



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:14 AM UTC

PDB ID : 6G5H / pdb\_00006g5h  
EMDB ID : EMD-4352  
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - Mature  
Authors : Ameismeier, M.; Cheng, J.; Berninghausen, O.; Beckmann, R.  
Deposited on : 2018-03-29  
Resolution : 3.60 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

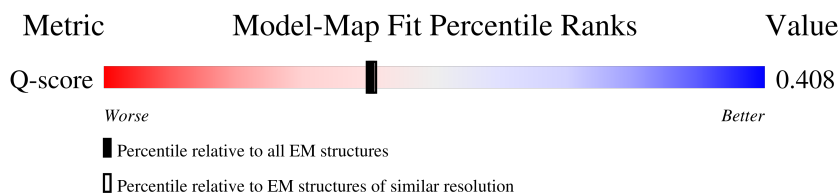
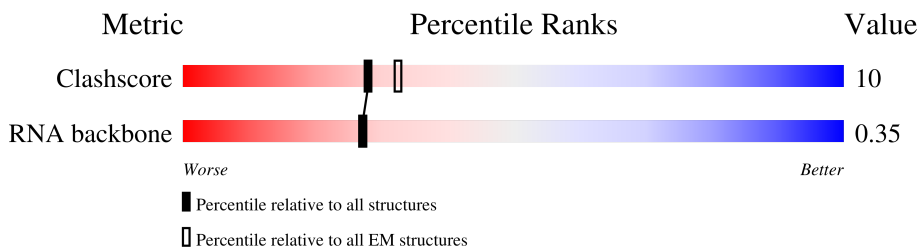
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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                       | -                                                        |
| RNA backbone | 8273                        | 3508                        | -                                                        |
| Q-score      | -                           | 25397                       | 12797 ( 3.10 - 4.10 )                                    |

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   | 2     | 1868   |                  |
| 2   | A     | 295    |                  |
| 3   | B     | 264    |                  |
| 4   | C     | 293    |                  |
| 5   | E     | 263    |                  |

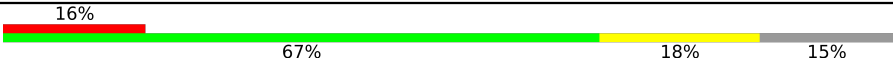
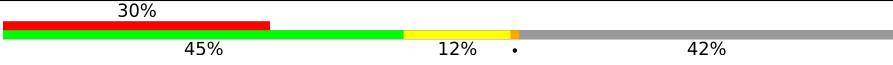
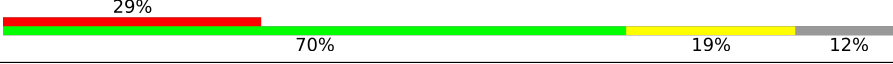
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | G     | 249    |                  |
| 7   | H     | 194    |                  |
| 8   | I     | 208    |                  |
| 9   | J     | 194    |                  |
| 10  | L     | 158    |                  |
| 11  | N     | 151    |                  |
| 12  | O     | 151    |                  |
| 13  | V     | 83     |                  |
| 14  | W     | 130    |                  |
| 15  | X     | 143    |                  |
| 16  | Y     | 133    |                  |
| 17  | a     | 115    |                  |
| 18  | b     | 84     |                  |
| 19  | d     | 56     |                  |
| 20  | e     | 59     |                  |
| 21  | h     | 25     |                  |
| 22  | D     | 243    |                  |
| 23  | F     | 204    |                  |
| 24  | K     | 165    |                  |
| 25  | M     | 132    |                  |
| 26  | P     | 145    |                  |
| 27  | Q     | 146    |                  |
| 28  | R     | 135    |                  |
| 29  | S     | 152    |                  |
| 30  | T     | 145    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 31  | U     | 119    |  |
| 32  | Z     | 125    |  |
| 33  | c     | 69     |  |
| 34  | f     | 156    |  |
| 35  | g     | 317    |  |

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 74342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | 2     | 1665     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 35552 | 15869 | 6385 | 11633 | 1665 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference |
|-------|---------|----------|--------|----------|-----------|
| 2     | 1772    | C        | G      | conflict | GB 337376 |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | A     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1035 | 287 | 294 | 8 |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | B     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1729  | 1098 | 309 | 308 | 14 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | C     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1682  | 1090 | 289 | 293 | 10 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | G     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1862  | 1164 | 371 | 320 | 7 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1501  | 957 | 276 | 267 | 1 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | I     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1682  | 1056 | 331 | 290 | 5 |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | J     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1499  | 955 | 300 | 242 | 2 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | L     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1229  | 782 | 230 | 211 | 6 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | N     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1202  | 770 | 228 | 203 | 1 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | O     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1006  | 616 | 198 | 186 | 6 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | V     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 384 | 116 | 120 | 5 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | W     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | X     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Y     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1014  | 641 | 198 | 170 | 5 |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | a     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 814   | 507 | 170 | 132 | 5 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | b     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 640   | 402 | 118 | 113 | 7 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | d     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 284 | 93 | 73 | 5 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20  | e     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 442   | 273 | 96 | 72 | 1 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 21  | h     | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 231   | 140 | 63 | 26 | 2 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | D     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1748  | 1115 | 315 | 311 | 7 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | F     | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 934 | 284 | 270 | 7 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | K     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 800   | 522 | 142 | 131 | 5 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | M     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 953   | 598 | 169 | 177 | 9 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | P     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 984   | 625 | 184 | 168 | 7 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Q     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1109  | 704 | 210 | 192 | 3 |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | R     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 669 | 199 | 194 | 4 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | S     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1184  | 743 | 240 | 200 | 1 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | T     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1122  | 703 | 217 | 199 | 3 |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | U     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 803   | 504 | 153 | 142 | 4 |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Z     | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 574   | 368 | 104 | 101 | 1 |         |       |

- Molecule 33 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | c     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 479   | 292 | 95 | 90 | 2 |         |       |

- Molecule 34 is a protein called Ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 34  | f     | 72       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 585   | 366 | 114 | 97 | 8 |         |       |

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 35  | g     | 314      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2440  | 1537 | 425 | 466 | 12 |         |       |

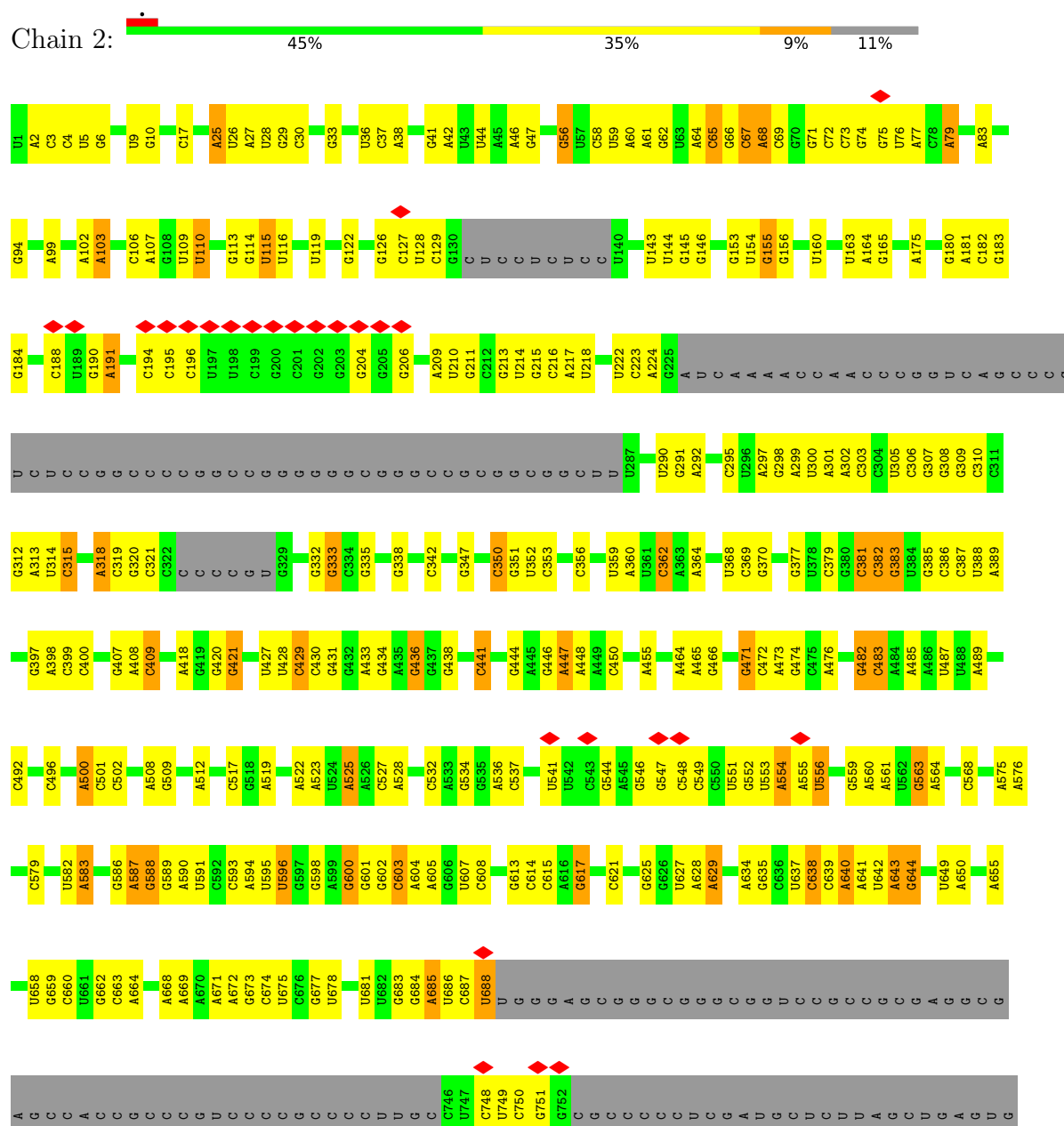
- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 36  | a     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 36  | d     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 36  | f     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

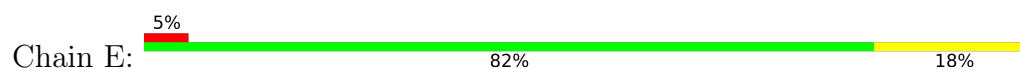
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

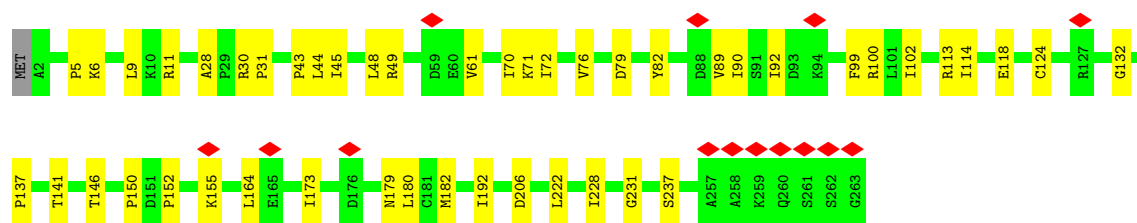
#### • Molecule 1: 18S ribosomal RNA



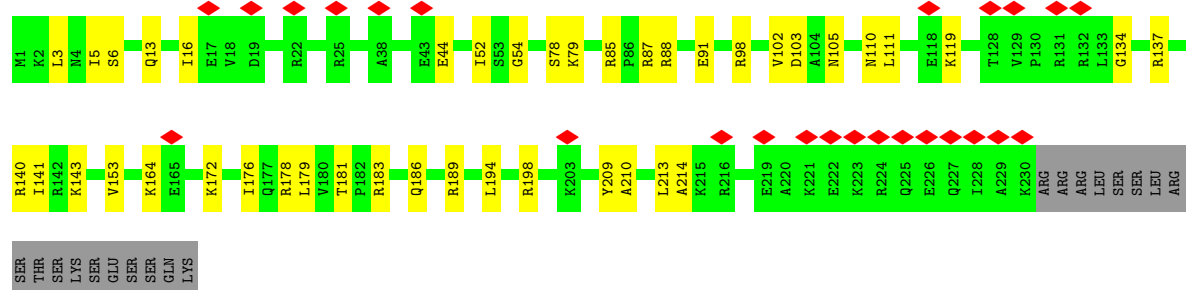
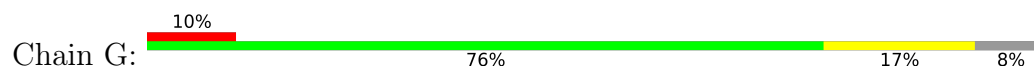


Chain A: 





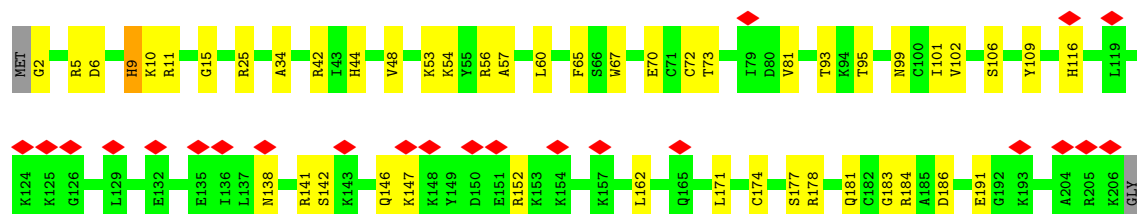
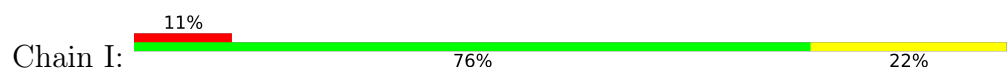
• Molecule 6: 40S ribosomal protein S6



• Molecule 7: 40S ribosomal protein S7

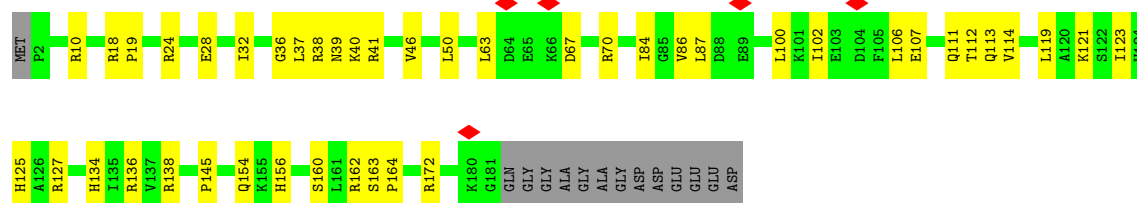


• Molecule 8: 40S ribosomal protein S8



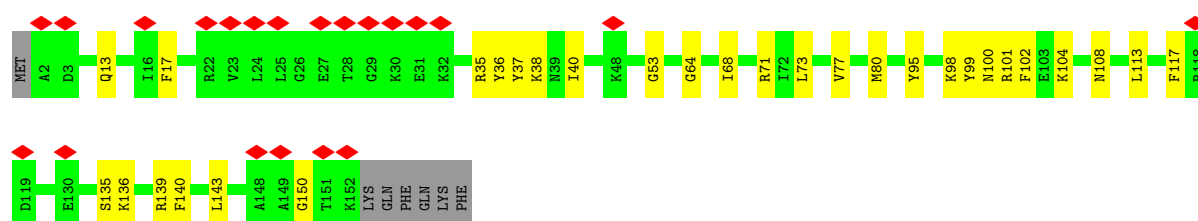
- Molecule 9: 40S ribosomal protein S9

Chain J: 



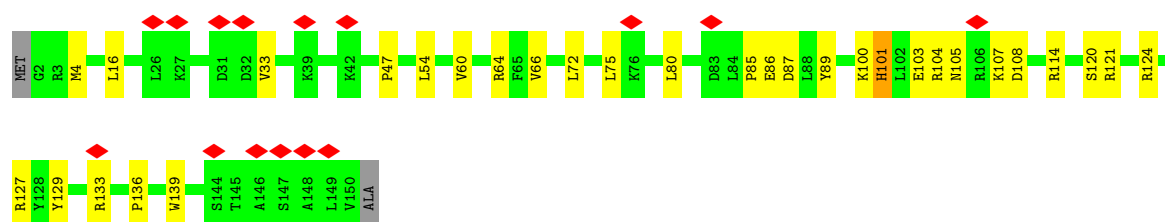
- Molecule 10: 40S ribosomal protein S11

Chain L: 



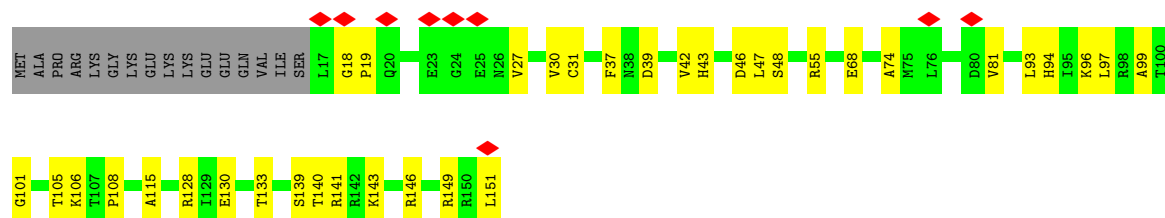
- Molecule 11: 40S ribosomal protein S13

Chain N: 



- Molecule 12: 40S ribosomal protein S14

Chain O: 



- Molecule 13: 40S ribosomal protein S21

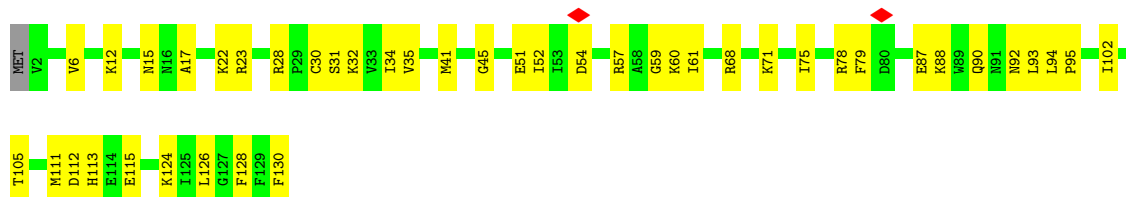
Chain V: 





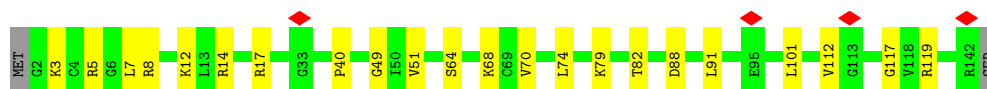
- Molecule 14: 40S ribosomal protein S15a

Chain W: 66% 33%



- Molecule 15: 40S ribosomal protein S23

Chain X: 83% 15%



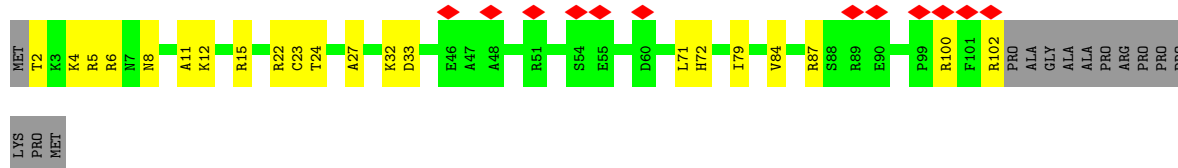
- Molecule 16: 40S ribosomal protein S24

Chain Y: 74% 19% 7%



- Molecule 17: 40S ribosomal protein S26

Chain a: 10% 70% 18% 12%

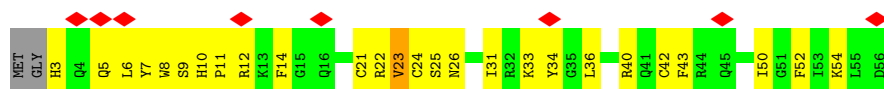


- Molecule 18: 40S ribosomal protein S27

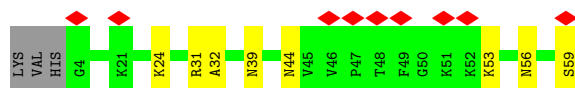
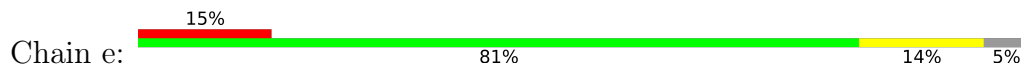
Chain b: 12% 76% 21%



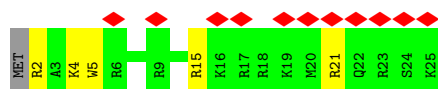
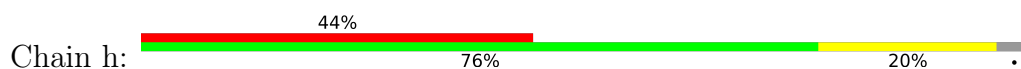
- Molecule 19: 40S ribosomal protein S29



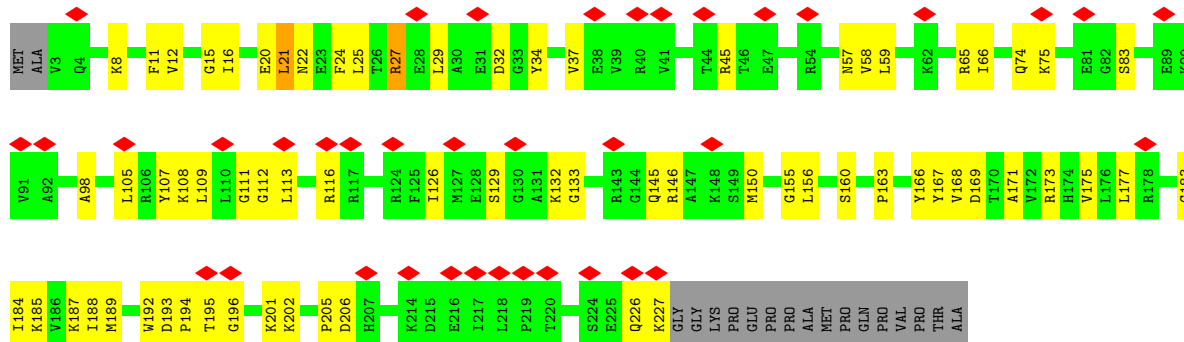
- Molecule 20: 40S ribosomal protein S30



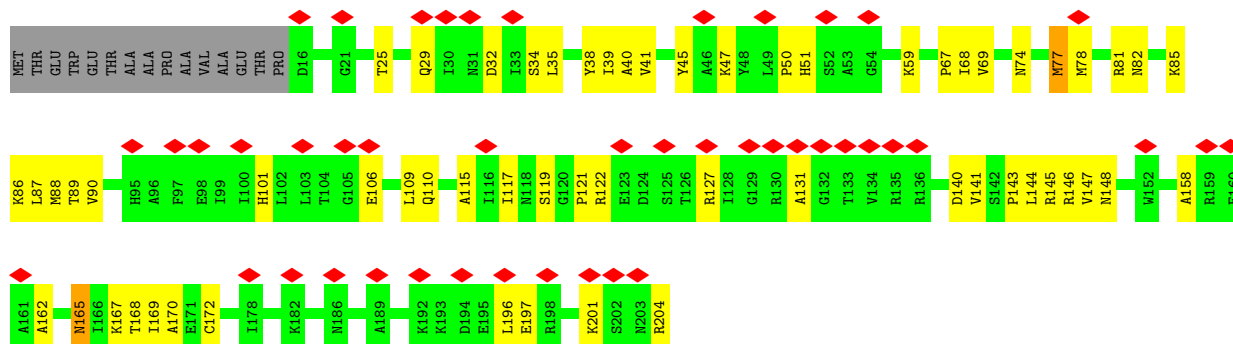
- Molecule 21: 60S ribosomal protein L41



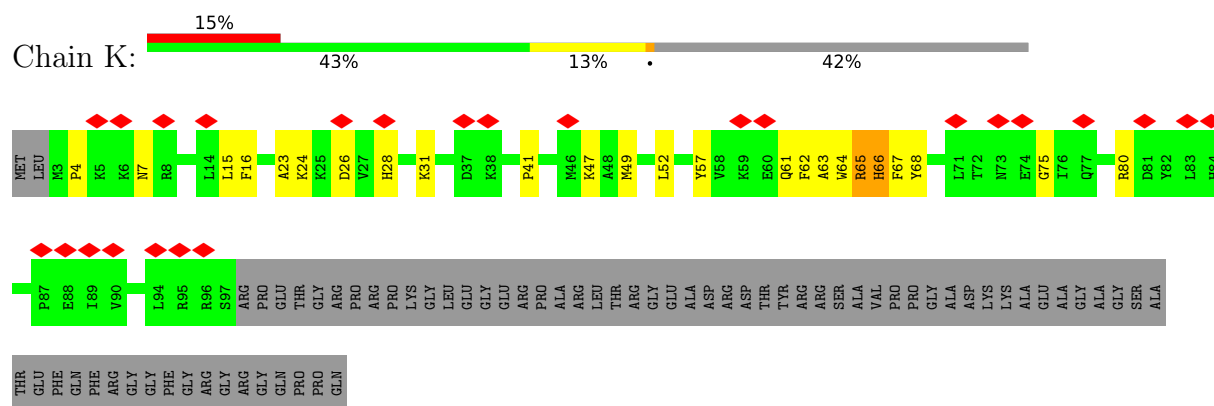
- Molecule 22: 40S ribosomal protein S3



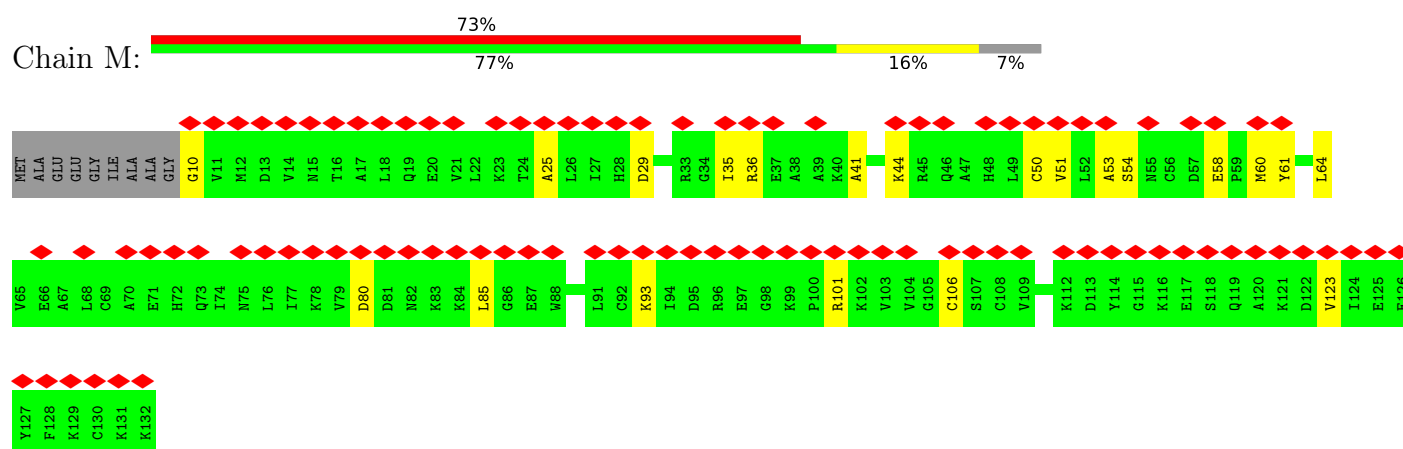
- Molecule 23: 40S ribosomal protein S5



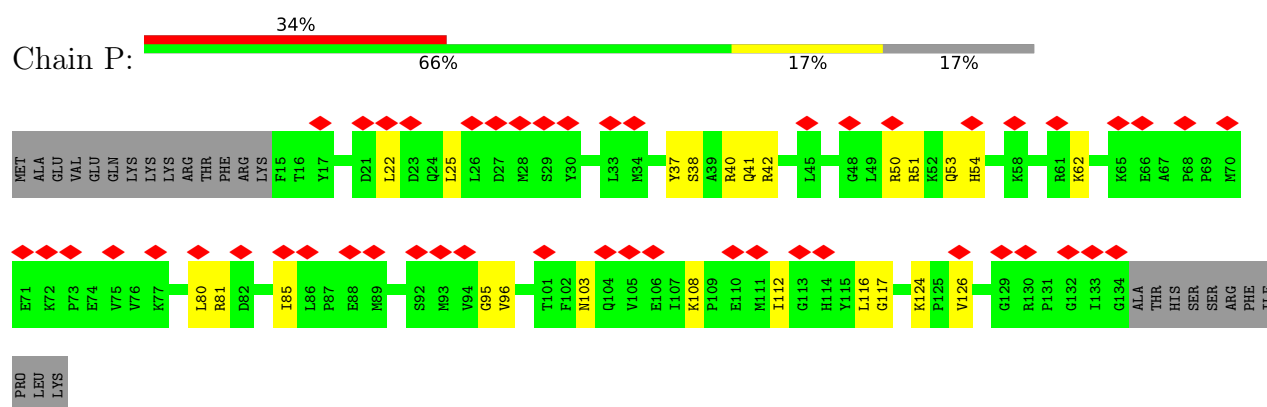
- Molecule 24: 40S ribosomal protein S10



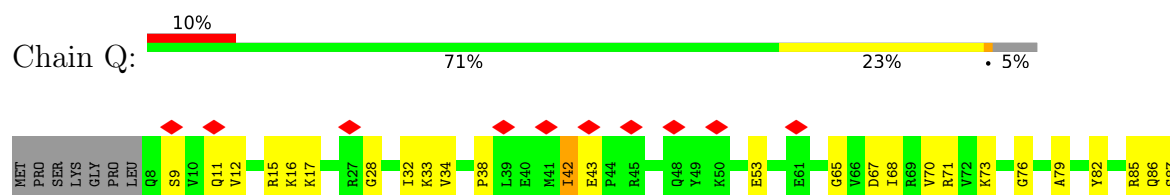
- Molecule 25: 40S ribosomal protein S12

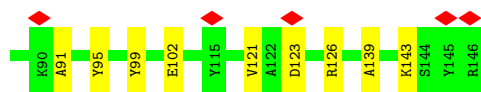


- Molecule 26: 40S ribosomal protein S15

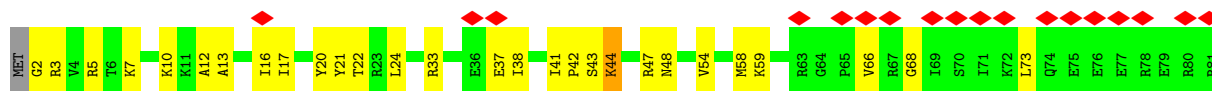
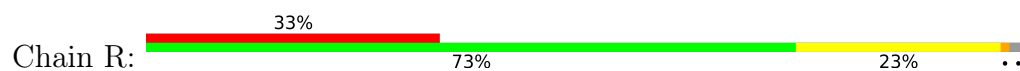


- Molecule 27: 40S ribosomal protein S16

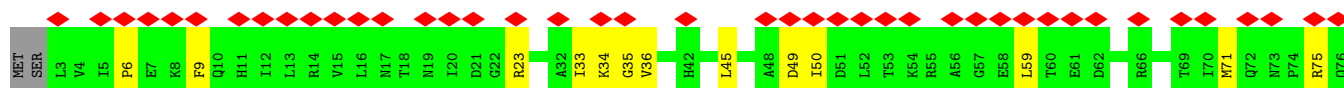
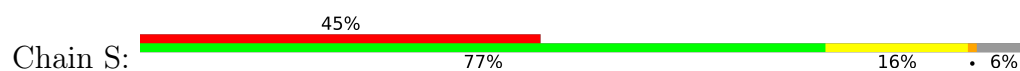




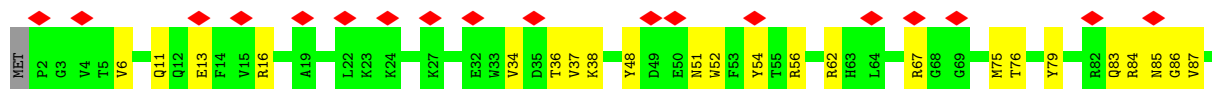
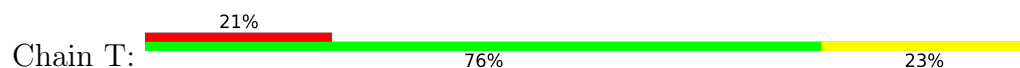
- Molecule 28: 40S ribosomal protein S17



- Molecule 29: 40S ribosomal protein S18



- Molecule 30: 40S ribosomal protein S19



- Molecule 31: 40S ribosomal protein S20



- Molecule 32: 40S ribosomal protein S25



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 70822                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 2.5                                     | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.372                                   | Depositor |
| Minimum map value                    | -0.186                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.017                                   | Depositor |
| Recommended contour level            | 0.06                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 390.24, 390.24, 390.24                  | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.084, 1.084, 1.084                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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   | 2     | 0.56         | 0/39755       | 0.61        | 16/61954 (0.0%) |
| 2   | A     | 0.57         | 0/1661        | 0.89        | 4/2259 (0.2%)   |
| 3   | B     | 0.54         | 0/1756        | 0.91        | 4/2350 (0.2%)   |
| 4   | C     | 0.66         | 0/1718        | 0.98        | 7/2322 (0.3%)   |
| 5   | E     | 0.67         | 1/2118 (0.0%) | 0.82        | 1/2849 (0.0%)   |
| 6   | G     | 0.49         | 0/1885        | 0.88        | 0/2510          |
| 7   | H     | 0.36         | 0/1524        | 0.81        | 1/2042 (0.0%)   |
| 8   | I     | 0.55         | 0/1711        | 0.87        | 3/2282 (0.1%)   |
| 9   | J     | 0.68         | 0/1524        | 0.93        | 0/2035          |
| 10  | L     | 0.63         | 0/1250        | 0.83        | 0/1673          |
| 11  | N     | 0.56         | 0/1226        | 0.88        | 0/1649          |
| 12  | O     | 0.55         | 0/1019        | 0.91        | 1/1367 (0.1%)   |
| 13  | V     | 0.56         | 0/631         | 0.83        | 0/844           |
| 14  | W     | 0.65         | 0/1051        | 0.93        | 0/1406          |
| 15  | X     | 0.63         | 0/1116        | 0.92        | 0/1490          |
| 16  | Y     | 0.60         | 0/1031        | 0.88        | 0/1370          |
| 17  | a     | 0.59         | 0/828         | 0.83        | 0/1109          |
| 18  | b     | 0.48         | 0/653         | 0.79        | 0/876           |
| 19  | d     | 0.51         | 0/466         | 0.85        | 1/618 (0.2%)    |
| 20  | e     | 0.52         | 0/447         | 0.85        | 2/587 (0.3%)    |
| 21  | h     | 0.45         | 0/232         | 1.01        | 0/295           |
| 22  | D     | 0.53         | 0/1776        | 0.96        | 7/2392 (0.3%)   |
| 23  | F     | 0.43         | 0/1516        | 0.89        | 2/2037 (0.1%)   |
| 24  | K     | 0.43         | 0/824         | 0.85        | 2/1112 (0.2%)   |
| 25  | M     | 0.30         | 0/963         | 0.76        | 0/1291          |
| 26  | P     | 0.36         | 0/1003        | 0.77        | 0/1341          |
| 27  | Q     | 0.49         | 0/1126        | 0.89        | 0/1506          |
| 28  | R     | 0.45         | 0/1080        | 0.94        | 6/1449 (0.4%)   |
| 29  | S     | 0.33         | 0/1202        | 0.80        | 2/1610 (0.1%)   |
| 30  | T     | 0.47         | 1/1142 (0.1%) | 0.80        | 0/1530          |
| 31  | U     | 0.50         | 0/813         | 1.01        | 3/1092 (0.3%)   |
| 32  | Z     | 0.34         | 0/580         | 0.86        | 2/780 (0.3%)    |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 33  | c     | 0.42         | 0/481          | 0.86        | 1/643 (0.2%)     |
| 34  | f     | 0.31         | 0/595          | 0.70        | 0/785            |
| 35  | g     | 0.39         | 0/2497         | 0.74        | 0/3399           |
| All | All   | 0.54         | 2/79200 (0.0%) | 0.74        | 65/114854 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 8   | I     | 0                   | 1                   |
| 11  | N     | 0                   | 1                   |
| 12  | O     | 0                   | 1                   |
| 15  | X     | 0                   | 1                   |
| 16  | Y     | 0                   | 1                   |
| 18  | b     | 0                   | 1                   |
| 22  | D     | 0                   | 1                   |
| 23  | F     | 0                   | 4                   |
| 27  | Q     | 0                   | 1                   |
| 30  | T     | 0                   | 1                   |
| 34  | f     | 0                   | 1                   |
| All | All   | 0                   | 14                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | E     | 237 | SER  | C-N   | -8.45 | 1.21        | 1.33     |
| 30  | T     | 87  | VAL  | C-N   | -7.08 | 1.23        | 1.33     |

All (65) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | 2     | 37  | C    | C1'-C2'-O2' | -10.20 | 93.10       | 108.40   |
| 19  | d     | 23  | VAL  | N-CA-C      | 10.05  | 120.87      | 110.72   |
| 7   | H     | 85  | LYS  | N-CA-C      | 9.34   | 121.45      | 111.28   |
| 1   | 2     | 37  | C    | C4'-C3'-O3' | 8.94   | 126.41      | 113.00   |
| 3   | B     | 64  | GLY  | N-CA-C      | 8.56   | 123.00      | 112.73   |
| 22  | D     | 27  | ARG  | N-CA-C      | 7.73   | 119.70      | 111.28   |
| 1   | 2     | 36  | U    | C4'-C3'-O3' | 7.62   | 124.43      | 113.00   |
| 3   | B     | 65  | ARG  | N-CA-C      | 7.55   | 120.62      | 110.35   |
| 22  | D     | 21  | LEU  | N-CA-C      | 7.47   | 119.21      | 111.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31  | U     | 29   | VAL  | N-CA-C      | 7.29  | 118.06      | 110.62   |
| 1   | 2     | 36   | U    | N1-C1'-C2'  | -7.04 | 101.44      | 112.00   |
| 2   | A     | 171  | VAL  | N-CA-C      | 6.99  | 117.75      | 110.62   |
| 4   | C     | 132  | ASP  | N-CA-C      | -6.62 | 97.73       | 108.52   |
| 1   | 2     | 37   | C    | N1-C1'-C2'  | -6.52 | 102.21      | 112.00   |
| 1   | 2     | 38   | A    | N9-C1'-C2'  | -6.38 | 102.42      | 112.00   |
| 24  | K     | 65   | ARG  | N-CA-C      | 6.26  | 121.05      | 113.17   |
| 2   | A     | 187  | GLY  | N-CA-C      | 6.17  | 121.25      | 114.40   |
| 32  | Z     | 61   | GLU  | CA-C-N      | 6.17  | 126.35      | 120.43   |
| 32  | Z     | 61   | GLU  | C-N-CA      | 6.17  | 126.35      | 120.43   |
| 2   | A     | 190  | SER  | N-CA-C      | 6.12  | 117.94      | 110.41   |
| 23  | F     | 141  | VAL  | CA-C-N      | 6.02  | 130.49      | 120.86   |
| 23  | F     | 141  | VAL  | C-N-CA      | 6.02  | 130.49      | 120.86   |
| 1   | 2     | 25   | A    | N9-C1'-C2'  | 5.96  | 120.95      | 112.00   |
| 22  | D     | 173  | ARG  | CA-C-N      | -5.94 | 114.40      | 123.07   |
| 22  | D     | 173  | ARG  | C-N-CA      | -5.94 | 114.40      | 123.07   |
| 4   | C     | 97   | PHE  | N-CA-C      | 5.90  | 117.58      | 111.03   |
| 1   | 2     | 37   | C    | C2'-C3'-O3' | -5.89 | 104.87      | 113.70   |
| 22  | D     | 183  | GLY  | N-CA-C      | -5.80 | 103.65      | 111.54   |
| 20  | e     | 39   | ASN  | CA-C-N      | 5.79  | 129.96      | 120.63   |
| 20  | e     | 39   | ASN  | C-N-CA      | 5.79  | 129.96      | 120.63   |
| 1   | 2     | 1565 | C    | P-O3'-C3'   | 5.75  | 128.83      | 120.20   |
| 8   | I     | 9    | HIS  | N-CA-C      | -5.73 | 106.09      | 112.57   |
| 31  | U     | 18   | HIS  | CA-C-N      | 5.71  | 130.47      | 122.08   |
| 31  | U     | 18   | HIS  | C-N-CA      | 5.71  | 130.47      | 122.08   |
| 1   | 2     | 1403 | C    | P-O3'-C3'   | 5.64  | 128.65      | 120.20   |
| 33  | c     | 22   | GLY  | N-CA-C      | -5.62 | 104.11      | 111.37   |
| 28  | R     | 43   | SER  | CA-C-N      | 5.58  | 129.19      | 120.82   |
| 28  | R     | 43   | SER  | C-N-CA      | 5.58  | 129.19      | 120.82   |
| 8   | I     | 138  | ASN  | CA-C-N      | 5.56  | 128.61      | 120.71   |
| 8   | I     | 138  | ASN  | C-N-CA      | 5.56  | 128.61      | 120.71   |
| 4   | C     | 78   | LEU  | N-CA-C      | 5.56  | 117.34      | 111.28   |
| 4   | C     | 196  | ILE  | N-CA-C      | -5.55 | 104.64      | 109.19   |
| 3   | B     | 219  | LYS  | CA-C-N      | -5.52 | 109.40      | 122.31   |
| 3   | B     | 219  | LYS  | C-N-CA      | -5.52 | 109.40      | 122.31   |
| 1   | 2     | 541  | U    | N1-C1'-C2'  | 5.47  | 120.21      | 112.00   |
| 29  | S     | 99   | LEU  | CA-C-N      | 5.46  | 128.38      | 120.79   |
| 29  | S     | 99   | LEU  | C-N-CA      | 5.46  | 128.38      | 120.79   |
| 5   | E     | 173  | ILE  | N-CA-C      | -5.42 | 104.14      | 110.05   |
| 1   | 2     | 1425 | G    | C2'-C3'-O3' | 5.38  | 121.77      | 113.70   |
| 1   | 2     | 547  | G    | P-O3'-C3'   | 5.35  | 128.23      | 120.20   |
| 28  | R     | 129  | LYS  | CA-C-N      | 5.35  | 127.92      | 120.65   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 28  | R     | 129  | LYS  | C-N-CA    | 5.35  | 127.92      | 120.65   |
| 1   | 2     | 1330 | G    | P-O3'-C3' | 5.32  | 128.19      | 120.20   |
| 28  | R     | 73   | LEU  | N-CA-C    | -5.26 | 105.99      | 112.72   |
| 1   | 2     | 1585 | U    | P-O3'-C3' | 5.23  | 128.05      | 120.20   |
| 22  | D     | 196  | GLY  | CA-C-N    | 5.20  | 131.48      | 121.54   |
| 22  | D     | 196  | GLY  | C-N-CA    | 5.20  | 131.48      | 121.54   |
| 1   | 2     | 1308 | U    | P-O3'-C3' | 5.18  | 127.96      | 120.20   |
| 2   | A     | 189  | ILE  | N-CA-C    | 5.12  | 116.83      | 109.51   |
| 28  | R     | 44   | LYS  | N-CA-C    | 5.08  | 119.76      | 111.37   |
| 24  | K     | 66   | HIS  | N-CA-C    | 5.08  | 117.34      | 108.76   |
| 12  | O     | 146  | ARG  | CG-CD-NE  | -5.03 | 100.93      | 112.00   |
| 4   | C     | 189  | GLY  | CA-C-N    | 5.02  | 129.97      | 122.74   |
| 4   | C     | 189  | GLY  | C-N-CA    | 5.02  | 129.97      | 122.74   |
| 4   | C     | 93   | ILE  | N-CA-C    | -5.00 | 105.67      | 110.72   |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 22  | D     | 194 | PRO  | Peptide |
| 23  | F     | 165 | ASN  | Peptide |
| 23  | F     | 40  | ALA  | Peptide |
| 23  | F     | 77  | MET  | Peptide |
| 23  | F     | 82  | ASN  | Peptide |
| 8   | I     | 101 | ILE  | Peptide |
| 11  | N     | 101 | HIS  | Peptide |
| 12  | O     | 93  | LEU  | Peptide |
| 27  | Q     | 42  | ILE  | Peptide |
| 30  | T     | 36  | THR  | Peptide |
| 15  | X     | 112 | VAL  | Peptide |
| 16  | Y     | 118 | ARG  | Peptide |
| 18  | b     | 52  | THR  | Peptide |
| 34  | f     | 87  | THR  | Peptide |

## 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   | 2     | 35552 | 0        | 17948    | 431     | 0            |
| 2   | A     | 1624  | 0        | 1634     | 60      | 0            |
| 3   | B     | 1729  | 0        | 1801     | 63      | 0            |
| 4   | C     | 1682  | 0        | 1769     | 57      | 0            |
| 5   | E     | 2076  | 0        | 2177     | 29      | 0            |
| 6   | G     | 1862  | 0        | 2018     | 28      | 0            |
| 7   | H     | 1501  | 0        | 1593     | 47      | 0            |
| 8   | I     | 1682  | 0        | 1769     | 31      | 0            |
| 9   | J     | 1499  | 0        | 1618     | 34      | 0            |
| 10  | L     | 1229  | 0        | 1302     | 23      | 0            |
| 11  | N     | 1202  | 0        | 1289     | 24      | 0            |
| 12  | O     | 1006  | 0        | 1030     | 23      | 0            |
| 13  | V     | 625   | 0        | 628      | 10      | 0            |
| 14  | W     | 1034  | 0        | 1080     | 44      | 0            |
| 15  | X     | 1098  | 0        | 1167     | 19      | 0            |
| 16  | Y     | 1014  | 0        | 1082     | 21      | 0            |
| 17  | a     | 814   | 0        | 864      | 20      | 0            |
| 18  | b     | 640   | 0        | 665      | 10      | 0            |
| 19  | d     | 455   | 0        | 446      | 86      | 0            |
| 20  | e     | 442   | 0        | 487      | 6       | 0            |
| 21  | h     | 231   | 0        | 277      | 4       | 0            |
| 22  | D     | 1748  | 0        | 1844     | 81      | 0            |
| 23  | F     | 1495  | 0        | 1549     | 40      | 0            |
| 24  | K     | 800   | 0        | 818      | 70      | 0            |
| 25  | M     | 953   | 0        | 990      | 14      | 0            |
| 26  | P     | 984   | 0        | 1028     | 17      | 0            |
| 27  | Q     | 1109  | 0        | 1174     | 27      | 0            |
| 28  | R     | 1066  | 0        | 1116     | 45      | 0            |
| 29  | S     | 1184  | 0        | 1244     | 18      | 0            |
| 30  | T     | 1122  | 0        | 1153     | 27      | 0            |
| 31  | U     | 803   | 0        | 873      | 48      | 0            |
| 32  | Z     | 574   | 0        | 627      | 10      | 0            |
| 33  | c     | 479   | 0        | 507      | 11      | 0            |
| 34  | f     | 585   | 0        | 616      | 11      | 0            |
| 35  | g     | 2440  | 0        | 2396     | 60      | 0            |
| 36  | a     | 1     | 0        | 0        | 0       | 0            |
| 36  | d     | 1     | 0        | 0        | 0       | 0            |
| 36  | f     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 74342 | 0        | 58579    | 1234    | 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 10.

All (1234) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:62:LEU:HD11   | 3:B:91:VAL:CG2    | 1.37                     | 1.53              |
| 19:d:23:VAL:HG23  | 24:K:64:TRP:CD1   | 1.42                     | 1.50              |
| 28:R:12:ALA:O     | 28:R:16:ILE:HG22  | 1.29                     | 1.31              |
| 19:d:21:CYS:SG    | 19:d:23:VAL:HG12  | 1.73                     | 1.28              |
| 7:H:58:LYS:HD2    | 7:H:90:LYS:NZ     | 1.50                     | 1.25              |
| 19:d:8:TRP:CD1    | 24:K:28:HIS:HB2   | 1.73                     | 1.23              |
| 3:B:62:LEU:CD1    | 3:B:91:VAL:HG22   | 1.67                     | 1.22              |
| 19:d:8:TRP:NE1    | 24:K:28:HIS:CB    | 2.05                     | 1.20              |
| 19:d:50:ILE:HG12  | 22:D:15:GLY:O     | 1.40                     | 1.19              |
| 19:d:43:PHE:HE2   | 31:U:80:PHE:CD2   | 1.63                     | 1.16              |
| 31:U:34:LYS:HA    | 31:U:34:LYS:HE2   | 1.28                     | 1.15              |
| 4:C:102:LEU:HD21  | 4:C:130:ILE:CD1   | 1.74                     | 1.15              |
| 19:d:8:TRP:CD1    | 24:K:28:HIS:CB    | 2.29                     | 1.14              |
| 19:d:52:PHE:HE2   | 31:U:63:ILE:HD12  | 0.99                     | 1.12              |
| 19:d:8:TRP:CE2    | 24:K:28:HIS:HB3   | 1.85                     | 1.11              |
| 1:2:1497:G:C5     | 24:K:62:PHE:CE2   | 2.38                     | 1.10              |
| 1:2:1497:G:C5     | 24:K:62:PHE:HE2   | 1.70                     | 1.10              |
| 19:d:52:PHE:CE2   | 31:U:63:ILE:HD12  | 1.86                     | 1.10              |
| 31:U:27:ARG:CD    | 31:U:82:MET:HE1   | 1.79                     | 1.10              |
| 3:B:63:LYS:O      | 3:B:88:THR:HG23   | 1.52                     | 1.10              |
| 19:d:23:VAL:HG23  | 24:K:64:TRP:NE1   | 1.67                     | 1.10              |
| 24:K:24:LYS:HA    | 24:K:66:HIS:CE1   | 1.87                     | 1.09              |
| 31:U:27:ARG:HD2   | 31:U:82:MET:CE    | 1.83                     | 1.09              |
| 19:d:43:PHE:CE2   | 31:U:80:PHE:CD2   | 2.42                     | 1.08              |
| 19:d:23:VAL:CG2   | 24:K:64:TRP:CD1   | 2.37                     | 1.07              |
| 1:2:1497:G:C4     | 24:K:62:PHE:CD2   | 2.42                     | 1.06              |
| 2:A:176:TRP:CD1   | 2:A:195:TRP:HZ3   | 1.73                     | 1.04              |
| 4:C:102:LEU:CD2   | 4:C:130:ILE:HD11  | 1.87                     | 1.04              |
| 22:D:105:LEU:HD23 | 22:D:184:ILE:CD1  | 1.86                     | 1.04              |
| 19:d:34:TYR:HB3   | 22:D:12:VAL:HG21  | 1.40                     | 1.03              |
| 3:B:62:LEU:HD11   | 3:B:91:VAL:HG21   | 1.33                     | 1.03              |
| 2:A:176:TRP:NE1   | 2:A:195:TRP:CZ3   | 2.27                     | 1.03              |
| 1:2:1729:U:H3     | 1:2:1805:G:H1     | 1.03                     | 1.01              |
| 19:d:52:PHE:HE2   | 31:U:63:ILE:CD1   | 1.75                     | 1.00              |
| 1:2:1497:G:C4     | 24:K:62:PHE:HD2   | 1.76                     | 1.00              |
| 1:2:1497:G:N7     | 24:K:62:PHE:HE2   | 1.57                     | 1.00              |
| 22:D:105:LEU:CD2  | 22:D:184:ILE:HD12 | 1.91                     | 1.00              |
| 4:C:102:LEU:HD21  | 4:C:130:ILE:HD11  | 1.02                     | 1.00              |
| 19:d:43:PHE:CE2   | 31:U:80:PHE:CE2   | 2.50                     | 1.00              |
| 24:K:24:LYS:HG3   | 24:K:66:HIS:CE1   | 1.96                     | 0.99              |
| 4:C:78:LEU:HD13   | 4:C:97:PHE:CE2    | 1.98                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:62:LEU:CD1    | 3:B:91:VAL:CG2    | 2.30                     | 0.98              |
| 1:2:925:G:H1      | 1:2:1017:U:H3     | 1.06                     | 0.97              |
| 1:2:1227:G:H1     | 1:2:1531:A:N6     | 1.60                     | 0.97              |
| 3:B:49:VAL:HG22   | 3:B:65:ARG:NH2    | 1.80                     | 0.97              |
| 19:d:8:TRP:NE1    | 24:K:28:HIS:HB2   | 1.73                     | 0.97              |
| 1:2:678:U:H3      | 1:2:1027:A:H62    | 1.12                     | 0.96              |
| 22:D:156:LEU:HB2  | 22:D:189:MET:HE1  | 1.46                     | 0.96              |
| 22:D:105:LEU:HD23 | 22:D:184:ILE:HD12 | 0.96                     | 0.95              |
| 19:d:8:TRP:NE1    | 24:K:28:HIS:HB3   | 1.74                     | 0.95              |
| 31:U:27:ARG:HD2   | 31:U:82:MET:HE1   | 0.97                     | 0.95              |
| 7:H:58:LYS:HD2    | 7:H:90:LYS:HZ1    | 1.16                     | 0.95              |
| 19:d:23:VAL:HG23  | 24:K:64:TRP:HD1   | 1.32                     | 0.94              |
| 14:W:75:ILE:HD11  | 14:W:93:LEU:CD1   | 1.98                     | 0.94              |
| 3:B:62:LEU:HD11   | 3:B:91:VAL:HG22   | 0.94                     | 0.94              |
| 3:B:63:LYS:C      | 3:B:88:THR:HG23   | 1.91                     | 0.94              |
| 3:B:63:LYS:O      | 3:B:88:THR:CG2    | 2.16                     | 0.93              |
| 4:C:78:LEU:HD13   | 4:C:97:PHE:CD2    | 2.02                     | 0.93              |
| 1:2:1332:A:H62    | 1:2:1493:C:H42    | 1.11                     | 0.93              |
| 1:2:1606:G:N2     | 1:2:1633:A:N7     | 2.16                     | 0.93              |
| 2:A:76:VAL:HG13   | 2:A:175:TRP:CH2   | 2.05                     | 0.92              |
| 2:A:90:PHE:CE2    | 2:A:175:TRP:HZ3   | 1.88                     | 0.92              |
| 2:A:176:TRP:CD1   | 2:A:195:TRP:CZ3   | 2.57                     | 0.91              |
| 1:2:1495:G:H4'    | 19:d:26:ASN:OD1   | 1.70                     | 0.91              |
| 19:d:43:PHE:HE2   | 31:U:80:PHE:CE2   | 1.87                     | 0.91              |
| 22:D:187:LYS:O    | 22:D:188:ILE:HD13 | 1.70                     | 0.91              |
| 2:A:58:LEU:HD21   | 2:A:174:MET:HE1   | 1.53                     | 0.91              |
| 24:K:24:LYS:HA    | 24:K:66:HIS:ND1   | 1.84                     | 0.90              |
| 24:K:24:LYS:HG3   | 24:K:66:HIS:HE1   | 1.32                     | 0.90              |
| 2:A:58:LEU:HD21   | 2:A:174:MET:CE    | 2.00                     | 0.90              |
| 4:C:134:ASN:C     | 4:C:134:ASN:HD22  | 1.78                     | 0.90              |
| 14:W:75:ILE:HD11  | 14:W:93:LEU:HD11  | 1.51                     | 0.90              |
| 19:d:8:TRP:CD1    | 24:K:28:HIS:HB3   | 2.06                     | 0.89              |
| 1:2:1332:A:H62    | 1:2:1493:C:N4     | 1.72                     | 0.88              |
| 1:2:1033:G:H1     | 1:2:1080:A:HO2'   | 1.12                     | 0.88              |
| 19:d:34:TYR:CZ    | 31:U:61:LEU:HB3   | 2.09                     | 0.88              |
| 19:d:23:VAL:CG2   | 24:K:64:TRP:NE1   | 2.37                     | 0.87              |
| 7:H:58:LYS:HB2    | 7:H:90:LYS:HD3    | 1.55                     | 0.87              |
| 19:d:43:PHE:CE2   | 31:U:80:PHE:HD2   | 1.86                     | 0.87              |
| 4:C:78:LEU:HD22   | 4:C:97:PHE:HB2    | 1.58                     | 0.86              |
| 7:H:58:LYS:HD2    | 7:H:90:LYS:HZ3    | 1.36                     | 0.86              |
| 31:U:24:LEU:HD12  | 31:U:36:CYS:HB2   | 1.57                     | 0.86              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:R:13:ALA:HA   | 28:R:16:ILE:CG2   | 2.05                     | 0.85              |
| 22:D:21:LEU:O    | 22:D:21:LEU:HD12  | 1.77                     | 0.85              |
| 14:W:94:LEU:HD21 | 14:W:102:ILE:HG13 | 1.59                     | 0.84              |
| 4:C:102:LEU:HD21 | 4:C:130:ILE:CG1   | 2.08                     | 0.84              |
| 1:2:1332:A:N6    | 1:2:1493:C:H42    | 1.76                     | 0.83              |
| 1:2:1513:C:OP1   | 19:d:10:HIS:HB3   | 1.78                     | 0.83              |
| 22:D:132:LYS:CB  | 22:D:189:MET:HE3  | 2.09                     | 0.83              |
| 4:C:83:LEU:O     | 4:C:83:LEU:HD12   | 1.77                     | 0.83              |
| 19:d:23:VAL:HG11 | 19:d:42:CYS:CB    | 2.08                     | 0.83              |
| 31:U:24:LEU:CD1  | 31:U:36:CYS:HB2   | 2.08                     | 0.83              |
| 1:2:1497:G:C4    | 24:K:62:PHE:CE2   | 2.64                     | 0.82              |
| 2:A:176:TRP:NE1  | 2:A:195:TRP:CE3   | 2.43                     | 0.82              |
| 1:2:1329:U:H3    | 1:2:1500:G:H1     | 1.23                     | 0.82              |
| 3:B:49:VAL:HG22  | 3:B:65:ARG:HH21   | 1.39                     | 0.81              |
| 7:H:58:LYS:CD    | 7:H:90:LYS:NZ     | 2.40                     | 0.81              |
| 4:C:78:LEU:HB2   | 4:C:97:PHE:CG     | 2.16                     | 0.81              |
| 1:2:1497:G:C8    | 24:K:62:PHE:HE2   | 1.98                     | 0.81              |
| 1:2:1618:C:N4    | 19:d:10:HIS:HE1   | 1.79                     | 0.81              |
| 19:d:34:TYR:CE2  | 31:U:61:LEU:HB3   | 2.16                     | 0.81              |
| 2:A:173:LEU:O    | 2:A:173:LEU:HD22  | 1.81                     | 0.80              |
| 19:d:21:CYS:SG   | 19:d:23:VAL:CG1   | 2.64                     | 0.80              |
| 1:2:678:U:H3     | 1:2:1027:A:N6     | 1.77                     | 0.80              |
| 22:D:132:LYS:HB2 | 22:D:189:MET:HE3  | 1.64                     | 0.80              |
| 22:D:187:LYS:C   | 22:D:188:ILE:HD13 | 2.07                     | 0.79              |
| 22:D:20:GLU:HB2  | 24:K:64:TRP:CZ3   | 2.18                     | 0.79              |
| 2:A:90:PHE:CE2   | 2:A:175:TRP:CZ3   | 2.70                     | 0.79              |
| 1:2:1618:C:N4    | 19:d:10:HIS:CE1   | 2.52                     | 0.78              |
| 14:W:94:LEU:HD21 | 14:W:102:ILE:CG1  | 2.13                     | 0.78              |
| 3:B:63:LYS:HA    | 3:B:88:THR:HG23   | 1.65                     | 0.78              |
| 23:F:158:ALA:O   | 23:F:162:ALA:HB3  | 1.84                     | 0.78              |
| 1:2:1661:A:C8    | 19:d:14:PHE:CD1   | 2.72                     | 0.78              |
| 22:D:167:TYR:O   | 22:D:189:MET:HA   | 1.82                     | 0.78              |
| 19:d:34:TYR:OH   | 31:U:61:LEU:HA    | 1.82                     | 0.78              |
| 31:U:32:LEU:O    | 31:U:32:LEU:HD12  | 1.83                     | 0.78              |
| 24:K:24:LYS:CA   | 24:K:66:HIS:CE1   | 2.68                     | 0.77              |
| 28:R:13:ALA:O    | 28:R:16:ILE:HG23  | 1.84                     | 0.77              |
| 1:2:1227:G:H1    | 1:2:1531:A:H61    | 0.80                     | 0.77              |
| 19:d:23:VAL:HG11 | 19:d:42:CYS:HB3   | 1.65                     | 0.77              |
| 1:2:164:A:H3'    | 1:2:165:G:H21     | 1.50                     | 0.77              |
| 1:2:1513:C:OP1   | 19:d:10:HIS:CB    | 2.33                     | 0.77              |
| 1:2:1497:G:N3    | 24:K:62:PHE:HD2   | 1.83                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1618:C:O2    | 19:d:11:PRO:HG3   | 1.84                     | 0.76              |
| 1:2:1606:G:N2    | 1:2:1633:A:C8     | 2.54                     | 0.76              |
| 2:A:93:ALA:HB1   | 2:A:183:LEU:HD11  | 1.68                     | 0.75              |
| 4:C:78:LEU:HD12  | 4:C:78:LEU:O      | 1.86                     | 0.75              |
| 19:d:8:TRP:CD2   | 24:K:28:HIS:HB3   | 2.21                     | 0.75              |
| 24:K:24:LYS:CG   | 24:K:66:HIS:HE1   | 1.99                     | 0.75              |
| 28:R:16:ILE:HD12 | 28:R:16:ILE:O     | 1.87                     | 0.75              |
| 19:d:50:ILE:HG23 | 22:D:15:GLY:HA3   | 1.68                     | 0.75              |
| 14:W:90:GLN:HA   | 14:W:102:ILE:HD11 | 1.69                     | 0.74              |
| 1:2:1497:G:C8    | 24:K:62:PHE:CE2   | 2.74                     | 0.74              |
| 2:A:90:PHE:CD1   | 2:A:179:ALA:HB2   | 2.23                     | 0.74              |
| 19:d:34:TYR:HB2  | 22:D:12:VAL:HG11  | 1.70                     | 0.74              |
| 1:2:444:G:H22    | 1:2:447:A:H5''    | 1.52                     | 0.74              |
| 22:D:20:GLU:HB2  | 24:K:64:TRP:CE3   | 2.22                     | 0.74              |
| 3:B:63:LYS:CA    | 3:B:88:THR:HG23   | 2.17                     | 0.74              |
| 1:2:1232:U:H3    | 1:2:1526:G:H1     | 1.35                     | 0.74              |
| 4:C:78:LEU:HD22  | 4:C:97:PHE:CD2    | 2.23                     | 0.73              |
| 4:C:131:GLY:HA3  | 4:C:216:MET:HB3   | 1.70                     | 0.72              |
| 3:B:62:LEU:O     | 3:B:88:THR:HG21   | 1.89                     | 0.72              |
| 1:2:677:G:N1     | 1:2:1027:A:OP2    | 2.23                     | 0.72              |
| 19:d:34:TYR:CB   | 22:D:12:VAL:HG21  | 2.18                     | 0.72              |
| 31:U:26:SER:OG   | 31:U:32:LEU:HB2   | 1.89                     | 0.72              |
| 19:d:43:PHE:CE2  | 31:U:80:PHE:HE2   | 2.04                     | 0.72              |
| 3:B:62:LEU:HD21  | 3:B:91:VAL:HG11   | 1.70                     | 0.71              |
| 1:2:1368:U:HO2'  | 28:R:2:GLY:N      | 1.88                     | 0.71              |
| 19:d:25:SER:HB2  | 24:K:65:ARG:HD2   | 1.71                     | 0.71              |
| 19:d:52:PHE:CE2  | 31:U:63:ILE:CD1   | 2.60                     | 0.71              |
| 2:A:76:VAL:HG13  | 2:A:175:TRP:HH2   | 1.53                     | 0.71              |
| 3:B:63:LYS:C     | 3:B:88:THR:CG2    | 2.62                     | 0.71              |
| 27:Q:87:SER:O    | 27:Q:91:ALA:HB2   | 1.89                     | 0.70              |
| 31:U:34:LYS:HA   | 31:U:34:LYS:CE    | 2.09                     | 0.70              |
| 4:C:78:LEU:HD22  | 4:C:97:PHE:CB     | 2.20                     | 0.70              |
| 19:d:34:TYR:CB   | 22:D:12:VAL:HG11  | 2.22                     | 0.70              |
| 1:2:1482:C:H5'   | 19:d:54:LYS:HE3   | 1.72                     | 0.70              |
| 1:2:1618:C:H42   | 19:d:10:HIS:CE1   | 2.09                     | 0.70              |
| 7:H:58:LYS:CD    | 7:H:90:LYS:HZ3    | 2.02                     | 0.69              |
| 14:W:112:ASP:HB2 | 14:W:115:GLU:H    | 1.57                     | 0.69              |
| 1:2:1100:A:H4'   | 28:R:132:ARG:HH12 | 1.58                     | 0.69              |
| 1:2:617:G:H4'    | 15:X:88:ASP:HB3   | 1.74                     | 0.69              |
| 2:A:173:LEU:HD13 | 2:A:173:LEU:C     | 2.17                     | 0.69              |
| 1:2:641:A:OP1    | 9:J:40:LYS:NZ     | 2.26                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 32:Z:68:ILE:HB   | 32:Z:109:TYR:HB2 | 1.75                     | 0.69              |
| 1:2:318:A:C2     | 1:2:333:G:C2     | 2.81                     | 0.69              |
| 3:B:65:ARG:HB3   | 12:O:48:SER:HB2  | 1.75                     | 0.69              |
| 14:W:75:ILE:CD1  | 14:W:93:LEU:HD11 | 2.22                     | 0.69              |
| 30:T:11:GLN:OE1  | 30:T:62:ARG:NH1  | 2.26                     | 0.68              |
| 1:2:1310:U:O4    | 34:f:95:ARG:NH2  | 2.26                     | 0.68              |
| 4:C:83:LEU:HD12  | 4:C:83:LEU:C     | 2.18                     | 0.68              |
| 1:2:1482:C:C5'   | 19:d:54:LYS:HE3  | 2.23                     | 0.68              |
| 1:2:110:U:H3     | 1:2:351:G:H1     | 1.40                     | 0.68              |
| 8:I:162:LEU:HD11 | 8:I:191:GLU:HG2  | 1.76                     | 0.68              |
| 1:2:1533:A:N6    | 1:2:1602:U:C2    | 2.62                     | 0.68              |
| 19:d:23:VAL:HG11 | 19:d:42:CYS:SG   | 2.34                     | 0.68              |
| 31:U:61:LEU:HD12 | 31:U:82:MET:CB   | 2.24                     | 0.68              |
| 1:2:350:C:O2'    | 1:2:383:G:N1     | 2.27                     | 0.67              |
| 14:W:75:ILE:HD11 | 14:W:93:LEU:HD13 | 1.77                     | 0.67              |
| 3:B:90:ASP:HB2   | 3:B:97:LEU:HB2   | 1.75                     | 0.67              |
| 19:d:36:LEU:HA   | 22:D:16:ILE:HD11 | 1.75                     | 0.67              |
| 35:g:256:ILE:HB  | 35:g:270:LEU:HB2 | 1.77                     | 0.67              |
| 1:2:1726:G:H1    | 1:2:1808:U:H3    | 1.42                     | 0.67              |
| 1:2:1310:U:OP2   | 25:M:36:ARG:NH2  | 2.28                     | 0.67              |
| 1:2:496:C:OP1    | 5:E:49:ARG:NH2   | 2.27                     | 0.66              |
| 14:W:92:ASN:N    | 14:W:92:ASN:HD22 | 1.93                     | 0.66              |
| 31:U:61:LEU:HD12 | 31:U:82:MET:CG   | 2.24                     | 0.66              |
| 2:A:76:VAL:CG1   | 2:A:175:TRP:CH2  | 2.76                     | 0.66              |
| 35:g:17:TRP:HB2  | 35:g:36:ARG:HG3  | 1.79                     | 0.66              |
| 1:2:1565:C:OP2   | 30:T:101:ARG:NH1 | 2.28                     | 0.65              |
| 1:2:1144:A:N3    | 1:2:1199:A:O2'   | 2.27                     | 0.65              |
| 1:2:1259:A:H61   | 1:2:1519:U:H5'   | 1.61                     | 0.65              |
| 1:2:1497:G:N7    | 24:K:62:PHE:CE2  | 2.50                     | 0.65              |
| 22:D:132:LYS:HB3 | 22:D:189:MET:HE3 | 1.78                     | 0.65              |
| 4:C:134:ASN:C    | 4:C:134:ASN:ND2  | 2.49                     | 0.65              |
| 31:U:61:LEU:HD12 | 31:U:82:MET:HB3  | 1.79                     | 0.65              |
| 18:b:40:CYS:SG   | 18:b:41:TYR:N    | 2.70                     | 0.65              |
| 1:2:1295:A:OP1   | 26:P:62:LYS:NZ   | 2.30                     | 0.64              |
| 1:2:1513:C:P     | 19:d:12:ARG:HH12 | 2.20                     | 0.64              |
| 22:D:21:LEU:HD12 | 22:D:21:LEU:C    | 2.20                     | 0.64              |
| 1:2:1549:U:OP2   | 22:D:8:LYS:NZ    | 2.30                     | 0.64              |
| 9:J:114:VAL:HG13 | 9:J:119:LEU:HB2  | 1.80                     | 0.64              |
| 18:b:56:CYS:HB3  | 18:b:61:THR:H    | 1.63                     | 0.64              |
| 1:2:1669:G:OP1   | 31:U:79:ARG:NH1  | 2.31                     | 0.64              |
| 19:d:8:TRP:NE1   | 24:K:28:HIS:CG   | 2.65                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:T:76:THR:HG22  | 30:T:94:ARG:HB3  | 1.80                     | 0.64              |
| 1:2:678:U:N3      | 1:2:1027:A:N6    | 2.40                     | 0.64              |
| 1:2:1351:G:H1     | 1:2:1360:U:H3    | 1.44                     | 0.64              |
| 1:2:1387:G:N2     | 22:D:206:ASP:OD1 | 2.29                     | 0.63              |
| 1:2:934:G:O6      | 1:2:1008:A:N1    | 2.31                     | 0.63              |
| 1:2:1455:A:OP1    | 28:R:5:ARG:NH2   | 2.31                     | 0.63              |
| 4:C:209:VAL:HG11  | 4:C:233:LEU:HD11 | 1.79                     | 0.63              |
| 11:N:4:MET:SD     | 11:N:124:ARG:NH1 | 2.72                     | 0.63              |
| 3:B:33:VAL:HA     | 3:B:96:CYS:HB2   | 1.78                     | 0.63              |
| 1:2:678:U:C2      | 1:2:1027:A:N6    | 2.66                     | 0.63              |
| 5:E:48:LEU:HD23   | 5:E:61:VAL:HG13  | 1.80                     | 0.63              |
| 7:H:134:VAL:HG12  | 7:H:137:SER:HB2  | 1.80                     | 0.63              |
| 35:g:154:VAL:O    | 35:g:155:ARG:NH1 | 2.30                     | 0.63              |
| 1:2:943:U:OP1     | 3:B:214:LYS:NZ   | 2.31                     | 0.62              |
| 1:2:1862:G:O2'    | 17:a:5:ARG:NH2   | 2.32                     | 0.62              |
| 22:D:22:ASN:ND2   | 22:D:34:TYR:OH   | 2.32                     | 0.62              |
| 22:D:27:ARG:HB3   | 24:K:61:GLN:HE21 | 1.62                     | 0.62              |
| 28:R:13:ALA:CA    | 28:R:16:ILE:CG2  | 2.76                     | 0.62              |
| 1:2:379:C:O2      | 8:I:5:ARG:NH1    | 2.33                     | 0.62              |
| 2:A:58:LEU:HD11   | 2:A:174:MET:HE1  | 1.80                     | 0.62              |
| 2:A:78:SER:HG     | 2:A:125:THR:HG1  | 1.48                     | 0.62              |
| 5:E:137:PRO:HG2   | 5:E:150:PRO:HD2  | 1.81                     | 0.62              |
| 17:a:22:ARG:NH1   | 17:a:27:ALA:O    | 2.32                     | 0.62              |
| 19:d:8:TRP:CG     | 24:K:28:HIS:HB3  | 2.35                     | 0.62              |
| 23:F:168:THR:HG22 | 23:F:170:ALA:H   | 1.64                     | 0.62              |
| 1:2:1010:G:H2'    | 1:2:1011:A:H8    | 1.64                     | 0.62              |
| 1:2:1138:C:OP1    | 2:A:155:ARG:NH1  | 2.32                     | 0.62              |
| 28:R:24:LEU:HD13  | 28:R:54:VAL:CG1  | 2.30                     | 0.62              |
| 2:A:165:ASN:HA    | 2:A:171:VAL:HG22 | 1.82                     | 0.62              |
| 1:2:190:G:O2'     | 1:2:209:A:N6     | 2.33                     | 0.62              |
| 19:d:43:PHE:CZ    | 31:U:80:PHE:HD2  | 2.17                     | 0.62              |
| 1:2:441:C:OP2     | 8:I:2:GLY:N      | 2.32                     | 0.62              |
| 1:2:1865:C:OP1    | 17:a:87:ARG:NH1  | 2.33                     | 0.61              |
| 28:R:12:ALA:C     | 28:R:16:ILE:HG22 | 2.20                     | 0.61              |
| 1:2:1148:A:OP2    | 17:a:6:ARG:NH2   | 2.34                     | 0.61              |
| 1:2:1407:U:OP1    | 27:Q:71:ARG:NH2  | 2.33                     | 0.61              |
| 9:J:113:GLN:OE1   | 9:J:154:GLN:NE2  | 2.33                     | 0.61              |
| 19:d:8:TRP:CE2    | 24:K:28:HIS:CB   | 2.62                     | 0.61              |
| 1:2:663:C:OP2     | 15:X:3:LYS:NZ    | 2.34                     | 0.61              |
| 3:B:179:ASN:HB3   | 3:B:183:GLU:HB2  | 1.83                     | 0.61              |
| 5:E:71:LYS:HG2    | 5:E:76:VAL:HG22  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:T:56:ARG:HH12 | 30:T:99:VAL:HG12  | 1.66                     | 0.61              |
| 1:2:1153:C:OP2   | 14:W:12:LYS:NZ    | 2.33                     | 0.61              |
| 35:g:110:SER:HB3 | 35:g:155:ARG:HH12 | 1.66                     | 0.61              |
| 1:2:1618:C:O2    | 19:d:11:PRO:CG    | 2.49                     | 0.61              |
| 29:S:34:LYS:HB2  | 29:S:100:ALA:HA   | 1.82                     | 0.61              |
| 1:2:919:A:H5''   | 11:N:64:ARG:HH12  | 1.66                     | 0.61              |
| 1:2:1466:G:OP2   | 28:R:5:ARG:NH1    | 2.34                     | 0.61              |
| 3:B:92:GLN:HB2   | 3:B:95:ASN:HB2    | 1.83                     | 0.61              |
| 31:U:27:ARG:CG   | 31:U:82:MET:HE1   | 2.29                     | 0.61              |
| 31:U:61:LEU:CG   | 31:U:82:MET:HB3   | 2.31                     | 0.61              |
| 32:Z:73:VAL:HG13 | 32:Z:77:LEU:HD12  | 1.82                     | 0.61              |
| 23:F:201:LYS:HD3 | 23:F:204:ARG:HE   | 1.66                     | 0.60              |
| 1:2:1208:A:O2'   | 1:2:1835:A:N7     | 2.30                     | 0.60              |
| 1:2:429:C:H2'    | 1:2:430:C:H6      | 1.65                     | 0.60              |
| 1:2:678:U:OP1    | 11:N:127:ARG:NH2  | 2.34                     | 0.60              |
| 26:P:37:TYR:HB3  | 26:P:41:GLN:HB2   | 1.83                     | 0.60              |
| 1:2:1415:C:O2'   | 30:T:132:ASP:OD2  | 2.20                     | 0.60              |
| 30:T:75:MET:HG3  | 30:T:104:LEU:HD21 | 1.83                     | 0.60              |
| 10:L:104:LYS:HE2 | 15:X:8:ARG:HD3    | 1.83                     | 0.60              |
| 1:2:579:C:O2     | 16:Y:61:ARG:NH2   | 2.34                     | 0.60              |
| 1:2:1005:G:OP2   | 3:B:162:ARG:NH2   | 2.34                     | 0.60              |
| 8:I:178:ARG:NH1  | 8:I:181:GLN:OE1   | 2.35                     | 0.60              |
| 14:W:88:LYS:O    | 14:W:92:ASN:ND2   | 2.34                     | 0.60              |
| 1:2:65:C:N4      | 6:G:134:GLY:O     | 2.35                     | 0.60              |
| 2:A:181:GLU:OE1  | 2:A:181:GLU:HA    | 2.02                     | 0.60              |
| 5:E:45:ILE:HG13  | 5:E:61:VAL:HG11   | 1.82                     | 0.60              |
| 8:I:11:ARG:NH1   | 8:I:15:GLY:O      | 2.34                     | 0.60              |
| 35:g:8:ARG:HB3   | 35:g:309:VAL:HG23 | 1.83                     | 0.60              |
| 4:C:222:CYS:SG   | 4:C:223:TYR:N     | 2.75                     | 0.60              |
| 3:B:179:ASN:ND2  | 3:B:183:GLU:OE1   | 2.35                     | 0.60              |
| 29:S:75:ARG:HH21 | 29:S:95:TYR:HB2   | 1.66                     | 0.60              |
| 4:C:102:LEU:HD11 | 4:C:130:ILE:HD13  | 1.82                     | 0.60              |
| 22:D:107:TYR:O   | 22:D:111:GLY:N    | 2.31                     | 0.60              |
| 1:2:1617:G:N1    | 1:2:1620:A:OP2    | 2.34                     | 0.59              |
| 9:J:38:ARG:HA    | 20:e:31:ARG:HG2   | 1.84                     | 0.59              |
| 1:2:862:A:N3     | 14:W:105:THR:OG1  | 2.35                     | 0.59              |
| 1:2:5:U:H2'      | 1:2:6:G:H8        | 1.67                     | 0.59              |
| 2:A:128:ARG:HD3  | 2:A:153:PRO:HD2   | 1.84                     | 0.59              |
| 23:F:144:LEU:HB3 | 33:c:49:PRO:HG2   | 1.84                     | 0.59              |
| 24:K:15:LEU:HD22 | 24:K:49:MET:HE1   | 1.83                     | 0.59              |
| 3:B:146:ARG:HB2  | 3:B:149:GLN:HB2   | 1.84                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:K:24:LYS:CB   | 24:K:66:HIS:HE1   | 2.15                     | 0.59              |
| 1:2:1606:G:H5'   | 30:T:86:GLY:HA2   | 1.85                     | 0.59              |
| 3:B:62:LEU:CD1   | 3:B:91:VAL:HG21   | 2.17                     | 0.59              |
| 8:I:177:SER:HB3  | 8:I:186:ASP:H     | 1.67                     | 0.59              |
| 22:D:25:LEU:HD13 | 22:D:34:TYR:CE1   | 2.37                     | 0.59              |
| 1:2:1192:U:OP2   | 15:X:119:ARG:NH2  | 2.35                     | 0.59              |
| 17:a:23:CYS:SG   | 17:a:24:THR:N     | 2.76                     | 0.59              |
| 31:U:32:LEU:HD12 | 31:U:32:LEU:C     | 2.24                     | 0.59              |
| 7:H:101:LEU:O    | 7:H:116:ARG:NH1   | 2.36                     | 0.59              |
| 23:F:143:PRO:HG3 | 33:c:54:ASP:HB3   | 1.85                     | 0.58              |
| 1:2:583:A:OP1    | 9:J:162:ARG:NH2   | 2.36                     | 0.58              |
| 30:T:51:ASN:HB3  | 30:T:54:TYR:HB2   | 1.84                     | 0.58              |
| 9:J:32:ILE:O     | 9:J:36:GLY:N      | 2.37                     | 0.58              |
| 19:d:34:TYR:HB3  | 22:D:12:VAL:CG2   | 2.26                     | 0.58              |
| 19:d:36:LEU:HD12 | 22:D:12:VAL:CG1   | 2.33                     | 0.58              |
| 23:F:121:PRO:HG2 | 23:F:196:LEU:HD12 | 1.84                     | 0.58              |
| 1:2:1036:A:N3    | 1:2:1844:U:O2'    | 2.36                     | 0.58              |
| 1:2:446:G:H21    | 5:E:5:PRO:HD2     | 1.67                     | 0.58              |
| 1:2:1086:G:OP2   | 17:a:12:LYS:NZ    | 2.36                     | 0.58              |
| 6:G:6:SER:HB3    | 6:G:13:GLN:HG3    | 1.85                     | 0.58              |
| 1:2:688:U:H5''   | 7:H:103:LYS:HD2   | 1.83                     | 0.58              |
| 1:2:1477:U:OP2   | 28:R:3:ARG:NH2    | 2.37                     | 0.58              |
| 6:G:98:ARG:HH12  | 6:G:105:ASN:HB3   | 1.68                     | 0.58              |
| 1:2:1286:G:O2'   | 1:2:1313:A:N6     | 2.36                     | 0.58              |
| 3:B:87:ILE:HG12  | 3:B:101:HIS:HB2   | 1.84                     | 0.58              |
| 7:H:58:LYS:HB2   | 7:H:90:LYS:CD     | 2.33                     | 0.58              |
| 4:C:78:LEU:HD22  | 4:C:97:PHE:CG     | 2.38                     | 0.58              |
| 8:I:99:ASN:ND2   | 8:I:174:CYS:SG    | 2.77                     | 0.58              |
| 11:N:101:HIS:O   | 11:N:105:ASN:ND2  | 2.36                     | 0.58              |
| 13:V:19:ALA:O    | 14:W:23:ARG:NH2   | 2.37                     | 0.58              |
| 35:g:107:ASP:OD2 | 35:g:125:ARG:NH1  | 2.33                     | 0.58              |
| 24:K:23:ALA:O    | 24:K:66:HIS:ND1   | 2.30                     | 0.57              |
| 1:2:1606:G:H1    | 1:2:1632:G:H2'    | 1.69                     | 0.57              |
| 2:A:31:ASP:HB3   | 2:A:34:MET:H      | 1.69                     | 0.57              |
| 2:A:90:PHE:CZ    | 2:A:175:TRP:CZ3   | 2.91                     | 0.57              |
| 1:2:1182:A:O3'   | 21:h:15:ARG:NH2   | 2.38                     | 0.57              |
| 1:2:1673:U:OP1   | 27:Q:79:ALA:N     | 2.38                     | 0.57              |
| 19:d:23:VAL:CG2  | 24:K:64:TRP:HE1   | 2.16                     | 0.57              |
| 19:d:23:VAL:CG1  | 19:d:42:CYS:SG    | 2.92                     | 0.57              |
| 23:F:162:ALA:HB1 | 23:F:169:ILE:HG12 | 1.84                     | 0.57              |
| 1:2:688:U:OP1    | 7:H:121:THR:OG1   | 2.21                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:N:33:VAL:HG21  | 11:N:66:VAL:HG11  | 1.86                     | 0.57              |
| 22:D:226:GLN:HE21 | 35:g:224:GLY:HA3  | 1.69                     | 0.57              |
| 1:2:309:G:OP2     | 8:I:53:LYS:NZ     | 2.36                     | 0.57              |
| 1:2:1497:G:C5     | 24:K:62:PHE:CD2   | 2.79                     | 0.57              |
| 1:2:1373:C:O2'    | 28:R:10:LYS:NZ    | 2.38                     | 0.57              |
| 23:F:85:LYS:HB3   | 23:F:88:MET:HB2   | 1.86                     | 0.57              |
| 1:2:587:A:O2'     | 1:2:588:G:N2      | 2.38                     | 0.57              |
| 1:2:1605:G:OP1    | 30:T:84:ARG:NH1   | 2.38                     | 0.57              |
| 2:A:85:ARG:NH2    | 28:R:82:ASP:O     | 2.38                     | 0.57              |
| 2:A:173:LEU:HD22  | 2:A:173:LEU:C     | 2.28                     | 0.57              |
| 19:d:25:SER:HB2   | 24:K:65:ARG:CD    | 2.34                     | 0.57              |
| 28:R:13:ALA:HA    | 28:R:16:ILE:HG21  | 1.86                     | 0.57              |
| 7:H:98:ARG:HB3    | 7:H:125:VAL:HG13  | 1.85                     | 0.57              |
| 28:R:20:TYR:CE2   | 28:R:38:ILE:HG21  | 2.39                     | 0.57              |
| 1:2:1516:G:O5'    | 26:P:81:ARG:NH1   | 2.37                     | 0.57              |
| 27:Q:86:GLN:NE2   | 27:Q:121:VAL:O    | 2.37                     | 0.57              |
| 31:U:56:MET:HB2   | 31:U:86:LYS:HB3   | 1.86                     | 0.57              |
| 35:g:42:MET:O     | 35:g:56:GLN:N     | 2.34                     | 0.57              |
| 1:2:1495:G:C4'    | 19:d:26:ASN:OD1   | 2.50                     | 0.56              |
| 4:C:102:LEU:C     | 4:C:102:LEU:HD23  | 2.30                     | 0.56              |
| 7:H:66:VAL:HA     | 7:H:69:LEU:HB2    | 1.87                     | 0.56              |
| 1:2:64:A:H2       | 1:2:83:A:H62      | 1.53                     | 0.56              |
| 1:2:927:C:O2      | 18:b:51:GLN:NE2   | 2.38                     | 0.56              |
| 16:Y:20:ARG:NH1   | 16:Y:74:MET:SD    | 2.78                     | 0.56              |
| 32:Z:91:LEU:HD22  | 32:Z:96:LEU:HD12  | 1.87                     | 0.56              |
| 1:2:643:A:OP1     | 9:J:39:ASN:ND2    | 2.38                     | 0.56              |
| 5:E:31:PRO:HG3    | 5:E:43:PRO:HG3    | 1.87                     | 0.56              |
| 5:E:44:LEU:HD13   | 5:E:72:ILE:HD11   | 1.86                     | 0.56              |
| 7:H:51:ILE:HD11   | 7:H:176:VAL:HG22  | 1.86                     | 0.56              |
| 9:J:107:GLU:O     | 9:J:113:GLN:NE2   | 2.34                     | 0.56              |
| 12:O:139:SER:OG   | 12:O:140:THR:N    | 2.38                     | 0.56              |
| 16:Y:114:MET:O    | 16:Y:122:LYS:NZ   | 2.39                     | 0.56              |
| 35:g:302:TYR:HB3  | 35:g:304:ASP:H    | 1.69                     | 0.56              |
| 1:2:1533:A:N6     | 1:2:1602:U:N3     | 2.51                     | 0.56              |
| 1:2:1238:U:H1'    | 26:P:126:VAL:HG13 | 1.86                     | 0.56              |
| 1:2:1589:A:N3     | 1:2:1653:U:O2'    | 2.36                     | 0.56              |
| 13:V:73:ALA:O     | 13:V:77:GLY:N     | 2.39                     | 0.56              |
| 15:X:51:VAL:HG13  | 15:X:70:VAL:HG13  | 1.86                     | 0.56              |
| 22:D:168:VAL:HA   | 22:D:188:ILE:O    | 2.05                     | 0.56              |
| 28:R:24:LEU:HD13  | 28:R:54:VAL:HG13  | 1.87                     | 0.56              |
| 1:2:1397:U:H3     | 27:Q:12:VAL:HA    | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:D:59:LEU:HA   | 22:D:66:ILE:HB   | 1.87                     | 0.56              |
| 6:G:181:THR:HG22 | 6:G:183:ARG:H    | 1.69                     | 0.56              |
| 12:O:96:LYS:HE2  | 12:O:130:GLU:HG2 | 1.86                     | 0.56              |
| 17:a:11:ALA:HB3  | 17:a:33:ASP:HB2  | 1.87                     | 0.56              |
| 35:g:226:HIS:HE2 | 35:g:229:THR:HG1 | 1.52                     | 0.56              |
| 2:A:90:PHE:CZ    | 2:A:175:TRP:HZ3  | 2.23                     | 0.56              |
| 24:K:24:LYS:CG   | 24:K:66:HIS:CE1  | 2.76                     | 0.56              |
| 28:R:37:GLU:HG3  | 35:g:150:TRP:HE1 | 1.71                     | 0.56              |
| 30:T:13:GLU:OE2  | 30:T:16:ARG:NH1  | 2.38                     | 0.56              |
| 1:2:297:A:H5'    | 5:E:132:GLY:HA2  | 1.88                     | 0.56              |
| 1:2:318:A:N1     | 1:2:333:G:C6     | 2.74                     | 0.56              |
| 4:C:135:GLY:O    | 4:C:165:VAL:HG22 | 2.06                     | 0.56              |
| 8:I:116:HIS:O    | 8:I:152:ARG:NH1  | 2.32                     | 0.56              |
| 1:2:1614:A:OP2   | 26:P:42:ARG:NH2  | 2.39                     | 0.55              |
| 1:2:1729:U:O2    | 1:2:1805:G:N2    | 2.31                     | 0.55              |
| 32:Z:58:LEU:HD12 | 32:Z:62:VAL:HG21 | 1.88                     | 0.55              |
| 4:C:179:THR:OG1  | 4:C:180:VAL:N    | 2.39                     | 0.55              |
| 7:H:58:LYS:CD    | 7:H:90:LYS:HZ1   | 2.04                     | 0.55              |
| 7:H:129:ILE:HG21 | 7:H:180:LEU:HD11 | 1.89                     | 0.55              |
| 27:Q:33:LYS:HE2  | 27:Q:38:PRO:HG3  | 1.88                     | 0.55              |
| 35:g:68:ASP:OD2  | 35:g:111:VAL:N   | 2.34                     | 0.55              |
| 1:2:163:U:OP2    | 6:G:87:ARG:NH2   | 2.38                     | 0.55              |
| 5:E:100:ARG:NH1  | 5:E:118:GLU:OE2  | 2.40                     | 0.55              |
| 8:I:34:ALA:HB3   | 8:I:56:ARG:HD2   | 1.89                     | 0.55              |
| 1:2:1674:G:OP1   | 23:F:51:HIS:NE2  | 2.33                     | 0.55              |
| 3:B:104:ASP:OD1  | 3:B:104:ASP:N    | 2.39                     | 0.55              |
| 12:O:39:ASP:HB3  | 12:O:68:GLU:HG2  | 1.88                     | 0.55              |
| 33:c:20:ARG:NH1  | 33:c:26:GLN:O    | 2.39                     | 0.55              |
| 1:2:1489:A:N3    | 22:D:146:ARG:NH1 | 2.55                     | 0.55              |
| 22:D:166:TYR:OH  | 22:D:202:LYS:NZ  | 2.36                     | 0.55              |
| 1:2:918:U:H3'    | 11:N:64:ARG:HH22 | 1.72                     | 0.55              |
| 1:2:1256:G:H21   | 1:2:1659:U:H5'   | 1.72                     | 0.55              |
| 9:J:134:HIS:HE1  | 9:J:164:PRO:HD2  | 1.71                     | 0.55              |
| 1:2:1661:A:C8    | 19:d:14:PHE:HD1  | 2.23                     | 0.55              |
| 3:B:120:MET:HG3  | 3:B:142:PHE:HE1  | 1.72                     | 0.55              |
| 5:E:11:ARG:HA    | 5:E:28:ALA:HB2   | 1.88                     | 0.55              |
| 14:W:90:GLN:HB2  | 14:W:94:LEU:HD12 | 1.89                     | 0.55              |
| 1:2:1231:C:H42   | 1:2:1527:C:H42   | 1.54                     | 0.55              |
| 3:B:31:TYR:CD2   | 3:B:62:LEU:HD22  | 2.42                     | 0.55              |
| 8:I:72:CYS:SG    | 8:I:73:THR:N     | 2.80                     | 0.55              |
| 11:N:103:GLU:OE2 | 11:N:104:ARG:NH1 | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:W:78:ARG:HB3   | 14:W:124:LYS:HB3  | 1.88                     | 0.55              |
| 29:S:138:THR:HG23 | 29:S:139:THR:HG23 | 1.88                     | 0.55              |
| 1:2:1588:A:H2'    | 1:2:1589:A:C8     | 2.42                     | 0.55              |
| 1:2:1741:U:OP1    | 8:I:42:ARG:NH1    | 2.39                     | 0.55              |
| 1:2:1407:U:O2'    | 27:Q:11:GLN:NE2   | 2.37                     | 0.55              |
| 24:K:67:PHE:O     | 24:K:68:TYR:CD1   | 2.60                     | 0.55              |
| 35:g:212:LYS:HA   | 35:g:235:ILE:HB   | 1.89                     | 0.55              |
| 1:2:1245:G:O2'    | 1:2:1492:U:OP1    | 2.23                     | 0.54              |
| 1:2:1256:G:H1     | 19:d:31:ILE:HG12  | 1.71                     | 0.54              |
| 1:2:1757:G:O6     | 1:2:1775:U:O2     | 2.25                     | 0.54              |
| 4:C:102:LEU:HD11  | 4:C:130:ILE:CD1   | 2.37                     | 0.54              |
| 22:D:156:LEU:HB2  | 22:D:189:MET:CE   | 2.29                     | 0.54              |
| 1:2:686:U:OP1     | 14:W:32:LYS:N     | 2.35                     | 0.54              |
| 12:O:19:PRO:HG2   | 12:O:27:VAL:HG11  | 1.89                     | 0.54              |
| 22:D:109:LEU:HB2  | 22:D:175:VAL:HG21 | 1.89                     | 0.54              |
| 1:2:67:C:OP2      | 6:G:172:LYS:NZ    | 2.32                     | 0.54              |
| 3:B:71:LEU:HD11   | 3:B:189:ILE:HG23  | 1.90                     | 0.54              |
| 5:E:152:PRO:O     | 5:E:155:LYS:NZ    | 2.37                     | 0.54              |
| 6:G:5:ILE:HG12    | 6:G:111:LEU:HB2   | 1.89                     | 0.54              |
| 16:Y:23:MET:HE2   | 16:Y:25:ILE:HD11  | 1.88                     | 0.54              |
| 1:2:637:U:OP2     | 20:e:24:LYS:NZ    | 2.41                     | 0.54              |
| 1:2:1329:U:O4     | 1:2:1500:G:O6     | 2.26                     | 0.54              |
| 2:A:176:TRP:CE3   | 2:A:199:PRO:HB3   | 2.42                     | 0.54              |
| 10:L:95:TYR:OH    | 10:L:100:ASN:ND2  | 2.40                     | 0.54              |
| 23:F:145:ARG:HB2  | 33:c:49:PRO:HD2   | 1.89                     | 0.54              |
| 25:M:25:ALA:O     | 25:M:29:ASP:N     | 2.40                     | 0.54              |
| 31:U:61:LEU:CD1   | 31:U:82:MET:HB3   | 2.37                     | 0.54              |
| 1:2:575:A:OP2     | 16:Y:93:ARG:NH2   | 2.41                     | 0.54              |
| 4:C:221:ASP:OD1   | 4:C:221:ASP:N     | 2.36                     | 0.54              |
| 12:O:74:ALA:HB1   | 12:O:115:ALA:HB2  | 1.89                     | 0.54              |
| 1:2:525:A:H5'     | 20:e:32:ALA:HB3   | 1.89                     | 0.54              |
| 1:2:1075:C:OP1    | 11:N:107:LYS:NZ   | 2.39                     | 0.54              |
| 1:2:1226:G:N1     | 1:2:1639:G:OP2    | 2.39                     | 0.54              |
| 1:2:1227:G:N2     | 1:2:1531:A:N1     | 2.48                     | 0.54              |
| 1:2:1276:A:H62    | 1:2:1321:G:H21    | 1.55                     | 0.54              |
| 1:2:1585:U:OP1    | 30:T:67:ARG:NH2   | 2.41                     | 0.54              |
| 2:A:84:GLN:HE22   | 2:A:101:GLY:H     | 1.55                     | 0.54              |
| 7:H:142:LYS:HB3   | 14:W:54:ASP:HB3   | 1.90                     | 0.54              |
| 10:L:135:SER:OG   | 10:L:136:LYS:N    | 2.38                     | 0.54              |
| 16:Y:86:GLU:OE2   | 16:Y:90:ARG:NH1   | 2.40                     | 0.54              |
| 31:U:27:ARG:CD    | 31:U:82:MET:CE    | 2.64                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:1612:G:H1'    | 29:S:87:GLN:HG3  | 1.90                     | 0.54              |
| 1:2:318:A:C2      | 1:2:333:G:N1     | 2.76                     | 0.54              |
| 1:2:1864:U:OP2    | 17:a:4:LYS:NZ    | 2.40                     | 0.54              |
| 3:B:90:ASP:HB3    | 3:B:92:GLN:HE21  | 1.73                     | 0.54              |
| 13:V:73:ALA:HB1   | 13:V:78:ILE:HB   | 1.88                     | 0.54              |
| 27:Q:53:GLU:OE1   | 27:Q:85:ARG:NH2  | 2.41                     | 0.54              |
| 35:g:70:VAL:O     | 35:g:79:LEU:N    | 2.40                     | 0.54              |
| 9:J:50:LEU:HD13   | 9:J:102:ILE:HD13 | 1.89                     | 0.54              |
| 22:D:116:ARG:HG2  | 22:D:150:MET:HE1 | 1.90                     | 0.54              |
| 35:g:124:SER:OG   | 35:g:125:ARG:N   | 2.38                     | 0.54              |
| 35:g:142:VAL:O    | 35:g:146:SER:OG  | 2.22                     | 0.54              |
| 3:B:152:LYS:HG3   | 28:R:133:GLY:HA2 | 1.90                     | 0.53              |
| 5:E:71:LYS:HA     | 5:E:76:VAL:HA    | 1.90                     | 0.53              |
| 1:2:115:U:OP1     | 1:2:382:C:O2'    | 2.25                     | 0.53              |
| 1:2:995:G:O3'     | 11:N:114:ARG:NH2 | 2.41                     | 0.53              |
| 3:B:62:LEU:HD21   | 3:B:91:VAL:CG1   | 2.37                     | 0.53              |
| 25:M:41:ALA:HA    | 25:M:44:LYS:HE3  | 1.90                     | 0.53              |
| 29:S:35:GLY:O     | 29:S:97:GLN:NE2  | 2.42                     | 0.53              |
| 8:I:141:ARG:HD3   | 8:I:146:GLN:HA   | 1.91                     | 0.53              |
| 1:2:5:U:H2'       | 1:2:6:G:C8       | 2.43                     | 0.53              |
| 1:2:900:C:H2'     | 1:2:901:G:H8     | 1.73                     | 0.53              |
| 27:Q:9:SER:N      | 27:Q:99:TYR:OH   | 2.40                     | 0.53              |
| 1:2:1650:A:H3'    | 1:2:1651:A:H8    | 1.73                     | 0.53              |
| 2:A:16:LEU:HD22   | 28:R:96:ILE:HD11 | 1.90                     | 0.53              |
| 10:L:113:LEU:HD11 | 10:L:117:PHE:HB2 | 1.91                     | 0.53              |
| 14:W:17:ALA:HB1   | 14:W:22:LYS:HB2  | 1.90                     | 0.53              |
| 33:c:13:ARG:HB2   | 33:c:33:GLU:HB3  | 1.91                     | 0.53              |
| 1:2:350:C:O2'     | 1:2:383:G:N2     | 2.41                     | 0.53              |
| 1:2:551:U:O2'     | 20:e:44:ASN:ND2  | 2.42                     | 0.53              |
| 1:2:1618:C:C2     | 19:d:11:PRO:HG3  | 2.43                     | 0.53              |
| 22:D:45:ARG:HG2   | 22:D:83:SER:HA   | 1.91                     | 0.53              |
| 1:2:1325:G:H1'    | 1:2:1510:G:H5''  | 1.90                     | 0.53              |
| 3:B:106:THR:HG22  | 3:B:108:ASP:H    | 1.74                     | 0.53              |
| 16:Y:55:ILE:HG22  | 16:Y:75:ILE:HG23 | 1.90                     | 0.53              |
| 19:d:33:LYS:NZ    | 31:U:62:ARG:O    | 2.36                     | 0.53              |
| 1:2:1863:A:OP2    | 17:a:4:LYS:NZ    | 2.37                     | 0.53              |
| 9:J:112:THR:HG22  | 9:J:123:ILE:HD11 | 1.90                     | 0.53              |
| 12:O:42:VAL:HG11  | 12:O:81:VAL:HG11 | 1.91                     | 0.53              |
| 1:2:145:G:O6      | 6:G:178:ARG:NH2  | 2.42                     | 0.53              |
| 3:B:63:LYS:O      | 3:B:88:THR:HG22  | 2.07                     | 0.53              |
| 23:F:39:ILE:HG23  | 23:F:68:ILE:HD12 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:K:24:LYS:CB    | 24:K:66:HIS:CE1   | 2.92                     | 0.53              |
| 34:f:132:MET:HE3  | 34:f:141:CYS:HB2  | 1.90                     | 0.53              |
| 35:g:236:ILE:HG23 | 35:g:251:ALA:H    | 1.74                     | 0.53              |
| 3:B:169:MET:O     | 3:B:173:THR:OG1   | 2.23                     | 0.52              |
| 8:I:67:TRP:CD1    | 8:I:70:GLU:H      | 2.26                     | 0.52              |
| 17:a:100:ARG:O    | 17:a:102:ARG:NH1  | 2.39                     | 0.52              |
| 1:2:1676:U:H1'    | 23:F:78:MET:HE3   | 1.91                     | 0.52              |
| 4:C:259:THR:HG21  | 13:V:15:ARG:HA    | 1.91                     | 0.52              |
| 6:G:194:LEU:O     | 6:G:198:ARG:NH1   | 2.41                     | 0.52              |
| 11:N:100:LYS:O    | 11:N:104:ARG:NH1  | 2.38                     | 0.52              |
| 31:U:34:LYS:HE2   | 31:U:34:LYS:CA    | 2.19                     | 0.52              |
| 28:R:59:LYS:HE2   | 35:g:282:GLU:HG3  | 1.91                     | 0.52              |
| 1:2:1536:G:H2'    | 1:2:1537:A:C8     | 2.45                     | 0.52              |
| 3:B:217:MET:HE2   | 3:B:220:LYS:HG2   | 1.92                     | 0.52              |
| 4:C:98:LEU:N      | 4:C:98:LEU:CD1    | 2.73                     | 0.52              |
| 25:M:10:GLY:HA2   | 25:M:123:VAL:HG22 | 1.91                     | 0.52              |
| 1:2:1719:A:N6     | 1:2:1814:G:O2'    | 2.42                     | 0.52              |
| 2:A:89:LYS:HE2    | 2:A:201:LEU:HD11  | 1.90                     | 0.52              |
| 4:C:134:ASN:ND2   | 4:C:134:ASN:O     | 2.42                     | 0.52              |
| 19:d:36:LEU:HA    | 22:D:16:ILE:CD1   | 2.40                     | 0.52              |
| 1:2:628:A:OP1     | 22:D:145:GLN:NE2  | 2.43                     | 0.52              |
| 1:2:1159:G:OP2    | 15:X:5:ARG:NH1    | 2.42                     | 0.52              |
| 1:2:1199:A:H5'    | 17:a:2:THR:HB     | 1.92                     | 0.52              |
| 1:2:1648:G:N2     | 1:2:1675:A:OP2    | 2.40                     | 0.52              |
| 1:2:1785:C:O2'    | 1:2:1786:U:O4'    | 2.28                     | 0.52              |
| 1:2:1866:A:H62    | 17:a:84:VAL:HG13  | 1.75                     | 0.52              |
| 1:2:1098:C:H2'    | 1:2:1099:G:C8     | 2.44                     | 0.52              |
| 1:2:1628:C:OP1    | 30:T:38:LYS:NZ    | 2.37                     | 0.52              |
| 4:C:103:LYS:HD2   | 4:C:133:TYR:HE2   | 1.74                     | 0.52              |
| 22:D:226:GLN:NE2  | 35:g:223:GLU:O    | 2.43                     | 0.52              |
| 1:2:1567:G:H1'    | 30:T:37:VAL:HG21  | 1.92                     | 0.52              |
| 1:2:1740:C:OP1    | 8:I:44:HIS:ND1    | 2.31                     | 0.52              |
| 1:2:922:A:OP1     | 14:W:28:ARG:NH1   | 2.42                     | 0.52              |
| 1:2:1275:G:O2'    | 1:2:1321:G:N2     | 2.38                     | 0.52              |
| 1:2:1286:G:H21    | 1:2:1287:A:H62    | 1.57                     | 0.52              |
| 1:2:1864:U:H5'    | 17:a:79:ILE:HD11  | 1.91                     | 0.52              |
| 3:B:73:ASP:OD1    | 12:O:128:ARG:NH2  | 2.43                     | 0.52              |
| 7:H:87:PHE:H      | 7:H:87:PHE:HD2    | 1.57                     | 0.52              |
| 22:D:74:GLN:HB2   | 22:D:75:LYS:HD2   | 1.92                     | 0.52              |
| 1:2:103:A:OP2     | 1:2:356:C:N4      | 2.43                     | 0.52              |
| 1:2:106:C:OP1     | 1:2:431:G:O2'     | 2.27                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:613:G:N1     | 1:2:629:A:OP1    | 2.37                     | 0.52              |
| 2:A:2:SER:HB3    | 2:A:59:LEU:HD12  | 1.92                     | 0.52              |
| 5:E:6:LYS:O      | 5:E:30:ARG:NH2   | 2.43                     | 0.52              |
| 26:P:50:ARG:O    | 26:P:54:HIS:N    | 2.37                     | 0.52              |
| 1:2:110:U:OP1    | 1:2:855:G:N2     | 2.42                     | 0.51              |
| 1:2:913:A:H62    | 7:H:119:SER:HB3  | 1.75                     | 0.51              |
| 2:A:42:LYS:HD3   | 2:A:48:ILE:HD11  | 1.92                     | 0.51              |
| 16:Y:15:ASN:ND2  | 16:Y:22:GLN:OE1  | 2.43                     | 0.51              |
| 1:2:145:G:H2'    | 1:2:146:G:C8     | 2.46                     | 0.51              |
| 1:2:409:C:N4     | 1:2:427:U:OP1    | 2.39                     | 0.51              |
| 1:2:961:G:OP1    | 12:O:149:ARG:NH2 | 2.42                     | 0.51              |
| 1:2:1274:G:H5'   | 24:K:47:LYS:HE2  | 1.92                     | 0.51              |
| 22:D:27:ARG:HB2  | 24:K:61:GLN:HG3  | 1.92                     | 0.51              |
| 22:D:98:ALA:HB3  | 22:D:169:ASP:HB2 | 1.93                     | 0.51              |
| 35:g:129:ILE:HB  | 35:g:142:VAL:HB  | 1.93                     | 0.51              |
| 35:g:131:LEU:HB2 | 35:g:139:LYS:HB2 | 1.91                     | 0.51              |
| 1:2:1300:U:H2'   | 26:P:51:ARG:HH21 | 1.76                     | 0.51              |
| 1:2:1615:U:O4    | 26:P:40:ARG:NH1  | 2.43                     | 0.51              |
| 1:2:1722:G:O6    | 1:2:1812:U:O2    | 2.28                     | 0.51              |
| 4:C:84:PHE:CE1   | 4:C:264:SER:HA   | 2.46                     | 0.51              |
| 22:D:133:GLY:HA2 | 22:D:155:GLY:HA3 | 1.93                     | 0.51              |
| 1:2:1729:U:O4    | 1:2:1805:G:O6    | 2.29                     | 0.51              |
| 19:d:23:VAL:HG13 | 19:d:24:CYS:N    | 2.25                     | 0.51              |
| 35:g:3:GLU:HG2   | 35:g:315:GLY:H   | 1.73                     | 0.51              |
| 1:2:1265:A:H2'   | 34:f:78:LYS:HZ1  | 1.76                     | 0.51              |
| 23:F:143:PRO:HD2 | 33:c:50:VAL:HG22 | 1.92                     | 0.51              |
| 1:2:1013:U:OP1   | 1:2:1129:G:O2'   | 2.24                     | 0.51              |
| 6:G:52:ILE:HD13  | 6:G:102:VAL:HG21 | 1.93                     | 0.51              |
| 31:U:32:LEU:HD21 | 31:U:87:ARG:HG2  | 1.92                     | 0.51              |
| 1:2:388:U:H2'    | 1:2:389:A:C8     | 2.46                     | 0.51              |
| 1:2:1776:G:H2'   | 1:2:1777:G:H8    | 1.75                     | 0.51              |
| 1:2:1396:A:O2'   | 1:2:1398:G:N7    | 2.43                     | 0.51              |
| 1:2:1512:C:O2'   | 19:d:7:TYR:O     | 2.25                     | 0.51              |
| 9:J:138:ARG:HG2  | 9:J:156:HIS:CD2  | 2.46                     | 0.51              |
| 13:V:55:ILE:HD13 | 13:V:65:SER:HB2  | 1.92                     | 0.51              |
| 14:W:92:ASN:HD22 | 14:W:92:ASN:H    | 1.59                     | 0.51              |
| 30:T:6:VAL:O     | 30:T:11:GLN:NE2  | 2.43                     | 0.51              |
| 1:2:982:G:N2     | 1:2:1045:U:O2    | 2.33                     | 0.51              |
| 1:2:1174:U:OP1   | 21:h:21:ARG:NH2  | 2.40                     | 0.51              |
| 13:V:17:CYS:SG   | 13:V:18:SER:N    | 2.84                     | 0.51              |
| 14:W:94:LEU:HD23 | 14:W:94:LEU:N    | 2.25                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:F:35:LEU:HD12  | 23:F:117:ILE:HG12 | 1.93                     | 0.51              |
| 23:F:50:PRO:HG3   | 23:F:69:VAL:HG12  | 1.93                     | 0.51              |
| 35:g:206:LEU:HD22 | 35:g:218:LEU:HD21 | 1.93                     | 0.51              |
| 1:2:919:A:OP2     | 11:N:64:ARG:NH2   | 2.44                     | 0.51              |
| 1:2:1096:G:OP2    | 14:W:22:LYS:NZ    | 2.39                     | 0.51              |
| 4:C:183:LYS:HD2   | 4:C:194:ARG:HE    | 1.76                     | 0.51              |
| 16:Y:23:MET:SD    | 16:Y:23:MET:N     | 2.83                     | 0.51              |
| 1:2:387:C:OP2     | 8:I:10:LYS:NZ     | 2.42                     | 0.50              |
| 1:2:1482:C:H5''   | 19:d:54:LYS:HE3   | 1.93                     | 0.50              |
| 19:d:23:VAL:CB    | 24:K:64:TRP:NE1   | 2.73                     | 0.50              |
| 27:Q:28:GLY:HA3   | 27:Q:67:ASP:HB2   | 1.93                     | 0.50              |
| 1:2:808:A:O2'     | 1:2:809:A:O5'     | 2.28                     | 0.50              |
| 4:C:136:HIS:HB3   | 4:C:162:ILE:HG23  | 1.93                     | 0.50              |
| 9:J:67:ASP:HB3    | 9:J:70:ARG:HB3    | 1.93                     | 0.50              |
| 1:2:1279:C:H2'    | 1:2:1280:G:H8     | 1.76                     | 0.50              |
| 2:A:90:PHE:CE1    | 2:A:175:TRP:HE3   | 2.30                     | 0.50              |
| 4:C:78:LEU:HB2    | 4:C:97:PHE:CD1    | 2.46                     | 0.50              |
| 9:J:18:ARG:O      | 9:J:24:ARG:NH1    | 2.42                     | 0.50              |
| 22:D:132:LYS:CB   | 22:D:189:MET:CE   | 2.87                     | 0.50              |
| 23:F:74:ASN:HA    | 23:F:77:MET:HE3   | 1.93                     | 0.50              |
| 1:2:522:A:H5''    | 9:J:145:PRO:HD2   | 1.93                     | 0.50              |
| 1:2:1232:U:O4     | 1:2:1526:G:O6     | 2.29                     | 0.50              |
| 9:J:134:HIS:HD1   | 9:J:163:SER:HB2   | 1.77                     | 0.50              |
| 35:g:7:LEU:HB2    | 35:g:272:GLN:HE22 | 1.76                     | 0.50              |
| 1:2:1060:A:O2'    | 1:2:1062:A:N7     | 2.36                     | 0.50              |
| 3:B:129:THR:OG1   | 3:B:132:GLY:N     | 2.45                     | 0.50              |
| 9:J:63:LEU:HB2    | 9:J:70:ARG:HD2    | 1.94                     | 0.50              |
| 18:b:45:THR:OG1   | 18:b:82:LYS:NZ    | 2.44                     | 0.50              |
| 19:d:6:LEU:HA     | 19:d:9:SER:HB3    | 1.94                     | 0.50              |
| 22:D:29:LEU:HD22  | 22:D:58:VAL:HG12  | 1.93                     | 0.50              |
| 22:D:226:GLN:HA   | 35:g:186:THR:HA   | 1.94                     | 0.50              |
| 27:Q:102:GLU:HG2  | 35:g:55:PRO:HB2   | 1.93                     | 0.50              |
| 29:S:114:LEU:O    | 29:S:118:ARG:N    | 2.45                     | 0.50              |
| 1:2:126:G:N2      | 1:2:180:G:H21     | 2.09                     | 0.50              |
| 2:A:6:ASP:HA      | 2:A:9:GLN:HB2     | 1.93                     | 0.50              |
| 27:Q:76:GLY:H     | 27:Q:79:ALA:HB3   | 1.77                     | 0.50              |
| 31:U:61:LEU:HG    | 31:U:82:MET:HB3   | 1.94                     | 0.50              |
| 1:2:1590:C:H5''   | 1:2:1591:C:H5     | 1.77                     | 0.50              |
| 13:V:60:ARG:HA    | 13:V:65:SER:HB3   | 1.93                     | 0.50              |
| 23:F:144:LEU:O    | 23:F:148:ASN:ND2  | 2.44                     | 0.50              |
| 1:2:1324:G:O2'    | 1:2:1510:G:O2'    | 2.28                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1373:C:P     | 28:R:7:LYS:HG3    | 2.52                     | 0.50              |
| 5:E:180:LEU:O    | 5:E:228:ILE:HB    | 2.12                     | 0.50              |
| 14:W:30:CYS:N    | 14:W:59:GLY:O     | 2.41                     | 0.50              |
| 14:W:90:GLN:HB2  | 14:W:94:LEU:CD1   | 2.41                     | 0.50              |
| 25:M:35:ILE:HG23 | 34:f:102:VAL:HG21 | 1.94                     | 0.50              |
| 34:f:125:GLU:O   | 34:f:143:LYS:NZ   | 2.44                     | 0.50              |
| 1:2:1259:A:O2'   | 1:2:1262:C:N4     | 2.45                     | 0.50              |
| 4:C:207:ALA:HB3  | 4:C:210:PRO:HD2   | 1.93                     | 0.50              |
| 12:O:31:CYS:O    | 12:O:96:LYS:N     | 2.44                     | 0.50              |
| 22:D:163:PRO:O   | 22:D:167:TYR:HB2  | 2.11                     | 0.50              |
| 1:2:919:A:H5'    | 11:N:16:LEU:HD12  | 1.94                     | 0.49              |
| 1:2:1568:C:O2    | 1:2:1627:C:O2'    | 2.28                     | 0.49              |
| 1:2:1608:U:O4    | 1:2:1632:G:N2     | 2.45                     | 0.49              |
| 4:C:102:LEU:CD2  | 4:C:130:ILE:CD1   | 2.65                     | 0.49              |
| 7:H:9:VAL:HG22   | 7:H:45:ILE:HD11   | 1.94                     | 0.49              |
| 7:H:145:ARG:HA   | 14:W:51:GLU:HA    | 1.93                     | 0.49              |
| 22:D:24:PHE:HA   | 24:K:63:ALA:HB2   | 1.94                     | 0.49              |
| 11:N:101:HIS:NE2 | 11:N:108:ASP:OD2  | 2.44                     | 0.49              |
| 1:2:913:A:H2     | 7:H:99:ARG:H      | 1.60                     | 0.49              |
| 11:N:129:TYR:O   | 11:N:133:ARG:N    | 2.45                     | 0.49              |
| 16:Y:103:SER:HB3 | 16:Y:106:GLN:HG2  | 1.94                     | 0.49              |
| 28:R:33:ARG:HH21 | 35:g:64:HIS:HE1   | 1.59                     | 0.49              |
| 1:2:223:C:H2'    | 1:2:224:A:C8      | 2.47                     | 0.49              |
| 1:2:1284:A:O2'   | 25:M:106:CYS:SG   | 2.60                     | 0.49              |
| 5:E:72:ILE:HG12  | 5:E:90:ILE:HG12   | 1.93                     | 0.49              |
| 31:U:27:ARG:CG   | 31:U:82:MET:CE    | 2.91                     | 0.49              |
| 1:2:429:C:H2'    | 1:2:430:C:C6      | 2.47                     | 0.49              |
| 1:2:1617:G:O2'   | 19:d:14:PHE:CZ    | 2.65                     | 0.49              |
| 1:2:1726:G:H2'   | 1:2:1727:G:C8     | 2.48                     | 0.49              |
| 4:C:128:VAL:HG11 | 4:C:155:ILE:HG12  | 1.95                     | 0.49              |
| 1:2:68:A:OP2     | 6:G:164:LYS:NZ    | 2.33                     | 0.49              |
| 1:2:1047:C:H1'   | 12:O:141:ARG:HD3  | 1.94                     | 0.49              |
| 9:J:121:LYS:H    | 9:J:125:HIS:HD2   | 1.60                     | 0.49              |
| 1:2:1464:C:O2'   | 1:2:1465:A:O4'    | 2.29                     | 0.49              |
| 1:2:1537:A:O3'   | 30:T:84:ARG:NH2   | 2.46                     | 0.49              |
| 7:H:160:LYS:HA   | 7:H:163:GLN:HB2   | 1.95                     | 0.49              |
| 1:2:126:G:H21    | 1:2:180:G:H21     | 1.61                     | 0.49              |
| 1:2:928:G:H2'    | 1:2:929:G:C8      | 2.48                     | 0.49              |
| 5:E:124:CYS:HB3  | 5:E:141:THR:HB    | 1.94                     | 0.49              |
| 16:Y:74:MET:HE2  | 16:Y:74:MET:HB3   | 1.74                     | 0.49              |
| 19:d:34:TYR:OH   | 31:U:61:LEU:CA    | 2.58                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:D:32:ASP:OD2  | 22:D:65:ARG:NH1   | 2.46                     | 0.49              |
| 22:D:169:ASP:O   | 22:D:187:LYS:HA   | 2.12                     | 0.49              |
| 23:F:25:THR:HG22 | 23:F:109:LEU:HD22 | 1.95                     | 0.49              |
| 1:2:106:C:H2'    | 1:2:107:A:H8      | 1.78                     | 0.49              |
| 1:2:659:G:H21    | 15:X:17:ARG:NH1   | 2.10                     | 0.49              |
| 1:2:1047:C:H5''  | 12:O:143:LYS:HA   | 1.95                     | 0.49              |
| 3:B:113:MET:O    | 3:B:118:GLN:NE2   | 2.46                     | 0.49              |
| 3:B:137:LEU:HD23 | 3:B:215:VAL:HG22  | 1.95                     | 0.49              |
| 16:Y:41:ARG:NH2  | 16:Y:52:PRO:O     | 2.45                     | 0.49              |
| 22:D:109:LEU:HB3 | 22:D:177:LEU:HD11 | 1.93                     | 0.49              |
| 31:U:32:LEU:HD21 | 31:U:87:ARG:CG    | 2.43                     | 0.49              |
| 33:c:13:ARG:NH2  | 33:c:53:GLY:O     | 2.45                     | 0.49              |
| 35:g:42:MET:HB3  | 35:g:57:ARG:H     | 1.78                     | 0.49              |
| 1:2:1473:G:N2    | 1:2:1476:A:OP2    | 2.42                     | 0.48              |
| 4:C:78:LEU:HB2   | 4:C:97:PHE:CB     | 2.43                     | 0.48              |
| 5:E:9:LEU:HB2    | 5:E:30:ARG:HD3    | 1.95                     | 0.48              |
| 9:J:28:GLU:HB3   | 9:J:40:LYS:HE3    | 1.95                     | 0.48              |
| 28:R:66:VAL:HG12 | 28:R:68:GLY:H     | 1.78                     | 0.48              |
| 29:S:99:LEU:O    | 29:S:103:LEU:N    | 2.46                     | 0.48              |
| 1:2:602:G:H3'    | 1:2:603:C:H2'     | 1.95                     | 0.48              |
| 1:2:1546:G:H22   | 1:2:1655:C:H1'    | 1.77                     | 0.48              |
| 5:E:70:ILE:HG12  | 5:E:92:ILE:HG12   | 1.96                     | 0.48              |
| 7:H:10:LYS:HD2   | 7:H:44:ASN:HD22   | 1.78                     | 0.48              |
| 19:d:50:ILE:CG1  | 22:D:15:GLY:O     | 2.35                     | 0.48              |
| 1:2:28:U:H2'     | 1:2:29:G:H8       | 1.78                     | 0.48              |
| 1:2:1401:A:H2'   | 1:2:1402:A:C8     | 2.48                     | 0.48              |
| 3:B:52:THR:HG22  | 3:B:54:GLY:H      | 1.78                     | 0.48              |
| 11:N:136:PRO:HG2 | 11:N:139:TRP:HB2  | 1.95                     | 0.48              |
| 1:2:122:G:H21    | 5:E:146:THR:HG21  | 1.79                     | 0.48              |
| 1:2:678:U:O4     | 1:2:1027:A:N7     | 2.46                     | 0.48              |
| 2:A:58:LEU:CD2   | 2:A:174:MET:HE1   | 2.33                     | 0.48              |
| 28:R:20:TYR:CZ   | 28:R:38:ILE:HG21  | 2.48                     | 0.48              |
| 30:T:56:ARG:HE   | 30:T:79:TYR:HE2   | 1.59                     | 0.48              |
| 31:U:34:LYS:CE   | 31:U:34:LYS:CA    | 2.85                     | 0.48              |
| 35:g:147:HIS:HD2 | 35:g:151:VAL:HG22 | 1.78                     | 0.48              |
| 1:2:1233:G:N3    | 1:2:1252:C:O2'    | 2.37                     | 0.48              |
| 1:2:1297:U:H1'   | 1:2:1301:A:H62    | 1.78                     | 0.48              |
| 30:T:124:THR:O   | 30:T:128:GLN:N    | 2.45                     | 0.48              |
| 35:g:259:TRP:HA  | 35:g:266:ILE:HA   | 1.95                     | 0.48              |
| 1:2:1275:G:N2    | 1:2:1506:A:OP2    | 2.35                     | 0.48              |
| 1:2:1538:C:O2    | 30:T:48:TYR:OH    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:144:THR:HB   | 2:A:158:ASP:H     | 1.79                     | 0.48              |
| 5:E:179:ASN:HD22 | 5:E:231:GLY:H     | 1.62                     | 0.48              |
| 7:H:130:LEU:HD21 | 7:H:156:VAL:HG21  | 1.96                     | 0.48              |
| 27:Q:34:VAL:HB   | 27:Q:42:ILE:HD11  | 1.95                     | 0.48              |
| 30:T:97:LYS:O    | 30:T:101:ARG:HB2  | 2.14                     | 0.48              |
| 1:2:992:A:H62    | 17:a:15:ARG:HH12  | 1.62                     | 0.48              |
| 1:2:30:C:O2'     | 1:2:596:U:OP1     | 2.27                     | 0.48              |
| 1:2:204:G:OP1    | 8:I:147:LYS:NZ    | 2.47                     | 0.48              |
| 1:2:433:A:H2'    | 1:2:434:G:C8      | 2.49                     | 0.48              |
| 1:2:1010:G:H2'   | 1:2:1011:A:C8     | 2.47                     | 0.48              |
| 1:2:1371:U:H4'   | 1:2:1372:U:H5     | 1.79                     | 0.48              |
| 1:2:1543:U:O2'   | 27:Q:43:GLU:OE1   | 2.22                     | 0.48              |
| 1:2:1856:C:H2'   | 1:2:1857:G:C8     | 2.49                     | 0.48              |
| 12:O:30:VAL:HA   | 12:O:94:HIS:HB2   | 1.95                     | 0.48              |
| 1:2:300:U:H2'    | 1:2:301:A:C8      | 2.49                     | 0.48              |
| 1:2:300:U:H2'    | 1:2:301:A:H8      | 1.79                     | 0.48              |
| 1:2:436:G:OP2    | 1:2:471:G:O2'     | 2.32                     | 0.48              |
| 1:2:1542:C:OP1   | 30:T:62:ARG:NH2   | 2.47                     | 0.48              |
| 1:2:1590:C:O2    | 1:2:1652:G:N2     | 2.43                     | 0.48              |
| 7:H:174:SER:O    | 7:H:178:LYS:N     | 2.43                     | 0.48              |
| 13:V:17:CYS:SG   | 13:V:19:ALA:N     | 2.87                     | 0.48              |
| 28:R:44:LYS:O    | 28:R:48:ASN:N     | 2.47                     | 0.48              |
| 35:g:215:GLN:HG2 | 35:g:231:ASP:HA   | 1.94                     | 0.48              |
| 1:2:397:G:OP2    | 10:L:108:ASN:ND2  | 2.45                     | 0.48              |
| 1:2:634:A:H2'    | 1:2:635:G:H8      | 1.79                     | 0.48              |
| 1:2:1161:U:OP1   | 15:X:12:LYS:NZ    | 2.47                     | 0.48              |
| 2:A:90:PHE:HD1   | 2:A:179:ALA:HB2   | 1.78                     | 0.48              |
| 1:2:1274:G:N2    | 1:2:1274:G:OP1    | 2.46                     | 0.47              |
| 12:O:99:ALA:H    | 12:O:133:THR:HG22 | 1.79                     | 0.47              |
| 29:S:45:LEU:O    | 29:S:49:ASP:N     | 2.47                     | 0.47              |
| 8:I:106:SER:HB2  | 8:I:171:LEU:HG    | 1.96                     | 0.47              |
| 26:P:96:VAL:HG21 | 26:P:116:LEU:HB3  | 1.95                     | 0.47              |
| 34:f:138:ARG:HA  | 34:f:149:CYS:HA   | 1.96                     | 0.47              |
| 1:2:359:U:H2'    | 1:2:362:C:H5      | 1.79                     | 0.47              |
| 1:2:798:G:H21    | 7:H:107:LYS:HG2   | 1.79                     | 0.47              |
| 1:2:1513:C:OP1   | 19:d:10:HIS:HB2   | 2.13                     | 0.47              |
| 1:2:1550:G:O2'   | 1:2:1558:C:O2     | 2.30                     | 0.47              |
| 3:B:107:ARG:NH1  | 12:O:133:THR:O    | 2.45                     | 0.47              |
| 3:B:157:GLN:O    | 3:B:161:VAL:N     | 2.43                     | 0.47              |
| 4:C:70:VAL:CG1   | 4:C:96:PHE:HD2    | 2.27                     | 0.47              |
| 4:C:98:LEU:N     | 4:C:98:LEU:HD13   | 2.28                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:G:88:ARG:HB2    | 6:G:91:GLU:HB2   | 1.95                     | 0.47              |
| 12:O:43:HIS:HD2   | 12:O:55:ARG:HB2  | 1.79                     | 0.47              |
| 1:2:1378:A:N6     | 2:A:136:GLU:OE2  | 2.47                     | 0.47              |
| 2:A:90:PHE:CD1    | 2:A:175:TRP:HE3  | 2.32                     | 0.47              |
| 7:H:9:VAL:HG12    | 7:H:11:PRO:HD3   | 1.96                     | 0.47              |
| 24:K:16:PHE:HZ    | 24:K:80:ARG:HE   | 1.61                     | 0.47              |
| 1:2:1092:G:H2'    | 1:2:1093:A:H8    | 1.80                     | 0.47              |
| 1:2:851:C:O2'     | 1:2:852:G:N2     | 2.48                     | 0.47              |
| 1:2:948:C:H2'     | 1:2:949:G:H8     | 1.79                     | 0.47              |
| 2:A:90:PHE:CE1    | 2:A:179:ALA:HB2  | 2.48                     | 0.47              |
| 9:J:46:VAL:HG11   | 9:J:106:LEU:HD12 | 1.96                     | 0.47              |
| 12:O:46:ASP:OD1   | 12:O:47:LEU:N    | 2.47                     | 0.47              |
| 15:X:82:THR:OG1   | 15:X:117:GLY:O   | 2.33                     | 0.47              |
| 22:D:57:ASN:O     | 22:D:65:ARG:NH1  | 2.48                     | 0.47              |
| 1:2:681:U:O2'     | 1:2:1160:U:OP1   | 2.32                     | 0.47              |
| 1:2:1217:A:H2'    | 1:2:1218:C:C6    | 2.49                     | 0.47              |
| 1:2:1513:C:H2'    | 1:2:1514:G:C8    | 2.50                     | 0.47              |
| 1:2:1622:U:OP1    | 29:S:120:HIS:ND1 | 2.47                     | 0.47              |
| 1:2:1736:G:H2'    | 1:2:1737:G:H8    | 1.80                     | 0.47              |
| 1:2:1753:C:H2'    | 1:2:1754:G:C8    | 2.48                     | 0.47              |
| 22:D:192:TRP:CG   | 22:D:193:ASP:H   | 2.33                     | 0.47              |
| 1:2:924:G:H21     | 11:N:87:ASP:HB3  | 1.80                     | 0.47              |
| 1:2:1087:A:OP2    | 17:a:8:ASN:ND2   | 2.48                     | 0.47              |
| 1:2:1394:G:OP1    | 27:Q:126:ARG:NH1 | 2.48                     | 0.47              |
| 1:2:1866:A:N6     | 17:a:84:VAL:HG13 | 2.30                     | 0.47              |
| 2:A:74:VAL:HG13   | 2:A:121:LEU:HD23 | 1.97                     | 0.47              |
| 7:H:58:LYS:HD2    | 7:H:90:LYS:CE    | 2.39                     | 0.47              |
| 7:H:83:LEU:HD23   | 7:H:92:VAL:HG11  | 1.97                     | 0.47              |
| 11:N:75:LEU:HD12  | 11:N:80:LEU:HB2  | 1.97                     | 0.47              |
| 22:D:195:THR:HG22 | 22:D:201:LYS:HD3 | 1.96                     | 0.47              |
| 23:F:101:HIS:ND1  | 23:F:106:GLU:O   | 2.40                     | 0.47              |
| 1:2:527:C:H2'     | 1:2:528:A:H8     | 1.80                     | 0.47              |
| 22:D:171:ALA:O    | 22:D:185:LYS:HA  | 2.15                     | 0.47              |
| 24:K:57:TYR:HD1   | 24:K:75:GLY:HA2  | 1.80                     | 0.47              |
| 34:f:120:GLU:OE2  | 34:f:128:ALA:N   | 2.47                     | 0.47              |
| 1:2:99:A:H61      | 1:2:433:A:H1'    | 1.80                     | 0.47              |
| 1:2:996:A:H2'     | 1:2:997:A:C8     | 2.49                     | 0.47              |
| 8:I:65:PHE:O      | 8:I:109:TYR:OH   | 2.33                     | 0.47              |
| 10:L:35:ARG:HG3   | 10:L:37:TYR:HD1  | 1.80                     | 0.47              |
| 1:2:381:C:OP2     | 8:I:54:LYS:NZ    | 2.47                     | 0.46              |
| 1:2:1607:A:N6     | 1:2:1632:G:O2'   | 2.47                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:63:LYS:HA     | 3:B:88:THR:CG2   | 2.39                     | 0.46              |
| 6:G:44:GLU:HA     | 6:G:119:LYS:HD2  | 1.96                     | 0.46              |
| 9:J:37:LEU:HD11   | 9:J:106:LEU:HD21 | 1.97                     | 0.46              |
| 10:L:38:LYS:NZ    | 10:L:64:GLY:O    | 2.47                     | 0.46              |
| 21:h:2:ARG:HD2    | 21:h:5:TRP:CD1   | 2.50                     | 0.46              |
| 23:F:115:ALA:O    | 23:F:119:SER:HB3 | 2.14                     | 0.46              |
| 1:2:508:A:H3'     | 1:2:509:G:H8     | 1.80                     | 0.46              |
| 1:2:948:C:H2'     | 1:2:949:G:C8     | 2.50                     | 0.46              |
| 10:L:99:TYR:HE2   | 15:X:14:ARG:HB3  | 1.80                     | 0.46              |
| 35:g:133:ASN:HD22 | 35:g:137:VAL:HB  | 1.79                     | 0.46              |
| 35:g:188:HIS:HB3  | 35:g:219:TRP:CE2 | 2.50                     | 0.46              |
| 1:2:1228:A:H2'    | 1:2:1229:G:H8    | 1.79                     | 0.46              |
| 1:2:1243:U:OP1    | 1:2:1518:C:O2'   | 2.29                     | 0.46              |
| 1:2:797:C:H2'     | 1:2:798:G:C4     | 2.51                     | 0.46              |
| 1:2:1101:U:H2'    | 1:2:1102:G:C8    | 2.50                     | 0.46              |
| 1:2:1368:U:O3'    | 28:R:2:GLY:N     | 2.48                     | 0.46              |
| 3:B:133:TYR:HD1   | 3:B:221:PRO:HD2  | 1.80                     | 0.46              |
| 8:I:142:SER:O     | 8:I:146:GLN:N    | 2.47                     | 0.46              |
| 14:W:31:SER:H     | 14:W:34:ILE:HB   | 1.80                     | 0.46              |
| 4:C:78:LEU:CD1    | 4:C:97:PHE:CD2   | 2.88                     | 0.46              |
| 7:H:156:VAL:HB    | 7:H:187:PHE:HE1  | 1.81                     | 0.46              |
| 10:L:101:ARG:HH21 | 14:W:79:PHE:HZ   | 1.62                     | 0.46              |
| 24:K:24:LYS:HD3   | 24:K:26:ASP:OD2  | 2.15                     | 0.46              |
| 26:P:22:LEU:HD23  | 26:P:25:LEU:HD12 | 1.98                     | 0.46              |
| 28:R:13:ALA:C     | 28:R:16:ILE:HG23 | 2.40                     | 0.46              |
| 35:g:131:LEU:O    | 35:g:139:LYS:N   | 2.39                     | 0.46              |
| 35:g:213:ASP:OD1  | 35:g:213:ASP:N   | 2.48                     | 0.46              |
| 35:g:226:HIS:NE2  | 35:g:228:TYR:O   | 2.49                     | 0.46              |
| 1:2:106:C:H2'     | 1:2:107:A:C8     | 2.49                     | 0.46              |
| 1:2:1869:A:N6     | 3:B:111:CYS:O    | 2.48                     | 0.46              |
| 18:b:46:VAL:HG13  | 18:b:54:VAL:HG21 | 1.97                     | 0.46              |
| 23:F:165:ASN:O    | 23:F:167:LYS:N   | 2.48                     | 0.46              |
| 26:P:38:SER:HB2   | 26:P:41:GLN:HG2  | 1.98                     | 0.46              |
| 29:S:36:VAL:HG21  | 29:S:71:MET:HE3  | 1.97                     | 0.46              |
| 1:2:1373:C:O2'    | 1:2:1465:A:O2'   | 2.31                     | 0.46              |
| 1:2:1779:G:H2'    | 1:2:1780:G:C8    | 2.51                     | 0.46              |
| 18:b:33:MET:HB2   | 18:b:79:PHE:HB2  | 1.97                     | 0.46              |
| 23:F:41:VAL:HA    | 23:F:45:TYR:HB2  | 1.96                     | 0.46              |
| 1:2:1256:G:N1     | 19:d:31:ILE:HG12 | 2.31                     | 0.46              |
| 1:2:1444:U:OP1    | 27:Q:15:ARG:NH2  | 2.49                     | 0.46              |
| 1:2:1533:A:HO2'   | 23:F:81:ARG:HH12 | 1.62                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:94:ILE:HG13   | 4:C:159:LYS:O     | 2.16                     | 0.46              |
| 31:U:61:LEU:HD12  | 31:U:82:MET:HG2   | 1.97                     | 0.46              |
| 1:2:925:G:O6      | 1:2:1017:U:O4     | 2.34                     | 0.46              |
| 1:2:1656:G:H2'    | 1:2:1657:G:H8     | 1.80                     | 0.46              |
| 2:A:178:LEU:O     | 2:A:182:VAL:HG12  | 2.16                     | 0.46              |
| 14:W:6:VAL:HG12   | 14:W:34:ILE:HD11  | 1.98                     | 0.46              |
| 19:d:3:HIS:CE1    | 19:d:5:GLN:HB2    | 2.51                     | 0.46              |
| 1:2:659:G:O4'     | 1:2:662:G:N2      | 2.48                     | 0.46              |
| 6:G:5:ILE:HD12    | 6:G:16:ILE:HD12   | 1.98                     | 0.46              |
| 22:D:132:LYS:HB2  | 22:D:189:MET:CE   | 2.41                     | 0.46              |
| 23:F:168:THR:O    | 23:F:172:CYS:N    | 2.41                     | 0.46              |
| 35:g:149:GLU:HB3  | 35:g:170:TRP:HB2  | 1.98                     | 0.46              |
| 1:2:857:U:H2'     | 1:2:858:A:C8      | 2.51                     | 0.45              |
| 1:2:1618:C:C2     | 19:d:11:PRO:CG    | 2.99                     | 0.45              |
| 1:2:1808:U:H2'    | 1:2:1809:A:C8     | 2.51                     | 0.45              |
| 9:J:19:PRO:O      | 9:J:24:ARG:NH2    | 2.49                     | 0.45              |
| 11:N:120:SER:O    | 11:N:124:ARG:HB3  | 2.15                     | 0.45              |
| 23:F:51:HIS:O     | 27:Q:82:TYR:OH    | 2.33                     | 0.45              |
| 35:g:17:TRP:CE2   | 35:g:303:THR:HG23 | 2.51                     | 0.45              |
| 5:E:114:ILE:HG23  | 5:E:118:GLU:HB3   | 1.97                     | 0.45              |
| 7:H:132:ASP:HA    | 7:H:135:PHE:HB2   | 1.97                     | 0.45              |
| 35:g:36:ARG:HD2   | 35:g:65:PHE:HB3   | 1.98                     | 0.45              |
| 1:2:561:A:H5''    | 9:J:164:PRO:HG2   | 1.99                     | 0.45              |
| 1:2:1430:C:H2'    | 1:2:1431:G:C8     | 2.51                     | 0.45              |
| 6:G:78:SER:OG     | 6:G:79:LYS:N      | 2.50                     | 0.45              |
| 15:X:101:LEU:HD12 | 15:X:101:LEU:HA   | 1.81                     | 0.45              |
| 23:F:140:ASP:HB2  | 33:c:46:VAL:HG12  | 1.99                     | 0.45              |
| 35:g:14:HIS:HD2   | 35:g:41:ILE:HD12  | 1.82                     | 0.45              |
| 6:G:209:TYR:O     | 6:G:213:LEU:HB2   | 2.16                     | 0.45              |
| 7:H:109:ARG:HG2   | 7:H:110:THR:H     | 1.81                     | 0.45              |
| 12:O:37:PHE:HE2   | 12:O:105:THR:HG21 | 1.81                     | 0.45              |
| 22:D:22:ASN:HD21  | 22:D:37:VAL:CG2   | 2.30                     | 0.45              |
| 22:D:126:ILE:HA   | 22:D:129:SER:HB3  | 1.99                     | 0.45              |
| 1:2:915:G:H5'     | 7:H:120:ARG:HH12  | 1.81                     | 0.45              |
| 1:2:1497:G:N9     | 24:K:62:PHE:CE2   | 2.84                     | 0.45              |
| 1:2:1856:C:H2'    | 1:2:1857:G:H8     | 1.82                     | 0.45              |
| 11:N:54:LEU:HB3   | 11:N:60:VAL:HB    | 1.99                     | 0.45              |
| 15:X:68:LYS:HB3   | 15:X:91:LEU:HD22  | 1.99                     | 0.45              |
| 29:S:34:LYS:HB3   | 29:S:103:LEU:HD23 | 1.99                     | 0.45              |
| 1:2:421:G:H5'     | 10:L:98:LYS:HG3   | 1.99                     | 0.45              |
| 1:2:455:A:O2'     | 1:2:1735:A:N3     | 2.38                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:600:G:H2'     | 1:2:601:G:H8      | 1.81                     | 0.45              |
| 1:2:1228:A:H2'    | 1:2:1229:G:C8     | 2.52                     | 0.45              |
| 1:2:1288:U:O2'    | 1:2:1315:U:O2'    | 2.28                     | 0.45              |
| 1:2:1655:C:OP1    | 30:T:92:PHE:N     | 2.49                     | 0.45              |
| 8:I:11:ARG:O      | 10:L:136:LYS:NZ   | 2.37                     | 0.45              |
| 13:V:31:SER:OG    | 13:V:32:ILE:N     | 2.46                     | 0.45              |
| 16:Y:27:VAL:O     | 16:Y:68:LYS:HA    | 2.17                     | 0.45              |
| 17:a:24:THR:HG21  | 17:a:71:LEU:HD22  | 1.98                     | 0.45              |
| 19:d:50:ILE:HG12  | 22:D:15:GLY:C     | 2.31                     | 0.45              |
| 23:F:87:LEU:HA    | 23:F:90:VAL:HG22  | 1.99                     | 0.45              |
| 30:T:83:GLN:NE2   | 30:T:85:ASN:OD1   | 2.50                     | 0.45              |
| 1:2:222:U:H5''    | 10:L:17:PHE:CG    | 2.51                     | 0.45              |
| 1:2:1776:G:H2'    | 1:2:1777:G:C8     | 2.52                     | 0.45              |
| 2:A:144:THR:OG1   | 13:V:60:ARG:NH2   | 2.49                     | 0.45              |
| 7:H:91:HIS:CD2    | 7:H:169:LYS:HG2   | 2.51                     | 0.45              |
| 1:2:28:U:H2'      | 1:2:29:G:C8       | 2.50                     | 0.45              |
| 2:A:205:ARG:HE    | 2:A:205:ARG:HA    | 1.82                     | 0.45              |
| 3:B:153:THR:HB    | 3:B:155:TYR:CE2   | 2.52                     | 0.45              |
| 22:D:132:LYS:HB3  | 22:D:189:MET:CE   | 2.43                     | 0.45              |
| 23:F:86:LYS:O     | 23:F:90:VAL:N     | 2.50                     | 0.45              |
| 28:R:21:TYR:O     | 28:R:21:TYR:CD1   | 2.70                     | 0.45              |
| 29:S:50:ILE:HD13  | 29:S:59:LEU:HD22  | 1.98                     | 0.45              |
| 1:2:638:C:O4'     | 20:e:56:ASN:ND2   | 2.50                     | 0.45              |
| 4:C:182:CYS:HB2   | 14:W:95:PRO:HB2   | 1.99                     | 0.45              |
| 4:C:196:ILE:HB    | 4:C:223:TYR:HB2   | 1.98                     | 0.45              |
| 35:g:57:ARG:NH1   | 35:g:94:THR:O     | 2.50                     | 0.45              |
| 35:g:289:LEU:HD11 | 35:g:298:LEU:HD22 | 1.98                     | 0.45              |
| 3:B:68:GLU:OE2    | 3:B:85:LYS:NZ     | 2.35                     | 0.45              |
| 19:d:40:ARG:NH2   | 31:U:69:PRO:O     | 2.50                     | 0.45              |
| 24:K:24:LYS:HA    | 24:K:66:HIS:HD1   | 1.76                     | 0.45              |
| 24:K:24:LYS:CD    | 24:K:26:ASP:OD2   | 2.65                     | 0.45              |
| 26:P:95:GLY:HA2   | 26:P:103:ASN:O    | 2.17                     | 0.45              |
| 27:Q:16:LYS:HG2   | 27:Q:17:LYS:H     | 1.82                     | 0.45              |
| 30:T:34:VAL:O     | 30:T:52:TRP:NE1   | 2.47                     | 0.45              |
| 1:2:688:U:OP1     | 7:H:122:LEU:N     | 2.44                     | 0.44              |
| 1:2:1279:C:H2'    | 1:2:1280:G:C8     | 2.51                     | 0.44              |
| 4:C:78:LEU:CD2    | 4:C:97:PHE:HB2    | 2.36                     | 0.44              |
| 10:L:135:SER:O    | 10:L:139:ARG:NH1  | 2.49                     | 0.44              |
| 24:K:52:LEU:HB3   | 24:K:57:TYR:HB2   | 1.99                     | 0.44              |
| 27:Q:32:ILE:HG12  | 27:Q:68:ILE:HB    | 1.99                     | 0.44              |
| 6:G:3:LEU:HD13    | 6:G:5:ILE:HD11    | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:W:31:SER:O    | 14:W:35:VAL:N     | 2.47                     | 0.44              |
| 1:2:1497:G:N9    | 24:K:62:PHE:CD2   | 2.84                     | 0.44              |
| 1:2:1513:C:OP1   | 19:d:12:ARG:NH1   | 2.50                     | 0.44              |
| 3:B:31:TYR:CE2   | 3:B:62:LEU:CD2    | 3.01                     | 0.44              |
| 4:C:182:CYS:SG   | 4:C:183:LYS:N     | 2.90                     | 0.44              |
| 8:I:93:THR:OG1   | 8:I:95:THR:OG1    | 2.30                     | 0.44              |
| 11:N:47:PRO:HG2  | 11:N:72:LEU:HD13  | 1.98                     | 0.44              |
| 14:W:87:GLU:HA   | 14:W:90:GLN:NE2   | 2.33                     | 0.44              |
| 21:h:2:ARG:HD3   | 21:h:4:LYS:H      | 1.82                     | 0.44              |
| 23:F:122:ARG:HA  | 23:F:146:ARG:HH21 | 1.82                     | 0.44              |
| 35:g:32:LEU:HD12 | 35:g:32:LEU:HA    | 1.85                     | 0.44              |
| 35:g:45:LEU:HD23 | 35:g:53:GLY:HA3   | 1.99                     | 0.44              |
| 1:2:482:G:N1     | 1:2:485:A:OP2     | 2.50                     | 0.44              |
| 1:2:913:A:H1'    | 7:H:66:VAL:HB     | 1.99                     | 0.44              |
| 1:2:929:G:N2     | 1:2:1013:U:O2     | 2.51                     | 0.44              |
| 1:2:1373:C:P     | 28:R:7:LYS:CG     | 3.05                     | 0.44              |
| 1:2:1628:C:H2'   | 1:2:1629:C:C6     | 2.52                     | 0.44              |
| 2:A:178:LEU:O    | 2:A:178:LEU:HD12  | 2.17                     | 0.44              |
| 6:G:176:ILE:HG22 | 6:G:179:LEU:HB2   | 2.00                     | 0.44              |
| 18:b:36:LYS:HE3  | 18:b:41:TYR:HA    | 1.99                     | 0.44              |
| 25:M:50:CYS:SG   | 25:M:51:VAL:N     | 2.91                     | 0.44              |
| 1:2:500:A:H3'    | 1:2:501:C:H6      | 1.82                     | 0.44              |
| 1:2:640:A:H2'    | 1:2:641:A:C8      | 2.52                     | 0.44              |
| 1:2:649:U:H2'    | 1:2:650:A:H8      | 1.83                     | 0.44              |
| 1:2:1325:G:O2'   | 1:2:1327:G:OP1    | 2.33                     | 0.44              |
| 1:2:1679:A:OP1   | 33:c:20:ARG:NH2   | 2.51                     | 0.44              |
| 4:C:102:LEU:CD2  | 4:C:130:ILE:CG1   | 2.90                     | 0.44              |
| 5:E:100:ARG:HG2  | 5:E:102:ILE:HG13  | 1.99                     | 0.44              |
| 6:G:85:ARG:HH22  | 16:Y:118:ARG:HD3  | 1.82                     | 0.44              |
| 8:I:48:VAL:HG11  | 8:I:54:LYS:HE3    | 2.00                     | 0.44              |
| 12:O:101:GLY:HA2 | 12:O:106:LYS:HD2  | 2.00                     | 0.44              |
| 1:2:886:A:C4     | 1:2:887:U:H1'     | 2.53                     | 0.44              |
| 1:2:925:G:OP1    | 11:N:121:ARG:NH1  | 2.51                     | 0.44              |
| 2:A:24:HIS:HB3   | 2:A:51:LEU:HD11   | 2.00                     | 0.44              |
| 4:C:107:LEU:HB2  | 4:C:127:PHE:HB2   | 2.00                     | 0.44              |
| 27:Q:87:SER:O    | 27:Q:91:ALA:CB    | 2.61                     | 0.44              |
| 28:R:24:LEU:HB3  | 28:R:58:MET:SD    | 2.58                     | 0.44              |
| 29:S:6:PRO:HB2   | 29:S:9:PHE:HB2    | 2.00                     | 0.44              |
| 33:c:32:VAL:O    | 33:c:41:SER:HA    | 2.17                     | 0.44              |
| 1:2:685:A:H62    | 1:2:918:U:H3      | 1.66                     | 0.44              |
| 1:2:830:A:OP2    | 1:2:846:G:N2      | 2.51                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:1215:C:H42    | 1:2:1220:A:H61   | 1.66                     | 0.44              |
| 1:2:1588:A:H2'    | 1:2:1589:A:H8    | 1.81                     | 0.44              |
| 18:b:49:HIS:CD2   | 18:b:70:LYS:HG2  | 2.52                     | 0.44              |
| 22:D:20:GLU:CB    | 24:K:64:TRP:CE3  | 2.97                     | 0.44              |
| 23:F:32:ASP:HB3   | 23:F:34:SER:H    | 1.82                     | 0.44              |
| 23:F:127:ARG:HH21 | 23:F:131:ALA:HA  | 1.82                     | 0.44              |
| 26:P:53:GLN:HG2   | 26:P:80:LEU:HD13 | 1.99                     | 0.44              |
| 1:2:1286:G:N2     | 1:2:1287:A:H62   | 2.16                     | 0.44              |
| 4:C:109:ILE:HG21  | 4:C:147:VAL:HG23 | 2.00                     | 0.44              |
| 14:W:28:ARG:HB3   | 14:W:60:LYS:HG2  | 2.00                     | 0.44              |
| 16:Y:56:PHE:HE2   | 16:Y:82:ALA:HB1  | 1.83                     | 0.44              |
| 19:d:34:TYR:HB3   | 22:D:12:VAL:HG11 | 1.99                     | 0.44              |
| 28:R:17:ILE:HD13  | 28:R:24:LEU:HD12 | 2.00                     | 0.44              |
| 1:2:210:U:H2'     | 1:2:211:G:H8     | 1.82                     | 0.44              |
| 1:2:519:A:O2'     | 9:J:10:ARG:O     | 2.32                     | 0.44              |
| 4:C:232:THR:O     | 4:C:232:THR:OG1  | 2.35                     | 0.44              |
| 5:E:182:MET:HE3   | 5:E:192:ILE:HD11 | 2.00                     | 0.44              |
| 8:I:25:ARG:HA     | 8:I:25:ARG:HD3   | 1.80                     | 0.44              |
| 24:K:65:ARG:O     | 24:K:65:ARG:HG3  | 2.18                     | 0.44              |
| 25:M:54:SER:HB2   | 25:M:80:ASP:HA   | 1.99                     | 0.44              |
| 1:2:642:U:OP1     | 9:J:41:ARG:N     | 2.51                     | 0.43              |
| 1:2:1533:A:N6     | 1:2:1602:U:H3    | 2.15                     | 0.43              |
| 2:A:58:LEU:HD21   | 2:A:174:MET:HE3  | 1.94                     | 0.43              |
| 28:R:44:LYS:HA    | 28:R:47:ARG:HB3  | 2.00                     | 0.43              |
| 1:2:27:A:O2'      | 1:2:483:C:O2'    | 2.36                     | 0.43              |
| 1:2:1174:U:H2'    | 1:2:1175:G:H8    | 1.83                     | 0.43              |
| 1:2:1253:A:O2'    | 1:2:1666:C:O2'   | 2.32                     | 0.43              |
| 1:2:1550:G:H3'    | 1:2:1579:A:H61   | 1.83                     | 0.43              |
| 27:Q:65:GLY:O     | 27:Q:95:TYR:OH   | 2.31                     | 0.43              |
| 1:2:94:G:O2'      | 1:2:508:A:O2'    | 2.34                     | 0.43              |
| 1:2:582:U:OP1     | 9:J:162:ARG:NH1  | 2.52                     | 0.43              |
| 1:2:871:U:H3'     | 1:2:872:A:H4'    | 2.00                     | 0.43              |
| 1:2:934:G:H1      | 1:2:1008:A:H2    | 1.64                     | 0.43              |
| 1:2:1231:C:H2'    | 1:2:1232:U:O4'   | 2.18                     | 0.43              |
| 1:2:1537:A:O2'    | 1:2:1604:G:OP1   | 2.36                     | 0.43              |
| 7:H:9:VAL:HG23    | 7:H:24:SER:HB3   | 1.99                     | 0.43              |
| 10:L:102:PHE:N    | 15:X:7:LEU:O     | 2.50                     | 0.43              |
| 16:Y:41:ARG:HA    | 16:Y:55:ILE:HD11 | 1.99                     | 0.43              |
| 23:F:85:LYS:HD2   | 23:F:88:MET:HG3  | 2.00                     | 0.43              |
| 1:2:563:G:N7      | 1:2:586:G:N2     | 2.67                     | 0.43              |
| 1:2:1633:A:H2'    | 1:2:1634:A:C8    | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:23:ASP:HB2   | 3:B:26:SER:HB2    | 2.01                     | 0.43              |
| 23:F:38:TYR:HB3  | 23:F:147:VAL:HG21 | 1.99                     | 0.43              |
| 23:F:146:ARG:NH1 | 33:c:57:THR:OG1   | 2.45                     | 0.43              |
| 25:M:64:LEU:HD11 | 34:f:103:LEU:HA   | 2.01                     | 0.43              |
| 28:R:16:ILE:HD12 | 28:R:16:ILE:C     | 2.40                     | 0.43              |
| 31:U:27:ARG:HG2  | 31:U:82:MET:CE    | 2.48                     | 0.43              |
| 1:2:1536:G:H2'   | 1:2:1537:A:H8     | 1.81                     | 0.43              |
| 1:2:1542:C:H5''  | 30:T:62:ARG:HH22  | 1.83                     | 0.43              |
| 11:N:85:PRO:O    | 11:N:89:TYR:N     | 2.51                     | 0.43              |
| 35:g:14:HIS:CD2  | 35:g:41:ILE:HD12  | 2.53                     | 0.43              |
| 35:g:71:ILE:HA   | 35:g:78:ALA:HA    | 2.00                     | 0.43              |
| 35:g:260:ASP:N   | 35:g:265:ILE:O    | 2.39                     | 0.43              |
| 7:H:60:ILE:HB    | 7:H:92:VAL:HG22   | 2.01                     | 0.43              |
| 9:J:136:ARG:HG2  | 9:J:160:SER:HA    | 2.00                     | 0.43              |
| 14:W:45:GLY:O    | 14:W:68:ARG:NH1   | 2.48                     | 0.43              |
| 19:d:22:ARG:NH1  | 22:D:16:ILE:HG21  | 2.33                     | 0.43              |
| 23:F:47:LYS:HD2  | 23:F:67:PRO:HG2   | 2.01                     | 0.43              |
| 2:A:178:LEU:C    | 2:A:178:LEU:CD1   | 2.92                     | 0.43              |
| 7:H:144:ILE:O    | 14:W:52:ILE:N     | 2.42                     | 0.43              |
| 9:J:40:LYS:HE2   | 9:J:40:LYS:HB3    | 1.73                     | 0.43              |
| 10:L:13:GLN:NE2  | 10:L:36:TYR:O     | 2.52                     | 0.43              |
| 10:L:68:ILE:HG21 | 10:L:143:LEU:HD11 | 2.00                     | 0.43              |
| 15:X:40:PRO:HB3  | 15:X:79:LYS:HG3   | 2.00                     | 0.43              |
| 27:Q:34:VAL:HG22 | 27:Q:70:VAL:HB    | 2.01                     | 0.43              |
| 1:2:1539:U:H2'   | 1:2:1540:G:C8     | 2.54                     | 0.43              |
| 1:2:1726:G:H2'   | 1:2:1727:G:H8     | 1.84                     | 0.43              |
| 12:O:149:ARG:NH1 | 12:O:151:LEU:O    | 2.52                     | 0.43              |
| 29:S:23:ARG:HB2  | 32:Z:48:VAL:HG21  | 2.01                     | 0.43              |
| 1:2:1373:C:OP1   | 28:R:7:LYS:N      | 2.52                     | 0.43              |
| 6:G:137:ARG:HB3  | 6:G:140:ARG:HG2   | 2.01                     | 0.43              |
| 26:P:85:ILE:HB   | 26:P:112:ILE:HA   | 2.01                     | 0.43              |
| 28:R:20:TYR:OH   | 28:R:38:ILE:HG23  | 2.18                     | 0.43              |
| 1:2:218:U:O2     | 8:I:184:ARG:NH1   | 2.52                     | 0.43              |
| 1:2:1101:U:H2'   | 1:2:1102:G:H8     | 1.83                     | 0.43              |
| 1:2:1810:U:H2'   | 1:2:1811:C:C6     | 2.54                     | 0.43              |
| 4:C:66:LEU:HG    | 4:C:93:ILE:CD1    | 2.49                     | 0.43              |
| 7:H:175:GLY:HA2  | 7:H:178:LYS:HB3   | 2.01                     | 0.43              |
| 10:L:77:VAL:HG11 | 10:L:80:MET:HE3   | 2.01                     | 0.43              |
| 10:L:101:ARG:HG3 | 15:X:7:LEU:HD23   | 2.00                     | 0.43              |
| 22:D:227:LYS:N   | 35:g:185:LYS:O    | 2.52                     | 0.43              |
| 31:U:53:PRO:HG3  | 31:U:89:ILE:HD12  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:586:G:C5      | 9:J:172:ARG:HD3   | 2.54                     | 0.42              |
| 1:2:625:G:N1      | 15:X:64:SER:O     | 2.41                     | 0.42              |
| 1:2:920:A:O2'     | 1:2:922:A:O5'     | 2.37                     | 0.42              |
| 1:2:1249:C:O2'    | 27:Q:143:LYS:NZ   | 2.37                     | 0.42              |
| 1:2:1497:G:N3     | 24:K:62:PHE:CD2   | 2.71                     | 0.42              |
| 1:2:1533:A:O2'    | 23:F:81:ARG:NH1   | 2.44                     | 0.42              |
| 5:E:99:PHE:HE1    | 5:E:113:ARG:HG2   | 1.84                     | 0.42              |
| 12:O:30:VAL:HG22  | 12:O:94:HIS:HB2   | 2.01                     | 0.42              |
| 22:D:108:LYS:O    | 22:D:112:GLY:N    | 2.52                     | 0.42              |
| 25:M:60:MET:HB3   | 34:f:103:LEU:HD13 | 2.01                     | 0.42              |
| 35:g:109:LEU:HD13 | 35:g:152:SER:HA   | 1.99                     | 0.42              |
| 35:g:114:SER:HB3  | 35:g:119:GLN:HB2  | 2.01                     | 0.42              |
| 1:2:1268:C:H2'    | 1:2:1269:G:C8     | 2.54                     | 0.42              |
| 1:2:1360:U:O2'    | 1:2:1379:A:OP2    | 2.34                     | 0.42              |
| 1:2:1634:A:O2'    | 29:S:142:ARG:NH1  | 2.46                     | 0.42              |
| 1:2:1808:U:H2'    | 1:2:1809:A:H8     | 1.83                     | 0.42              |
| 5:E:206:ASP:HB2   | 5:E:222:LEU:HB2   | 2.01                     | 0.42              |
| 18:b:24:LEU:HD12  | 18:b:24:LEU:HA    | 1.81                     | 0.42              |
| 22:D:22:ASN:ND2   | 22:D:37:VAL:HG23  | 2.34                     | 0.42              |
| 24:K:64:TRP:HB3   | 24:K:65:ARG:H     | 1.68                     | 0.42              |
| 1:2:925:G:H2'     | 1:2:926:A:H8      | 1.84                     | 0.42              |
| 1:2:989:C:O2      | 17:a:32:LYS:NZ    | 2.52                     | 0.42              |
| 5:E:164:LEU:HD23  | 5:E:164:LEU:HA    | 1.87                     | 0.42              |
| 8:I:57:ALA:HB2    | 8:I:183:GLY:HA2   | 2.02                     | 0.42              |
| 9:J:160:SER:O     | 9:J:162:ARG:N     | 2.52                     | 0.42              |
| 12:O:97:LEU:HD21  | 12:O:108:PRO:HG2  | 2.02                     | 0.42              |
| 17:a:22:ARG:HA    | 17:a:22:ARG:HD3   | 1.78                     | 0.42              |
| 22:D:27:ARG:CB    | 24:K:61:GLN:HG3   | 2.49                     | 0.42              |
| 32:Z:61:GLU:HG3   | 32:Z:65:TYR:HE1   | 1.84                     | 0.42              |
| 1:2:1126:G:OP2    | 28:R:129:LYS:NZ   | 2.37                     | 0.42              |
| 1:2:1377:U:H3'    | 2:A:102:ARG:HH22  | 1.84                     | 0.42              |
| 1:2:1428:G:N7     | 27:Q:73:LYS:NZ    | 2.66                     | 0.42              |
| 1:2:1659:U:O2     | 1:2:1664:A:N7     | 2.51                     | 0.42              |
| 1:2:1842:C:H2'    | 1:2:1843:G:H8     | 1.84                     | 0.42              |
| 3:B:31:TYR:HD2    | 3:B:62:LEU:HD22   | 1.85                     | 0.42              |
| 1:2:1174:U:H2'    | 1:2:1175:G:C8     | 2.55                     | 0.42              |
| 2:A:37:TYR:OH     | 2:A:57:LYS:NZ     | 2.33                     | 0.42              |
| 3:B:127:VAL:HG22  | 3:B:173:THR:HG23  | 2.01                     | 0.42              |
| 4:C:65:LYS:HD3    | 4:C:273:LEU:HD13  | 2.00                     | 0.42              |
| 4:C:102:LEU:CG    | 4:C:130:ILE:HG12  | 2.49                     | 0.42              |
| 6:G:186:GLN:HA    | 6:G:189:ARG:HD3   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:I:81:VAL:HG22   | 8:I:102:VAL:HG22 | 2.01                     | 0.42              |
| 14:W:105:THR:HG22 | 14:W:126:LEU:HG  | 2.01                     | 0.42              |
| 22:D:22:ASN:HD21  | 22:D:37:VAL:HG23 | 1.84                     | 0.42              |
| 26:P:81:ARG:NH2   | 26:P:117:GLY:O   | 2.39                     | 0.42              |
| 29:S:33:ILE:HB    | 29:S:100:ALA:HB2 | 2.02                     | 0.42              |
| 32:Z:48:VAL:HG22  | 32:Z:80:ARG:HG3  | 2.02                     | 0.42              |
| 1:2:964:A:H2'     | 1:2:965:U:H6     | 1.84                     | 0.42              |
| 1:2:1276:A:C6     | 1:2:1322:G:H1'   | 2.55                     | 0.42              |
| 3:B:62:LEU:HA     | 3:B:65:ARG:HE    | 1.85                     | 0.42              |
| 8:I:6:ASP:OD1     | 8:I:9:HIS:ND1    | 2.53                     | 0.42              |
| 11:N:86:GLU:H     | 11:N:86:GLU:HG3  | 1.64                     | 0.42              |
| 18:b:23:ARG:NH1   | 18:b:27:SER:HB2  | 2.35                     | 0.42              |
| 22:D:24:PHE:HA    | 24:K:63:ALA:CB   | 2.50                     | 0.42              |
| 25:M:58:GLU:HB3   | 25:M:61:TYR:HB2  | 2.00                     | 0.42              |
| 1:2:1386:A:OP2    | 22:D:160:SER:OG  | 2.34                     | 0.42              |
| 1:2:1716:C:H2'    | 1:2:1717:C:C6    | 2.55                     | 0.42              |
| 1:2:1753:C:H2'    | 1:2:1754:G:H8    | 1.85                     | 0.42              |
| 2:A:176:TRP:HA    | 2:A:202:TYR:CE2  | 2.55                     | 0.42              |
| 22:D:11:PHE:HD2   | 31:U:84:ILE:HG12 | 1.85                     | 0.42              |
| 28:R:13:ALA:HA    | 28:R:16:ILE:HG23 | 1.94                     | 0.42              |
| 1:2:500:A:H3'     | 1:2:501:C:C6     | 2.54                     | 0.42              |
| 1:2:1213:C:H2'    | 1:2:1214:A:C8    | 2.55                     | 0.42              |
| 1:2:1470:C:OP2    | 23:F:59:LYS:NZ   | 2.39                     | 0.42              |
| 5:E:89:VAL:HG22   | 5:E:100:ARG:HE   | 1.84                     | 0.42              |
| 6:G:54:GLY:H      | 6:G:110:ASN:HB2  | 1.85                     | 0.42              |
| 22:D:24:PHE:CE1   | 24:K:68:TYR:HD2  | 2.37                     | 0.42              |
| 1:2:1430:C:H2'    | 1:2:1431:G:H8    | 1.83                     | 0.42              |
| 1:2:1645:C:H5'    | 27:Q:139:ALA:HA  | 2.02                     | 0.42              |
| 1:2:1703:C:H2'    | 1:2:1704:C:O4'   | 2.19                     | 0.42              |
| 1:2:1735:A:H62    | 1:2:1799:G:H21   | 1.66                     | 0.42              |
| 3:B:82:ARG:NH1    | 3:B:188:LEU:O    | 2.40                     | 0.42              |
| 22:D:22:ASN:ND2   | 22:D:37:VAL:CG2  | 2.83                     | 0.42              |
| 35:g:106:LYS:HB3  | 35:g:125:ARG:HB2 | 2.00                     | 0.42              |
| 35:g:174:VAL:HB   | 35:g:188:HIS:HB2 | 2.02                     | 0.42              |
| 10:L:40:ILE:HD12  | 10:L:40:ILE:HA   | 1.83                     | 0.42              |
| 22:D:108:LYS:O    | 22:D:113:LEU:N   | 2.49                     | 0.42              |
| 32:Z:90:GLU:O     | 32:Z:93:SER:OG   | 2.32                     | 0.42              |
| 35:g:193:GLY:HA3  | 35:g:212:LYS:HB3 | 2.02                     | 0.42              |
| 1:2:981:A:H2'     | 1:2:982:G:C8     | 2.55                     | 0.41              |
| 4:C:102:LEU:HG    | 4:C:130:ILE:HG12 | 2.02                     | 0.41              |
| 6:G:85:ARG:HE     | 6:G:87:ARG:NH1   | 2.18                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:D:24:PHE:HB2   | 24:K:63:ALA:CB    | 2.50                     | 0.41              |
| 27:Q:16:LYS:NZ    | 27:Q:123:ASP:OD2  | 2.52                     | 0.41              |
| 1:2:625:G:O6      | 15:X:64:SER:N     | 2.46                     | 0.41              |
| 1:2:1373:C:OP1    | 28:R:7:LYS:CG     | 2.68                     | 0.41              |
| 5:E:79:ASP:HB3    | 5:E:82:TYR:HB2    | 2.02                     | 0.41              |
| 10:L:35:ARG:NH2   | 10:L:53:GLY:O     | 2.53                     | 0.41              |
| 24:K:31:LYS:HA    | 24:K:41:PRO:HA    | 2.02                     | 0.41              |
| 1:2:194:C:H2'     | 1:2:195:C:H6      | 1.85                     | 0.41              |
| 1:2:352:U:H2'     | 1:2:353:C:C6      | 2.55                     | 0.41              |
| 1:2:920:A:H4'     | 14:W:57:ARG:HG2   | 2.01                     | 0.41              |
| 1:2:1600:G:C5     | 1:2:1602:U:H1'    | 2.55                     | 0.41              |
| 3:B:48:LEU:O      | 3:B:65:ARG:NH2    | 2.53                     | 0.41              |
| 17:a:24:THR:N     | 17:a:72:HIS:O     | 2.53                     | 0.41              |
| 23:F:29:GLN:N     | 23:F:110:GLN:OE1  | 2.36                     | 0.41              |
| 25:M:53:ALA:HB2   | 25:M:85:LEU:HD12  | 2.00                     | 0.41              |
| 32:Z:103:HIS:CD2  | 32:Z:104:ARG:H    | 2.38                     | 0.41              |
| 35:g:270:LEU:HD13 | 35:g:310:TRP:CE2  | 2.55                     | 0.41              |
| 1:2:895:G:H2'     | 1:2:896:U:C6      | 2.55                     | 0.41              |
| 1:2:1253:A:N6     | 1:2:1665:G:O2'    | 2.53                     | 0.41              |
| 1:2:1378:A:OP2    | 2:A:102:ARG:NH2   | 2.54                     | 0.41              |
| 3:B:144:LYS:HG2   | 3:B:208:HIS:HD2   | 1.86                     | 0.41              |
| 7:H:84:GLU:HA     | 7:H:87:PHE:HE2    | 1.86                     | 0.41              |
| 20:e:53:LYS:NZ    | 20:e:59:SER:OXT   | 2.46                     | 0.41              |
| 28:R:41:ILE:HD13  | 28:R:47:ARG:HB2   | 2.03                     | 0.41              |
| 35:g:82:SER:OG    | 35:g:83:TRP:N     | 2.54                     | 0.41              |
| 1:2:1275:G:H4'    | 1:2:1322:G:H22    | 1.85                     | 0.41              |
| 2:A:104:THR:O     | 2:A:107:THR:OG1   | 2.29                     | 0.41              |
| 7:H:159:ASP:OD1   | 7:H:160:LYS:N     | 2.53                     | 0.41              |
| 10:L:73:LEU:HD12  | 10:L:140:PHE:HE2  | 1.85                     | 0.41              |
| 14:W:111:MET:HE2  | 14:W:111:MET:HB3  | 1.79                     | 0.41              |
| 1:2:1306:U:H2'    | 1:2:1307:U:O4'    | 2.20                     | 0.41              |
| 3:B:28:LYS:HD2    | 3:B:48:LEU:HG     | 2.02                     | 0.41              |
| 3:B:133:TYR:CD1   | 3:B:221:PRO:HD2   | 2.56                     | 0.41              |
| 6:G:210:ALA:O     | 6:G:214:ALA:N     | 2.53                     | 0.41              |
| 10:L:150:GLY:HA3  | 11:N:133:ARG:HH21 | 1.85                     | 0.41              |
| 15:X:7:LEU:HD23   | 15:X:7:LEU:HA     | 1.81                     | 0.41              |
| 24:K:52:LEU:HD23  | 24:K:52:LEU:HA    | 1.89                     | 0.41              |
| 35:g:51:ASN:OD1   | 35:g:51:ASN:N     | 2.53                     | 0.41              |
| 1:2:298:G:H2'     | 1:2:299:A:H8      | 1.85                     | 0.41              |
| 1:2:674:C:H2'     | 1:2:675:U:C6      | 2.55                     | 0.41              |
| 1:2:1301:A:H2'    | 1:2:1303:C:C6     | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1562:C:H2'   | 1:2:1563:G:H8    | 1.85                     | 0.41              |
| 1:2:1587:G:C6    | 30:T:67:ARG:HD3  | 2.56                     | 0.41              |
| 3:B:216:LYS:HB3  | 3:B:217:MET:H    | 1.66                     | 0.41              |
| 6:G:141:ILE:HG21 | 6:G:153:VAL:HG13 | 2.02                     | 0.41              |
| 7:H:58:LYS:O     | 7:H:90:LYS:HB3   | 2.20                     | 0.41              |
| 9:J:84:ILE:HG13  | 9:J:86:VAL:HG23  | 2.03                     | 0.41              |
| 22:D:22:ASN:HD22 | 22:D:22:ASN:HA   | 1.65                     | 0.41              |
| 25:M:64:LEU:HD13 | 34:f:106:TYR:HB2 | 2.03                     | 0.41              |
| 28:R:13:ALA:C    | 28:R:16:ILE:CG2  | 2.93                     | 0.41              |
| 31:U:34:LYS:HD3  | 31:U:34:LYS:C    | 2.46                     | 0.41              |
| 1:2:527:C:H2'    | 1:2:528:A:C8     | 2.55                     | 0.41              |
| 1:2:1362:U:H5''  | 1:2:1363:C:C5    | 2.55                     | 0.41              |
| 2:A:90:PHE:CD2   | 2:A:175:TRP:CZ3  | 3.08                     | 0.41              |
| 9:J:36:GLY:HA3   | 9:J:111:GLN:HE22 | 1.85                     | 0.41              |
| 9:J:111:GLN:NE2  | 9:J:127:ARG:HB2  | 2.36                     | 0.41              |
| 14:W:75:ILE:CD1  | 14:W:93:LEU:CD1  | 2.84                     | 0.41              |
| 23:F:197:GLU:O   | 23:F:201:LYS:NZ  | 2.44                     | 0.41              |
| 24:K:4:PRO:HD2   | 24:K:7:ASN:HD22  | 1.86                     | 0.41              |
| 1:2:146:G:OP1    | 6:G:143:LYS:NZ   | 2.53                     | 0.41              |
| 1:2:155:G:H2'    | 1:2:156:G:C8     | 2.56                     | 0.41              |
| 1:2:218:U:O4     | 1:2:303:C:N3     | 2.54                     | 0.41              |
| 1:2:314:U:H2'    | 1:2:315:C:H6     | 1.86                     | 0.41              |
| 1:2:643:A:H4'    | 1:2:644:G:H5'    | 2.03                     | 0.41              |
| 1:2:1239:U:H4'   | 26:P:124:LYS:HB3 | 2.03                     | 0.41              |
| 1:2:1266:C:OP1   | 34:f:80:ARG:NH2  | 2.53                     | 0.41              |
| 2:A:58:LEU:CD1   | 2:A:174:MET:HE1  | 2.50                     | 0.41              |
| 2:A:90:PHE:CE1   | 2:A:175:TRP:CE3  | 3.08                     | 0.41              |
| 7:H:116:ARG:HA   | 7:H:117:PRO:HD3  | 1.96                     | 0.41              |
| 15:X:49:GLY:HA2  | 15:X:74:LEU:HA   | 2.03                     | 0.41              |
| 16:Y:61:ARG:HA   | 16:Y:61:ARG:HD2  | 1.82                     | 0.41              |
| 19:d:23:VAL:HB   | 24:K:64:TRP:NE1  | 2.36                     | 0.41              |
| 22:D:24:PHE:CE1  | 24:K:68:TYR:CD2  | 3.09                     | 0.41              |
| 30:T:116:ASP:OD2 | 30:T:122:LYS:N   | 2.54                     | 0.41              |
| 31:U:27:ARG:HG2  | 31:U:82:MET:HE1  | 2.01                     | 0.41              |
| 35:g:112:ALA:HB2 | 35:g:155:ARG:HA  | 2.03                     | 0.41              |
| 1:2:109:U:O2'    | 10:L:71:ARG:NH2  | 2.51                     | 0.41              |
| 1:2:1410:C:H2'   | 1:2:1411:G:C8    | 2.56                     | 0.41              |
| 1:2:1482:C:H5''  | 19:d:54:LYS:CE   | 2.51                     | 0.41              |
| 1:2:1543:U:OP2   | 30:T:62:ARG:NH2  | 2.54                     | 0.41              |
| 1:2:1667:U:H2'   | 1:2:1668:U:C6    | 2.56                     | 0.41              |
| 2:A:77:ILE:HD12  | 2:A:122:LEU:HD11 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:G:85:ARG:NH2   | 16:Y:118:ARG:HD3  | 2.35                     | 0.41              |
| 7:H:144:ILE:HB   | 14:W:52:ILE:HB    | 2.03                     | 0.41              |
| 14:W:128:PHE:HE2 | 14:W:130:PHE:HE1  | 1.69                     | 0.41              |
| 1:2:191:A:OP2    | 8:I:142:SER:OG    | 2.39                     | 0.40              |
| 1:2:1091:C:N4    | 1:2:1092:G:O6     | 2.54                     | 0.40              |
| 1:2:1373:C:OP1   | 28:R:7:LYS:HG3    | 2.20                     | 0.40              |
| 1:2:685:A:N7     | 1:2:918:U:O2      | 2.55                     | 0.40              |
| 1:2:1082:A:HO2'  | 1:2:1842:C:HO2'   | 1.60                     | 0.40              |
| 1:2:1569:A:O2'   | 1:2:1626:C:O2     | 2.36                     | 0.40              |
| 2:A:63:ARG:HG2   | 2:A:185:MET:HE1   | 2.02                     | 0.40              |
| 3:B:32:ASP:O     | 3:B:96:CYS:N      | 2.51                     | 0.40              |
| 6:G:98:ARG:HH22  | 6:G:103:ASP:HB2   | 1.86                     | 0.40              |
| 14:W:41:MET:O    | 14:W:45:GLY:N     | 2.53                     | 0.40              |
| 27:Q:12:VAL:HG21 | 27:Q:91:ALA:HA    | 2.01                     | 0.40              |
| 28:R:22:THR:HA   | 35:g:212:LYS:HE3  | 2.02                     | 0.40              |
| 1:2:56:G:OP1     | 16:Y:111:LYS:NZ   | 2.54                     | 0.40              |
| 2:A:122:LEU:HD12 | 2:A:122:LEU:HA    | 1.85                     | 0.40              |
| 4:C:63:VAL:N     | 4:C:90:GLU:OE2    | 2.44                     | 0.40              |
| 8:I:60:LEU:HA    | 8:I:60:LEU:HD23   | 1.90                     | 0.40              |
| 1:2:1256:G:O6    | 19:d:31:ILE:HD11  | 2.22                     | 0.40              |
| 1:2:1598:G:H5'   | 32:Z:80:ARG:HE    | 1.87                     | 0.40              |
| 4:C:83:LEU:C     | 4:C:83:LEU:CD1    | 2.89                     | 0.40              |
| 14:W:61:ILE:HD13 | 14:W:61:ILE:HG21  | 1.90                     | 0.40              |
| 16:Y:10:ARG:HH11 | 16:Y:10:ARG:HD2   | 1.76                     | 0.40              |
| 23:F:85:LYS:O    | 23:F:89:THR:OG1   | 2.33                     | 0.40              |
| 26:P:108:LYS:NZ  | 29:S:116:LYS:O    | 2.37                     | 0.40              |
| 28:R:13:ALA:O    | 28:R:16:ILE:CG2   | 2.65                     | 0.40              |
| 1:2:71:G:H1'     | 1:2:79:A:H61      | 1.86                     | 0.40              |
| 1:2:554:A:H2'    | 1:2:556:U:C6      | 2.56                     | 0.40              |
| 1:2:1402:A:H2'   | 1:2:1405:A:H62    | 1.87                     | 0.40              |
| 1:2:1634:A:H4'   | 29:S:142:ARG:HH22 | 1.86                     | 0.40              |
| 2:A:121:LEU:HD12 | 2:A:143:PRO:HB2   | 2.02                     | 0.40              |
| 3:B:30:TRP:HE1   | 12:O:18:GLY:HA2   | 1.85                     | 0.40              |
| 3:B:129:THR:OG1  | 3:B:131:ASP:OD1   | 2.32                     | 0.40              |
| 4:C:95:ASP:O     | 4:C:99:GLY:HA2    | 2.22                     | 0.40              |
| 4:C:136:HIS:ND1  | 4:C:136:HIS:N     | 2.69                     | 0.40              |
| 7:H:60:ILE:N     | 7:H:91:HIS:O      | 2.52                     | 0.40              |
| 9:J:87:LEU:HD21  | 9:J:100:LEU:HD11  | 2.03                     | 0.40              |
| 14:W:15:ASN:HD21 | 14:W:71:LYS:HD2   | 1.87                     | 0.40              |
| 14:W:102:ILE:HB  | 14:W:113:HIS:HB3  | 2.03                     | 0.40              |
| 16:Y:105:LYS:HD2 | 16:Y:105:LYS:HA   | 1.91                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:D:205:PRO:HA   | 28:R:42:PRO:HG3   | 2.04                     | 0.40              |
| 25:M:93:LYS:HB3   | 25:M:101:ARG:HE   | 1.85                     | 0.40              |
| 35:g:201:SER:HB2  | 35:g:206:LEU:HB2  | 2.03                     | 0.40              |
| 35:g:218:LEU:HD23 | 35:g:227:LEU:HD23 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 2     | 1654/1868 (88%) | 530 (32%)         | 0               |

All (530) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 2   | A    |
| 1   | 2     | 3   | C    |
| 1   | 2     | 4   | C    |
| 1   | 2     | 9   | U    |
| 1   | 2     | 10  | G    |
| 1   | 2     | 17  | C    |
| 1   | 2     | 25  | A    |
| 1   | 2     | 26  | U    |
| 1   | 2     | 33  | G    |
| 1   | 2     | 41  | G    |
| 1   | 2     | 42  | A    |
| 1   | 2     | 44  | U    |
| 1   | 2     | 46  | A    |
| 1   | 2     | 47  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 56  | G    |
| 1   | 2     | 58  | C    |
| 1   | 2     | 59  | U    |
| 1   | 2     | 60  | A    |
| 1   | 2     | 61  | A    |
| 1   | 2     | 62  | G    |
| 1   | 2     | 65  | C    |
| 1   | 2     | 66  | G    |
| 1   | 2     | 67  | C    |
| 1   | 2     | 68  | A    |
| 1   | 2     | 69  | C    |
| 1   | 2     | 72  | C    |
| 1   | 2     | 73  | C    |
| 1   | 2     | 74  | G    |
| 1   | 2     | 75  | G    |
| 1   | 2     | 76  | U    |
| 1   | 2     | 77  | A    |
| 1   | 2     | 79  | A    |
| 1   | 2     | 102 | A    |
| 1   | 2     | 103 | A    |
| 1   | 2     | 110 | U    |
| 1   | 2     | 113 | G    |
| 1   | 2     | 114 | G    |
| 1   | 2     | 115 | U    |
| 1   | 2     | 116 | U    |
| 1   | 2     | 119 | U    |
| 1   | 2     | 127 | C    |
| 1   | 2     | 128 | U    |
| 1   | 2     | 129 | C    |
| 1   | 2     | 143 | U    |
| 1   | 2     | 144 | U    |
| 1   | 2     | 153 | G    |
| 1   | 2     | 154 | U    |
| 1   | 2     | 155 | G    |
| 1   | 2     | 160 | U    |
| 1   | 2     | 175 | A    |
| 1   | 2     | 181 | A    |
| 1   | 2     | 182 | C    |
| 1   | 2     | 183 | G    |
| 1   | 2     | 184 | G    |
| 1   | 2     | 188 | C    |
| 1   | 2     | 191 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 196 | C    |
| 1   | 2     | 206 | G    |
| 1   | 2     | 213 | G    |
| 1   | 2     | 214 | U    |
| 1   | 2     | 215 | G    |
| 1   | 2     | 216 | C    |
| 1   | 2     | 217 | A    |
| 1   | 2     | 290 | U    |
| 1   | 2     | 291 | G    |
| 1   | 2     | 292 | A    |
| 1   | 2     | 295 | C    |
| 1   | 2     | 302 | A    |
| 1   | 2     | 305 | U    |
| 1   | 2     | 306 | C    |
| 1   | 2     | 307 | G    |
| 1   | 2     | 308 | G    |
| 1   | 2     | 310 | C    |
| 1   | 2     | 312 | G    |
| 1   | 2     | 313 | A    |
| 1   | 2     | 315 | C    |
| 1   | 2     | 318 | A    |
| 1   | 2     | 319 | C    |
| 1   | 2     | 320 | G    |
| 1   | 2     | 321 | C    |
| 1   | 2     | 332 | G    |
| 1   | 2     | 333 | G    |
| 1   | 2     | 335 | G    |
| 1   | 2     | 338 | G    |
| 1   | 2     | 342 | C    |
| 1   | 2     | 347 | G    |
| 1   | 2     | 350 | C    |
| 1   | 2     | 360 | A    |
| 1   | 2     | 362 | C    |
| 1   | 2     | 364 | A    |
| 1   | 2     | 368 | U    |
| 1   | 2     | 369 | C    |
| 1   | 2     | 370 | G    |
| 1   | 2     | 377 | G    |
| 1   | 2     | 381 | C    |
| 1   | 2     | 382 | C    |
| 1   | 2     | 383 | G    |
| 1   | 2     | 385 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 386 | C    |
| 1   | 2     | 398 | A    |
| 1   | 2     | 399 | C    |
| 1   | 2     | 400 | C    |
| 1   | 2     | 407 | G    |
| 1   | 2     | 408 | A    |
| 1   | 2     | 409 | C    |
| 1   | 2     | 418 | A    |
| 1   | 2     | 420 | G    |
| 1   | 2     | 421 | G    |
| 1   | 2     | 428 | U    |
| 1   | 2     | 429 | C    |
| 1   | 2     | 436 | G    |
| 1   | 2     | 438 | G    |
| 1   | 2     | 441 | C    |
| 1   | 2     | 447 | A    |
| 1   | 2     | 448 | A    |
| 1   | 2     | 450 | C    |
| 1   | 2     | 464 | A    |
| 1   | 2     | 465 | A    |
| 1   | 2     | 466 | G    |
| 1   | 2     | 471 | G    |
| 1   | 2     | 472 | C    |
| 1   | 2     | 473 | A    |
| 1   | 2     | 474 | G    |
| 1   | 2     | 476 | A    |
| 1   | 2     | 482 | G    |
| 1   | 2     | 483 | C    |
| 1   | 2     | 487 | U    |
| 1   | 2     | 489 | A    |
| 1   | 2     | 492 | C    |
| 1   | 2     | 500 | A    |
| 1   | 2     | 502 | C    |
| 1   | 2     | 512 | A    |
| 1   | 2     | 517 | C    |
| 1   | 2     | 523 | A    |
| 1   | 2     | 525 | A    |
| 1   | 2     | 532 | C    |
| 1   | 2     | 534 | G    |
| 1   | 2     | 536 | A    |
| 1   | 2     | 537 | C    |
| 1   | 2     | 544 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 546 | G    |
| 1   | 2     | 548 | C    |
| 1   | 2     | 549 | C    |
| 1   | 2     | 552 | G    |
| 1   | 2     | 553 | U    |
| 1   | 2     | 554 | A    |
| 1   | 2     | 555 | A    |
| 1   | 2     | 556 | U    |
| 1   | 2     | 559 | G    |
| 1   | 2     | 560 | A    |
| 1   | 2     | 563 | G    |
| 1   | 2     | 564 | A    |
| 1   | 2     | 568 | C    |
| 1   | 2     | 576 | A    |
| 1   | 2     | 583 | A    |
| 1   | 2     | 587 | A    |
| 1   | 2     | 588 | G    |
| 1   | 2     | 589 | G    |
| 1   | 2     | 590 | A    |
| 1   | 2     | 591 | U    |
| 1   | 2     | 593 | C    |
| 1   | 2     | 594 | A    |
| 1   | 2     | 595 | U    |
| 1   | 2     | 596 | U    |
| 1   | 2     | 598 | G    |
| 1   | 2     | 600 | G    |
| 1   | 2     | 603 | C    |
| 1   | 2     | 604 | A    |
| 1   | 2     | 605 | A    |
| 1   | 2     | 607 | U    |
| 1   | 2     | 608 | C    |
| 1   | 2     | 614 | C    |
| 1   | 2     | 615 | C    |
| 1   | 2     | 617 | G    |
| 1   | 2     | 621 | C    |
| 1   | 2     | 627 | U    |
| 1   | 2     | 629 | A    |
| 1   | 2     | 638 | C    |
| 1   | 2     | 639 | C    |
| 1   | 2     | 640 | A    |
| 1   | 2     | 643 | A    |
| 1   | 2     | 644 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 655 | A    |
| 1   | 2     | 658 | U    |
| 1   | 2     | 660 | C    |
| 1   | 2     | 664 | A    |
| 1   | 2     | 668 | A    |
| 1   | 2     | 669 | A    |
| 1   | 2     | 671 | A    |
| 1   | 2     | 672 | A    |
| 1   | 2     | 673 | G    |
| 1   | 2     | 683 | G    |
| 1   | 2     | 684 | G    |
| 1   | 2     | 685 | A    |
| 1   | 2     | 687 | C    |
| 1   | 2     | 688 | U    |
| 1   | 2     | 748 | C    |
| 1   | 2     | 749 | U    |
| 1   | 2     | 750 | C    |
| 1   | 2     | 751 | G    |
| 1   | 2     | 792 | C    |
| 1   | 2     | 793 | G    |
| 1   | 2     | 794 | A    |
| 1   | 2     | 797 | C    |
| 1   | 2     | 798 | G    |
| 1   | 2     | 801 | U    |
| 1   | 2     | 809 | A    |
| 1   | 2     | 810 | A    |
| 1   | 2     | 812 | A    |
| 1   | 2     | 821 | G    |
| 1   | 2     | 822 | U    |
| 1   | 2     | 823 | U    |
| 1   | 2     | 824 | C    |
| 1   | 2     | 827 | A    |
| 1   | 2     | 830 | A    |
| 1   | 2     | 834 | C    |
| 1   | 2     | 844 | U    |
| 1   | 2     | 847 | A    |
| 1   | 2     | 852 | G    |
| 1   | 2     | 856 | C    |
| 1   | 2     | 859 | G    |
| 1   | 2     | 869 | A    |
| 1   | 2     | 871 | U    |
| 1   | 2     | 872 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 873 | G    |
| 1   | 2     | 874 | G    |
| 1   | 2     | 878 | G    |
| 1   | 2     | 879 | C    |
| 1   | 2     | 880 | G    |
| 1   | 2     | 882 | U    |
| 1   | 2     | 887 | U    |
| 1   | 2     | 888 | U    |
| 1   | 2     | 890 | U    |
| 1   | 2     | 894 | G    |
| 1   | 2     | 898 | U    |
| 1   | 2     | 903 | A    |
| 1   | 2     | 909 | G    |
| 1   | 2     | 912 | C    |
| 1   | 2     | 913 | A    |
| 1   | 2     | 914 | U    |
| 1   | 2     | 915 | G    |
| 1   | 2     | 917 | U    |
| 1   | 2     | 918 | U    |
| 1   | 2     | 919 | A    |
| 1   | 2     | 920 | A    |
| 1   | 2     | 921 | G    |
| 1   | 2     | 926 | A    |
| 1   | 2     | 933 | G    |
| 1   | 2     | 934 | G    |
| 1   | 2     | 938 | A    |
| 1   | 2     | 943 | U    |
| 1   | 2     | 952 | G    |
| 1   | 2     | 954 | U    |
| 1   | 2     | 959 | G    |
| 1   | 2     | 962 | A    |
| 1   | 2     | 963 | A    |
| 1   | 2     | 967 | C    |
| 1   | 2     | 969 | U    |
| 1   | 2     | 970 | G    |
| 1   | 2     | 971 | G    |
| 1   | 2     | 973 | C    |
| 1   | 2     | 978 | G    |
| 1   | 2     | 981 | A    |
| 1   | 2     | 982 | G    |
| 1   | 2     | 988 | C    |
| 1   | 2     | 989 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 990  | A    |
| 1   | 2     | 992  | A    |
| 1   | 2     | 999  | G    |
| 1   | 2     | 1001 | A    |
| 1   | 2     | 1002 | U    |
| 1   | 2     | 1017 | U    |
| 1   | 2     | 1023 | A    |
| 1   | 2     | 1027 | A    |
| 1   | 2     | 1029 | G    |
| 1   | 2     | 1030 | A    |
| 1   | 2     | 1040 | G    |
| 1   | 2     | 1041 | G    |
| 1   | 2     | 1042 | A    |
| 1   | 2     | 1045 | U    |
| 1   | 2     | 1049 | A    |
| 1   | 2     | 1050 | A    |
| 1   | 2     | 1053 | C    |
| 1   | 2     | 1060 | A    |
| 1   | 2     | 1067 | C    |
| 1   | 2     | 1081 | U    |
| 1   | 2     | 1083 | A    |
| 1   | 2     | 1085 | C    |
| 1   | 2     | 1088 | U    |
| 1   | 2     | 1096 | G    |
| 1   | 2     | 1114 | U    |
| 1   | 2     | 1115 | U    |
| 1   | 2     | 1116 | C    |
| 1   | 2     | 1118 | C    |
| 1   | 2     | 1119 | A    |
| 1   | 2     | 1120 | U    |
| 1   | 2     | 1121 | G    |
| 1   | 2     | 1123 | C    |
| 1   | 2     | 1133 | A    |
| 1   | 2     | 1137 | U    |
| 1   | 2     | 1138 | C    |
| 1   | 2     | 1139 | C    |
| 1   | 2     | 1143 | A    |
| 1   | 2     | 1148 | A    |
| 1   | 2     | 1149 | A    |
| 1   | 2     | 1153 | C    |
| 1   | 2     | 1154 | U    |
| 1   | 2     | 1156 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1157 | G    |
| 1   | 2     | 1166 | G    |
| 1   | 2     | 1168 | G    |
| 1   | 2     | 1170 | A    |
| 1   | 2     | 1171 | G    |
| 1   | 2     | 1195 | A    |
| 1   | 2     | 1198 | G    |
| 1   | 2     | 1207 | G    |
| 1   | 2     | 1208 | A    |
| 1   | 2     | 1211 | G    |
| 1   | 2     | 1215 | C    |
| 1   | 2     | 1217 | A    |
| 1   | 2     | 1221 | G    |
| 1   | 2     | 1224 | G    |
| 1   | 2     | 1227 | G    |
| 1   | 2     | 1232 | U    |
| 1   | 2     | 1235 | G    |
| 1   | 2     | 1236 | G    |
| 1   | 2     | 1238 | U    |
| 1   | 2     | 1242 | U    |
| 1   | 2     | 1243 | U    |
| 1   | 2     | 1245 | G    |
| 1   | 2     | 1251 | A    |
| 1   | 2     | 1253 | A    |
| 1   | 2     | 1254 | C    |
| 1   | 2     | 1257 | G    |
| 1   | 2     | 1259 | A    |
| 1   | 2     | 1260 | A    |
| 1   | 2     | 1261 | C    |
| 1   | 2     | 1270 | G    |
| 1   | 2     | 1274 | G    |
| 1   | 2     | 1275 | G    |
| 1   | 2     | 1283 | C    |
| 1   | 2     | 1284 | A    |
| 1   | 2     | 1286 | G    |
| 1   | 2     | 1288 | U    |
| 1   | 2     | 1294 | G    |
| 1   | 2     | 1298 | G    |
| 1   | 2     | 1301 | A    |
| 1   | 2     | 1302 | G    |
| 1   | 2     | 1303 | C    |
| 1   | 2     | 1304 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1308 | U    |
| 1   | 2     | 1309 | C    |
| 1   | 2     | 1313 | A    |
| 1   | 2     | 1314 | U    |
| 1   | 2     | 1315 | U    |
| 1   | 2     | 1317 | C    |
| 1   | 2     | 1320 | G    |
| 1   | 2     | 1321 | G    |
| 1   | 2     | 1322 | G    |
| 1   | 2     | 1323 | U    |
| 1   | 2     | 1327 | G    |
| 1   | 2     | 1329 | U    |
| 1   | 2     | 1330 | G    |
| 1   | 2     | 1331 | C    |
| 1   | 2     | 1343 | U    |
| 1   | 2     | 1344 | A    |
| 1   | 2     | 1348 | G    |
| 1   | 2     | 1354 | G    |
| 1   | 2     | 1358 | U    |
| 1   | 2     | 1363 | C    |
| 1   | 2     | 1364 | U    |
| 1   | 2     | 1366 | G    |
| 1   | 2     | 1369 | A    |
| 1   | 2     | 1371 | U    |
| 1   | 2     | 1373 | C    |
| 1   | 2     | 1377 | U    |
| 1   | 2     | 1378 | A    |
| 1   | 2     | 1380 | C    |
| 1   | 2     | 1382 | A    |
| 1   | 2     | 1401 | A    |
| 1   | 2     | 1402 | A    |
| 1   | 2     | 1403 | C    |
| 1   | 2     | 1404 | U    |
| 1   | 2     | 1405 | A    |
| 1   | 2     | 1406 | G    |
| 1   | 2     | 1411 | G    |
| 1   | 2     | 1414 | A    |
| 1   | 2     | 1415 | C    |
| 1   | 2     | 1416 | C    |
| 1   | 2     | 1426 | U    |
| 1   | 2     | 1428 | G    |
| 1   | 2     | 1429 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1430 | C    |
| 1   | 2     | 1431 | G    |
| 1   | 2     | 1432 | U    |
| 1   | 2     | 1439 | A    |
| 1   | 2     | 1441 | U    |
| 1   | 2     | 1442 | U    |
| 1   | 2     | 1444 | U    |
| 1   | 2     | 1446 | A    |
| 1   | 2     | 1452 | A    |
| 1   | 2     | 1454 | A    |
| 1   | 2     | 1462 | U    |
| 1   | 2     | 1463 | U    |
| 1   | 2     | 1465 | A    |
| 1   | 2     | 1466 | G    |
| 1   | 2     | 1474 | A    |
| 1   | 2     | 1476 | A    |
| 1   | 2     | 1477 | U    |
| 1   | 2     | 1478 | U    |
| 1   | 2     | 1486 | A    |
| 1   | 2     | 1487 | A    |
| 1   | 2     | 1489 | A    |
| 1   | 2     | 1494 | U    |
| 1   | 2     | 1495 | G    |
| 1   | 2     | 1498 | A    |
| 1   | 2     | 1500 | G    |
| 1   | 2     | 1505 | U    |
| 1   | 2     | 1506 | A    |
| 1   | 2     | 1507 | G    |
| 1   | 2     | 1510 | G    |
| 1   | 2     | 1512 | C    |
| 1   | 2     | 1516 | G    |
| 1   | 2     | 1517 | G    |
| 1   | 2     | 1518 | C    |
| 1   | 2     | 1519 | U    |
| 1   | 2     | 1520 | G    |
| 1   | 2     | 1521 | C    |
| 1   | 2     | 1522 | A    |
| 1   | 2     | 1523 | C    |
| 1   | 2     | 1524 | G    |
| 1   | 2     | 1526 | G    |
| 1   | 2     | 1531 | A    |
| 1   | 2     | 1533 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1534 | C    |
| 1   | 2     | 1535 | U    |
| 1   | 2     | 1536 | G    |
| 1   | 2     | 1544 | C    |
| 1   | 2     | 1548 | G    |
| 1   | 2     | 1559 | C    |
| 1   | 2     | 1560 | U    |
| 1   | 2     | 1566 | G    |
| 1   | 2     | 1567 | G    |
| 1   | 2     | 1570 | G    |
| 1   | 2     | 1572 | C    |
| 1   | 2     | 1573 | G    |
| 1   | 2     | 1574 | C    |
| 1   | 2     | 1579 | A    |
| 1   | 2     | 1580 | A    |
| 1   | 2     | 1581 | C    |
| 1   | 2     | 1582 | C    |
| 1   | 2     | 1585 | U    |
| 1   | 2     | 1586 | U    |
| 1   | 2     | 1587 | G    |
| 1   | 2     | 1588 | A    |
| 1   | 2     | 1598 | G    |
| 1   | 2     | 1599 | U    |
| 1   | 2     | 1600 | G    |
| 1   | 2     | 1601 | A    |
| 1   | 2     | 1602 | U    |
| 1   | 2     | 1603 | G    |
| 1   | 2     | 1606 | G    |
| 1   | 2     | 1607 | A    |
| 1   | 2     | 1612 | G    |
| 1   | 2     | 1615 | U    |
| 1   | 2     | 1617 | G    |
| 1   | 2     | 1618 | C    |
| 1   | 2     | 1619 | A    |
| 1   | 2     | 1621 | U    |
| 1   | 2     | 1623 | A    |
| 1   | 2     | 1630 | A    |
| 1   | 2     | 1631 | U    |
| 1   | 2     | 1632 | G    |
| 1   | 2     | 1635 | C    |
| 1   | 2     | 1648 | G    |
| 1   | 2     | 1649 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1650 | A    |
| 1   | 2     | 1654 | G    |
| 1   | 2     | 1660 | C    |
| 1   | 2     | 1663 | A    |
| 1   | 2     | 1665 | G    |
| 1   | 2     | 1671 | G    |
| 1   | 2     | 1675 | A    |
| 1   | 2     | 1678 | A    |
| 1   | 2     | 1683 | C    |
| 1   | 2     | 1695 | A    |
| 1   | 2     | 1698 | C    |
| 1   | 2     | 1699 | A    |
| 1   | 2     | 1701 | C    |
| 1   | 2     | 1704 | C    |
| 1   | 2     | 1719 | A    |
| 1   | 2     | 1721 | U    |
| 1   | 2     | 1722 | G    |
| 1   | 2     | 1725 | U    |
| 1   | 2     | 1728 | U    |
| 1   | 2     | 1729 | U    |
| 1   | 2     | 1730 | U    |
| 1   | 2     | 1748 | G    |
| 1   | 2     | 1757 | G    |
| 1   | 2     | 1761 | U    |
| 1   | 2     | 1778 | C    |
| 1   | 2     | 1783 | C    |
| 1   | 2     | 1784 | G    |
| 1   | 2     | 1785 | C    |
| 1   | 2     | 1786 | U    |
| 1   | 2     | 1799 | G    |
| 1   | 2     | 1807 | C    |
| 1   | 2     | 1813 | A    |
| 1   | 2     | 1824 | A    |
| 1   | 2     | 1825 | A    |
| 1   | 2     | 1829 | G    |
| 1   | 2     | 1831 | A    |
| 1   | 2     | 1835 | A    |
| 1   | 2     | 1836 | G    |
| 1   | 2     | 1838 | U    |
| 1   | 2     | 1839 | U    |
| 1   | 2     | 1840 | U    |
| 1   | 2     | 1849 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1850 | A    |
| 1   | 2     | 1852 | C    |
| 1   | 2     | 1856 | C    |
| 1   | 2     | 1859 | A    |
| 1   | 2     | 1860 | A    |
| 1   | 2     | 1861 | G    |
| 1   | 2     | 1862 | G    |
| 1   | 2     | 1863 | A    |
| 1   | 2     | 1865 | C    |
| 1   | 2     | 1866 | A    |
| 1   | 2     | 1868 | U    |
| 1   | 2     | 1869 | A    |

There are no RNA pucker outliers to report.

## 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 [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

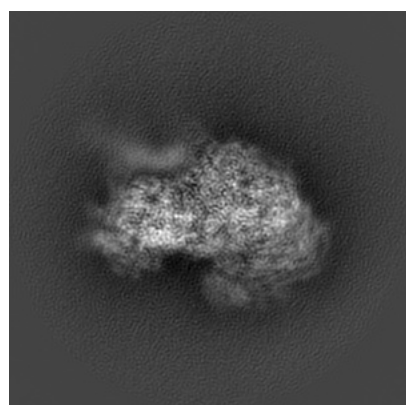
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4352. These allow visual inspection of the internal detail of the map and identification of artifacts.

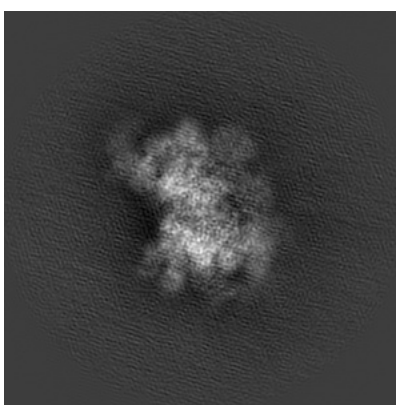
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

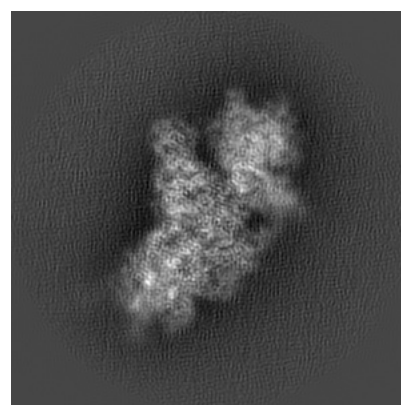
#### 6.1.1 Primary map



X



Y

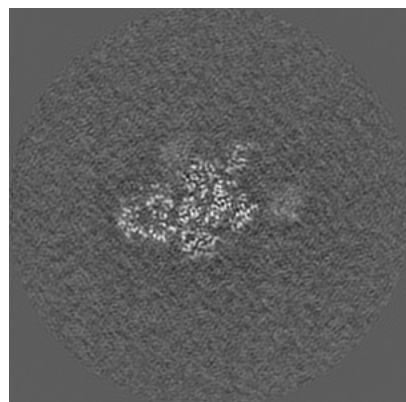


Z

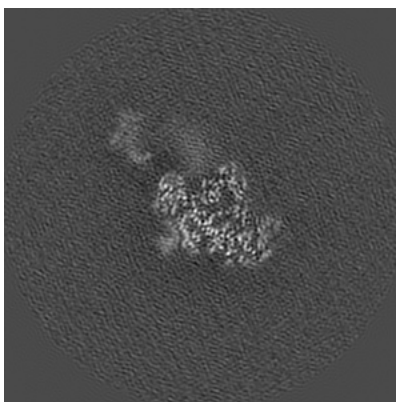
The images above show the map projected in three orthogonal directions.

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

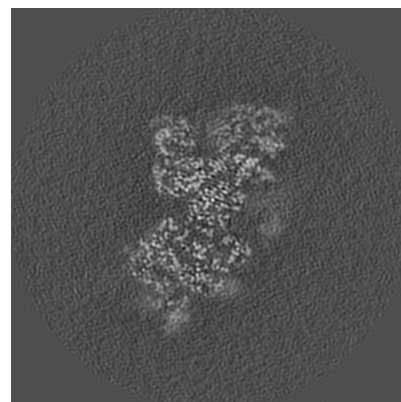
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

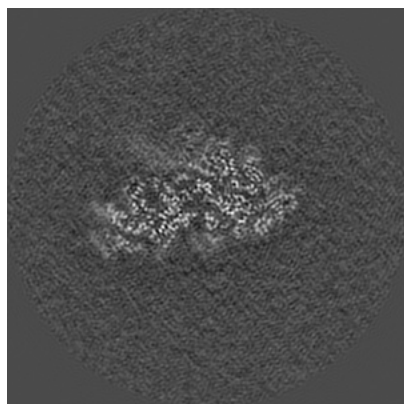


Z Index: 180

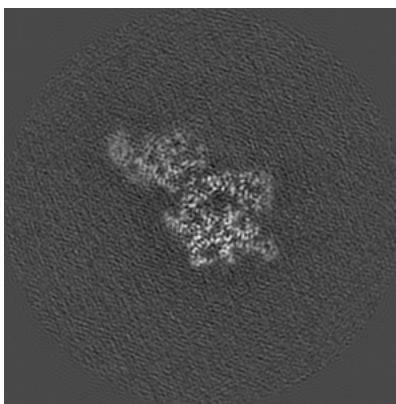
The images above show central slices of the map in three orthogonal directions.

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

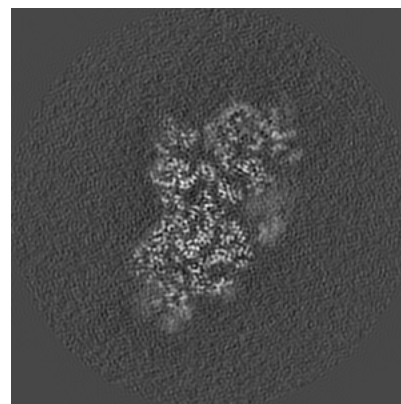
### 6.3.1 Primary map



X Index: 154



Y Index: 203

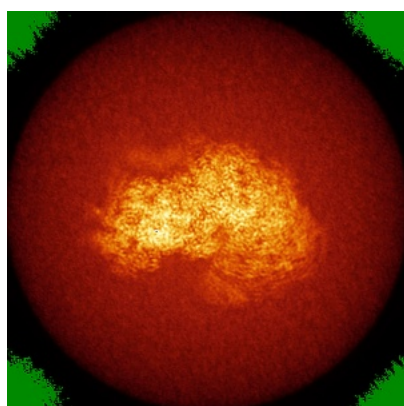


Z Index: 175

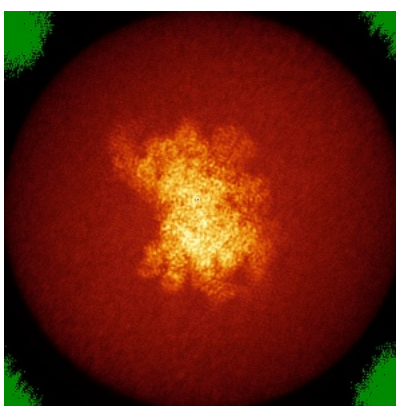
The images above show the largest variance slices of the map in three orthogonal directions.

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

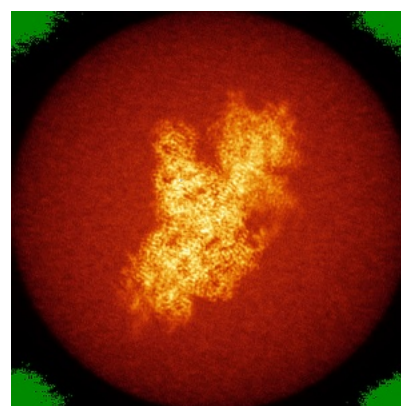
### 6.4.1 Primary map



X



Y

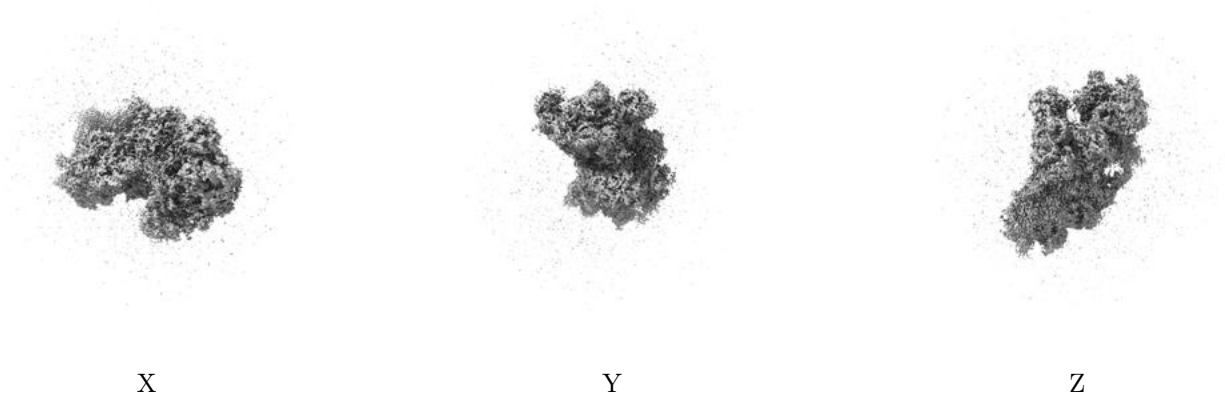


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

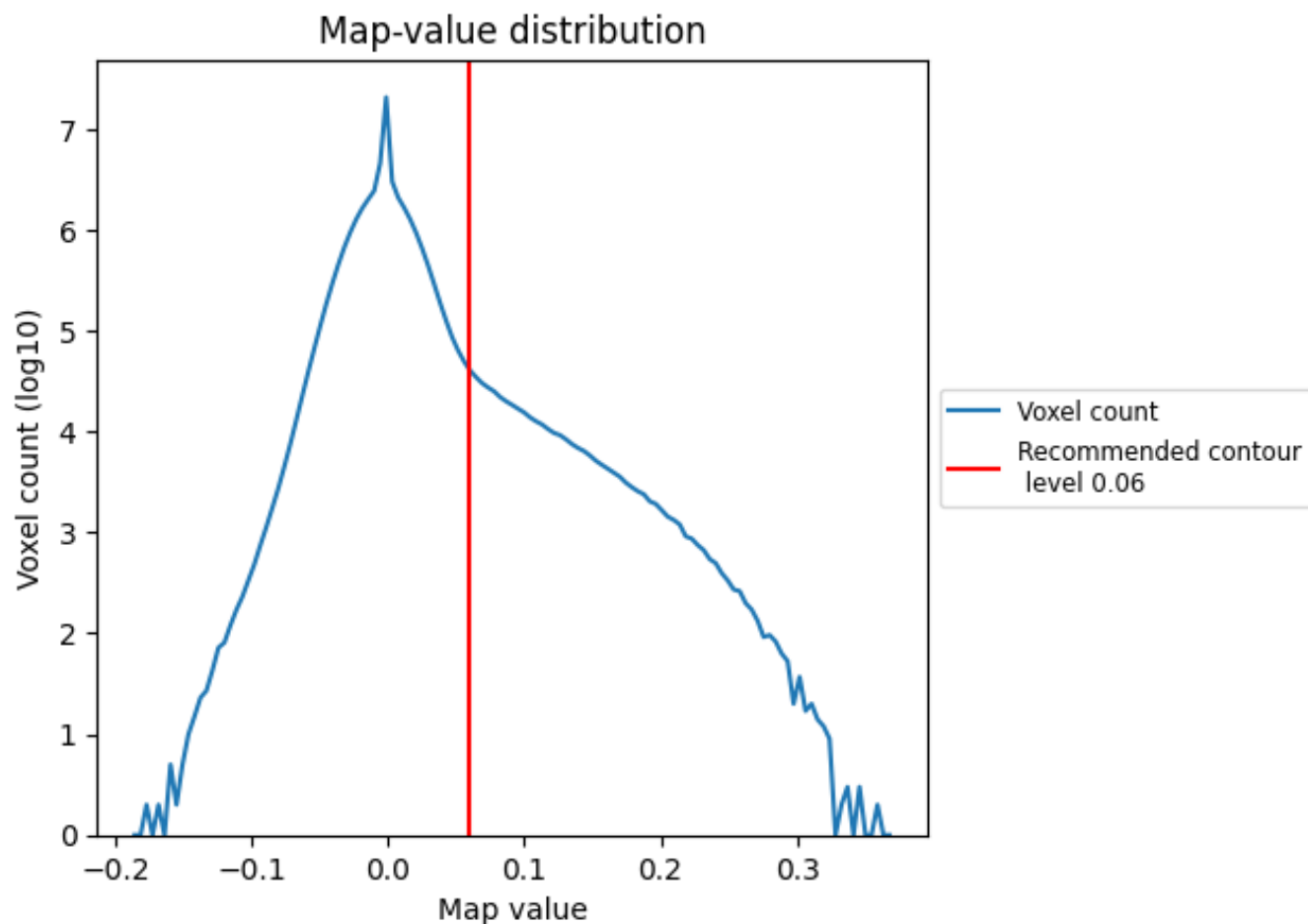
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

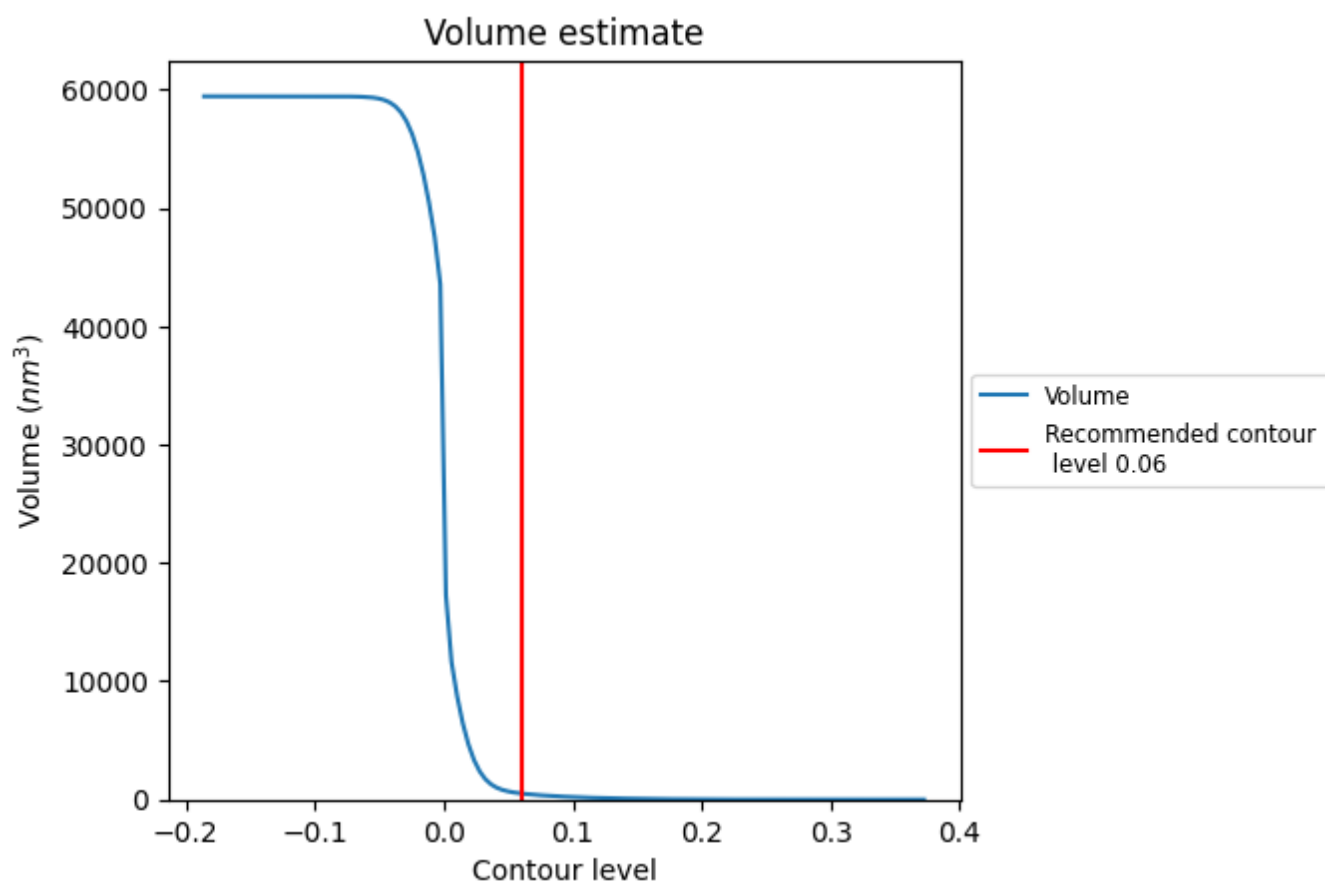
This section contains the results of statistical analysis of the map.

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



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

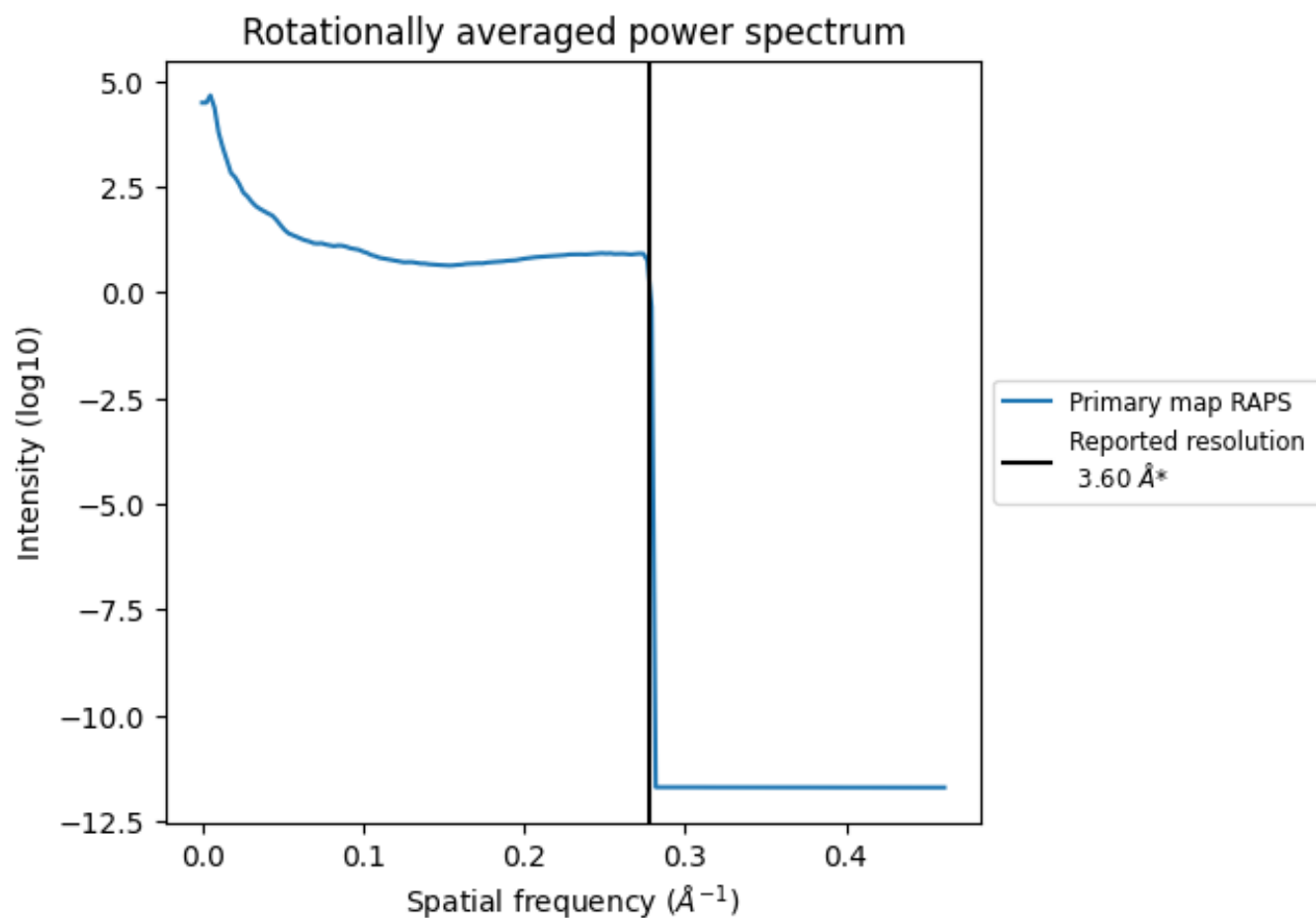
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm<sup>3</sup>; this corresponds to an approximate mass of 467 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 ⓘ

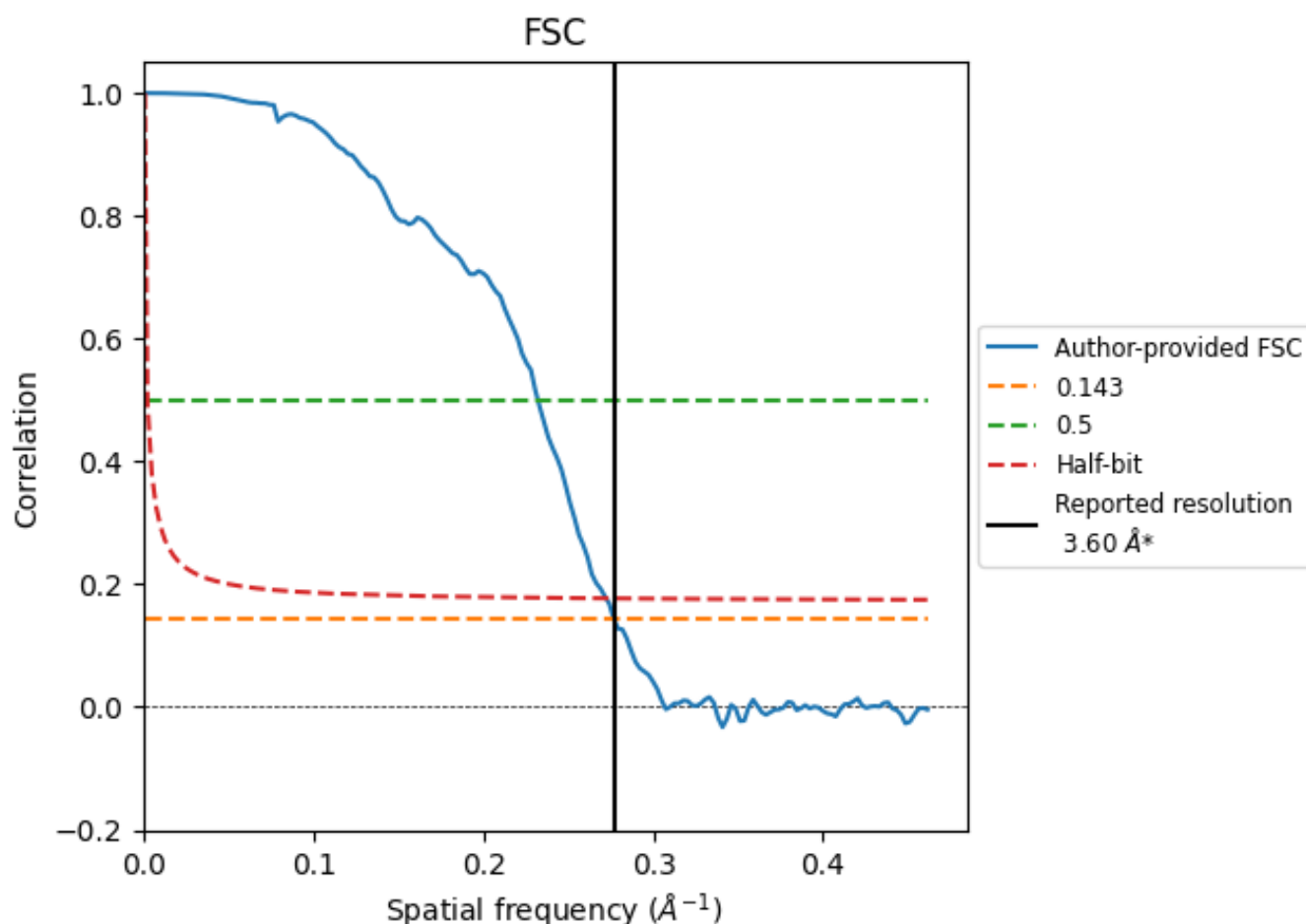


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

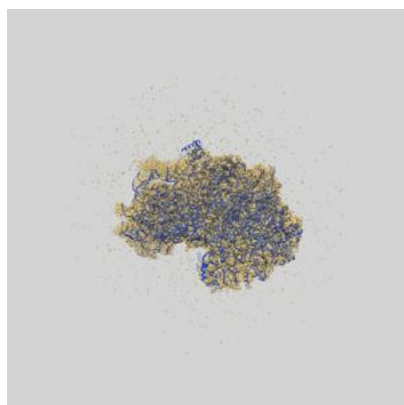
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.60                               | -    | -        |
| Author-provided FSC curve | 3.61                               | 4.31 | 3.67     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

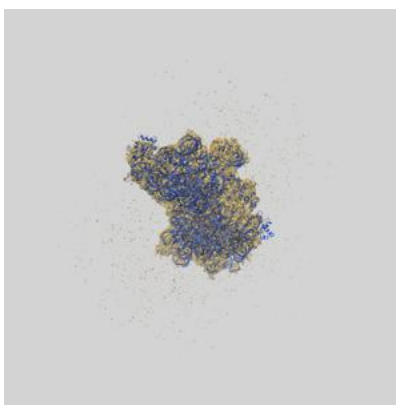
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4352 and PDB model 6G5H. Per-residue inclusion information can be found in section 3 on page 11.

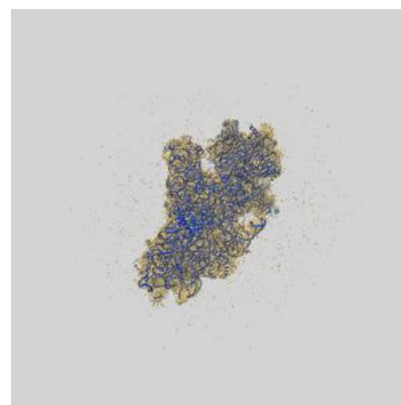
### 9.1 Map-model overlay [i](#)



X



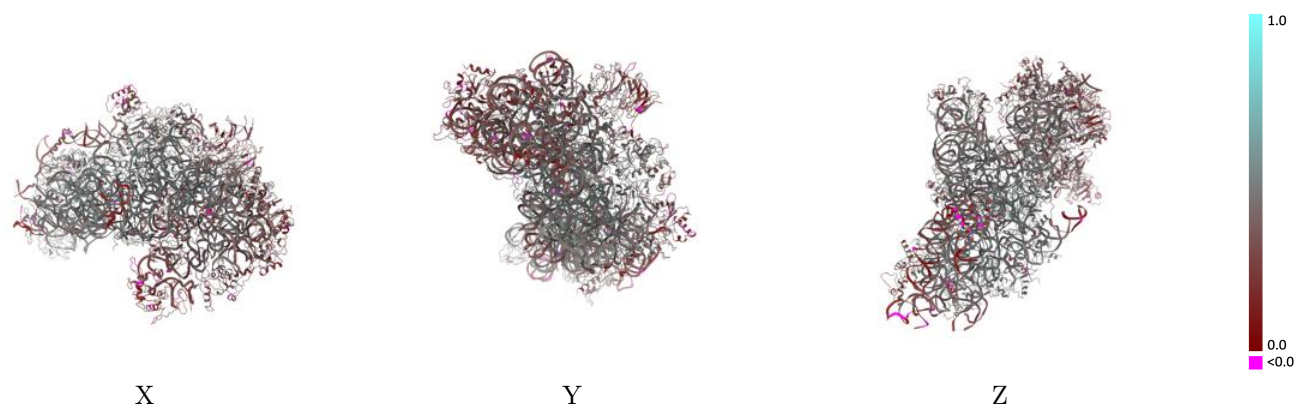
Y



Z

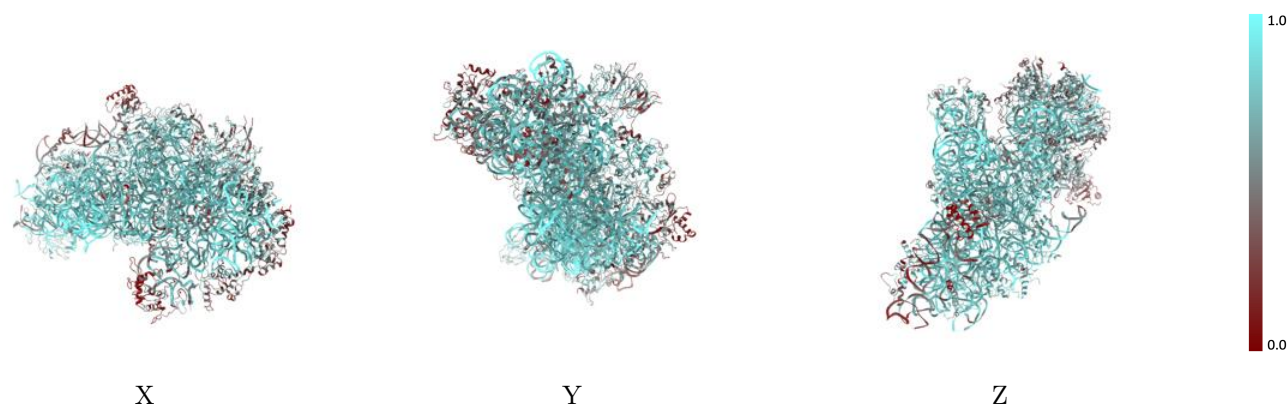
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



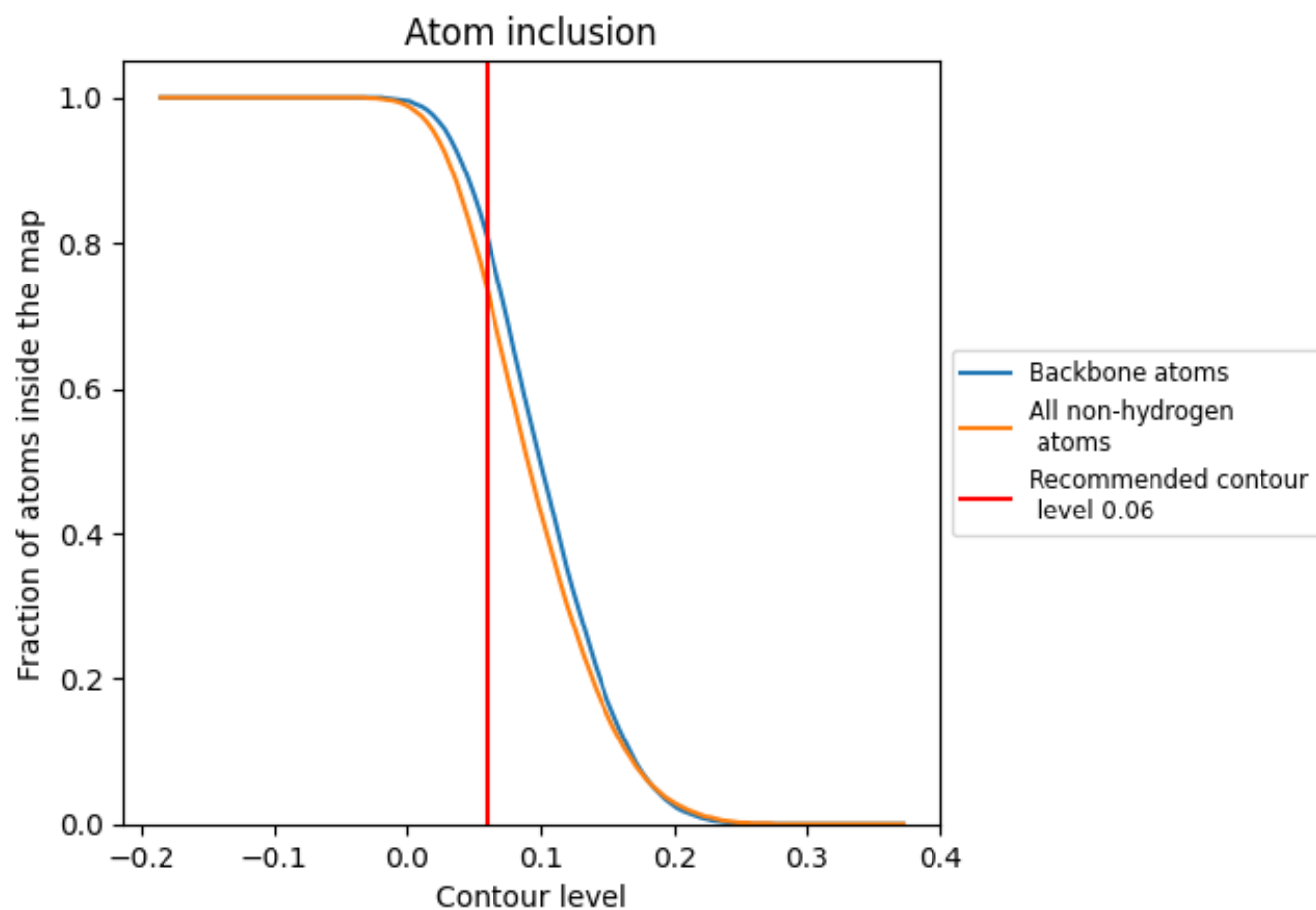
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.06) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7340   |  0.4080   |
| 2     |  0.8500   |  0.4210   |
| A     |  0.7190   |  0.4440   |
| B     |  0.6950   |  0.4180   |
| C     |  0.7560   |  0.4730   |
| D     |  0.6010   |  0.3750   |
| E     |  0.7450   |  0.4740   |
| F     |  0.5610   |  0.3440   |
| G     |  0.7000   |  0.4190   |
| H     |  0.3080   |  0.2870   |
| I     |  0.6990   |  0.4310   |
| J     |  0.7940   |  0.4690   |
| K     |  0.5820   |  0.3390   |
| L     |  0.7010   |  0.4600   |
| M     |  0.2150  |  0.2100  |
| N     |  0.7070 |  0.4380 |
| O     |  0.7070 |  0.4280 |
| P     |  0.4600 |  0.3250 |
| Q     |  0.6290 |  0.3780 |
| R     |  0.5240 |  0.3770 |
| S     |  0.4440 |  0.2990 |
| T     |  0.5660 |  0.3400 |
| U     |  0.5880 |  0.3890 |
| V     |  0.7400 |  0.4640 |
| W     |  0.7610 |  0.4890 |
| X     |  0.7670 |  0.4900 |
| Y     |  0.7720 |  0.4620 |
| Z     |  0.4010 |  0.2570 |
| a     |  0.7110 |  0.4550 |
| b     |  0.6150 |  0.4260 |
| c     |  0.5050 |  0.3770 |
| d     |  0.6370 |  0.3480 |
| e     |  0.6700 |  0.4400 |
| f     |  0.3090 |  0.2460 |
| g     |  0.5750 |  0.3320 |
| h     |  0.4430 |  0.3480 |

