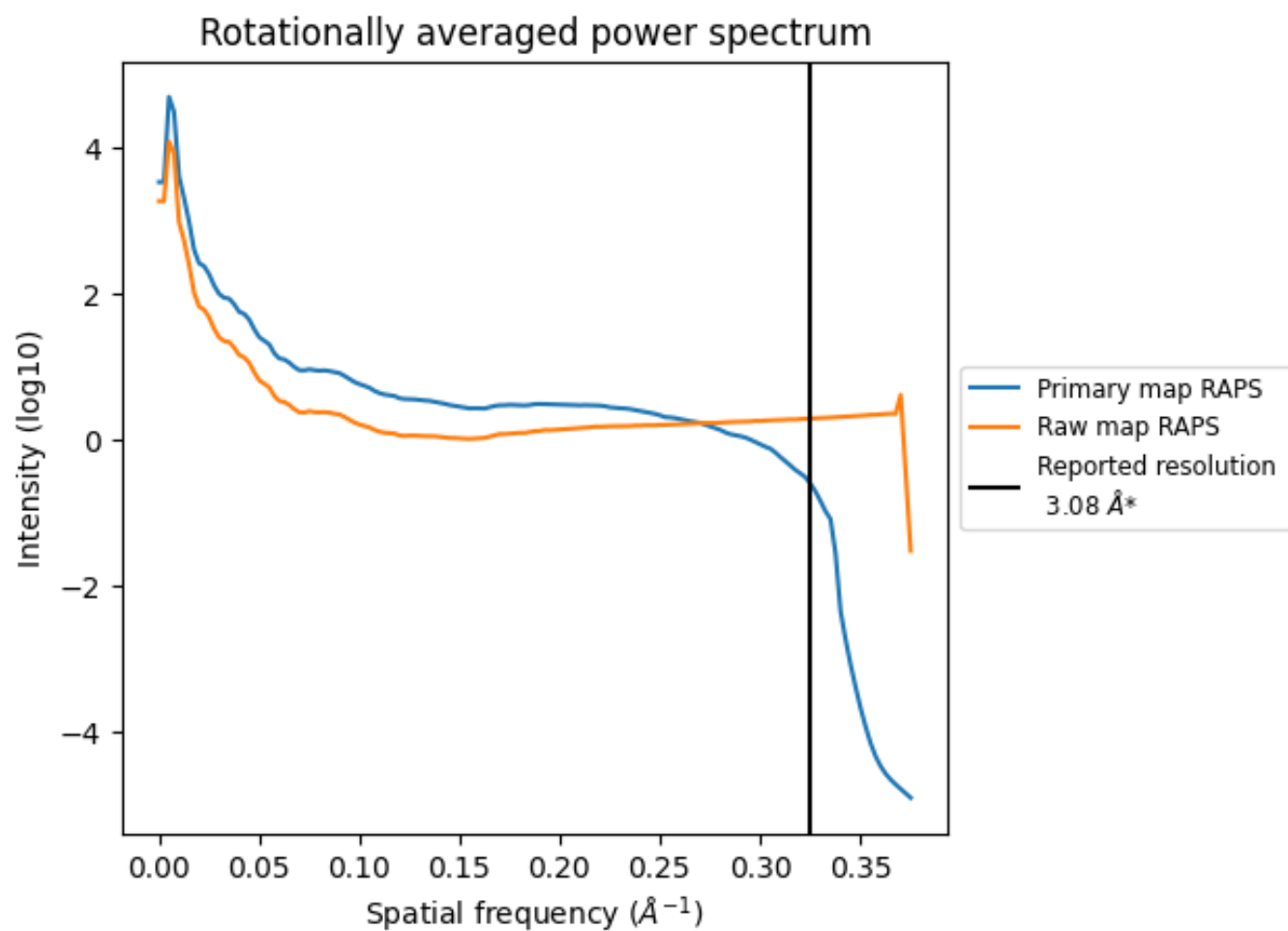
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm<sup>3</sup>; this corresponds to an approximate mass of 744 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 ⓘ

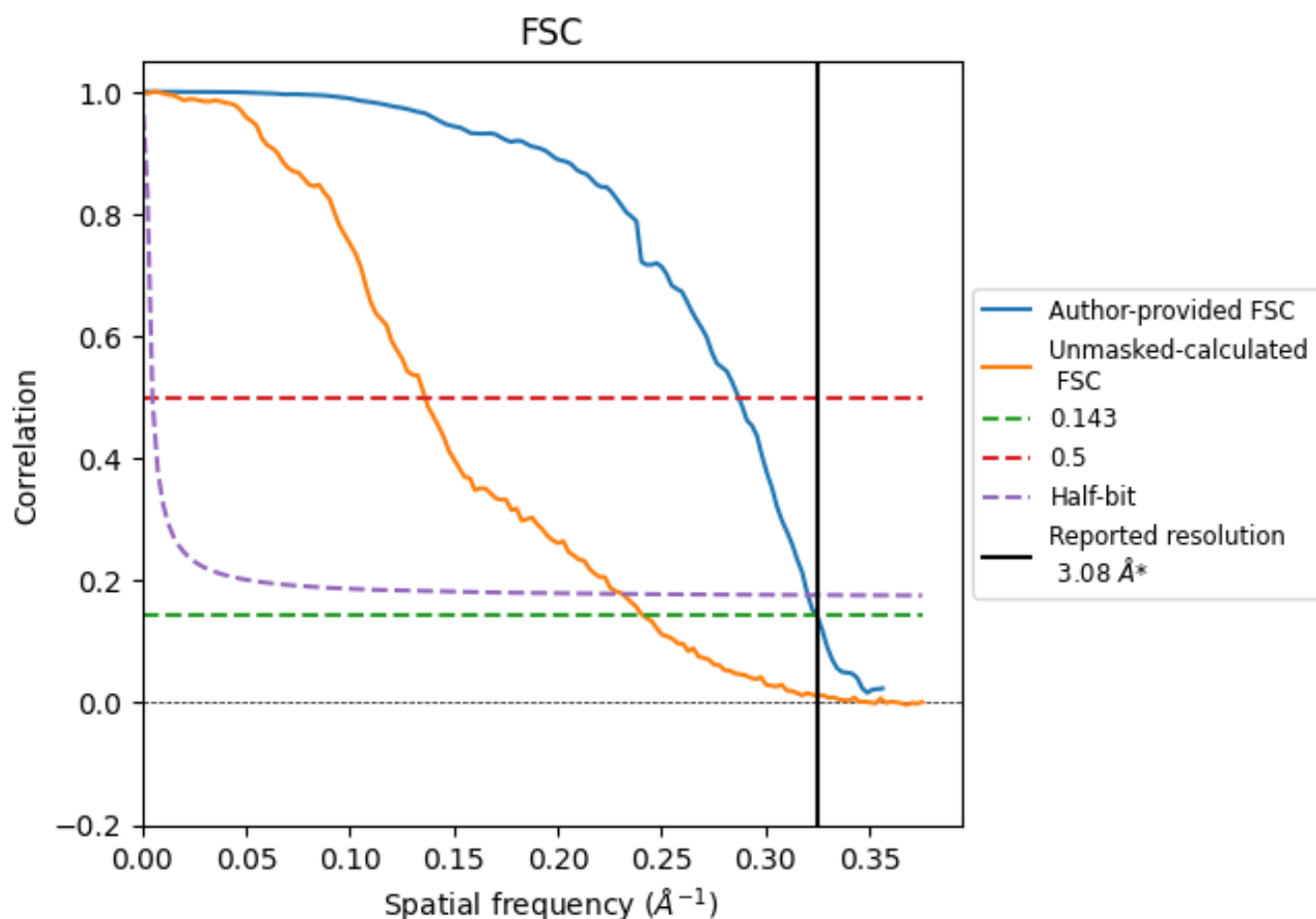


\*Reported resolution corresponds to spatial frequency of 0.325 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.325  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

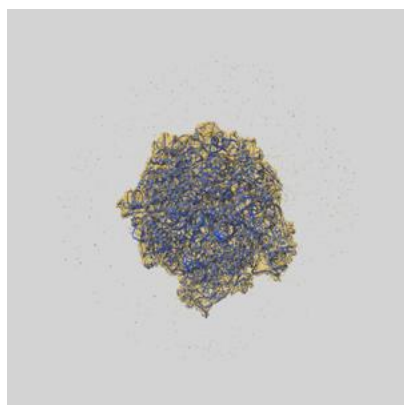
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.08                               | -    | -        |
| Author-provided FSC curve | 3.08                               | 3.48 | 3.12     |
| Unmasked-calculated*      | 4.15                               | 7.34 | 4.33     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.08 by more than 10 %

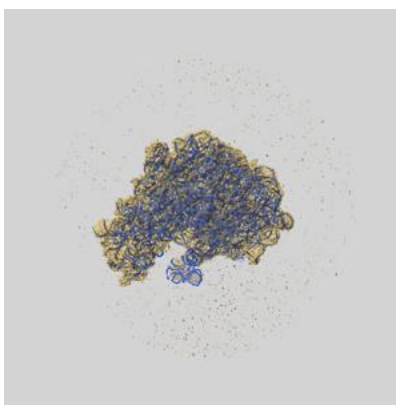
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51978 and PDB model 9HA6. Per-residue inclusion information can be found in section [3](#) on page [10](#).

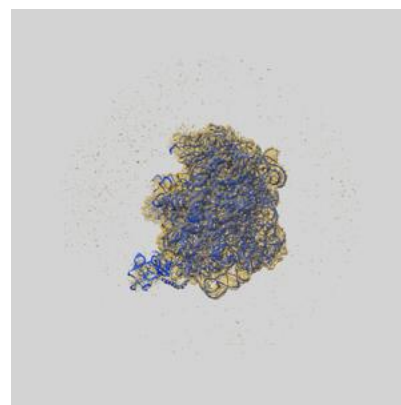
### 9.1 Map-model overlay [i](#)



X



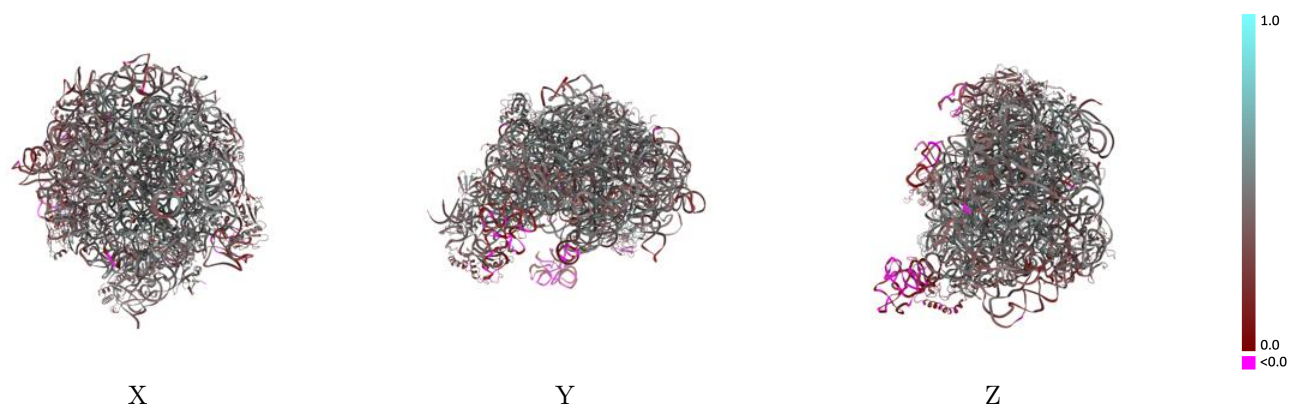
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

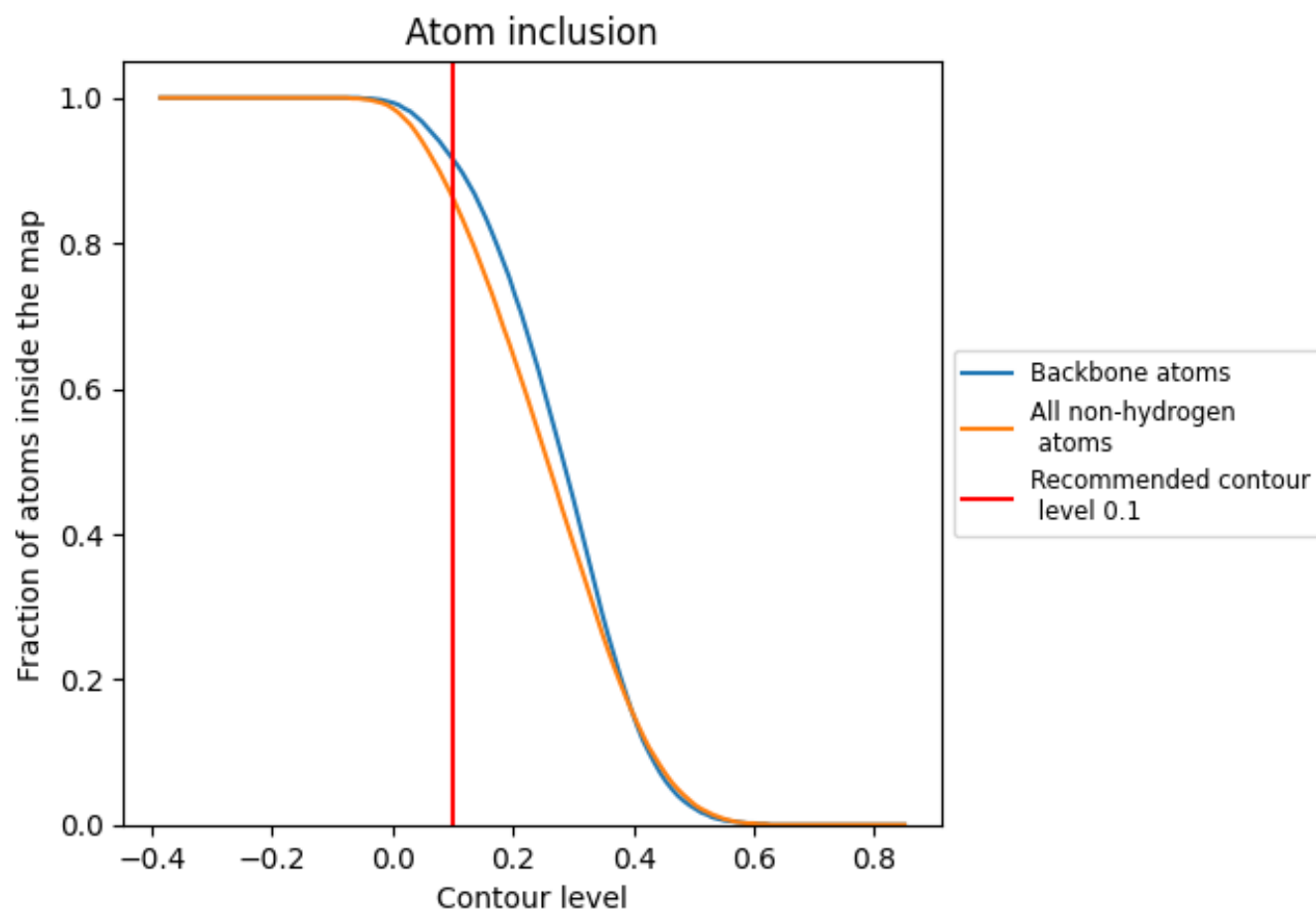


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8630   |  0.4120   |
| 0     |  0.8670   |  0.4750   |
| 1     |  0.6680   |  0.4040   |
| 2     |  0.8900   |  0.4910   |
| 3     |  0.8530   |  0.4570   |
| 4     |  0.7840   |  0.4130   |
| A     |  0.8950   |  0.4150   |
| B     |  0.9310   |  0.4110   |
| C     |  0.8560   |  0.4680   |
| D     |  0.8220   |  0.4430   |
| E     |  0.7800   |  0.3860   |
| F     |  0.6700   |  0.2910   |
| G     |  0.7310   |  0.3400   |
| H     |  0.2230   |  0.1780   |
| J     |  0.8640  |  0.4700  |
| K     |  0.7340 |  0.3650 |
| L     |  0.8030 |  0.4030 |
| M     |  0.8370 |  0.4500 |
| N     |  0.8620 |  0.4520 |
| O     |  0.7970 |  0.3850 |
| P     |  0.7340 |  0.3880 |
| Q     |  0.8810 |  0.4770 |
| R     |  0.8180 |  0.4260 |
| S     |  0.8460 |  0.4630 |
| T     |  0.8100 |  0.4360 |
| U     |  0.7900 |  0.3910 |
| V     |  0.8280 |  0.4170 |
| W     |  0.8610 |  0.4820 |
| X     |  0.8550 |  0.4540 |
| Y     |  0.7470 |  0.3460 |
| Z     |  0.8120 |  0.4540 |
| y     |  0.4100 |  0.2240 |
| z     |  0.4460 |  0.3410 |

