



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:41 PM UTC

PDB ID : 6WDR / pdb\_00006wdr  
EMDB ID : EMD-21644  
Title : Subunit joining exposes nascent pre-40S rRNA for processing and quality control  
Authors : Rai, J.; Parker, M.D.; Huang, H.; Choy, S.; Ghalei, H.; Johnson, M.C.; Karbstein, K.; Stroupe, M.E.  
Deposited on : 2020-04-01  
Resolution : 3.70 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:

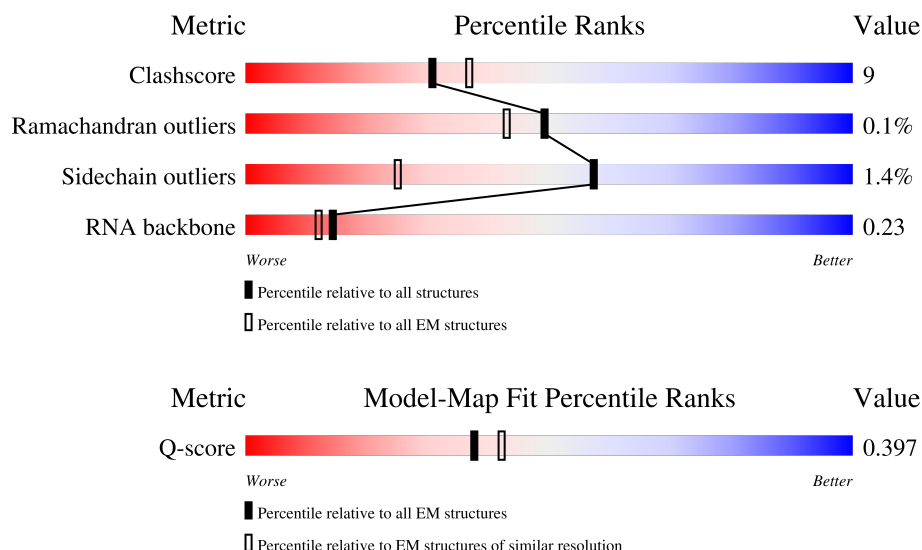
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



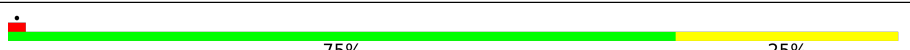
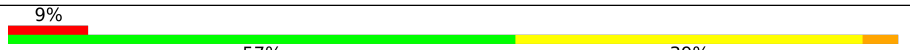
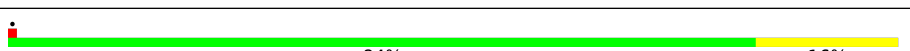
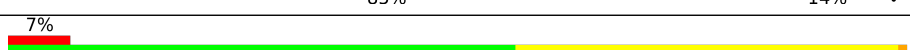
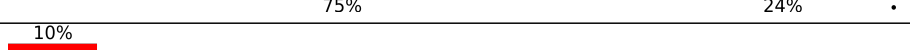
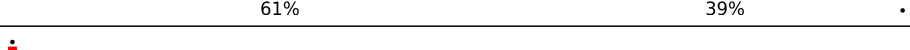
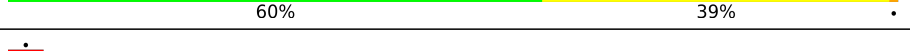
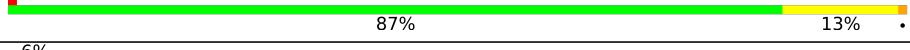
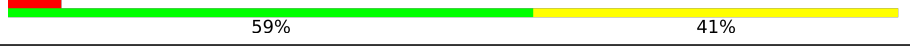
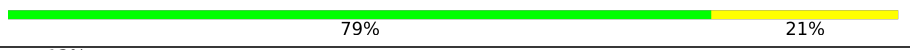
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11569 ( 3.20 - 4.20 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 206    |                  |
| 2   | C     | 217    |                  |
| 3   | D     | 223    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | E     | 260    |    |
| 5   | F     | 206    |    |
| 6   | G     | 232    |    |
| 7   | H     | 184    |    |
| 8   | I     | 199    |    |
| 9   | J     | 185    |    |
| 10  | K     | 96     |    |
| 11  | L     | 140    |    |
| 12  | M     | 125    |    |
| 13  | N     | 150    |    |
| 14  | P     | 127    |    |
| 15  | Q     | 127    |    |
| 16  | R     | 125    |  |
| 17  | S     | 135    |  |
| 18  | T     | 143    |  |
| 19  | U     | 103    |  |
| 20  | V     | 87     |  |
| 21  | W     | 129    |  |
| 22  | X     | 144    |  |
| 23  | Y     | 134    |  |
| 24  | Z     | 63     |  |
| 25  | b     | 81     |  |
| 26  | c     | 63     |  |
| 27  | d     | 37     |  |
| 28  | e     | 63     |  |

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| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 29  | f     | 71     | <div><div></div><div>32%</div><div>75%</div><div>25%</div></div>               |
| 30  | g     | 317    | <div><div></div><div>70%</div><div>30%</div></div>                             |
| 31  | k     | 788    | <div><div></div><div>29%</div><div>61%</div><div>20%</div><div>19%</div></div> |
| 32  | 2     | 1910   | <div><div></div><div>40%</div><div>34%</div><div>12%</div><div>14%</div></div> |

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 74473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1611  | 1036 | 285 | 288 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 206     | PHE      | ASP    | conflict | UNP P32905 |

- Molecule 2 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | C     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | D     | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | E     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | F     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | G     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1873  | 1172 | 366 | 332 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |   |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | I     | 188      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | J     | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | K     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 529 | 133 | 153 | 2 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | L     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 724 | 215 | 187 | 3 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | M     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 941   | 591 | 166 | 182 | 2 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | N     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | P     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1001  | 637 | 186 | 171 | 7 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | Q     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 993   | 640 | 177 | 176 |   |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | R     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1000  | 625 | 188 | 185 | 2 |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | S     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1110  | 696 | 215 | 197 | 2 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | T     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | U     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 819   | 519 | 148 | 151 | 1 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | V     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | W     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | X     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Y     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |   |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 24  | Z     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 512   | 328 | 94 | 90 |   |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | b     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | c     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S29-A.



| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | d     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 186 | 62 | 50 | 4 |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | e     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 384   | 242 | 81 | 59 | 2 |         |       |

- Molecule 29 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | f     | 71       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 498   | 309 | 93 | 92 | 4 |         |       |

- Molecule 30 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | g     | 317      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2431  | 1538 | 417 | 468 | 8 |         |       |

- Molecule 31 is a protein called Ribosome biogenesis protein TSR1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 31  | k     | 638      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5154  | 3291 | 896 | 953 | 14 |         |       |

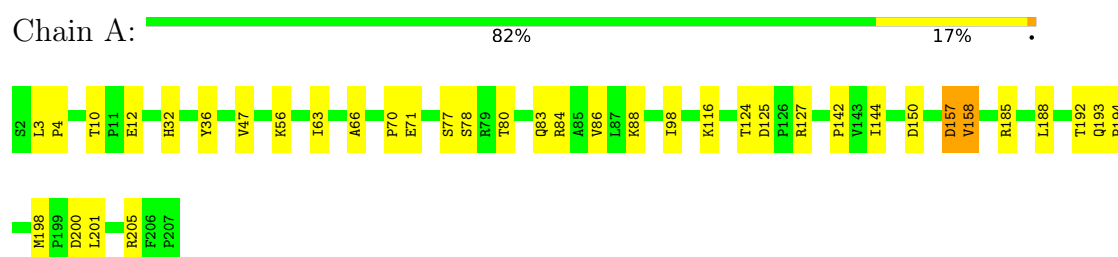
- Molecule 32 is a RNA chain called 20S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 32  | 2     | 1647     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 35078 | 15682 | 6196 | 11553 | 1647 |         |       |

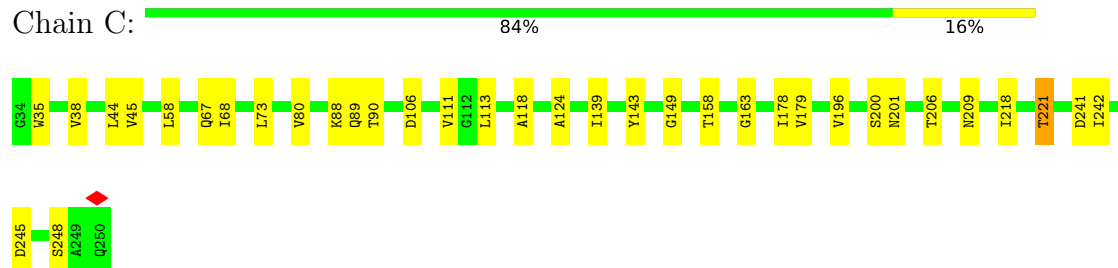
### 3 Residue-property plots

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

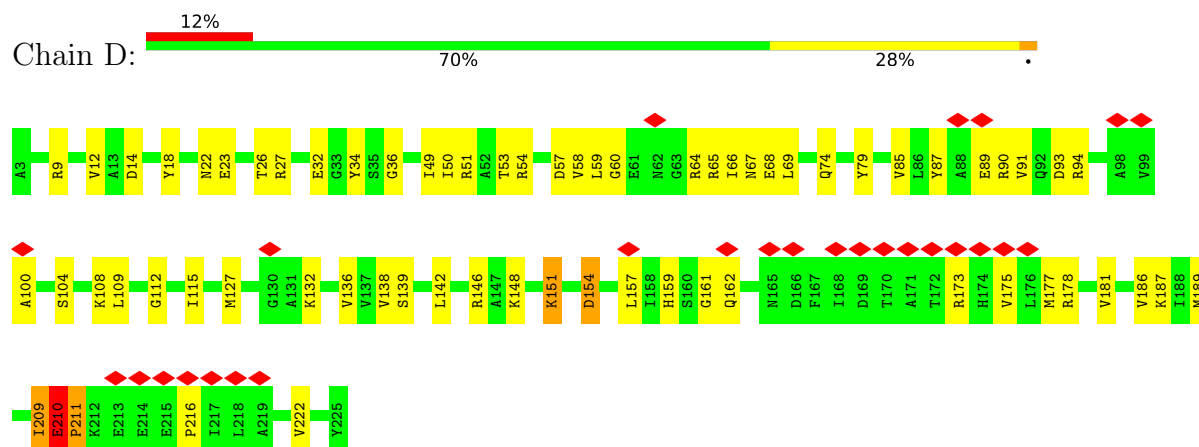
#### • Molecule 1: 40S ribosomal protein S0-A



#### • Molecule 2: 40S ribosomal protein S2

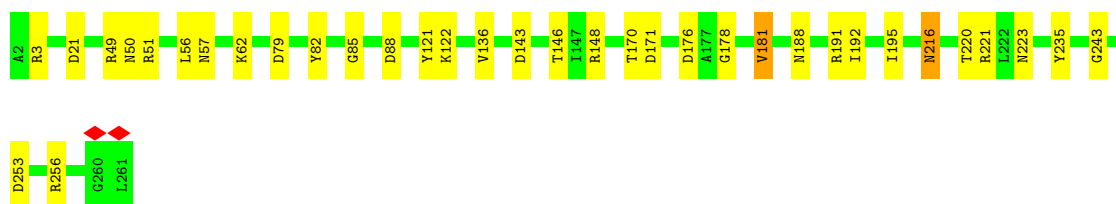


#### • Molecule 3: 40S ribosomal protein S3



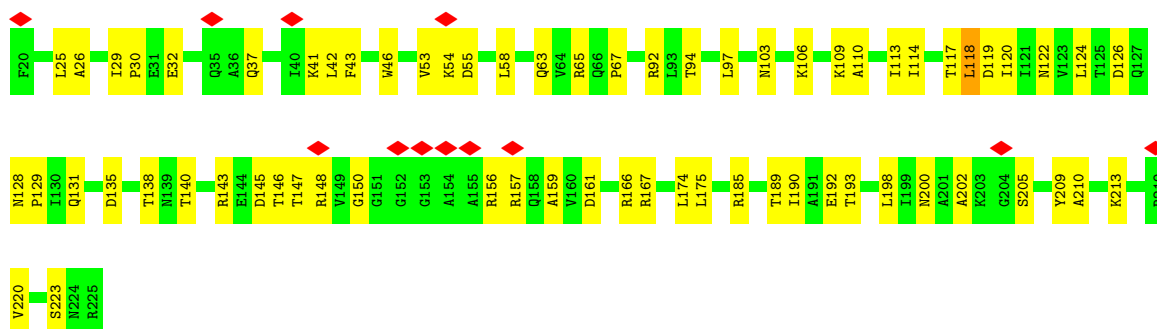
#### • Molecule 4: 40S ribosomal protein S4-A

Chain E:  87% 13%



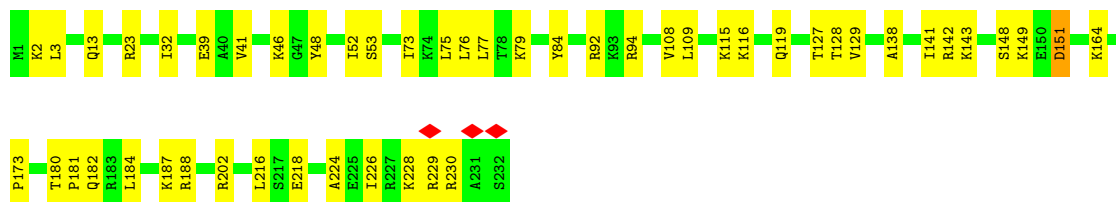
- Molecule 5: 40S ribosomal protein S5

Chain F:  6% 67% 32%



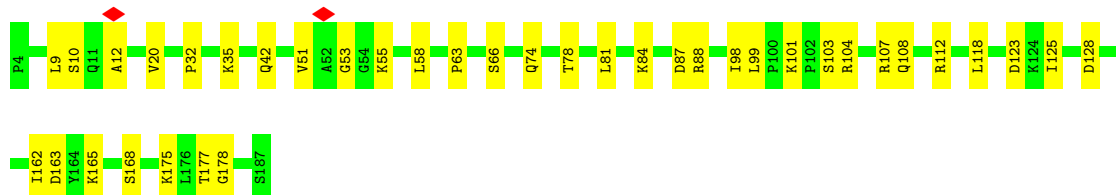
- Molecule 6: 40S ribosomal protein S6-A

Chain G:  78% 21%



- Molecule 7: 40S ribosomal protein S7-A

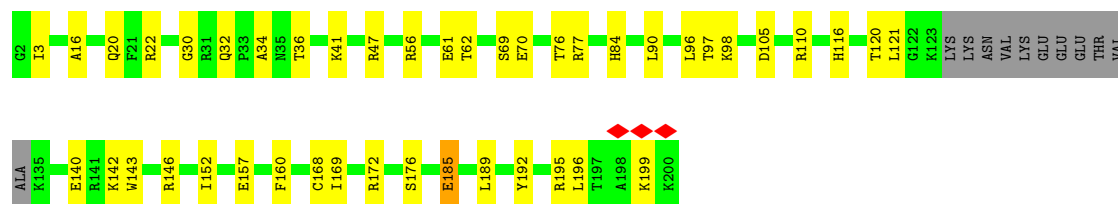
Chain H:  79% 21%



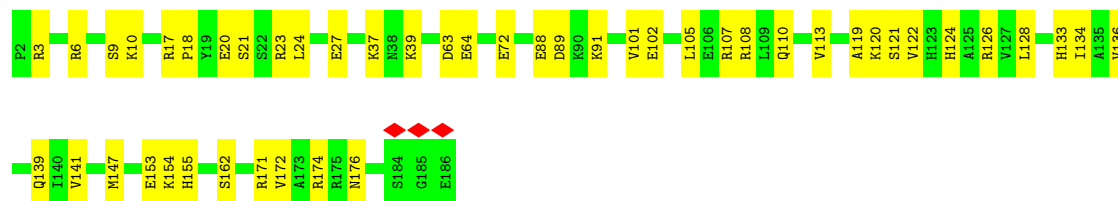
- Molecule 8: 40S ribosomal protein S8-A

Chain I:  72% 22% 6%

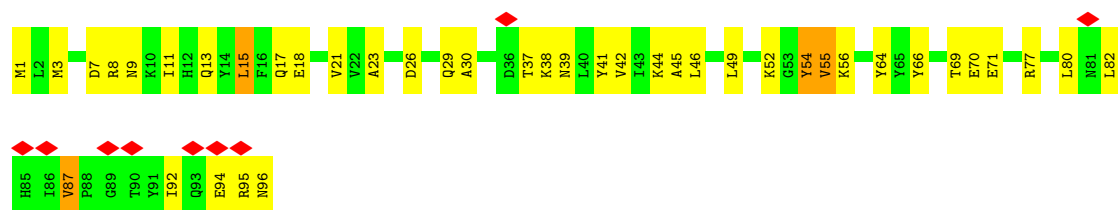




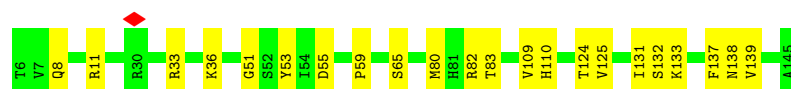
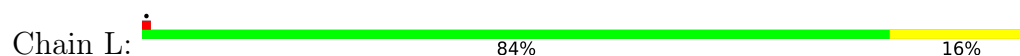
• Molecule 9: 40S ribosomal protein S9-A



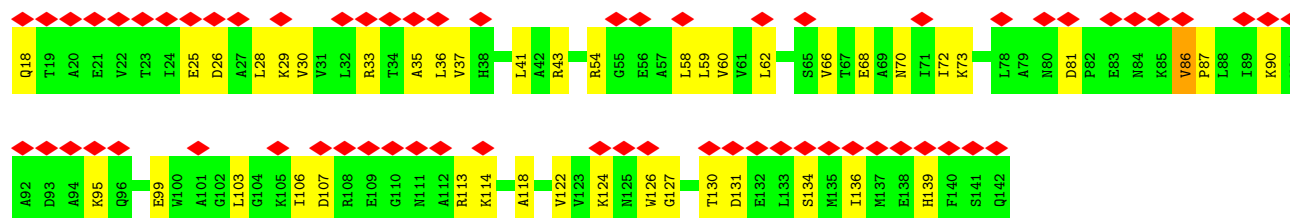
• Molecule 10: 40S ribosomal protein S10-A



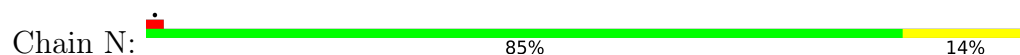
• Molecule 11: 40S ribosomal protein S11-A



• Molecule 12: 40S ribosomal protein S12

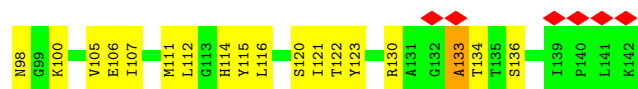


• Molecule 13: 40S ribosomal protein S13

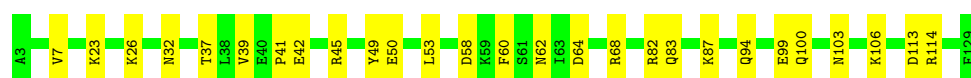
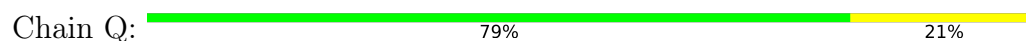




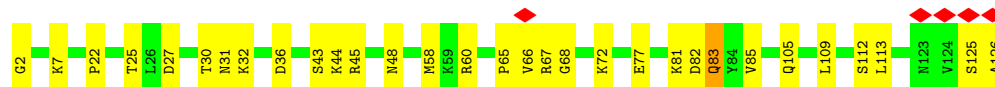
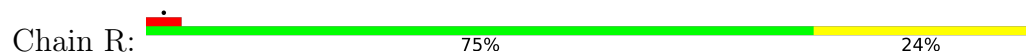
- Molecule 14: 40S ribosomal protein S15



- Molecule 15: 40S ribosomal protein S16-A



- Molecule 16: 40S ribosomal protein S17-A



- Molecule 17: 40S ribosomal protein S18-A

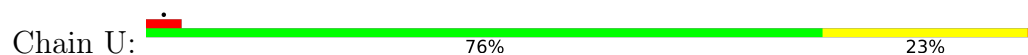


- Molecule 18: 40S ribosomal protein S19-A

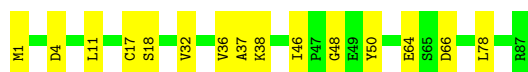
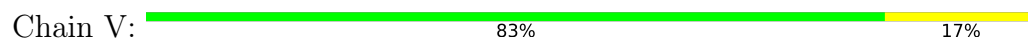




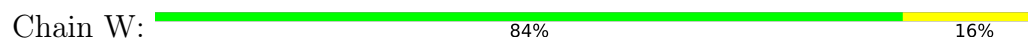
- Molecule 19: 40S ribosomal protein S20



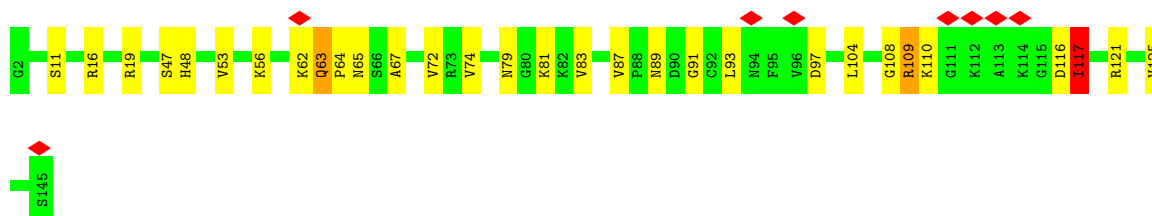
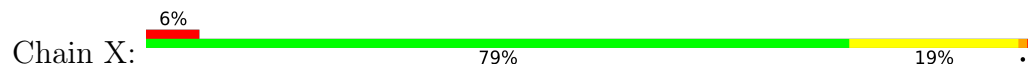
- Molecule 20: 40S ribosomal protein S21-A



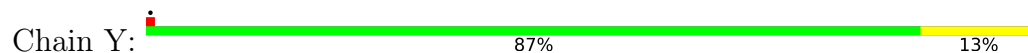
- Molecule 21: 40S ribosomal protein S22-A



- Molecule 22: 40S ribosomal protein S23-A



- Molecule 23: 40S ribosomal protein S24-A



- Molecule 24: 40S ribosomal protein S25-A



- Molecule 25: 40S ribosomal protein S27-A

Chain b:  79% 21%



- Molecule 26: 40S ribosomal protein S28-A

Chain c:  13% 71% 29%



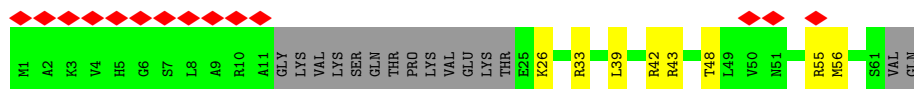
- Molecule 27: 40S ribosomal protein S29-A

Chain d:  78% 19% .



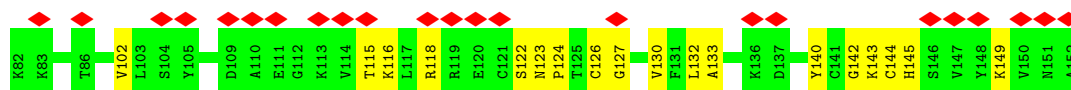
- Molecule 28: 40S ribosomal protein S30-A

Chain e:  22% 63% 13% 24%



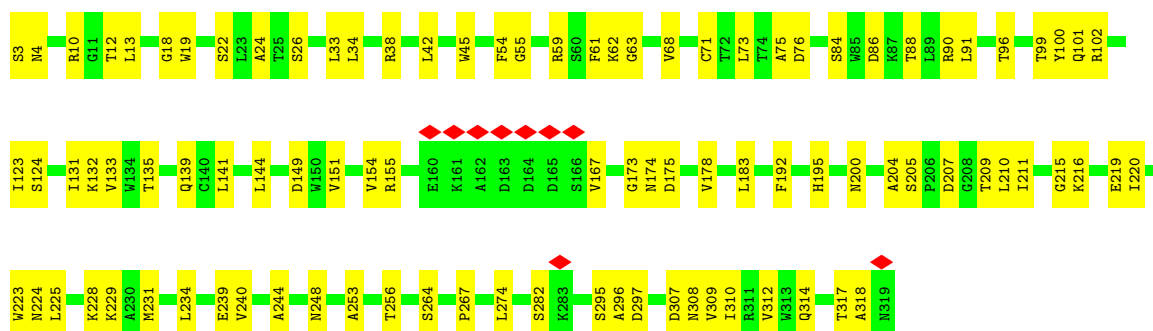
- Molecule 29: Ubiquitin-40S ribosomal protein S31

Chain f:  32% 75% 25%

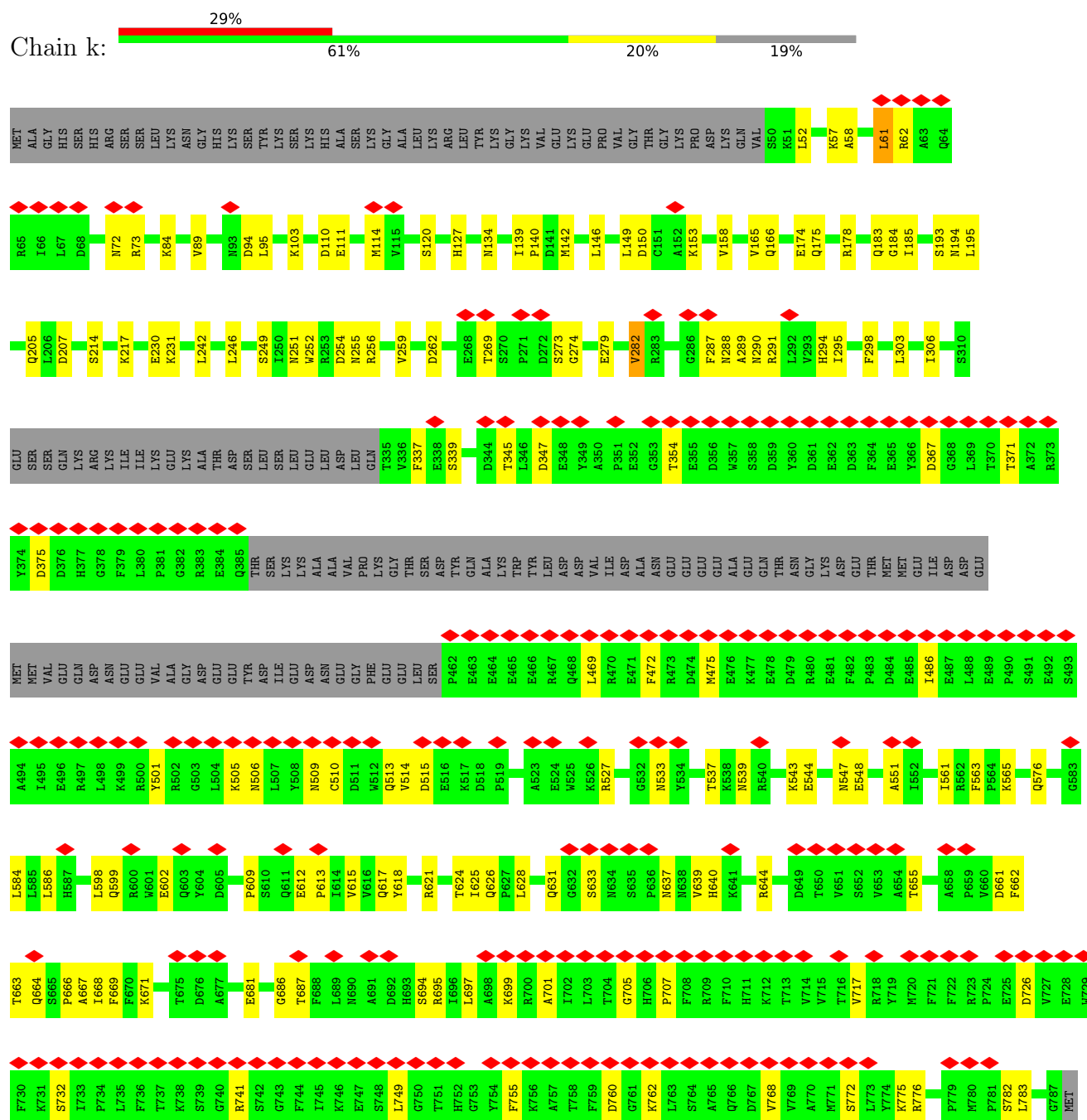


- Molecule 30: Guanine nucleotide-binding protein subunit beta-like protein

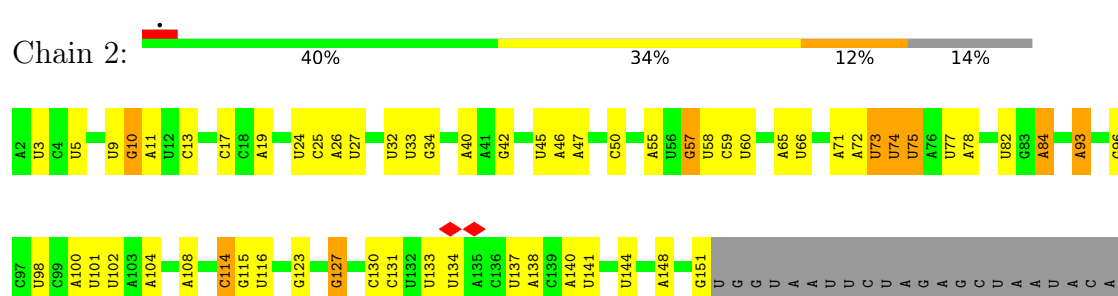
Chain g:  70% 30%



• Molecule 31: Ribosome biogenesis protein TSR1



• Molecule 32: 20S ribosomal RNA





|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G1365 | G1366 | C1367 | C1368 | A1369 | G1370 | A1371 | C1372 | A1373 | C1374 | A1375 | A1376 | A1377 | A1378 | A1379 | C1380 | G1381 | A1382 | U1383 | U1384 | U1385 | A1386 | C1387 | A1388 | U1389 | U1390 | C1391 | U1392 | U1393 | A1394 | C1395 | A1396 | C1397 | C1398 | U1399 | C1400 | U1403 | C1404 | U1405 | U1406 | G1407 | A1408 | U1409 | U1410 | U1411 | U1412 | G1413 | U1414 | G1415 | G1416 | G1417 | G1418 | G1419 | G1420 | U1421 | G1422 | G1423 | U1424 | C1425 | C1426 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A1299 | C1300 | G1301 | G1302 | G1216 | A1304 | G1225 | C1307 | C1308 | A1309 | C1310 | C1311 | U1312 | U1313 | U1314 | U1315 | U1316 | U1317 | U1318 | U1319 | U1320 | G1321 | G1322 | U1327 | U1328 | C1329 | G1330 | G1331 | C1332 | U1333 | U1334 | U1335 | A1336 | U1337 | U1338 | U1339 | U1340 | A1341 | C1342 | U1343 | U1344 | A1346 | A1347 | A1348 | C1349 | G1350 | G1351 | G1352 | G1353 | A1354 | A1355 | U1356 | C1357 | U1358 | U1359 | A1360 | C1361 | C1362 | A1363 | G1364 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A1213 | A1214 | U1215 | U1216 | A1217 | C1218 | G1225 | G1226 | A1228 | C1229 | C1230 | U1231 | U1232 | A1233 | C1234 | G1235 | A1244 | C1248 | U1249 | G1252 | G1253 | G1254 | U1255 | U1256 | C1257 | G1263 | G1264 | A1265 | G1266 | U1269 | G1270 | G1271 | G1274 | C1275 | A1276 | A1277 | G1278 | G1279 | A1280 | U1281 | G1282 | A1283 | A1284 | A1285 | C1286 | G1289 | A1290 | A1295 | U1296 | U1297 | U1298 | U1299 | U1300 |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G1118 | G1122 | G1123 | G1124 | C1131 | U1132 | U1133 | U1134 | U1135 | G1142 | C1143 | A1144 | C1149 | C1150 | A1151 | U1159 | U1160 | U1161 | C1162 | A1166 | A1167 | U1168 | C1169 | U1170 | U1171 | A1172 | C1173 | C1174 | A1175 | U1176 | A1177 | A1178 | U1179 | U1180 | U1181 | C1182 | C1186 | G1192 | G1193 | G1194 | G1202 | G1203 | U1204 | G1205 | U1206 | U1207 | U1208 | U1209 | U1210 | U1211 | U1212 |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A959  | G960  | U961  | C962  | C963  | U964  | U965  | G966  | U967  | G968  | G969  | C970  | U971  | G972  | U973  | U974  | G975  | C976  | C977  | A980  | G984  | G985  | G986  | U987  | U988  | U989  | G997  | A998  | A999  | A1000 | G1007 | G1011 | U1012 | U1013 | C1014 | A1015 | A1016 | A1017 | A1020 | G1021 | G1022 | G1023 | G1024 | U1025 | A1026 | U1027 | U1028 | C954  | G955  | U956  | U957  | U958  |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U1040 | G1048 | A1049 | A1050 | U1051 | A1052 | A1053 | G1056 | A1057 | A1058 | U1059 | A1060 | G1062 | A1063 | G1064 | U1065 | U1066 | U1067 | U1068 | G1069 | G1070 | U1071 | U1072 | C1073 | U1074 | A1075 | U1076 | U1077 | U1078 | U1079 | U1085 | U1086 | U1087 | C1088 | U1089 | G1091 | C1095 | A1096 | U1097 | C1098 | G1099 | U1100 | A1101 | A1102 | U1106 | U1107 | A1108 | A1109 | G1112 | A1115 |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A879  | U880  | A883  | A884  | A885  | A886  | G887  | C888  | U889  | C890  | G891  | U892  | U893  | G904  | G905  | G906  | G910  | G915  | C916  | G917  | A833  | G834  | C835  | C836  | G837  | C838  | G839  | G840  | U841  | A842  | A843  | U844  | U845  | A848  | G849  | C850  | U851  | C852  | C853  | A854  | U855  | U856  | A857  | U858  | C859  | A869  | U872  | G873  | U874  | U875  | U876  | U877  | U878  | U879  | U880  |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U415  | A420  | U421  | U422  | U426  | U441  | U446  | U447  | U448  | U449  | U450  | U451  | U452  | U453  | U454  | U455  | U456  | U457  | U458  | U459  | U460  | U461  | U466  | U478  | U479  | U480  | U481  | U482  | U485  | U486  | U487  | U488  | U489  | U490  | U492  | U493  | U494  | U495  | U496  | U497  | U498  | U499  | U500  | U501  | U502  | U503  | U504  | U505  | C513  | A514  |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A519  | A520  | U523  | A623  | U525  | C526  | A529  | U530  | A534  | U535  | U536  | U537  | U538  | U539  | U540  | U541  | U542  | U543  | U544  | U545  | U546  | U547  | A551  | A558  | A562  | C568  | C571  | C572  | C573  | C577  | A576  | A579  | C584  | U585  | U587  | U588  | U589  | U590  | A591  | U592  | U599  | U600  | C601  | A604  | U605  | C606  | A615  |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A616  | C617  | A622  | G623  | C624  | G625  | U626  | U631  | U635  | U636  | U644  | U647  | U648  | U649  | U650  | U651  | U652  | U653  | U654  | U655  | U656  | U657  | U658  | U659  | U660  | U661  | U662  | U663  | U664  | U665  | U666  | U667  | U668  | U669  | U670  | U671  | U672  | U673  | U674  | U675  | U676  | U677  | U678  | U679  | U680  | U681  | U682  | U683  | U684  | U685  | U686  | U687  | U688  | U689  | U690  | U691  | U692  | U693  | U694  | U695  | U696 | U697 | U698 | U699 | U700 | U701 | U702 | U703 | U704 | U705 | U706 | U707 | U708 | U709 | U710 | U711 | U712 | U713 | U714 | U715 | U716 | U717 | U718 | U719 | U720 | U721 | U722 | U723 | U724 | U725 | U726 | U727 | U728 | U729 | U730 | U731 | U732 | U733 | U734 | U735 | U736 | U737 | U738 | U739 | U740 | U741 | U742 | U743 | U744 | U745 | U746 | U747 | U748 | U749 | U750 | U751 | U752 | U753 | U754 | U755 | U756 | U757 | U758 | U759 | U760 | U761 | U762 | U763 | U764 | U765 | U766 | U767 | U768 | U769 | U770 | U771 | U772 | U773 | U774 | U775 | U776 | U777 | U778 | U779 | U780 | U781 | U782 | U783 | U784 | U785 | U786 | U787 | U788 | U789 | U790 | U791 | U792 | U793 | U794 | U795 | U796 | U797 | U798 | U799 | U800 | U801 | U802 | U803 | U804 | U805 | U806 | U807 | U808 | U809 | U810 | U811 | U812 | U813 | U814 | U815 | U816 | U817 | U818 | U819 | U820 | U821 | U822 | U823 | U824 | U825 | U826 | U827 | U828 | U829 | U830 | U831 | U832 | U833 | U834 | U835 | U836 | U837 | U838 | U839 | U840 | U841 | U842 | U843 | U844 | U845 | U846 | U847 | U848 | U849 | U850 | U851 | U852 | U853 | U854 | U855 | U856 | U857 | U858 | U859 | U860 | U861 | U862 | U863 | U864 | U865 | U866 | U867 | U868 | U869 | U870 | U871 | U872 | U873 | U874 | U875 | U876 | U877 | U878 | U879 | U880 | U881 | U882 | U883 | U884 | U885 | U886 | U887 | U888 | U889 | U890 | U891 | U892 | U893 | U894 | U895 | U896 | U897 | U898 | U899 | U900 | U901 | U902 | U903 | U904 | U905 | U906 | U907 | U908 | U909 | U910 | U911 | U912 | U913 | U914 | U915 | U916 | U917 | U918 | U919 | U920 | U921 | U922 | U923 | U924 | U925 | U926 | U927 | U928 | U929 | U930 | U931 | U932 | U933 | U934 | U935 | U936 | U937 | U938 | U939 | U940 | U941 | U942 | U943 | U944 | U945 | U946 | U947 | U948 | U949 | U950 | U951 | U952 | U953 | U954 | U955 | U956 | U957 | U958 | U959 | U960 | U961 | U962 | U963 | U964 | U965 | U966 | U967 | U968 | U969 | U970 | U971 | U972 | U973 | U974 | U975 | U976 | U977 | U978 | U979 | U980 | U981 | U982 | U983 | U984 | U985 | U986 | U987 | U988 | U989 | U990 | U991 | U992 | U993 | U994 | U995 | U996 | U997 | U998 | U999 | U1000 | U1001 | U1002 | U1003 | U1004 | U1005 | U1006 | U1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | U1043 | U1044 | U1045 | U1046 | U1047 | U1048 | U1049 | U1050 | U1051 | U1052 | U1053 | U1054 | U1055 | U1056 | U1057 | U1058 | U1059 | U1060 | U1061 | U1062 | U1063 | U1064 | U1065 | U1066 | U1067 | U1068 | U1069 | U1070 | U1071 | U1072 | U1073 | U1074 | U1075 | U1076 | U1077 | U1078 | U1079 | U1080 | U1081 | U1082 | U1083 | U1084 | U1085 | U1086 | U1087 | U1088 | U1089 | U1090 | U1091 | U1092 | U1093 | U1094 | U1095 | U1096 | U1097 | U1098 | U1099 | U1100 | U1101 | U1102 | U1103 | U1104 | U1105 | U1106 | U1107 | U1108 | U1109 | U1110 | U1111 | U1112 | U1113 | U1114 | U1115 | U1116 | U1117 | U1118 | U1119 | U1120 | U1121 | U1122 | U1123 | U1124 | U1125 | U1126 | U1127 | U1128 | U1129 | U1130 | U1131 | U1132 | U1133 | U1134 | U1135 | U1136 | U1137 | U1138 | U1139 | U1140 | U1141 | U1142 | U1143 | U1144 | U1145 | U1146 | U1147 | U1148 | U1149 | U1150 | U1151 | U1152 | U1153 | U1154 | U1155 | U1156 | U1157 | U1158 | U1159 | U1160 | U1161 | U1162 | U1163 | U1164 | U1165 | U1166 | U1167 | U1168 | U1169 | U1170 | U1171 | U1172 | U1173 | U1174 | U1175 | U1176 | U1177 | U1178 | U1179 | U1180 | U1181 | U1182 | U1183 | U1184 | U1185 | U1186 | U1187 | U1188 | U1189 | U1190 | U1191 | U1192 | U1193 | U1194 | U1195 | U1196 | U1197 | U1198 | U1199 | U1200 | U1201 | U1202 | U1203 | U1204 | U1205 | U1206 | U1207 | U1208 | U1209 | U1210 | U1211 | U1212 |



## 4 Experimental information

| Property                             | Value                                                                            | Source    |
|--------------------------------------|----------------------------------------------------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                                                  | Depositor |
| Imposed symmetry                     | POINT, POINT                                                                     | Depositor |
| Number of particles used             | 90692, 90692                                                                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF                                             | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                                                                  | Depositor |
| Voltage (kV)                         | 300                                                                              | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 25.00                                                                            | Depositor |
| Minimum defocus (nm)                 | Not provided                                                                     |           |
| Maximum defocus (nm)                 | Not provided                                                                     |           |
| Magnification                        | Not provided                                                                     |           |
| Image detector                       | DIRECT ELECTRON DE-64 (8k x 8k)                                                  | Depositor |
| Maximum map value                    | 0.172                                                                            | Depositor |
| Minimum map value                    | -0.087                                                                           | Depositor |
| Average map value                    | 0.000                                                                            | Depositor |
| Map value standard deviation         | 0.004                                                                            | Depositor |
| Recommended contour level            | 0.018                                                                            | Depositor |
| Map size ( $\text{\AA}$ )            | 476.16, 476.16, 476.16                                                           | wwPDB     |
| Map dimensions                       | 384, 384, 384                                                                    | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                                                                 | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.24, 1.24, 1.24                                                                 | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.68         | 0/1653         | 0.68        | 0/2261           |
| 2   | C     | 0.78         | 0/1665         | 0.75        | 1/2263 (0.0%)    |
| 3   | D     | 0.43         | 0/1758         | 0.87        | 7/2365 (0.3%)    |
| 4   | E     | 0.78         | 0/2109         | 0.70        | 0/2839           |
| 5   | F     | 0.34         | 0/1628         | 0.58        | 0/2199           |
| 6   | G     | 0.54         | 0/1897         | 0.59        | 0/2532           |
| 7   | H     | 0.52         | 0/1506         | 0.60        | 0/2028           |
| 8   | I     | 0.70         | 0/1514         | 0.65        | 0/2021           |
| 9   | J     | 0.77         | 0/1519         | 0.72        | 0/2035           |
| 10  | K     | 0.31         | 0/836          | 0.70        | 2/1128 (0.2%)    |
| 11  | L     | 0.85         | 0/1155         | 0.76        | 0/1557           |
| 12  | M     | 0.21         | 0/949          | 0.56        | 1/1284 (0.1%)    |
| 13  | N     | 0.63         | 0/1215         | 0.63        | 0/1638           |
| 14  | P     | 0.30         | 0/1019         | 0.62        | 0/1363           |
| 15  | Q     | 0.41         | 0/1011         | 0.62        | 0/1362           |
| 16  | R     | 0.49         | 0/1010         | 0.64        | 0/1355           |
| 17  | S     | 0.26         | 0/1128         | 0.58        | 0/1518           |
| 18  | T     | 0.32         | 0/1130         | 0.54        | 0/1517           |
| 19  | U     | 0.37         | 0/829          | 0.60        | 0/1121           |
| 20  | V     | 0.73         | 0/693          | 0.74        | 0/935            |
| 21  | W     | 1.03         | 0/1038         | 0.90        | 0/1395           |
| 22  | X     | 0.77         | 0/1139         | 0.89        | 3/1518 (0.2%)    |
| 23  | Y     | 0.67         | 0/1087         | 0.70        | 0/1449           |
| 24  | Z     | 0.26         | 0/519          | 0.56        | 0/696            |
| 25  | b     | 0.61         | 0/620          | 0.61        | 0/838            |
| 26  | c     | 0.29         | 0/499          | 0.56        | 0/670            |
| 27  | d     | 0.52         | 0/306          | 0.80        | 0/404            |
| 28  | e     | 0.52         | 0/390          | 0.72        | 0/517            |
| 29  | f     | 0.25         | 0/502          | 0.61        | 0/673            |
| 30  | g     | 0.30         | 0/2484         | 0.58        | 0/3382           |
| 31  | k     | 0.28         | 0/5273         | 0.55        | 0/7129           |
| 32  | 2     | 0.75         | 2/39196 (0.0%) | 0.63        | 16/60993 (0.0%)  |
| All | All   | 0.66         | 2/79277 (0.0%) | 0.64        | 30/114985 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 2   | C     | 0                   | 1                   |
| 3   | D     | 0                   | 1                   |
| 8   | I     | 0                   | 1                   |
| 9   | J     | 0                   | 1                   |
| 10  | K     | 0                   | 1                   |
| 14  | P     | 0                   | 2                   |
| 16  | R     | 0                   | 1                   |
| 18  | T     | 0                   | 1                   |
| 19  | U     | 0                   | 1                   |
| 22  | X     | 0                   | 4                   |
| 27  | d     | 0                   | 1                   |
| All | All   | 0                   | 16                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 32  | 2     | 1168 | U    | P-O5'   | 5.34 | 1.67        | 1.59     |
| 32  | 2     | 1168 | U    | C3'-O3' | 5.19 | 1.50        | 1.42     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | 2     | 1168 | U    | OP1-P-OP2   | -6.96 | 98.73       | 119.60   |
| 32  | 2     | 1168 | U    | P-O5'-C5'   | 6.90  | 131.25      | 120.90   |
| 32  | 2     | 835  | C    | O3'-P-O5'   | 6.68  | 114.02      | 104.00   |
| 32  | 2     | 1168 | U    | O3'-P-O5'   | 6.56  | 113.83      | 104.00   |
| 32  | 2     | 1168 | U    | P-O3'-C3'   | 6.24  | 129.56      | 120.20   |
| 32  | 2     | 1168 | U    | O5'-P-OP2   | 6.03  | 126.09      | 108.00   |
| 32  | 2     | 1168 | U    | C4'-C3'-O3' | 5.96  | 121.94      | 113.00   |
| 3   | D     | 210  | GLU  | N-CA-C      | 5.87  | 122.78      | 109.81   |
| 22  | X     | 93   | LEU  | CA-CB-CG    | 5.52  | 135.63      | 116.30   |
| 32  | 2     | 835  | C    | P-O3'-C3'   | -5.50 | 111.95      | 120.20   |
| 32  | 2     | 836  | C    | O5'-C5'-C4' | 5.49  | 119.73      | 111.50   |
| 22  | X     | 91   | GLY  | CA-C-N      | 5.41  | 131.88      | 121.18   |
| 22  | X     | 91   | GLY  | C-N-CA      | 5.41  | 131.88      | 121.18   |
| 32  | 2     | 1181 | U    | P-O3'-C3'   | 5.35  | 128.23      | 120.20   |
| 32  | 2     | 1168 | U    | C5'-C4'-O4' | -5.32 | 101.81      | 109.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | 2     | 1731 | U    | C2-N1-C1'   | 5.30  | 133.60      | 117.70   |
| 32  | 2     | 1643 | U    | P-O3'-C3'   | 5.29  | 128.14      | 120.20   |
| 12  | M     | 30   | VAL  | N-CA-C      | -5.29 | 108.69      | 113.71   |
| 10  | K     | 80   | LEU  | CA-C-N      | 5.20  | 131.47      | 121.54   |
| 10  | K     | 80   | LEU  | C-N-CA      | 5.20  | 131.47      | 121.54   |
| 32  | 2     | 999  | A    | C4'-C3'-O3' | 5.19  | 120.79      | 113.00   |
| 3   | D     | 211  | PRO  | CA-C-N      | 5.12  | 128.35      | 120.82   |
| 3   | D     | 211  | PRO  | C-N-CA      | 5.12  | 128.35      | 120.82   |
| 32  | 2     | 1437 | U    | C2-N1-C1'   | 5.09  | 132.96      | 117.70   |
| 2   | C     | 38   | VAL  | N-CA-C      | -5.04 | 108.22      | 113.10   |
| 3   | D     | 151  | LYS  | CA-C-N      | 5.03  | 130.83      | 121.62   |
| 3   | D     | 151  | LYS  | C-N-CA      | 5.03  | 130.83      | 121.62   |
| 32  | 2     | 1167 | A    | C4'-C3'-O3' | 5.02  | 120.53      | 113.00   |
| 3   | D     | 209  | ILE  | CA-C-N      | 5.02  | 134.05      | 121.80   |
| 3   | D     | 209  | ILE  | C-N-CA      | 5.02  | 134.05      | 121.80   |

There are no chirality outliers.

All (16) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 158 | VAL  | Peptide |
| 2   | C     | 106 | ASP  | Peptide |
| 3   | D     | 210 | GLU  | Peptide |
| 8   | I     | 185 | GLU  | Peptide |
| 9   | J     | 20  | GLU  | Peptide |
| 10  | K     | 87  | VAL  | Peptide |
| 14  | P     | 111 | MET  | Peptide |
| 14  | P     | 133 | ALA  | Peptide |
| 16  | R     | 83  | GLN  | Peptide |
| 18  | T     | 79  | LEU  | Peptide |
| 19  | U     | 77  | LYS  | Peptide |
| 22  | X     | 108 | GLY  | Peptide |
| 22  | X     | 109 | ARG  | Peptide |
| 22  | X     | 117 | ILE  | Peptide |
| 22  | X     | 63  | GLN  | Peptide |
| 27  | d     | 23  | VAL  | 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   | A     | 1611  | 0        | 1616     | 27      | 0            |
| 2   | C     | 1635  | 0        | 1723     | 19      | 0            |
| 3   | D     | 1734  | 0        | 1816     | 53      | 0            |
| 4   | E     | 2068  | 0        | 2154     | 25      | 0            |
| 5   | F     | 1609  | 0        | 1674     | 51      | 0            |
| 6   | G     | 1873  | 0        | 1980     | 34      | 0            |
| 7   | H     | 1481  | 0        | 1572     | 29      | 0            |
| 8   | I     | 1489  | 0        | 1525     | 28      | 0            |
| 9   | J     | 1494  | 0        | 1573     | 31      | 0            |
| 10  | K     | 817   | 0        | 803      | 27      | 0            |
| 11  | L     | 1129  | 0        | 1196     | 14      | 0            |
| 12  | M     | 941   | 0        | 982      | 34      | 0            |
| 13  | N     | 1192  | 0        | 1255     | 17      | 0            |
| 14  | P     | 1001  | 0        | 1040     | 45      | 0            |
| 15  | Q     | 993   | 0        | 1051     | 22      | 0            |
| 16  | R     | 1000  | 0        | 1063     | 25      | 0            |
| 17  | S     | 1110  | 0        | 1134     | 39      | 0            |
| 18  | T     | 1112  | 0        | 1124     | 45      | 0            |
| 19  | U     | 819   | 0        | 885      | 18      | 0            |
| 20  | V     | 684   | 0        | 672      | 12      | 0            |
| 21  | W     | 1021  | 0        | 1060     | 11      | 0            |
| 22  | X     | 1121  | 0        | 1196     | 14      | 0            |
| 23  | Y     | 1073  | 0        | 1132     | 13      | 0            |
| 24  | Z     | 512   | 0        | 551      | 21      | 0            |
| 25  | b     | 610   | 0        | 633      | 12      | 0            |
| 26  | c     | 497   | 0        | 535      | 12      | 0            |
| 27  | d     | 302   | 0        | 301      | 8       | 0            |
| 28  | e     | 384   | 0        | 423      | 8       | 0            |
| 29  | f     | 498   | 0        | 438      | 19      | 0            |
| 30  | g     | 2431  | 0        | 2381     | 72      | 0            |
| 31  | k     | 5154  | 0        | 5025     | 102     | 0            |
| 32  | 2     | 35078 | 0        | 17686    | 330     | 0            |
| All | All   | 74473 | 0        | 58199    | 1060    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1060) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 14:P:78:THR:HG1   | 14:P:80:MET:N    | 1.78                     | 0.81              |
| 32:2:749:G:H1     | 32:2:764:U:H3    | 1.29                     | 0.79              |
| 17:S:73:MET:HE1   | 17:S:99:HIS:HB3  | 1.70                     | 0.74              |
| 32:2:910:G:H22    | 32:2:933:G:H1    | 1.37                     | 0.72              |
| 32:2:945:U:H3     | 32:2:985:G:H1    | 1.39                     | 0.71              |
| 6:G:23:ARG:HB3    | 6:G:41:VAL:HG23  | 1.74                     | 0.69              |
| 30:g:132:LYS:HZ1  | 30:g:141:LEU:H   | 1.40                     | 0.69              |
| 29:f:132:LEU:HD22 | 29:f:140:TYR:H   | 1.57                     | 0.69              |
| 3:D:58:VAL:HG12   | 3:D:66:ILE:HD13  | 1.74                     | 0.69              |
| 22:X:62:LYS:H     | 22:X:116:ASP:HB2 | 1.58                     | 0.69              |
| 27:d:20:GLN:HE21  | 27:d:22:ARG:HB2  | 1.59                     | 0.68              |
| 22:X:67:ALA:HB3   | 32:2:831:G:H2'   | 1.75                     | 0.67              |
| 32:2:1616:G:H2'   | 32:2:1617:C:H42  | 1.59                     | 0.67              |
| 32:2:1395:G:N2    | 32:2:1397:G:N3   | 2.42                     | 0.67              |
| 30:g:224:ASN:HB3  | 30:g:228:LYS:H   | 1.59                     | 0.67              |
| 2:C:163:GLY:HA3   | 2:C:209:ASN:HD21 | 1.59                     | 0.67              |
| 12:M:43:ARG:HH21  | 32:2:1379:A:H61  | 1.42                     | 0.66              |
| 32:2:1418:U:H3'   | 32:2:1419:G:H8   | 1.59                     | 0.66              |
| 32:2:1842:G:N2    | 32:2:1864:A:N7   | 2.43                     | 0.66              |
| 6:G:39:GLU:HG2    | 6:G:46:LYS:HA    | 1.78                     | 0.66              |
| 27:d:40:ARG:HH21  | 32:2:1351:G:H5'' | 1.61                     | 0.66              |
| 3:D:58:VAL:HA     | 3:D:65:ARG:HB2   | 1.76                     | 0.66              |
| 31:k:354:THR:HB   | 31:k:527:ARG:HG2 | 1.78                     | 0.66              |
| 7:H:103:SER:H     | 32:2:942:C:H42   | 1.44                     | 0.65              |
| 32:2:857:A:O2'    | 32:2:858:G:N2    | 2.29                     | 0.65              |
| 5:F:103:ASN:HD22  | 32:2:1625:U:H3   | 1.44                     | 0.65              |
| 3:D:154:ASP:N     | 3:D:154:ASP:OD1  | 2.29                     | 0.65              |
| 14:P:50:THR:HB    | 14:P:53:PRO:HG2  | 1.77                     | 0.65              |
| 32:2:1207:U:H3    | 32:2:1216:G:H1   | 1.43                     | 0.65              |
| 1:A:10:THR:HG22   | 1:A:12:GLU:H     | 1.62                     | 0.65              |
| 15:Q:83:GLN:HE21  | 15:Q:87:LYS:HD2  | 1.61                     | 0.64              |
| 27:d:41:GLN:NE2   | 32:2:1583:C:OP2  | 2.31                     | 0.64              |
| 30:g:200:ASN:H    | 30:g:215:GLY:HA2 | 1.62                     | 0.64              |
| 7:H:51:VAL:HG23   | 7:H:53:GLY:H     | 1.63                     | 0.64              |
| 28:e:43:ARG:NH2   | 32:2:853:C:OP1   | 2.31                     | 0.64              |
| 8:I:76:THR:OG1    | 8:I:77:ARG:N     | 2.30                     | 0.64              |
| 8:I:140:GLU:HA    | 8:I:143:TRP:HB2  | 1.80                     | 0.64              |
| 15:Q:39:VAL:HG12  | 15:Q:41:PRO:HD2  | 1.80                     | 0.64              |
| 5:F:122:ASN:HB3   | 5:F:129:PRO:HG3  | 1.80                     | 0.63              |
| 25:b:47:PHE:HB3   | 25:b:50:ALA:HB2  | 1.81                     | 0.63              |
| 16:R:36:ASP:N     | 16:R:36:ASP:OD1  | 2.29                     | 0.63              |
| 13:N:124:ARG:HH22 | 32:2:1166:A:H62  | 1.45                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:2:1742:G:N2    | 32:2:1744:A:OP1   | 2.31                     | 0.63              |
| 13:N:60:VAL:HG23  | 13:N:66:ILE:HD12  | 1.80                     | 0.63              |
| 19:U:68:ARG:NH1   | 19:U:70:THR:O     | 2.32                     | 0.63              |
| 22:X:89:ASN:ND2   | 32:2:833:A:N1     | 2.42                     | 0.63              |
| 32:2:1374:C:H1'   | 32:2:1415:G:H22   | 1.63                     | 0.63              |
| 3:D:181:VAL:H     | 32:2:1588:A:H8    | 1.46                     | 0.63              |
| 29:f:142:GLY:HA2  | 32:2:1403:U:H3    | 1.63                     | 0.63              |
| 1:A:198:MET:HG3   | 1:A:200:ASP:H     | 1.64                     | 0.62              |
| 3:D:14:ASP:N      | 3:D:14:ASP:OD1    | 2.30                     | 0.62              |
| 32:2:1379:A:N6    | 32:2:1408:A:N7    | 2.47                     | 0.62              |
| 32:2:1375:A:N6    | 32:2:1410:U:O4    | 2.32                     | 0.62              |
| 32:2:1746:G:N1    | 32:2:1755:U:O4    | 2.30                     | 0.62              |
| 14:P:61:ARG:HH21  | 14:P:64:LYS:HG2   | 1.64                     | 0.62              |
| 32:2:1167:A:N6    | 32:2:1169:C:OP2   | 2.31                     | 0.62              |
| 32:2:1073:C:O2    | 32:2:1091:G:N2    | 2.33                     | 0.62              |
| 32:2:1309:A:N6    | 32:2:1312:A:N3    | 2.47                     | 0.62              |
| 11:L:33:ARG:NH2   | 11:L:51:GLY:O     | 2.33                     | 0.62              |
| 12:M:36:LEU:HD23  | 12:M:37:VAL:HB    | 1.82                     | 0.62              |
| 31:k:617:GLN:HB3  | 31:k:668:ILE:HB   | 1.81                     | 0.61              |
| 7:H:107:ARG:HD2   | 32:2:988:U:H1'    | 1.81                     | 0.61              |
| 32:2:960:G:N1     | 32:2:970:C:N3     | 2.42                     | 0.61              |
| 10:K:46:LEU:HA    | 10:K:49:LEU:HB2   | 1.81                     | 0.61              |
| 30:g:240:VAL:HA   | 30:g:256:THR:HA   | 1.82                     | 0.61              |
| 32:2:10:G:O6      | 32:2:11:A:N6      | 2.33                     | 0.61              |
| 32:2:1511:C:O2    | 32:2:1516:G:N1    | 2.34                     | 0.61              |
| 31:k:195:LEU:O    | 31:k:205:GLN:NE2  | 2.34                     | 0.61              |
| 32:2:1022:G:H1    | 32:2:1030:C:H42   | 1.46                     | 0.61              |
| 7:H:123:ASP:N     | 7:H:123:ASP:OD1   | 2.29                     | 0.61              |
| 8:I:152:ILE:HD11  | 8:I:157:GLU:HB3   | 1.81                     | 0.61              |
| 18:T:132:LEU:HD13 | 18:T:135:ILE:HD11 | 1.82                     | 0.61              |
| 10:K:23:ALA:HB3   | 10:K:64:TYR:HB2   | 1.81                     | 0.61              |
| 13:N:102:LEU:O    | 13:N:106:ARG:NH2  | 2.34                     | 0.61              |
| 32:2:1423:G:H1    | 32:2:1592:C:H1'   | 1.66                     | 0.60              |
| 11:L:132:SER:OG   | 11:L:133:LYS:N    | 2.34                     | 0.60              |
| 30:g:24:ALA:HB3   | 30:g:34:LEU:HB3   | 1.83                     | 0.60              |
| 5:F:126:ASP:OD1   | 5:F:126:ASP:N     | 2.35                     | 0.60              |
| 32:2:1491:C:O2'   | 32:2:1493:A:N7    | 2.33                     | 0.60              |
| 29:f:116:LYS:HE2  | 29:f:132:LEU:H    | 1.65                     | 0.60              |
| 30:g:3:SER:N      | 30:g:317:THR:OG1  | 2.35                     | 0.60              |
| 32:2:1513:U:H2'   | 32:2:1514:U:H2'   | 1.83                     | 0.60              |
| 32:2:1636:G:O2'   | 32:2:1758:C:O2'   | 2.20                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:60:VAL:HA    | 12:M:122:VAL:HG12 | 1.82                     | 0.60              |
| 30:g:3:SER:N      | 30:g:317:THR:HG1  | 2.00                     | 0.60              |
| 31:k:506:ASN:ND2  | 31:k:510:CYS:SG   | 2.74                     | 0.60              |
| 7:H:101:LYS:O     | 32:2:942:C:N4     | 2.35                     | 0.60              |
| 14:P:97:TYR:OH    | 32:2:1394:A:N3    | 2.32                     | 0.60              |
| 20:V:17:CYS:SG    | 20:V:18:SER:N     | 2.74                     | 0.60              |
| 29:f:133:ALA:HB3  | 29:f:140:TYR:HB3  | 1.82                     | 0.60              |
| 3:D:142:LEU:O     | 3:D:146:ARG:NH1   | 2.35                     | 0.60              |
| 30:g:18:GLY:O     | 30:g:308:ASN:ND2  | 2.35                     | 0.60              |
| 5:F:118:LEU:O     | 5:F:122:ASN:ND2   | 2.34                     | 0.59              |
| 9:J:21:SER:HA     | 9:J:24:LEU:HD12   | 1.83                     | 0.59              |
| 32:2:751:G:H21    | 32:2:762:U:H3     | 1.50                     | 0.59              |
| 12:M:66:VAL:HG11  | 12:M:72:ILE:HG21  | 1.85                     | 0.59              |
| 32:2:1365:G:N2    | 32:2:1603:C:N3    | 2.44                     | 0.59              |
| 5:F:94:THR:HG22   | 5:F:114:ILE:HG13  | 1.84                     | 0.59              |
| 32:2:1366:U:O2    | 32:2:1603:C:N4    | 2.35                     | 0.59              |
| 3:D:181:VAL:HB    | 32:2:1588:A:H1'   | 1.83                     | 0.59              |
| 16:R:25:THR:HG22  | 16:R:27:ASP:H     | 1.67                     | 0.59              |
| 24:Z:47:TYR:O     | 24:Z:52:LYS:NZ    | 2.36                     | 0.59              |
| 32:2:892:U:H5'    | 32:2:1166:A:H2'   | 1.84                     | 0.59              |
| 8:I:20:GLN:NE2    | 8:I:22:ARG:O      | 2.36                     | 0.59              |
| 10:K:37:THR:HB    | 10:K:42:VAL:HG12  | 1.85                     | 0.59              |
| 27:d:20:GLN:HE21  | 27:d:22:ARG:HE    | 1.49                     | 0.59              |
| 31:k:697:LEU:HB3  | 31:k:699:LYS:HZ2  | 1.66                     | 0.59              |
| 32:2:918:G:H4'    | 32:2:919:G:H5'    | 1.85                     | 0.59              |
| 4:E:253:ASP:OD1   | 4:E:253:ASP:N     | 2.33                     | 0.59              |
| 5:F:110:ALA:HA    | 5:F:113:ILE:HD12  | 1.84                     | 0.59              |
| 7:H:9:LEU:HD13    | 7:H:12:ALA:H      | 1.67                     | 0.59              |
| 32:2:756:U:H2'    | 32:2:757:U:H2'    | 1.83                     | 0.59              |
| 6:G:115:LYS:NZ    | 6:G:116:LYS:O     | 2.36                     | 0.59              |
| 16:R:44:LYS:NZ    | 32:2:1539:G:N7    | 2.42                     | 0.59              |
| 10:K:8:ARG:HA     | 10:K:11:ILE:HB    | 1.85                     | 0.58              |
| 32:2:828:C:H2'    | 32:2:829:C:H2'    | 1.85                     | 0.58              |
| 10:K:9:ASN:HA     | 10:K:13:GLN:HB2   | 1.85                     | 0.58              |
| 11:L:109:VAL:HG12 | 11:L:137:PHE:HB2  | 1.85                     | 0.58              |
| 14:P:80:MET:SD    | 14:P:98:ASN:ND2   | 2.76                     | 0.58              |
| 15:Q:32:ASN:OD1   | 15:Q:68:ARG:NH1   | 2.35                     | 0.58              |
| 32:2:747:C:O2     | 32:2:766:G:N2     | 2.33                     | 0.58              |
| 32:2:1351:G:N2    | 32:2:1746:G:O2'   | 2.36                     | 0.58              |
| 32:2:1497:A:O2'   | 32:2:1500:A:N7    | 2.35                     | 0.58              |
| 32:2:1624:C:H4'   | 32:2:1625:U:H5'   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:107:SER:HB2  | 32:2:1048:G:H21   | 1.69                     | 0.58              |
| 24:Z:72:GLY:H     | 24:Z:75:LEU:HD12  | 1.69                     | 0.58              |
| 29:f:124:PRO:HA   | 29:f:130:VAL:HG21 | 1.84                     | 0.58              |
| 32:2:1467:U:OP1   | 32:2:1480:G:N2    | 2.35                     | 0.58              |
| 32:2:1796:C:H2'   | 32:2:1909:G:H1    | 1.69                     | 0.58              |
| 12:M:106:ILE:O    | 12:M:114:LYS:NZ   | 2.36                     | 0.58              |
| 16:R:60:ARG:NH1   | 32:2:1552:A:OP2   | 2.37                     | 0.58              |
| 29:f:140:TYR:HA   | 29:f:149:LYS:HE2  | 1.86                     | 0.58              |
| 31:k:543:LYS:O    | 31:k:547:ASN:ND2  | 2.36                     | 0.58              |
| 3:D:162:GLN:H     | 32:2:1485:C:H4'   | 1.68                     | 0.58              |
| 31:k:288:ASN:ND2  | 31:k:548:GLU:O    | 2.37                     | 0.58              |
| 8:I:61:GLU:HG2    | 8:I:62:THR:HG23   | 1.85                     | 0.58              |
| 7:H:74:GLN:O      | 7:H:78:THR:OG1    | 2.22                     | 0.58              |
| 19:U:35:GLU:OE2   | 19:U:57:ARG:NH2   | 2.37                     | 0.58              |
| 32:2:906:G:H1     | 32:2:937:C:H42    | 1.52                     | 0.58              |
| 32:2:1328:G:N1    | 32:2:1616:G:O3'   | 2.36                     | 0.57              |
| 6:G:2:LYS:HB2     | 6:G:108:VAL:HG12  | 1.86                     | 0.57              |
| 32:2:884:A:OP2    | 32:2:1181:U:N3    | 2.37                     | 0.57              |
| 23:Y:55:VAL:HG23  | 23:Y:75:VAL:HB    | 1.86                     | 0.57              |
| 28:e:26:LYS:NZ    | 32:2:850:C:OP1    | 2.37                     | 0.57              |
| 31:k:57:LYS:O     | 31:k:61:LEU:N     | 2.38                     | 0.57              |
| 32:2:1182:A:H61   | 32:2:1257:C:H42   | 1.53                     | 0.57              |
| 15:Q:37:THR:O     | 15:Q:45:ARG:NH1   | 2.37                     | 0.57              |
| 18:T:74:GLY:HA2   | 18:T:77:ASN:HD22  | 1.70                     | 0.57              |
| 32:2:824:G:N2     | 32:2:825:G:O4'    | 2.38                     | 0.57              |
| 3:D:100:ALA:O     | 3:D:104:SER:N     | 2.38                     | 0.57              |
| 3:D:157:LEU:HD13  | 3:D:189:MET:HE3   | 1.84                     | 0.57              |
| 31:k:486:ILE:HD12 | 31:k:701:ALA:HB1  | 1.87                     | 0.57              |
| 6:G:180:THR:HG22  | 6:G:182:GLN:H     | 1.69                     | 0.57              |
| 11:L:33:ARG:NH1   | 11:L:53:TYR:O     | 2.37                     | 0.57              |
| 31:k:475:MET:SD   | 31:k:644:ARG:NH1  | 2.78                     | 0.57              |
| 31:k:631:GLN:O    | 31:k:640:HIS:ND1  | 2.37                     | 0.57              |
| 31:k:726:ASP:N    | 31:k:726:ASP:OD1  | 2.38                     | 0.57              |
| 30:g:19:TRP:H     | 30:g:38:ARG:HB2   | 1.69                     | 0.57              |
| 1:A:142:PRO:HG3   | 20:V:32:VAL:HG13  | 1.86                     | 0.57              |
| 8:I:3:ILE:O       | 8:I:30:GLY:N      | 2.35                     | 0.57              |
| 8:I:41:LYS:NZ     | 32:2:523:U:OP2    | 2.38                     | 0.57              |
| 14:P:85:ILE:HG22  | 14:P:116:LEU:HD23 | 1.85                     | 0.57              |
| 32:2:1335:A:N3    | 32:2:1363:A:N6    | 2.53                     | 0.57              |
| 32:2:1742:G:O6    | 32:2:1757:G:N1    | 2.38                     | 0.57              |
| 2:C:218:ILE:O     | 2:C:221:THR:OG1   | 2.19                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:55:ASP:OD2   | 11:L:82:ARG:NH1   | 2.38                     | 0.56              |
| 20:V:66:ASP:OD1   | 20:V:66:ASP:N     | 2.34                     | 0.56              |
| 30:g:178:VAL:HB   | 30:g:192:PHE:HB2  | 1.85                     | 0.56              |
| 31:k:165:VAL:HG23 | 31:k:166:GLN:HG3  | 1.87                     | 0.56              |
| 20:V:38:LYS:NZ    | 20:V:50:TYR:O     | 2.38                     | 0.56              |
| 31:k:371:THR:HG21 | 31:k:732:SER:H    | 1.70                     | 0.56              |
| 3:D:222:VAL:HG23  | 30:g:192:PHE:HA   | 1.88                     | 0.56              |
| 9:J:154:LYS:HG3   | 9:J:155:HIS:HD2   | 1.71                     | 0.56              |
| 9:J:171:ARG:HH21  | 9:J:174:ARG:HG3   | 1.70                     | 0.56              |
| 11:L:36:LYS:NZ    | 11:L:59:PRO:O     | 2.32                     | 0.56              |
| 14:P:56:PHE:O     | 14:P:60:LEU:N     | 2.38                     | 0.56              |
| 15:Q:32:ASN:HA    | 15:Q:68:ARG:HG2   | 1.86                     | 0.56              |
| 17:S:114:GLU:HA   | 17:S:117:LYS:HB3  | 1.86                     | 0.56              |
| 30:g:101:GLN:NE2  | 30:g:102:ARG:O    | 2.37                     | 0.56              |
| 30:g:132:LYS:NZ   | 30:g:133:VAL:O    | 2.37                     | 0.56              |
| 3:D:90:ARG:NH2    | 3:D:91:VAL:O      | 2.39                     | 0.56              |
| 7:H:128:ASP:N     | 7:H:128:ASP:OD1   | 2.34                     | 0.56              |
| 22:X:11:SER:O     | 22:X:11:SER:OG    | 2.18                     | 0.56              |
| 10:K:37:THR:OG1   | 10:K:41:TYR:N     | 2.38                     | 0.56              |
| 28:e:55:ARG:NH2   | 32:2:820:G:OP2    | 2.37                     | 0.56              |
| 1:A:98:ILE:HD11   | 1:A:116:LYS:HE2   | 1.86                     | 0.56              |
| 2:C:45:VAL:HG11   | 2:C:68:ILE:HG23   | 1.87                     | 0.56              |
| 10:K:7:ASP:N      | 10:K:7:ASP:OD1    | 2.37                     | 0.56              |
| 10:K:26:ASP:OD2   | 10:K:29:GLN:NE2   | 2.38                     | 0.56              |
| 23:Y:19:ALA:HB1   | 23:Y:77:ASN:HD21  | 1.70                     | 0.56              |
| 23:Y:34:ASN:ND2   | 32:2:795:U:O2     | 2.39                     | 0.56              |
| 31:k:705:GLY:H    | 31:k:768:VAL:HG11 | 1.70                     | 0.56              |
| 32:2:1426:C:H5'   | 32:2:1587:G:C5    | 2.41                     | 0.56              |
| 18:T:129:GLN:NE2  | 32:2:1509:A:N3    | 2.53                     | 0.56              |
| 2:C:206:THR:O     | 2:C:206:THR:OG1   | 2.24                     | 0.56              |
| 32:2:1811:A:H61   | 32:2:1894:U:H3    | 1.52                     | 0.56              |
| 4:E:50:ASN:O      | 4:E:51:ARG:NH1    | 2.39                     | 0.56              |
| 15:Q:82:ARG:NH2   | 15:Q:113:ASP:OD2  | 2.39                     | 0.56              |
| 32:2:960:G:N2     | 32:2:971:U:O2'    | 2.39                     | 0.56              |
| 2:C:241:ASP:N     | 2:C:241:ASP:OD1   | 2.34                     | 0.55              |
| 14:P:40:ARG:NH1   | 32:2:1709:U:OP1   | 2.39                     | 0.55              |
| 32:2:1851:G:H2'   | 32:2:1853:A:H62   | 1.71                     | 0.55              |
| 10:K:52:LYS:NZ    | 32:2:1371:A:O3'   | 2.38                     | 0.55              |
| 22:X:19:ARG:NH2   | 32:2:872:U:O2     | 2.39                     | 0.55              |
| 22:X:47:SER:OG    | 22:X:48:HIS:N     | 2.39                     | 0.55              |
| 32:2:140:A:N6     | 32:2:544:G:OP2    | 2.39                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:Q:23:LYS:HB3  | 15:Q:64:ASP:HB3   | 1.89                     | 0.55              |
| 32:2:963:C:N4    | 32:2:966:G:OP2    | 2.39                     | 0.55              |
| 11:L:80:MET:SD   | 11:L:83:THR:OG1   | 2.64                     | 0.55              |
| 14:P:94:VAL:N    | 14:P:105:VAL:O    | 2.39                     | 0.55              |
| 24:Z:77:ARG:NH1  | 32:2:1685:C:OP2   | 2.39                     | 0.55              |
| 32:2:1582:U:H1'  | 32:2:1585:G:C5    | 2.41                     | 0.55              |
| 30:g:84:SER:OG   | 30:g:88:THR:OG1   | 2.25                     | 0.55              |
| 9:J:176:ASN:ND2  | 32:2:774:A:OP2    | 2.39                     | 0.55              |
| 10:K:1:MET:HB3   | 10:K:44:LYS:HD3   | 1.88                     | 0.55              |
| 12:M:127:GLY:H   | 12:M:130:THR:HG23 | 1.72                     | 0.55              |
| 15:Q:49:TYR:HB3  | 15:Q:53:LEU:HD13  | 1.86                     | 0.55              |
| 16:R:82:ASP:HA   | 16:R:85:VAL:HG23  | 1.87                     | 0.55              |
| 19:U:22:ILE:HG22 | 19:U:118:VAL:HG23 | 1.88                     | 0.55              |
| 29:f:116:LYS:HG3 | 29:f:118:ARG:H    | 1.72                     | 0.55              |
| 3:D:157:LEU:HD22 | 3:D:189:MET:HB2   | 1.89                     | 0.55              |
| 9:J:113:VAL:HG21 | 9:J:134:ILE:HD13  | 1.89                     | 0.55              |
| 12:M:54:ARG:NH1  | 29:f:126:CYS:O    | 2.39                     | 0.55              |
| 32:2:1695:A:N6   | 32:2:1720:C:O2'   | 2.39                     | 0.55              |
| 1:A:66:ALA:HB2   | 20:V:37:ALA:HB2   | 1.88                     | 0.55              |
| 3:D:22:ASN:OD1   | 3:D:22:ASN:N      | 2.40                     | 0.55              |
| 6:G:138:ALA:HA   | 6:G:141:ILE:HD12  | 1.88                     | 0.55              |
| 18:T:8:ASP:N     | 18:T:8:ASP:OD1    | 2.39                     | 0.55              |
| 18:T:39:THR:OG1  | 18:T:43:ASN:ND2   | 2.40                     | 0.55              |
| 3:D:127:MET:HE3  | 3:D:132:LYS:HD2   | 1.89                     | 0.55              |
| 15:Q:26:LYS:NZ   | 15:Q:26:LYS:O     | 2.40                     | 0.55              |
| 14:P:133:ALA:O   | 32:2:1331:G:N2    | 2.39                     | 0.55              |
| 30:g:220:ILE:HB  | 30:g:234:LEU:HB3  | 1.88                     | 0.55              |
| 9:J:17:ARG:NH2   | 32:2:3:U:O2       | 2.40                     | 0.54              |
| 32:2:1673:G:O2'  | 32:2:1675:G:OP2   | 2.25                     | 0.54              |
| 12:M:43:ARG:NE   | 32:2:1379:A:N1    | 2.56                     | 0.54              |
| 32:2:919:G:O2'   | 32:2:924:A:N6     | 2.41                     | 0.54              |
| 26:c:10:ALA:HB3  | 26:c:54:LEU:HB2   | 1.89                     | 0.54              |
| 30:g:12:THR:HG23 | 30:g:309:VAL:HG23 | 1.89                     | 0.54              |
| 30:g:59:ARG:NH1  | 30:g:96:THR:O     | 2.38                     | 0.54              |
| 30:g:154:VAL:O   | 30:g:155:ARG:NH1  | 2.37                     | 0.54              |
| 31:k:633:SER:O   | 31:k:640:HIS:NE2  | 2.41                     | 0.54              |
| 31:k:699:LYS:HB2 | 31:k:775:LYS:HB2  | 1.89                     | 0.54              |
| 5:F:157:ARG:HH22 | 5:F:220:VAL:HG13  | 1.72                     | 0.54              |
| 8:I:110:ARG:HG3  | 8:I:121:LEU:HD12  | 1.90                     | 0.54              |
| 14:P:29:SER:OG   | 14:P:30:THR:N     | 2.39                     | 0.54              |
| 26:c:9:LEU:HG    | 26:c:33:LEU:HD13  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:108:GLN:HE21  | 32:2:1056:G:H21   | 1.54                     | 0.54              |
| 10:K:30:ALA:H     | 10:K:39:ASN:HB2   | 1.73                     | 0.54              |
| 31:k:84:LYS:NZ    | 31:k:242:LEU:O    | 2.40                     | 0.54              |
| 3:D:53:THR:HA     | 3:D:90:ARG:HG3    | 1.89                     | 0.54              |
| 13:N:108:ASP:OD1  | 32:2:1124:G:O2'   | 2.24                     | 0.54              |
| 19:U:113:ASP:OD1  | 19:U:113:ASP:N    | 2.40                     | 0.54              |
| 31:k:251:ASN:O    | 31:k:255:ASN:ND2  | 2.40                     | 0.54              |
| 31:k:501:TYR:HA   | 31:k:775:LYS:HD3  | 1.90                     | 0.54              |
| 32:2:1277:A:C5    | 32:2:1278:G:H1'   | 2.42                     | 0.54              |
| 8:I:47:ARG:NH1    | 32:2:660:A:OP2    | 2.41                     | 0.54              |
| 14:P:122:THR:HG22 | 17:S:126:ARG:HH21 | 1.72                     | 0.54              |
| 17:S:53:ASP:O     | 17:S:56:LYS:NZ    | 2.40                     | 0.54              |
| 4:E:85:GLY:N      | 4:E:88:ASP:OD2    | 2.40                     | 0.54              |
| 14:P:120:SER:OG   | 14:P:121:ILE:N    | 2.41                     | 0.54              |
| 18:T:84:LYS:HG3   | 18:T:94:ILE:HA    | 1.90                     | 0.54              |
| 18:T:122:ARG:HH21 | 32:2:1651:G:H5''  | 1.73                     | 0.54              |
| 32:2:1427:A:N6    | 32:2:1588:A:OP2   | 2.41                     | 0.54              |
| 16:R:45:ARG:HA    | 16:R:48:ASN:HD22  | 1.73                     | 0.54              |
| 25:b:74:SER:OG    | 25:b:75:GLU:N     | 2.38                     | 0.54              |
| 27:d:31:ILE:HD11  | 27:d:40:ARG:HB3   | 1.90                     | 0.54              |
| 32:2:1677:A:N3    | 32:2:1741:C:O2'   | 2.41                     | 0.54              |
| 3:D:67:ASN:HB3    | 10:K:96:ASN:HB2   | 1.90                     | 0.53              |
| 26:c:18:ARG:NH2   | 32:2:1767:C:OP1   | 2.41                     | 0.53              |
| 32:2:753:C:O2'    | 32:2:760:G:N2     | 2.41                     | 0.53              |
| 4:E:181:VAL:HG21  | 4:E:195:ILE:HD11  | 1.90                     | 0.53              |
| 5:F:138:THR:O     | 5:F:143:ARG:NH2   | 2.41                     | 0.53              |
| 5:F:148:ARG:HH22  | 5:F:166:ARG:HH21  | 1.56                     | 0.53              |
| 6:G:187:LYS:NZ    | 32:2:140:A:OP2    | 2.38                     | 0.53              |
| 18:T:13:ASP:HA    | 18:T:16:ASN:HD22  | 1.73                     | 0.53              |
| 31:k:249:SER:OG   | 31:k:254:ASP:OD2  | 2.26                     | 0.53              |
| 32:2:893:A:N7     | 32:2:1166:A:O2'   | 2.39                     | 0.53              |
| 32:2:1271:G:H22   | 32:2:1280:A:H2    | 1.56                     | 0.53              |
| 18:T:126:GLU:OE1  | 18:T:130:ARG:NH2  | 2.40                     | 0.53              |
| 30:g:68:VAL:HA    | 30:g:84:SER:HA    | 1.90                     | 0.53              |
| 30:g:91:LEU:HB2   | 30:g:100:TYR:HB3  | 1.89                     | 0.53              |
| 30:g:244:ALA:HB3  | 30:g:253:ALA:HB3  | 1.91                     | 0.53              |
| 32:2:1301:G:O2'   | 32:2:1302:G:N2    | 2.40                     | 0.53              |
| 12:M:66:VAL:HG22  | 12:M:68:GLU:H     | 1.72                     | 0.53              |
| 14:P:41:VAL:HA    | 14:P:44:ARG:HB3   | 1.91                     | 0.53              |
| 17:S:109:LEU:HD23 | 17:S:110:ARG:HG3  | 1.89                     | 0.53              |
| 19:U:36:ASN:O     | 19:U:40:ASN:ND2   | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:Y:36:SER:OG   | 23:Y:37:LYS:N    | 2.41                     | 0.53              |
| 32:2:1651:G:N2   | 32:2:1662:U:O2   | 2.34                     | 0.53              |
| 12:M:33:ARG:O    | 12:M:33:ARG:NH1  | 2.35                     | 0.53              |
| 14:P:43:ARG:NH2  | 32:2:1704:U:OP2  | 2.40                     | 0.53              |
| 17:S:71:GLN:NE2  | 17:S:79:TYR:OH   | 2.41                     | 0.53              |
| 18:T:106:GLN:NE2 | 32:2:1652:C:OP2  | 2.36                     | 0.53              |
| 29:f:123:ASN:ND2 | 29:f:144:CYS:SG  | 2.82                     | 0.53              |
| 31:k:214:SER:HA  | 31:k:217:LYS:HD2 | 1.90                     | 0.53              |
| 32:2:74:U:O2'    | 32:2:75:U:O3'    | 2.26                     | 0.53              |
| 5:F:55:ASP:OD2   | 5:F:167:ARG:NH2  | 2.41                     | 0.53              |
| 7:H:53:GLY:O     | 7:H:55:LYS:NZ    | 2.42                     | 0.53              |
| 8:I:142:LYS:NZ   | 32:2:449:C:OP2   | 2.38                     | 0.53              |
| 31:k:662:PHE:O   | 31:k:664:GLN:NE2 | 2.41                     | 0.53              |
| 32:2:1355:A:OP1  | 32:2:1608:C:N4   | 2.42                     | 0.53              |
| 5:F:32:GLU:O     | 5:F:37:GLN:NE2   | 2.36                     | 0.53              |
| 5:F:92:ARG:NH2   | 32:2:1765:U:OP1  | 2.42                     | 0.53              |
| 32:2:831:G:N7    | 32:2:838:C:N4    | 2.57                     | 0.53              |
| 32:2:1783:A:O2'  | 32:2:1784:C:OP2  | 2.25                     | 0.53              |
| 9:J:18:PRO:O     | 9:J:23:ARG:NH2   | 2.42                     | 0.53              |
| 14:P:42:ARG:NH2  | 32:2:1701:C:OP2  | 2.38                     | 0.53              |
| 16:R:44:LYS:O    | 16:R:48:ASN:ND2  | 2.42                     | 0.53              |
| 30:g:200:ASN:ND2 | 30:g:240:VAL:O   | 2.38                     | 0.53              |
| 31:k:539:ASN:O   | 31:k:543:LYS:NZ  | 2.41                     | 0.53              |
| 9:J:119:ALA:HB1  | 9:J:124:HIS:HB3  | 1.90                     | 0.53              |
| 17:S:83:ALA:O    | 17:S:89:GLN:NE2  | 2.42                     | 0.53              |
| 2:C:245:ASP:N    | 2:C:245:ASP:OD1  | 2.40                     | 0.52              |
| 4:E:56:LEU:O     | 4:E:57:ASN:ND2   | 2.42                     | 0.52              |
| 5:F:145:ASP:OD1  | 5:F:145:ASP:N    | 2.40                     | 0.52              |
| 5:F:209:TYR:O    | 5:F:213:LYS:NZ   | 2.43                     | 0.52              |
| 9:J:72:GLU:OE2   | 32:2:1007:G:O2'  | 2.23                     | 0.52              |
| 21:W:30:SER:OG   | 21:W:31:SER:N    | 2.40                     | 0.52              |
| 21:W:55:ASP:HB3  | 25:b:25:VAL:HG22 | 1.91                     | 0.52              |
| 32:2:1298:G:N2   | 32:2:1298:G:OP1  | 2.42                     | 0.52              |
| 6:G:224:ALA:O    | 6:G:228:LYS:NZ   | 2.42                     | 0.52              |
| 16:R:2:GLY:N     | 32:2:1555:C:OP1  | 2.42                     | 0.52              |
| 17:S:2:SER:OG    | 17:S:3:LEU:N     | 2.43                     | 0.52              |
| 18:T:5:SER:OG    | 18:T:6:VAL:N     | 2.43                     | 0.52              |
| 32:2:826:U:H4'   | 32:2:827:G:H4'   | 1.92                     | 0.52              |
| 5:F:119:ASP:N    | 5:F:119:ASP:OD1  | 2.40                     | 0.52              |
| 6:G:202:ARG:NH2  | 32:2:127:G:O6    | 2.41                     | 0.52              |
| 30:g:248:ASN:ND2 | 30:g:297:ASP:O   | 2.43                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:k:146:LEU:HD13 | 31:k:149:LEU:HD12 | 1.91                     | 0.52              |
| 32:2:1274:G:N2    | 32:2:1277:A:OP2   | 2.43                     | 0.52              |
| 32:2:1514:U:O2    | 32:2:1515:U:N3    | 2.42                     | 0.52              |
| 32:2:1699:A:N6    | 32:2:1717:C:N3    | 2.57                     | 0.52              |
| 10:K:21:VAL:HB    | 10:K:66:TYR:HB2   | 1.90                     | 0.52              |
| 32:2:1807:A:N6    | 32:2:1898:A:N3    | 2.57                     | 0.52              |
| 4:E:216:ASN:OD1   | 4:E:216:ASN:N     | 2.39                     | 0.52              |
| 9:J:128:LEU:HD23  | 9:J:134:ILE:HD11  | 1.92                     | 0.52              |
| 12:M:59:LEU:HG    | 12:M:124:LYS:HE3  | 1.92                     | 0.52              |
| 18:T:65:ILE:HD13  | 18:T:71:VAL:HG23  | 1.91                     | 0.52              |
| 24:Z:94:LYS:HA    | 24:Z:99:ALA:HA    | 1.92                     | 0.52              |
| 32:2:1455:U:O2'   | 32:2:1474:A:OP2   | 2.25                     | 0.52              |
| 32:2:1802:U:H3    | 32:2:1902:A:H61   | 1.57                     | 0.52              |
| 32:2:1866:A:H2'   | 32:2:1867:G:H8    | 1.75                     | 0.52              |
| 3:D:146:ARG:HG3   | 3:D:148:LYS:HB2   | 1.91                     | 0.52              |
| 5:F:143:ARG:HD2   | 26:c:55:VAL:HG11  | 1.91                     | 0.52              |
| 7:H:163:ASP:N     | 7:H:163:ASP:OD1   | 2.43                     | 0.52              |
| 16:R:22:PRO:O     | 30:g:216:LYS:NZ   | 2.43                     | 0.52              |
| 30:g:63:GLY:O     | 30:g:90:ARG:NH2   | 2.41                     | 0.52              |
| 32:2:1522:U:H1'   | 32:2:1523:A:H5'   | 1.91                     | 0.52              |
| 3:D:175:VAL:HG11  | 3:D:181:VAL:HG22  | 1.92                     | 0.52              |
| 9:J:133:HIS:ND1   | 9:J:162:SER:OG    | 2.32                     | 0.52              |
| 17:S:111:ASP:OD1  | 17:S:111:ASP:N    | 2.41                     | 0.52              |
| 32:2:767:U:H2'    | 32:2:768:A:H8     | 1.75                     | 0.52              |
| 32:2:1844:G:N2    | 32:2:1863:C:O4'   | 2.42                     | 0.52              |
| 7:H:63:PRO:O      | 7:H:66:SER:OG     | 2.28                     | 0.52              |
| 10:K:15:LEU:HA    | 10:K:18:GLU:HB2   | 1.92                     | 0.52              |
| 17:S:40:ARG:HH22  | 32:2:1720:C:H41   | 1.56                     | 0.52              |
| 21:W:53:ILE:HD11  | 25:b:8:LEU:HD11   | 1.92                     | 0.52              |
| 24:Z:74:SER:OG    | 24:Z:77:ARG:NH2   | 2.42                     | 0.52              |
| 4:E:171:ASP:OD1   | 4:E:171:ASP:N     | 2.41                     | 0.52              |
| 14:P:52:LYS:NZ    | 32:2:1396:A:O5'   | 2.43                     | 0.52              |
| 18:T:22:LEU:HA    | 18:T:25:GLN:HG2   | 1.91                     | 0.52              |
| 30:g:13:LEU:HB2   | 30:g:310:ILE:HB   | 1.92                     | 0.52              |
| 30:g:211:ILE:HB   | 30:g:223:TRP:HB2  | 1.90                     | 0.52              |
| 3:D:50:ILE:O      | 3:D:89:GLU:N      | 2.43                     | 0.52              |
| 5:F:159:ALA:O     | 26:c:43:ASN:ND2   | 2.43                     | 0.52              |
| 7:H:177:THR:OG1   | 7:H:178:GLY:N     | 2.42                     | 0.52              |
| 13:N:99:ARG:HA    | 13:N:102:LEU:HD12 | 1.92                     | 0.52              |
| 14:P:122:THR:HG23 | 14:P:123:TYR:HD1  | 1.76                     | 0.52              |
| 18:T:25:GLN:HB3   | 18:T:27:LYS:HG2   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:2:1426:C:C4    | 32:2:1589:U:H5'   | 2.45                     | 0.52              |
| 11:L:110:HIS:HB3  | 11:L:138:ASN:HB3  | 1.91                     | 0.51              |
| 14:P:18:ARG:NH2   | 14:P:35:LYS:O     | 2.39                     | 0.51              |
| 1:A:80:THR:HA     | 1:A:83:GLN:HE21   | 1.74                     | 0.51              |
| 5:F:41:LYS:NZ     | 5:F:43:PHE:O      | 2.43                     | 0.51              |
| 29:f:115:THR:OG1  | 29:f:116:LYS:N    | 2.44                     | 0.51              |
| 30:g:220:ILE:HD12 | 30:g:234:LEU:HD22 | 1.90                     | 0.51              |
| 31:k:103:LYS:NZ   | 31:k:230:GLU:OE2  | 2.43                     | 0.51              |
| 31:k:514:VAL:HG13 | 31:k:776:ARG:HH12 | 1.75                     | 0.51              |
| 32:2:1359:C:N4    | 32:2:1607:G:O6    | 2.33                     | 0.51              |
| 9:J:27:GLU:OE1    | 9:J:39:LYS:NZ     | 2.38                     | 0.51              |
| 13:N:142:GLU:O    | 13:N:146:ALA:N    | 2.43                     | 0.51              |
| 30:g:84:SER:OG    | 30:g:86:ASP:OD1   | 2.27                     | 0.51              |
| 32:2:504:U:O2'    | 32:2:505:U:O4'    | 2.28                     | 0.51              |
| 32:2:1808:U:H3    | 32:2:1897:G:H1    | 1.58                     | 0.51              |
| 30:g:131:ILE:HB   | 30:g:144:LEU:HB3  | 1.93                     | 0.51              |
| 30:g:211:ILE:O    | 30:g:223:TRP:N    | 2.39                     | 0.51              |
| 8:I:195:ARG:HE    | 8:I:199:LYS:HD2   | 1.75                     | 0.51              |
| 9:J:107:ARG:NH1   | 9:J:153:GLU:OE2   | 2.43                     | 0.51              |
| 9:J:120:LYS:NZ    | 32:2:742:C:O2'    | 2.43                     | 0.51              |
| 15:Q:42:GLU:OE1   | 15:Q:45:ARG:NH2   | 2.43                     | 0.51              |
| 13:N:87:ASP:N     | 13:N:87:ASP:OD1   | 2.40                     | 0.51              |
| 32:2:959:A:N6     | 32:2:968:G:OP1    | 2.43                     | 0.51              |
| 32:2:1385:G:N2    | 32:2:1404:C:O4'   | 2.43                     | 0.51              |
| 8:I:116:HIS:O     | 8:I:146:ARG:NH1   | 2.43                     | 0.51              |
| 12:M:113:ARG:HH12 | 32:2:1376:A:H8    | 1.59                     | 0.51              |
| 16:R:125:SER:OG   | 16:R:126:ALA:N    | 2.44                     | 0.51              |
| 32:2:1593:C:H5''  | 32:2:1598:A:H5'   | 1.91                     | 0.51              |
| 32:2:1641:U:O2    | 32:2:1665:G:N2    | 2.44                     | 0.51              |
| 18:T:43:ASN:OD1   | 18:T:43:ASN:N     | 2.43                     | 0.51              |
| 18:T:68:ARG:NH2   | 32:2:1673:G:O6    | 2.42                     | 0.51              |
| 18:T:117:SER:HB3  | 18:T:123:ARG:HG2  | 1.92                     | 0.51              |
| 32:2:1334:U:O2'   | 32:2:1336:A:N7    | 2.40                     | 0.51              |
| 32:2:1755:U:H5    | 32:2:1756:U:C2    | 2.29                     | 0.51              |
| 24:Z:78:ILE:HA    | 24:Z:81:ARG:HB2   | 1.92                     | 0.51              |
| 10:K:42:VAL:HA    | 10:K:45:ALA:HB3   | 1.93                     | 0.51              |
| 17:S:45:LEU:O     | 17:S:49:LYS:N     | 2.41                     | 0.51              |
| 31:k:295:ILE:HG23 | 31:k:298:PHE:HB2  | 1.93                     | 0.51              |
| 1:A:205:ARG:HB3   | 16:R:83:GLN:HE22  | 1.76                     | 0.50              |
| 5:F:174:LEU:HB3   | 5:F:213:LYS:HE2   | 1.92                     | 0.50              |
| 13:N:142:GLU:N    | 13:N:145:THR:OG1  | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:93:VAL:HA    | 14:P:106:GLU:HA   | 1.93                     | 0.50              |
| 32:2:1589:U:OP1   | 32:2:1592:C:N4    | 2.44                     | 0.50              |
| 32:2:1462:U:H2'   | 32:2:1463:U:H6    | 1.76                     | 0.50              |
| 32:2:1510:G:O6    | 32:2:1516:G:N1    | 2.44                     | 0.50              |
| 12:M:26:ASP:HA    | 12:M:29:LYS:HD2   | 1.94                     | 0.50              |
| 26:c:8:THR:HB     | 26:c:56:LEU:HB3   | 1.92                     | 0.50              |
| 31:k:120:SER:O    | 31:k:576:GLN:NE2  | 2.44                     | 0.50              |
| 31:k:599:GLN:HG3  | 31:k:686:GLY:HA2  | 1.94                     | 0.50              |
| 32:2:693:G:H21    | 32:2:694:C:H3'    | 1.76                     | 0.50              |
| 32:2:1640:G:N2    | 32:2:1647:C:O2'   | 2.44                     | 0.50              |
| 1:A:192:THR:HG23  | 1:A:193:GLN:HE21  | 1.75                     | 0.50              |
| 3:D:159:HIS:O     | 3:D:161:GLY:N     | 2.44                     | 0.50              |
| 17:S:15:LEU:O     | 17:S:21:ASN:ND2   | 2.39                     | 0.50              |
| 22:X:56:LYS:NZ    | 32:2:1906:A:N7    | 2.56                     | 0.50              |
| 31:k:207:ASP:OD1  | 31:k:207:ASP:N    | 2.39                     | 0.50              |
| 32:2:486:U:O2     | 32:2:1085:U:N3    | 2.44                     | 0.50              |
| 32:2:1803:A:N7    | 32:2:1804:C:N4    | 2.60                     | 0.50              |
| 5:F:63:GLN:OE1    | 5:F:65:ARG:NH1    | 2.45                     | 0.50              |
| 31:k:625:ILE:HD13 | 31:k:782:SER:HB2  | 1.94                     | 0.50              |
| 32:2:802:G:OP2    | 32:2:802:G:N2     | 2.34                     | 0.50              |
| 8:I:157:GLU:HA    | 8:I:160:PHE:HD2   | 1.77                     | 0.50              |
| 9:J:88:GLU:O      | 9:J:91:LYS:NZ     | 2.44                     | 0.50              |
| 29:f:122:SER:OG   | 29:f:123:ASN:N    | 2.45                     | 0.50              |
| 31:k:544:GLU:HA   | 31:k:547:ASN:HD22 | 1.76                     | 0.50              |
| 6:G:52:ILE:HG22   | 6:G:109:LEU:HD21  | 1.94                     | 0.50              |
| 18:T:35:ASP:OD1   | 18:T:35:ASP:N     | 2.43                     | 0.50              |
| 5:F:140:THR:HG21  | 5:F:175:LEU:HD21  | 1.94                     | 0.50              |
| 7:H:87:ASP:OD1    | 7:H:88:ARG:NH1    | 2.44                     | 0.50              |
| 16:R:32:LYS:NZ    | 32:2:1540:A:OP2   | 2.45                     | 0.50              |
| 31:k:150:ASP:HA   | 31:k:153:LYS:HG2  | 1.94                     | 0.50              |
| 7:H:99:LEU:O      | 7:H:112:ARG:NH1   | 2.45                     | 0.50              |
| 9:J:121:SER:OG    | 9:J:122:VAL:N     | 2.45                     | 0.50              |
| 10:K:17:GLN:NE2   | 10:K:92:ILE:O     | 2.45                     | 0.50              |
| 18:T:130:ARG:NE   | 32:2:1510:G:OP1   | 2.42                     | 0.50              |
| 31:k:94:ASP:OD1   | 31:k:94:ASP:N     | 2.35                     | 0.50              |
| 3:D:34:TYR:HA     | 3:D:91:VAL:HG21   | 1.93                     | 0.49              |
| 18:T:12:GLN:O     | 18:T:16:ASN:ND2   | 2.45                     | 0.49              |
| 31:k:175:GLN:NE2  | 31:k:602:GLU:OE2  | 2.45                     | 0.49              |
| 32:2:1385:G:N3    | 32:2:1386:A:N6    | 2.60                     | 0.49              |
| 1:A:32:HIS:NE2    | 20:V:64:GLU:OE2   | 2.46                     | 0.49              |
| 5:F:150:GLY:O     | 5:F:156:ARG:N     | 2.41                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 24:Z:57:TYR:O     | 24:Z:103:ARG:NE  | 2.40                     | 0.49              |
| 32:2:426:G:OP2    | 32:2:426:G:N2    | 2.42                     | 0.49              |
| 1:A:84:ARG:NH1    | 16:R:83:GLN:OE1  | 2.43                     | 0.49              |
| 31:k:193:SER:OG   | 31:k:194:ASN:OD1 | 2.31                     | 0.49              |
| 31:k:269:THR:OG1  | 31:k:273:SER:O   | 2.30                     | 0.49              |
| 32:2:1193:G:N2    | 32:2:1230:C:O2   | 2.45                     | 0.49              |
| 18:T:7:ARG:NH2    | 32:2:1519:G:OP1  | 2.45                     | 0.49              |
| 19:U:88:LYS:NZ    | 32:2:1668:A:OP1  | 2.42                     | 0.49              |
| 30:g:175:ASP:OD1  | 30:g:175:ASP:N   | 2.40                     | 0.49              |
| 32:2:11:A:H61     | 32:2:1296:U:H3   | 1.61                     | 0.49              |
| 3:D:32:GLU:O      | 3:D:94:ARG:NH1   | 2.44                     | 0.49              |
| 7:H:32:PRO:HA     | 7:H:35:LYS:HE3   | 1.95                     | 0.49              |
| 19:U:76:SER:OG    | 32:2:1434:U:O3'  | 2.30                     | 0.49              |
| 31:k:174:GLU:OE2  | 31:k:178:ARG:NE  | 2.37                     | 0.49              |
| 31:k:741:ARG:HH12 | 31:k:762:LYS:HE3 | 1.76                     | 0.49              |
| 1:A:63:ILE:HG12   | 20:V:36:VAL:HG12 | 1.94                     | 0.49              |
| 3:D:109:LEU:H     | 3:D:177:MET:HE2  | 1.77                     | 0.49              |
| 24:Z:83:LEU:HD12  | 24:Z:86:GLU:HB2  | 1.94                     | 0.49              |
| 32:2:1393:G:N2    | 32:2:1395:G:OP2  | 2.44                     | 0.49              |
| 32:2:1617:C:OP1   | 32:2:1731:U:O2'  | 2.30                     | 0.49              |
| 3:D:34:TYR:OH     | 3:D:49:ILE:O     | 2.18                     | 0.49              |
| 6:G:13:GLN:HE22   | 32:2:151:G:H21   | 1.59                     | 0.49              |
| 13:N:147:SER:HA   | 13:N:151:ASN:HB3 | 1.95                     | 0.49              |
| 19:U:23:ARG:N     | 19:U:117:VAL:O   | 2.45                     | 0.49              |
| 2:C:201:ASN:ND2   | 32:2:1249:U:O4   | 2.34                     | 0.49              |
| 17:S:36:LYS:HE3   | 32:2:1719:U:H5'' | 1.95                     | 0.49              |
| 32:2:803:G:O2'    | 32:2:805:A:OP2   | 2.25                     | 0.49              |
| 32:2:1387:C:O2    | 32:2:1388:A:N6   | 2.46                     | 0.49              |
| 11:L:11:ARG:NH2   | 32:2:605:C:O2'   | 2.45                     | 0.49              |
| 21:W:102:VAL:HG12 | 21:W:128:PHE:HB3 | 1.94                     | 0.49              |
| 29:f:145:HIS:HA   | 29:f:149:LYS:HZ2 | 1.78                     | 0.49              |
| 30:g:135:THR:OG1  | 30:g:139:GLN:N   | 2.46                     | 0.49              |
| 31:k:598:LEU:HA   | 31:k:669:PHE:HE2 | 1.78                     | 0.49              |
| 4:E:122:LYS:NZ    | 4:E:143:ASP:OD2  | 2.33                     | 0.49              |
| 5:F:148:ARG:NH2   | 32:2:1315:A:O3'  | 2.46                     | 0.49              |
| 7:H:98:ILE:HD13   | 7:H:118:LEU:HD12 | 1.95                     | 0.49              |
| 14:P:94:VAL:HB    | 14:P:105:VAL:HB  | 1.94                     | 0.49              |
| 29:f:102:VAL:HG11 | 32:2:1381:G:H3'  | 1.95                     | 0.49              |
| 31:k:306:ILE:HB   | 31:k:337:PHE:HB2 | 1.94                     | 0.49              |
| 32:2:1616:G:N2    | 32:2:1617:C:O2   | 2.46                     | 0.49              |
| 12:M:95:LYS:O     | 12:M:99:GLU:N    | 2.45                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:S:44:ASN:OD1   | 17:S:44:ASN:N     | 2.46                     | 0.48              |
| 3:D:112:GLY:HA2   | 3:D:178:ARG:HH21  | 1.77                     | 0.48              |
| 15:Q:114:ARG:NH2  | 32:2:1561:G:N7    | 2.61                     | 0.48              |
| 31:k:671:LYS:O    | 31:k:681:GLU:N    | 2.43                     | 0.48              |
| 32:2:736:A:O2'    | 32:2:1014:C:N3    | 2.46                     | 0.48              |
| 32:2:1426:C:H5    | 32:2:1587:G:H5'   | 1.79                     | 0.48              |
| 3:D:23:GLU:O      | 3:D:26:THR:OG1    | 2.23                     | 0.48              |
| 4:E:121:TYR:OH    | 4:E:235:TYR:O     | 2.30                     | 0.48              |
| 5:F:103:ASN:ND2   | 32:2:1625:U:H3    | 2.09                     | 0.48              |
| 9:J:139:GLN:NE2   | 23:Y:64:PHE:O     | 2.46                     | 0.48              |
| 12:M:58:LEU:HD23  | 12:M:124:LYS:HG2  | 1.95                     | 0.48              |
| 16:R:30:THR:OG1   | 16:R:31:ASN:N     | 2.47                     | 0.48              |
| 28:e:56:MET:SD    | 28:e:56:MET:N     | 2.85                     | 0.48              |
| 31:k:252:TRP:HE3  | 31:k:256:ARG:HH12 | 1.60                     | 0.48              |
| 32:2:1515:U:H3'   | 32:2:1516:G:H8    | 1.78                     | 0.48              |
| 5:F:103:ASN:HA    | 5:F:106:LYS:HD2   | 1.94                     | 0.48              |
| 14:P:61:ARG:NH1   | 14:P:88:GLU:OE1   | 2.47                     | 0.48              |
| 14:P:112:LEU:H    | 17:S:122:HIS:CD2  | 2.31                     | 0.48              |
| 24:Z:90:LYS:N     | 24:Z:102:THR:O    | 2.44                     | 0.48              |
| 29:f:145:HIS:O    | 29:f:145:HIS:ND1  | 2.46                     | 0.48              |
| 32:2:1423:G:N1    | 32:2:1592:C:H1'   | 2.29                     | 0.48              |
| 32:2:1605:G:O2'   | 32:2:1606:G:O4'   | 2.31                     | 0.48              |
| 8:I:97:THR:OG1    | 8:I:98:LYS:O      | 2.32                     | 0.48              |
| 31:k:612:GLU:N    | 31:k:626:GLN:OE1  | 2.47                     | 0.48              |
| 32:2:73:U:O2'     | 32:2:74:U:O4'     | 2.32                     | 0.48              |
| 32:2:1442:U:H2'   | 32:2:1443:G:C8    | 2.48                     | 0.48              |
| 14:P:39:ALA:HA    | 14:P:42:ARG:HB2   | 1.95                     | 0.48              |
| 14:P:85:ILE:HG12  | 14:P:114:HIS:H    | 1.77                     | 0.48              |
| 18:T:133:ASP:O    | 18:T:137:ALA:N    | 2.45                     | 0.48              |
| 30:g:90:ARG:HD3   | 30:g:99:THR:HG21  | 1.95                     | 0.48              |
| 31:k:375:ASP:OD1  | 31:k:375:ASP:N    | 2.46                     | 0.48              |
| 32:2:451:A:N6     | 32:2:460:A:O2'    | 2.46                     | 0.48              |
| 4:E:170:THR:OG1   | 4:E:171:ASP:OD1   | 2.27                     | 0.48              |
| 14:P:136:SER:OG   | 32:2:1330:G:N2    | 2.47                     | 0.48              |
| 18:T:129:GLN:O    | 32:2:1510:G:O2'   | 2.30                     | 0.48              |
| 19:U:27:THR:O     | 19:U:27:THR:OG1   | 2.29                     | 0.48              |
| 23:Y:112:LYS:NZ   | 32:2:57:G:OP1     | 2.37                     | 0.48              |
| 24:Z:94:LYS:NZ    | 32:2:1683:G:OP1   | 2.47                     | 0.48              |
| 32:2:1637:C:O2'   | 32:2:1638:G:O4'   | 2.28                     | 0.48              |
| 3:D:36:GLY:O      | 3:D:51:ARG:NH2    | 2.47                     | 0.48              |
| 12:M:103:LEU:HD13 | 32:2:1378:A:H8    | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:2:454:C:N4     | 32:2:458:G:O6     | 2.43                     | 0.48              |
| 32:2:1307:G:H1    | 32:2:1775:C:H42   | 1.61                     | 0.48              |
| 18:T:89:ARG:NH1   | 32:2:1753:G:N7    | 2.62                     | 0.48              |
| 22:X:97:ASP:N     | 22:X:97:ASP:OD1   | 2.46                     | 0.48              |
| 31:k:628:LEU:O    | 31:k:655:THR:N    | 2.43                     | 0.48              |
| 32:2:1610:G:OP2   | 32:2:1610:G:N2    | 2.39                     | 0.48              |
| 21:W:55:ASP:OD1   | 21:W:55:ASP:N     | 2.44                     | 0.48              |
| 32:2:1699:A:H61   | 32:2:1717:C:H42   | 1.60                     | 0.48              |
| 3:D:109:LEU:HB3   | 3:D:177:MET:SD    | 2.54                     | 0.47              |
| 5:F:190:ILE:O     | 5:F:193:THR:OG1   | 2.27                     | 0.47              |
| 21:W:2:THR:OG1    | 21:W:3:ARG:N      | 2.42                     | 0.47              |
| 31:k:158:VAL:HG21 | 31:k:185:ILE:HD11 | 1.96                     | 0.47              |
| 32:2:1386:A:H2'   | 32:2:1387:C:H4'   | 1.95                     | 0.47              |
| 32:2:1442:U:H2'   | 32:2:1443:G:H8    | 1.79                     | 0.47              |
| 30:g:307:ASP:OD1  | 30:g:307:ASP:N    | 2.36                     | 0.47              |
| 32:2:1205:G:H1    | 32:2:1218:C:H42   | 1.62                     | 0.47              |
| 14:P:21:ASP:H     | 14:P:24:LYS:HE2   | 1.77                     | 0.47              |
| 25:b:34:ASP:HB3   | 25:b:43:ILE:HD11  | 1.96                     | 0.47              |
| 32:2:1801:G:O6    | 32:2:1902:A:N6    | 2.48                     | 0.47              |
| 8:I:172:ARG:O     | 8:I:176:SER:OG    | 2.31                     | 0.47              |
| 31:k:73:ARG:HH22  | 31:k:246:LEU:H    | 1.63                     | 0.47              |
| 31:k:695:ARG:HH21 | 31:k:697:LEU:HD12 | 1.79                     | 0.47              |
| 32:2:1274:G:O2'   | 32:2:1276:A:N7    | 2.42                     | 0.47              |
| 32:2:1626:G:H2'   | 32:2:1627:A:H8    | 1.80                     | 0.47              |
| 17:S:2:SER:O      | 24:Z:82:HIS:ND1   | 2.47                     | 0.47              |
| 17:S:38:VAL:HG13  | 17:S:42:TYR:HD1   | 1.80                     | 0.47              |
| 31:k:291:ARG:HB3  | 31:k:586:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:71:GLU:N      | 1:A:71:GLU:OE2    | 2.47                     | 0.47              |
| 2:C:143:TYR:OH    | 2:C:149:GLY:O     | 2.26                     | 0.47              |
| 4:E:223:ASN:N     | 4:E:223:ASN:OD1   | 2.46                     | 0.47              |
| 9:J:63:ASP:OD1    | 9:J:64:GLU:N      | 2.48                     | 0.47              |
| 10:K:82:LEU:HD11  | 10:K:87:VAL:HB    | 1.97                     | 0.47              |
| 11:L:125:VAL:HG12 | 11:L:139:VAL:HA   | 1.96                     | 0.47              |
| 18:T:84:LYS:HE3   | 18:T:94:ILE:HA    | 1.96                     | 0.47              |
| 30:g:151:VAL:HA   | 30:g:173:GLY:HA2  | 1.95                     | 0.47              |
| 30:g:295:SER:OG   | 30:g:296:ALA:N    | 2.44                     | 0.47              |
| 32:2:873:G:HO2'   | 32:2:876:G:HO2'   | 1.57                     | 0.47              |
| 32:2:1269:U:H2'   | 32:2:1270:G:C8    | 2.50                     | 0.47              |
| 32:2:1702:A:N6    | 32:2:1713:U:O4    | 2.48                     | 0.47              |
| 1:A:127:ARG:NH2   | 1:A:150:ASP:O     | 2.48                     | 0.47              |
| 3:D:222:VAL:O     | 30:g:229:LYS:NZ   | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:38:PRO:HA    | 14:P:42:ARG:HH21  | 1.79                     | 0.47              |
| 30:g:86:ASP:OD1   | 30:g:86:ASP:N     | 2.36                     | 0.47              |
| 30:g:200:ASN:ND2  | 30:g:239:GLU:OE1  | 2.47                     | 0.47              |
| 9:J:147:MET:HB3   | 9:J:147:MET:HE3   | 1.74                     | 0.47              |
| 10:K:3:MET:O      | 32:2:1409:U:O2'   | 2.26                     | 0.47              |
| 13:N:2:GLY:N      | 32:2:1112:G:OP1   | 2.48                     | 0.47              |
| 22:X:74:VAL:HG11  | 22:X:104:LEU:HD11 | 1.96                     | 0.47              |
| 30:g:10:ARG:HB2   | 30:g:312:VAL:HG13 | 1.97                     | 0.47              |
| 30:g:195:HIS:NE2  | 30:g:219:GLU:O    | 2.37                     | 0.47              |
| 3:D:9:ARG:HH12    | 32:2:1641:U:P     | 2.38                     | 0.47              |
| 24:Z:83:LEU:HD11  | 24:Z:88:ILE:HB    | 1.96                     | 0.47              |
| 31:k:274:GLY:N    | 31:k:563:PHE:O    | 2.46                     | 0.47              |
| 32:2:945:U:O2     | 32:2:985:G:N2     | 2.40                     | 0.47              |
| 5:F:220:VAL:O     | 5:F:223:SER:OG    | 2.29                     | 0.46              |
| 18:T:49:ASP:OD1   | 18:T:52:GLY:N     | 2.48                     | 0.46              |
| 24:Z:64:VAL:O     | 24:Z:68:ARG:NH1   | 2.45                     | 0.46              |
| 29:f:143:LYS:HZ1  | 32:2:1404:C:H4'   | 1.78                     | 0.46              |
| 32:2:65:A:H2      | 32:2:84:A:H62     | 1.62                     | 0.46              |
| 1:A:188:LEU:HD13  | 1:A:188:LEU:HA    | 1.77                     | 0.46              |
| 9:J:37:LYS:HB2    | 28:e:33:ARG:HE    | 1.80                     | 0.46              |
| 30:g:86:ASP:OD1   | 30:g:88:THR:OG1   | 2.34                     | 0.46              |
| 8:I:32:GLN:HE21   | 32:2:1879:G:H21   | 1.63                     | 0.46              |
| 14:P:79:HIS:HA    | 32:2:1604:U:H4'   | 1.98                     | 0.46              |
| 1:A:144:ILE:HG12  | 1:A:158:VAL:HG13  | 1.97                     | 0.46              |
| 4:E:79:ASP:HB3    | 4:E:82:TYR:HB2    | 1.98                     | 0.46              |
| 4:E:192:ILE:HG13  | 4:E:243:GLY:HA3   | 1.97                     | 0.46              |
| 5:F:185:ARG:NH2   | 32:2:1623:A:OP1   | 2.49                     | 0.46              |
| 11:L:132:SER:OG   | 32:2:588:G:OP1    | 2.29                     | 0.46              |
| 32:2:491:G:N1     | 32:2:502:C:OP2    | 2.48                     | 0.46              |
| 32:2:535:U:O2'    | 32:2:536:G:O4'    | 2.32                     | 0.46              |
| 4:E:253:ASP:HA    | 4:E:256:ARG:HB2   | 1.97                     | 0.46              |
| 14:P:40:ARG:NH2   | 14:P:115:TYR:OH   | 2.48                     | 0.46              |
| 19:U:90:TYR:OH    | 32:2:1499:U:OP1   | 2.34                     | 0.46              |
| 24:Z:83:LEU:HG    | 24:Z:89:ILE:HG13  | 1.97                     | 0.46              |
| 31:k:127:HIS:ND1  | 31:k:134:ASN:OD1  | 2.34                     | 0.46              |
| 31:k:295:ILE:HG12 | 31:k:298:PHE:HD2  | 1.79                     | 0.46              |
| 5:F:189:THR:HG23  | 5:F:192:GLU:H     | 1.80                     | 0.46              |
| 17:S:127:HIS:HD2  | 17:S:132:ARG:HH22 | 1.63                     | 0.46              |
| 26:c:12:VAL:HA    | 26:c:30:VAL:HA    | 1.97                     | 0.46              |
| 32:2:1308:C:H1'   | 32:2:1309:A:H5'   | 1.98                     | 0.46              |
| 15:Q:100:GLN:NE2  | 30:g:55:GLY:O     | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:R:58:MET:HE3   | 16:R:58:MET:HB3   | 1.74                     | 0.46              |
| 18:T:65:ILE:HG23  | 18:T:124:ILE:HD11 | 1.98                     | 0.46              |
| 18:T:97:SER:OG    | 32:2:1656:G:OP1   | 2.33                     | 0.46              |
| 24:Z:93:SER:O     | 24:Z:100:ILE:N    | 2.42                     | 0.46              |
| 30:g:76:ASP:OD1   | 30:g:76:ASP:N     | 2.45                     | 0.46              |
| 20:V:36:VAL:HG21  | 20:V:78:LEU:HD21  | 1.97                     | 0.46              |
| 3:D:139:SER:O     | 32:2:1430:G:N2    | 2.40                     | 0.46              |
| 4:E:176:ASP:N     | 4:E:176:ASP:OD1   | 2.49                     | 0.46              |
| 12:M:107:ASP:N    | 12:M:107:ASP:OD1  | 2.45                     | 0.46              |
| 16:R:72:LYS:O     | 16:R:77:GLU:N     | 2.40                     | 0.46              |
| 27:d:20:GLN:NE2   | 27:d:22:ARG:HE    | 2.13                     | 0.46              |
| 32:2:1807:A:H61   | 32:2:1898:A:H2'   | 1.81                     | 0.46              |
| 32:2:1887:U:H2'   | 32:2:1888:G:C8    | 2.51                     | 0.46              |
| 1:A:47:VAL:HG21   | 16:R:105:GLN:HE22 | 1.81                     | 0.46              |
| 7:H:104:ARG:NH2   | 32:2:1051:U:O4    | 2.49                     | 0.46              |
| 8:I:34:ALA:HB2    | 8:I:56:ARG:HD3    | 1.98                     | 0.46              |
| 10:K:69:THR:OG1   | 10:K:70:GLU:N     | 2.43                     | 0.46              |
| 21:W:87:GLU:HA    | 21:W:90:THR:HG22  | 1.97                     | 0.46              |
| 7:H:81:LEU:HA     | 7:H:84:LYS:HB3    | 1.98                     | 0.45              |
| 12:M:136:ILE:HG22 | 12:M:139:HIS:HD1  | 1.82                     | 0.45              |
| 14:P:75:PRO:HB3   | 14:P:95:GLY:H     | 1.81                     | 0.45              |
| 14:P:136:SER:HA   | 32:2:1330:G:H22   | 1.81                     | 0.45              |
| 17:S:24:GLY:HA3   | 17:S:58:ALA:HB2   | 1.99                     | 0.45              |
| 31:k:513:GLN:NE2  | 31:k:515:ASP:OD2  | 2.49                     | 0.45              |
| 32:2:757:U:O2'    | 32:2:758:C:O4'    | 2.33                     | 0.45              |
| 1:A:124:THR:OG1   | 1:A:125:ASP:N     | 2.50                     | 0.45              |
| 26:c:13:ILE:HG22  | 26:c:14:LYS:HG2   | 1.98                     | 0.45              |
| 31:k:259:VAL:HG22 | 31:k:282:VAL:HA   | 1.98                     | 0.45              |
| 5:F:26:ALA:HB2    | 15:Q:26:LYS:HB3   | 1.98                     | 0.45              |
| 5:F:124:LEU:HD13  | 24:Z:58:ARG:HG2   | 1.99                     | 0.45              |
| 12:M:25:GLU:HA    | 12:M:28:LEU:HB2   | 1.99                     | 0.45              |
| 13:N:27:LYS:HA    | 13:N:27:LYS:HD3   | 1.81                     | 0.45              |
| 19:U:40:ASN:HA    | 19:U:43:LYS:HB2   | 1.97                     | 0.45              |
| 26:c:40:ILE:HA    | 26:c:64:ARG:HH12  | 1.80                     | 0.45              |
| 31:k:345:THR:OG1  | 31:k:347:ASP:OD1  | 2.30                     | 0.45              |
| 5:F:166:ARG:HB2   | 26:c:47:PRO:HD2   | 1.99                     | 0.45              |
| 32:2:735:U:O2'    | 32:2:1015:A:N3    | 2.49                     | 0.45              |
| 2:C:88:LYS:HG3    | 2:C:90:THR:HG23   | 1.98                     | 0.45              |
| 5:F:200:ASN:OD1   | 5:F:205:SER:OG    | 2.26                     | 0.45              |
| 10:K:54:TYR:HB3   | 10:K:71:GLU:HG2   | 1.98                     | 0.45              |
| 11:L:131:ILE:HD13 | 11:L:131:ILE:HA   | 1.80                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:S:35:ILE:HB   | 17:S:102:ALA:HB2  | 1.98                     | 0.45              |
| 32:2:1393:G:N7   | 32:2:1394:A:N6    | 2.65                     | 0.45              |
| 32:2:1395:G:N2   | 32:2:1396:A:N7    | 2.65                     | 0.45              |
| 32:2:1507:C:H5   | 32:2:1520:G:H21   | 1.65                     | 0.45              |
| 8:I:120:THR:OG1  | 8:I:121:LEU:N     | 2.50                     | 0.45              |
| 9:J:102:GLU:HA   | 9:J:105:LEU:HB2   | 1.98                     | 0.45              |
| 32:2:1685:C:H4'  | 32:2:1691:G:H1    | 1.82                     | 0.45              |
| 1:A:88:LYS:HZ1   | 16:R:81:LYS:HA    | 1.82                     | 0.45              |
| 4:E:21:ASP:N     | 4:E:21:ASP:OD1    | 2.38                     | 0.45              |
| 6:G:3:LEU:HD23   | 6:G:3:LEU:HA      | 1.80                     | 0.45              |
| 6:G:226:ILE:HG23 | 6:G:229:ARG:HH12  | 1.82                     | 0.45              |
| 15:Q:58:ASP:OD1  | 15:Q:58:ASP:N     | 2.36                     | 0.45              |
| 19:U:35:GLU:OE1  | 19:U:89:ARG:NH1   | 2.50                     | 0.45              |
| 21:W:88:LYS:O    | 21:W:92:ASN:ND2   | 2.49                     | 0.45              |
| 31:k:61:LEU:HD12 | 31:k:62:ARG:HB3   | 1.99                     | 0.45              |
| 31:k:72:ASN:OD1  | 31:k:72:ASN:N     | 2.50                     | 0.45              |
| 31:k:699:LYS:HZ3 | 31:k:776:ARG:HA   | 1.82                     | 0.45              |
| 6:G:142:ARG:HH12 | 6:G:149:LYS:HD3   | 1.82                     | 0.45              |
| 7:H:165:LYS:O    | 7:H:168:SER:OG    | 2.27                     | 0.45              |
| 17:S:27:LYS:HB2  | 17:S:30:TYR:HD2   | 1.80                     | 0.45              |
| 17:S:61:LEU:O    | 17:S:63:GLN:NE2   | 2.50                     | 0.45              |
| 25:b:68:GLY:H    | 32:2:1118:G:H1'   | 1.81                     | 0.45              |
| 31:k:639:VAL:HA  | 31:k:695:ARG:HH12 | 1.80                     | 0.45              |
| 32:2:1423:G:N1   | 32:2:1592:C:O2    | 2.39                     | 0.45              |
| 5:F:198:LEU:O    | 5:F:202:ALA:N     | 2.49                     | 0.45              |
| 6:G:76:LEU:HD13  | 6:G:94:ARG:HH21   | 1.82                     | 0.45              |
| 6:G:79:LYS:HB3   | 6:G:79:LYS:HE2    | 1.72                     | 0.45              |
| 8:I:168:CYS:SG   | 8:I:169:ILE:N     | 2.89                     | 0.45              |
| 9:J:126:ARG:HD3  | 28:e:33:ARG:HH11  | 1.82                     | 0.45              |
| 23:Y:34:ASN:HD21 | 32:2:795:U:H1'    | 1.80                     | 0.45              |
| 32:2:1629:G:H2'  | 32:2:1630:G:H8    | 1.82                     | 0.45              |
| 6:G:216:LEU:HD21 | 32:2:504:U:H4'    | 1.98                     | 0.45              |
| 8:I:36:THR:HB    | 8:I:96:LEU:HB2    | 1.98                     | 0.45              |
| 17:S:129:TRP:HA  | 17:S:132:ARG:HB2  | 1.99                     | 0.45              |
| 21:W:9:ASP:HA    | 21:W:12:ASN:HB3   | 1.98                     | 0.45              |
| 4:E:146:THR:HG21 | 32:2:123:G:H21    | 1.82                     | 0.44              |
| 6:G:226:ILE:O    | 6:G:230:ARG:N     | 2.43                     | 0.44              |
| 27:d:22:ARG:HG3  | 27:d:23:VAL:HG22  | 1.99                     | 0.44              |
| 30:g:26:SER:OG   | 30:g:75:ALA:O     | 2.27                     | 0.44              |
| 31:k:110:ASP:OD1 | 31:k:111:GLU:N    | 2.46                     | 0.44              |
| 32:2:1841:A:H3'  | 32:2:1842:G:H8    | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:3:ARG:HD3     | 9:J:6:ARG:HH12    | 1.82                     | 0.44              |
| 14:P:77:ARG:NE    | 32:2:1395:G:N7    | 2.65                     | 0.44              |
| 18:T:27:LYS:O     | 18:T:110:LYS:NZ   | 2.34                     | 0.44              |
| 18:T:73:VAL:O     | 18:T:77:ASN:ND2   | 2.50                     | 0.44              |
| 23:Y:27:VAL:HG21  | 23:Y:35:VAL:HG11  | 1.98                     | 0.44              |
| 29:f:127:GLY:N    | 32:2:1405:U:OP1   | 2.40                     | 0.44              |
| 30:g:149:ASP:HB3  | 30:g:174:ASN:HB3  | 1.99                     | 0.44              |
| 32:2:1497:A:H8    | 32:2:1500:A:C6    | 2.35                     | 0.44              |
| 3:D:59:LEU:O      | 3:D:64:ARG:N      | 2.39                     | 0.44              |
| 4:E:188:ASN:HB3   | 4:E:191:ARG:HD3   | 2.00                     | 0.44              |
| 6:G:173:PRO:O     | 32:2:78:A:O2'     | 2.36                     | 0.44              |
| 14:P:78:THR:OG1   | 14:P:80:MET:N     | 2.46                     | 0.44              |
| 15:Q:103:ASN:HA   | 15:Q:106:LYS:HB3  | 1.98                     | 0.44              |
| 1:A:70:PRO:HB3    | 1:A:185:ARG:HH22  | 1.82                     | 0.44              |
| 1:A:157:ASP:N     | 1:A:157:ASP:OD1   | 2.45                     | 0.44              |
| 22:X:79:ASN:HB3   | 22:X:81:LYS:HG2   | 1.99                     | 0.44              |
| 5:F:53:VAL:HA     | 5:F:58:LEU:HD11   | 2.00                     | 0.44              |
| 15:Q:23:LYS:O     | 15:Q:64:ASP:N     | 2.49                     | 0.44              |
| 31:k:262:ASP:N    | 31:k:279:GLU:O    | 2.40                     | 0.44              |
| 32:2:802:G:H4'    | 32:2:803:G:H5'    | 1.99                     | 0.44              |
| 6:G:77:LEU:HD13   | 6:G:84:TYR:HB2    | 1.98                     | 0.44              |
| 6:G:228:LYS:HA    | 6:G:228:LYS:HD3   | 1.84                     | 0.44              |
| 17:S:130:GLY:H    | 17:S:132:ARG:HH21 | 1.65                     | 0.44              |
| 18:T:4:VAL:HG21   | 18:T:140:LEU:HD21 | 1.99                     | 0.44              |
| 19:U:45:ALA:O     | 19:U:49:ASN:N     | 2.51                     | 0.44              |
| 31:k:73:ARG:HH12  | 31:k:246:LEU:HB3  | 1.82                     | 0.44              |
| 31:k:367:ASP:OD2  | 31:k:367:ASP:N    | 2.51                     | 0.44              |
| 31:k:615:VAL:HA   | 31:k:624:THR:HA   | 1.99                     | 0.44              |
| 32:2:1100:U:O2'   | 32:2:1101:A:O4'   | 2.34                     | 0.44              |
| 32:2:1623:A:H62   | 32:2:1690:U:H3    | 1.65                     | 0.44              |
| 2:C:89:GLN:OE1    | 32:2:10:G:N2      | 2.51                     | 0.44              |
| 2:C:118:ALA:HB3   | 2:C:124:ALA:HB2   | 1.98                     | 0.44              |
| 13:N:106:ARG:HA   | 13:N:106:ARG:HD3  | 1.85                     | 0.44              |
| 14:P:64:LYS:HG3   | 14:P:65:LEU:HG    | 1.99                     | 0.44              |
| 17:S:115:ARG:HH22 | 17:S:122:HIS:HB2  | 1.82                     | 0.44              |
| 19:U:70:THR:OG1   | 19:U:72:ASN:O     | 2.26                     | 0.44              |
| 23:Y:37:LYS:NZ    | 32:2:786:G:OP2    | 2.34                     | 0.44              |
| 25:b:40:CYS:HB3   | 25:b:59:CYS:HB2   | 2.00                     | 0.44              |
| 31:k:671:LYS:HB3  | 31:k:681:GLU:HB2  | 1.99                     | 0.44              |
| 32:2:659:G:N2     | 32:2:662:A:OP2    | 2.46                     | 0.44              |
| 32:2:1062:G:H2'   | 32:2:1063:A:H8    | 1.83                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 32:2:1649:U:O4    | 32:2:1662:U:N3   | 2.42                     | 0.44              |
| 32:2:1651:G:N1    | 32:2:1661:C:N3   | 2.66                     | 0.44              |
| 3:D:65:ARG:HD3    | 3:D:69:LEU:HD21  | 2.00                     | 0.44              |
| 5:F:114:ILE:O     | 5:F:117:THR:OG1  | 2.34                     | 0.44              |
| 9:J:9:SER:OG      | 32:2:1017:A:OP1  | 2.35                     | 0.44              |
| 9:J:89:ASP:OD1    | 9:J:89:ASP:N     | 2.36                     | 0.44              |
| 17:S:6:GLN:HB3    | 24:Z:43:ASP:HA   | 1.99                     | 0.44              |
| 30:g:274:LEU:HD12 | 30:g:274:LEU:HA  | 1.84                     | 0.44              |
| 31:k:183:GLN:NE2  | 31:k:184:GLY:O   | 2.51                     | 0.44              |
| 32:2:1192:G:O6    | 32:2:1230:C:N4   | 2.51                     | 0.44              |
| 3:D:9:ARG:HA      | 3:D:12:VAL:HG22  | 2.00                     | 0.44              |
| 3:D:57:ASP:OD1    | 3:D:57:ASP:N     | 2.49                     | 0.44              |
| 10:K:42:VAL:HG22  | 10:K:46:LEU:HG   | 2.00                     | 0.44              |
| 15:Q:62:ASN:OD1   | 15:Q:62:ASN:N    | 2.48                     | 0.44              |
| 22:X:109:ARG:HG3  | 22:X:110:LYS:HE2 | 1.99                     | 0.44              |
| 24:Z:74:SER:OG    | 32:2:1686:G:OP2  | 2.30                     | 0.44              |
| 30:g:264:SER:OG   | 30:g:267:PRO:O   | 2.26                     | 0.44              |
| 31:k:613:PRO:O    | 31:k:624:THR:OG1 | 2.36                     | 0.44              |
| 31:k:661:ASP:OD1  | 31:k:661:ASP:N   | 2.50                     | 0.44              |
| 32:2:1375:A:N1    | 32:2:1412:U:N3   | 2.64                     | 0.43              |
| 2:C:245:ASP:O     | 2:C:248:SER:OG   | 2.36                     | 0.43              |
| 3:D:14:ASP:O      | 3:D:18:TYR:N     | 2.49                     | 0.43              |
| 5:F:97:LEU:HD12   | 5:F:110:ALA:HB1  | 2.00                     | 0.43              |
| 13:N:16:ILE:HG23  | 13:N:62:GLN:HE22 | 1.83                     | 0.43              |
| 30:g:33:LEU:HB3   | 30:g:45:TRP:HB2  | 2.01                     | 0.43              |
| 32:2:1610:G:H5'   | 32:2:1611:C:H5   | 1.83                     | 0.43              |
| 3:D:34:TYR:O      | 3:D:173:ARG:NH2  | 2.51                     | 0.43              |
| 23:Y:10:ARG:NH2   | 32:2:1024:G:H22  | 2.16                     | 0.43              |
| 31:k:153:LYS:HB3  | 31:k:153:LYS:HE3 | 1.84                     | 0.43              |
| 31:k:469:LEU:HA   | 31:k:472:PHE:HB2 | 1.98                     | 0.43              |
| 31:k:775:LYS:HD2  | 31:k:775:LYS:HA  | 1.79                     | 0.43              |
| 32:2:1405:U:H2'   | 32:2:1406:U:H4'  | 2.00                     | 0.43              |
| 32:2:1427:A:H62   | 32:2:1588:A:P    | 2.41                     | 0.43              |
| 2:C:242:ILE:HD13  | 2:C:242:ILE:HA   | 1.85                     | 0.43              |
| 6:G:143:LYS:NZ    | 32:2:144:U:OP1   | 2.51                     | 0.43              |
| 10:K:94:GLU:OE2   | 10:K:95:ARG:NH1  | 2.51                     | 0.43              |
| 12:M:131:ASP:O    | 12:M:134:SER:OG  | 2.35                     | 0.43              |
| 13:N:145:THR:HA   | 13:N:148:ALA:HB3 | 1.99                     | 0.43              |
| 16:R:31:ASN:N     | 16:R:31:ASN:OD1  | 2.51                     | 0.43              |
| 18:T:141:GLU:OE1  | 18:T:141:GLU:N   | 2.50                     | 0.43              |
| 20:V:46:ILE:HG22  | 20:V:48:GLY:H    | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:83:LEU:HA    | 24:Z:86:GLU:HG2   | 2.00                     | 0.43              |
| 30:g:133:VAL:HG13 | 30:g:141:LEU:HB2  | 2.00                     | 0.43              |
| 32:2:17:C:O2'     | 32:2:1289:A:N6    | 2.52                     | 0.43              |
| 32:2:1379:A:H4'   | 32:2:1380:G:H8    | 1.82                     | 0.43              |
| 32:2:1632:G:N2    | 32:2:1680:U:O2    | 2.52                     | 0.43              |
| 3:D:65:ARG:HA     | 3:D:68:GLU:HB3    | 1.99                     | 0.43              |
| 12:M:113:ARG:HD2  | 32:2:1375:A:H5''  | 2.01                     | 0.43              |
| 16:R:43:SER:OG    | 16:R:44:LYS:N     | 2.47                     | 0.43              |
| 19:U:69:LYS:NZ    | 19:U:78:THR:H     | 2.17                     | 0.43              |
| 32:2:1322:G:H1    | 32:2:1621:A:N6    | 2.16                     | 0.43              |
| 32:2:1676:A:H2'   | 32:2:1677:A:C8    | 2.53                     | 0.43              |
| 5:F:63:GLN:HG3    | 5:F:65:ARG:HD2    | 2.00                     | 0.43              |
| 6:G:92:ARG:O      | 32:2:668:C:O2'    | 2.36                     | 0.43              |
| 7:H:10:SER:OG     | 7:H:42:GLN:OE1    | 2.37                     | 0.43              |
| 9:J:10:LYS:NZ     | 32:2:24:U:OP1     | 2.51                     | 0.43              |
| 12:M:35:ALA:HB1   | 12:M:41:LEU:HD22  | 2.01                     | 0.43              |
| 14:P:100:LYS:HD2  | 32:2:1363:A:C8    | 2.53                     | 0.43              |
| 14:P:114:HIS:NE2  | 17:S:123:ARG:O    | 2.52                     | 0.43              |
| 32:2:1180:C:O2'   | 32:2:1181:U:OP1   | 2.28                     | 0.43              |
| 8:I:76:THR:OG1    | 8:I:105:ASP:OD1   | 2.37                     | 0.43              |
| 12:M:33:ARG:HA    | 12:M:33:ARG:HD2   | 1.85                     | 0.43              |
| 13:N:149:LEU:HD12 | 13:N:150:VAL:HG23 | 2.00                     | 0.43              |
| 15:Q:50:GLU:OE1   | 15:Q:82:ARG:NH1   | 2.52                     | 0.43              |
| 25:b:32:PHE:HB2   | 25:b:82:LYS:HD3   | 2.00                     | 0.43              |
| 31:k:289:ALA:HB1  | 31:k:339:SER:HA   | 2.00                     | 0.43              |
| 32:2:1167:A:C5    | 32:2:1168:U:H4'   | 2.53                     | 0.43              |
| 4:E:49:ARG:NH1    | 32:2:710:U:OP1    | 2.50                     | 0.43              |
| 12:M:86:VAL:HG22  | 12:M:87:PRO:HD2   | 2.01                     | 0.43              |
| 14:P:100:LYS:HB3  | 32:2:1363:A:C4    | 2.54                     | 0.43              |
| 24:Z:73:GLY:HA3   | 32:2:1686:G:C8    | 2.54                     | 0.43              |
| 25:b:56:CYS:SG    | 25:b:57:GLU:N     | 2.92                     | 0.43              |
| 27:d:25:SER:O     | 27:d:25:SER:OG    | 2.32                     | 0.43              |
| 32:2:1301:G:N2    | 32:2:1303:A:OP2   | 2.52                     | 0.43              |
| 32:2:1391:U:H3'   | 32:2:1392:U:H3'   | 2.01                     | 0.43              |
| 32:2:1637:C:C2    | 32:2:1638:G:H8    | 2.36                     | 0.43              |
| 12:M:54:ARG:NH2   | 29:f:124:PRO:O    | 2.52                     | 0.43              |
| 12:M:81:ASP:OD1   | 12:M:81:ASP:N     | 2.52                     | 0.43              |
| 16:R:65:PRO:O     | 16:R:67:ARG:NH1   | 2.50                     | 0.43              |
| 18:T:70:GLN:HB3   | 18:T:121:GLY:HA3  | 1.99                     | 0.43              |
| 31:k:58:ALA:O     | 31:k:61:LEU:N     | 2.52                     | 0.43              |
| 32:2:497:G:N1     | 32:2:498:G:N3     | 2.67                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 32:2:1841:A:H3'   | 32:2:1842:G:C8   | 2.53                     | 0.43              |
| 6:G:148:SER:N     | 6:G:151:ASP:OD2  | 2.51                     | 0.43              |
| 7:H:175:LYS:HD2   | 7:H:175:LYS:HA   | 1.80                     | 0.43              |
| 10:K:37:THR:HB    | 10:K:42:VAL:H    | 1.84                     | 0.43              |
| 11:L:65:SER:OG    | 32:2:114:C:O2    | 2.31                     | 0.43              |
| 28:e:42:ARG:HH22  | 32:2:852:C:H5'   | 1.83                     | 0.43              |
| 32:2:1431:C:HO2'  | 32:2:1432:C:P    | 2.42                     | 0.43              |
| 32:2:1844:G:N2    | 32:2:1863:C:OP2  | 2.49                     | 0.43              |
| 3:D:32:GLU:OE2    | 3:D:54:ARG:NH2   | 2.52                     | 0.42              |
| 5:F:29:ILE:HD12   | 5:F:30:PRO:HD2   | 2.01                     | 0.42              |
| 7:H:148:LYS:HE2   | 7:H:148:LYS:HB3  | 1.84                     | 0.42              |
| 31:k:472:PHE:HE2  | 31:k:609:PRO:HD3 | 1.83                     | 0.42              |
| 7:H:162:ILE:HD12  | 7:H:165:LYS:HD2  | 2.00                     | 0.42              |
| 14:P:44:ARG:HA    | 14:P:47:ARG:HB3  | 2.01                     | 0.42              |
| 18:T:39:THR:H     | 18:T:43:ASN:HD21 | 1.66                     | 0.42              |
| 31:k:114:MET:SD   | 31:k:114:MET:N   | 2.92                     | 0.42              |
| 3:D:108:LYS:HA    | 3:D:108:LYS:HD2  | 1.79                     | 0.42              |
| 6:G:48:TYR:OH     | 6:G:119:GLN:O    | 2.32                     | 0.42              |
| 8:I:84:HIS:CD2    | 8:I:90:LEU:HD12  | 2.54                     | 0.42              |
| 9:J:126:ARG:NE    | 28:e:33:ARG:HD2  | 2.35                     | 0.42              |
| 2:C:35:TRP:NE1    | 2:C:67:GLN:OE1   | 2.52                     | 0.42              |
| 3:D:159:HIS:NE2   | 3:D:189:MET:SD   | 2.92                     | 0.42              |
| 9:J:172:VAL:O     | 9:J:176:ASN:N    | 2.47                     | 0.42              |
| 15:Q:94:GLN:HB3   | 30:g:62:LYS:HZ1  | 1.84                     | 0.42              |
| 26:c:11:LYS:HE2   | 26:c:11:LYS:HB2  | 1.81                     | 0.42              |
| 30:g:10:ARG:HG3   | 30:g:314:GLN:HG3 | 2.02                     | 0.42              |
| 30:g:167:VAL:HG23 | 30:g:183:LEU:HB3 | 2.00                     | 0.42              |
| 31:k:290:ASN:OD1  | 31:k:290:ASN:N   | 2.49                     | 0.42              |
| 4:E:220:THR:OG1   | 4:E:221:ARG:N    | 2.53                     | 0.42              |
| 12:M:73:LYS:HA    | 12:M:73:LYS:HD3  | 1.84                     | 0.42              |
| 20:V:1:MET:HE3    | 20:V:1:MET:HB2   | 1.89                     | 0.42              |
| 32:2:590:U:H2'    | 32:2:591:A:C8    | 2.54                     | 0.42              |
| 3:D:26:THR:OG1    | 3:D:27:ARG:N     | 2.51                     | 0.42              |
| 18:T:77:ASN:HA    | 18:T:96:ALA:HB3  | 2.02                     | 0.42              |
| 25:b:43:ILE:HD12  | 25:b:43:ILE:HA   | 1.85                     | 0.42              |
| 31:k:515:ASP:OD2  | 31:k:515:ASP:N   | 2.50                     | 0.42              |
| 32:2:456:U:H2'    | 32:2:457:U:H2'   | 2.02                     | 0.42              |
| 5:F:175:LEU:HD23  | 5:F:210:ALA:HB1  | 2.02                     | 0.42              |
| 6:G:181:PRO:HA    | 6:G:184:LEU:HD12 | 2.02                     | 0.42              |
| 7:H:108:GLN:NE2   | 32:2:1056:G:H21  | 2.18                     | 0.42              |
| 13:N:43:LYS:HA    | 13:N:43:LYS:HD3  | 1.84                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:2:1379:A:HI'  | 32:2:1381:G:C2    | 2.55                     | 0.42              |
| 32:2:1407:G:HI'  | 32:2:1408:A:C8    | 2.55                     | 0.42              |
| 2:C:44:LEU:HD23  | 2:C:44:LEU:HA     | 1.85                     | 0.42              |
| 2:C:178:ILE:HG23 | 2:C:196:VAL:HG12  | 2.02                     | 0.42              |
| 3:D:50:ILE:N     | 3:D:87:TYR:O      | 2.52                     | 0.42              |
| 5:F:109:LYS:HE3  | 5:F:109:LYS:HB3   | 1.89                     | 0.42              |
| 5:F:146:THR:OG1  | 5:F:147:THR:N     | 2.53                     | 0.42              |
| 6:G:73:ILE:HD12  | 6:G:73:ILE:HA     | 1.93                     | 0.42              |
| 8:I:185:GLU:O    | 8:I:189:LEU:N     | 2.47                     | 0.42              |
| 9:J:108:ARG:NH1  | 9:J:110:GLN:OE1   | 2.53                     | 0.42              |
| 14:P:44:ARG:HD3  | 14:P:84:ILE:HD11  | 2.00                     | 0.42              |
| 21:W:4:SER:OG    | 21:W:5:SER:N      | 2.52                     | 0.42              |
| 30:g:132:LYS:HZ1 | 30:g:141:LEU:N    | 2.13                     | 0.42              |
| 30:g:209:THR:HA  | 30:g:225:LEU:HB3  | 2.00                     | 0.42              |
| 31:k:252:TRP:HB2 | 31:k:663:THR:HB   | 2.02                     | 0.42              |
| 31:k:741:ARG:HB3 | 31:k:760:ASP:HB2  | 2.01                     | 0.42              |
| 6:G:32:ILE:HA    | 6:G:52:ILE:HG13   | 2.02                     | 0.42              |
| 6:G:75:LEU:HA    | 6:G:75:LEU:HD23   | 1.86                     | 0.42              |
| 7:H:107:ARG:NH1  | 32:2:987:C:O2     | 2.47                     | 0.42              |
| 12:M:72:ILE:HG23 | 12:M:73:LYS:HE2   | 2.01                     | 0.42              |
| 17:S:84:TRP:CE2  | 32:2:1655:A:H8    | 2.38                     | 0.42              |
| 17:S:96:LYS:HB2  | 17:S:96:LYS:HE2   | 1.87                     | 0.42              |
| 30:g:4:ASN:O     | 30:g:318:ALA:N    | 2.52                     | 0.42              |
| 30:g:22:SER:OG   | 30:g:71:CYS:SG    | 2.78                     | 0.42              |
| 30:g:62:LYS:HE2  | 30:g:62:LYS:HB2   | 1.82                     | 0.42              |
| 30:g:90:ARG:HH11 | 30:g:99:THR:HG21  | 1.84                     | 0.42              |
| 32:2:1312:A:O2'  | 32:2:1313:C:O4'   | 2.37                     | 0.42              |
| 4:E:178:GLY:H    | 4:E:195:ILE:HB    | 1.84                     | 0.42              |
| 5:F:119:ASP:HA   | 5:F:122:ASN:HD21  | 1.84                     | 0.42              |
| 10:K:38:LYS:H    | 10:K:41:TYR:HD1   | 1.68                     | 0.42              |
| 10:K:77:ARG:HG3  | 10:K:87:VAL:HG11  | 2.01                     | 0.42              |
| 12:M:126:TRP:HE3 | 12:M:130:THR:HA   | 1.85                     | 0.42              |
| 16:R:66:VAL:HG22 | 16:R:68:GLY:H     | 1.84                     | 0.42              |
| 17:S:117:LYS:HG2 | 17:S:118:LYS:HG2  | 2.02                     | 0.42              |
| 30:g:205:SER:HG  | 30:g:209:THR:H    | 1.63                     | 0.42              |
| 31:k:195:LEU:HA  | 31:k:195:LEU:HD23 | 1.84                     | 0.42              |
| 31:k:631:GLN:HB2 | 31:k:640:HIS:HB3  | 2.02                     | 0.42              |
| 32:2:1554:G:H2'  | 32:2:1555:C:C6    | 2.55                     | 0.42              |
| 32:2:1623:A:C5   | 32:2:1692:G:HI'   | 2.54                     | 0.42              |
| 5:F:54:LYS:HE3   | 5:F:135:ASP:HA    | 2.01                     | 0.41              |
| 6:G:188:ARG:NH2  | 32:2:547:G:N7     | 2.65                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:I:96:LEU:HD23  | 8:I:96:LEU:HA     | 1.83                     | 0.41              |
| 20:V:11:LEU:HD23 | 20:V:11:LEU:HA    | 1.90                     | 0.41              |
| 32:2:485:A:H62   | 32:2:1079:U:H3    | 1.67                     | 0.41              |
| 32:2:754:C:H42   | 32:2:759:G:N2     | 2.17                     | 0.41              |
| 32:2:1358:U:H2'  | 32:2:1359:C:C6    | 2.55                     | 0.41              |
| 7:H:58:LEU:HD13  | 7:H:58:LEU:HA     | 1.93                     | 0.41              |
| 8:I:16:ALA:HB2   | 32:2:617:C:H5''   | 2.02                     | 0.41              |
| 17:S:15:LEU:HB2  | 17:S:22:VAL:H     | 1.85                     | 0.41              |
| 18:T:134:ARG:HA  | 18:T:134:ARG:HD2  | 1.92                     | 0.41              |
| 22:X:110:LYS:NZ  | 22:X:121:ARG:HH12 | 2.18                     | 0.41              |
| 5:F:128:ASN:HD22 | 5:F:131:GLN:HB2   | 1.85                     | 0.41              |
| 6:G:53:SER:O     | 6:G:53:SER:OG     | 2.33                     | 0.41              |
| 12:M:118:ALA:HA  | 32:2:1379:A:H5''  | 2.01                     | 0.41              |
| 17:S:70:VAL:HG22 | 17:S:74:GLN:HG2   | 2.02                     | 0.41              |
| 17:S:75:ASN:HB3  | 17:S:78:HIS:CG    | 2.56                     | 0.41              |
| 31:k:62:ARG:H    | 31:k:62:ARG:HD3   | 1.85                     | 0.41              |
| 31:k:618:TYR:HD2 | 31:k:621:ARG:HH21 | 1.68                     | 0.41              |
| 31:k:707:PRO:HB3 | 31:k:717:VAL:HG12 | 2.02                     | 0.41              |
| 32:2:856:U:O2'   | 32:2:857:A:O4'    | 2.37                     | 0.41              |
| 32:2:955:C:N4    | 32:2:971:U:H3     | 2.18                     | 0.41              |
| 32:2:1676:A:O2'  | 32:2:1743:C:OP1   | 2.38                     | 0.41              |
| 32:2:1805:C:O2'  | 32:2:1806:G:O4'   | 2.38                     | 0.41              |
| 4:E:3:ARG:HB2    | 32:2:93:A:H1'     | 2.02                     | 0.41              |
| 4:E:57:ASN:HD22  | 4:E:57:ASN:HA     | 1.69                     | 0.41              |
| 17:S:46:VAL:HA   | 17:S:49:LYS:HB2   | 2.03                     | 0.41              |
| 32:2:590:U:H2'   | 32:2:591:A:H8     | 1.84                     | 0.41              |
| 1:A:36:TYR:OH    | 1:A:56:LYS:NZ     | 2.39                     | 0.41              |
| 1:A:83:GLN:HA    | 1:A:86:VAL:HG12   | 2.02                     | 0.41              |
| 3:D:74:GLN:HG2   | 3:D:79:TYR:HB3    | 2.02                     | 0.41              |
| 3:D:74:GLN:NE2   | 3:D:79:TYR:O      | 2.42                     | 0.41              |
| 12:M:18:GLN:HE21 | 12:M:90:LYS:HB3   | 1.85                     | 0.41              |
| 18:T:11:ALA:HA   | 18:T:63:ARG:HH21  | 1.84                     | 0.41              |
| 18:T:133:ASP:OD1 | 18:T:133:ASP:N    | 2.53                     | 0.41              |
| 30:g:205:SER:N   | 30:g:210:LEU:O    | 2.54                     | 0.41              |
| 31:k:95:LEU:HD23 | 31:k:95:LEU:HA    | 1.86                     | 0.41              |
| 5:F:25:LEU:HD11  | 15:Q:60:PHE:HB2   | 2.03                     | 0.41              |
| 8:I:192:TYR:O    | 8:I:196:LEU:N     | 2.53                     | 0.41              |
| 14:P:77:ARG:HA   | 14:P:98:ASN:HB3   | 2.01                     | 0.41              |
| 14:P:89:MET:HB2  | 14:P:107:ILE:HG13 | 2.02                     | 0.41              |
| 18:T:84:LYS:HE3  | 18:T:95:ASP:H     | 1.85                     | 0.41              |
| 20:V:18:SER:O    | 20:V:18:SER:OG    | 2.38                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:b:8:LEU:HA     | 25:b:8:LEU:HD12   | 1.85                     | 0.41              |
| 25:b:36:LYS:HB2   | 25:b:36:LYS:HE3   | 1.86                     | 0.41              |
| 30:g:102:ARG:NH1  | 32:2:1493:A:O2'   | 2.49                     | 0.41              |
| 31:k:666:PRO:HA   | 31:k:687:THR:HA   | 2.02                     | 0.41              |
| 32:2:1428:U:C4    | 32:2:1588:A:H2'   | 2.56                     | 0.41              |
| 6:G:127:THR:OG1   | 6:G:128:THR:N     | 2.52                     | 0.41              |
| 12:M:106:ILE:HG12 | 12:M:114:LYS:HD3  | 2.03                     | 0.41              |
| 19:U:59:PRO:HG3   | 32:2:1533:U:H4'   | 2.01                     | 0.41              |
| 32:2:1087:U:H2'   | 32:2:1088:C:O4'   | 2.20                     | 0.41              |
| 32:2:1307:G:H1    | 32:2:1775:C:N4    | 2.19                     | 0.41              |
| 32:2:1418:U:H3'   | 32:2:1419:G:C8    | 2.48                     | 0.41              |
| 8:I:121:LEU:HA    | 8:I:121:LEU:HD23  | 1.82                     | 0.41              |
| 12:M:62:LEU:HD11  | 12:M:90:LYS:HE2   | 2.03                     | 0.41              |
| 13:N:72:MET:HE3   | 13:N:72:MET:HB3   | 1.80                     | 0.41              |
| 16:R:7:LYS:N      | 32:2:1468:G:OP1   | 2.54                     | 0.41              |
| 16:R:109:LEU:O    | 16:R:112:SER:OG   | 2.32                     | 0.41              |
| 17:S:41:ARG:HD2   | 17:S:41:ARG:HA    | 1.83                     | 0.41              |
| 29:f:132:LEU:HD23 | 29:f:132:LEU:HA   | 1.91                     | 0.41              |
| 32:2:679:A:H5'    | 32:2:680:A:C8     | 2.55                     | 0.41              |
| 32:2:957:U:OP2    | 32:2:967:U:N3     | 2.54                     | 0.41              |
| 32:2:1266:G:O2'   | 32:2:1282:G:O6    | 2.37                     | 0.41              |
| 32:2:1629:G:H2'   | 32:2:1630:G:C8    | 2.56                     | 0.41              |
| 32:2:1858:C:N4    | 32:2:1860:U:O4    | 2.40                     | 0.41              |
| 1:A:84:ARG:NH2    | 1:A:201:LEU:O     | 2.44                     | 0.41              |
| 2:C:73:LEU:HA     | 2:C:73:LEU:HD23   | 1.85                     | 0.41              |
| 3:D:142:LEU:HB3   | 3:D:146:ARG:HH11  | 1.86                     | 0.41              |
| 3:D:186:VAL:C     | 3:D:187:LYS:HZ2   | 2.29                     | 0.41              |
| 5:F:120:ILE:HD12  | 5:F:120:ILE:HA    | 1.90                     | 0.41              |
| 7:H:125:ILE:HD12  | 7:H:125:ILE:HA    | 1.95                     | 0.41              |
| 14:P:90:ILE:HG13  | 14:P:91:GLY:H     | 1.85                     | 0.41              |
| 29:f:142:GLY:HA2  | 32:2:1403:U:N3    | 2.33                     | 0.41              |
| 30:g:24:ALA:HB1   | 30:g:73:LEU:HD22  | 2.02                     | 0.41              |
| 30:g:123:ILE:HD12 | 30:g:123:ILE:HA   | 1.90                     | 0.41              |
| 30:g:231:MET:HE2  | 30:g:231:MET:HB2  | 1.85                     | 0.41              |
| 30:g:282:SER:N    | 32:2:1546:G:OP1   | 2.45                     | 0.41              |
| 31:k:139:ILE:HD12 | 31:k:140:PRO:HD2  | 2.01                     | 0.41              |
| 31:k:303:LEU:HA   | 31:k:561:ILE:HG13 | 2.02                     | 0.41              |
| 31:k:565:LYS:HE2  | 31:k:565:LYS:HB3  | 1.78                     | 0.41              |
| 31:k:782:SER:OG   | 31:k:783:LEU:N    | 2.53                     | 0.41              |
| 32:2:1362:C:H2'   | 32:2:1363:A:C8    | 2.56                     | 0.41              |
| 32:2:1626:G:H2'   | 32:2:1627:A:C8    | 2.55                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:193:GLN:HA   | 1:A:194:PRO:HD3   | 1.96                     | 0.41              |
| 3:D:139:SER:N    | 32:2:1430:G:OP2   | 2.34                     | 0.41              |
| 5:F:46:TRP:CE2   | 5:F:129:PRO:HG2   | 2.56                     | 0.41              |
| 14:P:130:ARG:NH1 | 32:2:1333:U:OP1   | 2.53                     | 0.41              |
| 17:S:27:LYS:HA   | 17:S:27:LYS:HD3   | 1.92                     | 0.41              |
| 17:S:106:GLU:HB2 | 17:S:110:ARG:NH1  | 2.35                     | 0.41              |
| 18:T:56:LYS:HD3  | 18:T:56:LYS:HA    | 1.92                     | 0.41              |
| 19:U:36:ASN:OD1  | 19:U:36:ASN:N     | 2.53                     | 0.41              |
| 22:X:63:GLN:O    | 22:X:65:ASN:N     | 2.54                     | 0.41              |
| 30:g:132:LYS:HA  | 30:g:132:LYS:HD2  | 1.88                     | 0.41              |
| 31:k:294:HIS:HB3 | 31:k:584:LEU:HD21 | 2.02                     | 0.41              |
| 31:k:506:ASN:ND2 | 31:k:509:ASN:OD1  | 2.54                     | 0.41              |
| 1:A:3:LEU:HA     | 1:A:4:PRO:HD3     | 1.91                     | 0.40              |
| 3:D:209:ILE:HG13 | 3:D:210:GLU:H     | 1.87                     | 0.40              |
| 10:K:55:VAL:HB   | 10:K:66:TYR:HD1   | 1.86                     | 0.40              |
| 14:P:134:THR:H   | 14:P:134:THR:HG23 | 1.65                     | 0.40              |
| 18:T:19:ALA:O    | 18:T:23:GLN:N     | 2.52                     | 0.40              |
| 18:T:86:ARG:NH1  | 32:2:1753:G:OP1   | 2.50                     | 0.40              |
| 30:g:124:SER:N   | 30:g:132:LYS:O    | 2.54                     | 0.40              |
| 31:k:140:PRO:HG2 | 31:k:142:MET:HE1  | 2.03                     | 0.40              |
| 31:k:533:ASN:O   | 31:k:537:THR:OG1  | 2.31                     | 0.40              |
| 31:k:749:LEU:H   | 31:k:755:PHE:HA   | 1.86                     | 0.40              |
| 32:2:1430:G:H1'  | 32:2:1581:G:O6    | 2.21                     | 0.40              |
| 1:A:80:THR:HA    | 1:A:83:GLN:NE2    | 2.36                     | 0.40              |
| 4:E:136:VAL:HG21 | 4:E:148:ARG:HH21  | 1.86                     | 0.40              |
| 5:F:42:LEU:HD13  | 5:F:67:PRO:HB3    | 2.03                     | 0.40              |
| 18:T:80:TYR:HD1  | 18:T:80:TYR:HA    | 1.72                     | 0.40              |
| 23:Y:17:LEU:HD23 | 23:Y:17:LEU:HA    | 1.91                     | 0.40              |
| 23:Y:62:THR:OG1  | 23:Y:69:SER:OG    | 2.38                     | 0.40              |
| 30:g:13:LEU:HD21 | 30:g:54:PHE:HB2   | 2.03                     | 0.40              |
| 31:k:287:PHE:H   | 31:k:551:ALA:HB3  | 1.85                     | 0.40              |
| 31:k:667:ALA:O   | 31:k:686:GLY:N    | 2.54                     | 0.40              |
| 32:2:33:U:O2     | 32:2:731:A:N6     | 2.54                     | 0.40              |
| 32:2:1074:U:O4   | 32:2:1075:A:N6    | 2.54                     | 0.40              |
| 1:A:77:SER:OG    | 1:A:78:SER:N      | 2.54                     | 0.40              |
| 5:F:120:ILE:HD13 | 24:Z:100:ILE:HG23 | 2.03                     | 0.40              |
| 6:G:184:LEU:HD23 | 6:G:184:LEU:HA    | 1.87                     | 0.40              |
| 7:H:74:GLN:O     | 7:H:74:GLN:NE2    | 2.55                     | 0.40              |
| 9:J:154:LYS:HG3  | 9:J:155:HIS:CD2   | 2.53                     | 0.40              |
| 12:M:70:ASN:OD1  | 12:M:70:ASN:N     | 2.54                     | 0.40              |
| 15:Q:99:GLU:O    | 15:Q:103:ASN:ND2  | 2.54                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:R:82:ASP:OD1  | 16:R:85:VAL:N     | 2.33                     | 0.40              |
| 17:S:70:VAL:HA   | 17:S:73:MET:HB3   | 2.02                     | 0.40              |
| 19:U:68:ARG:HG3  | 19:U:77:LYS:NZ    | 2.37                     | 0.40              |
| 23:Y:41:ARG:NH2  | 23:Y:52:LYS:O     | 2.51                     | 0.40              |
| 26:c:14:LYS:HB2  | 26:c:29:ARG:HB3   | 2.02                     | 0.40              |
| 31:k:231:LYS:HA  | 31:k:231:LYS:HD3  | 1.92                     | 0.40              |
| 32:2:692:G:C2    | 32:2:693:G:H8     | 2.39                     | 0.40              |
| 32:2:1388:A:N6   | 32:2:1400:C:H42   | 2.20                     | 0.40              |
| 32:2:1904:U:H2'  | 32:2:1905:A:C8    | 2.57                     | 0.40              |
| 2:C:200:SER:O    | 2:C:200:SER:OG    | 2.39                     | 0.40              |
| 3:D:138:VAL:H    | 3:D:151:LYS:HE2   | 1.87                     | 0.40              |
| 4:E:62:LYS:HB2   | 4:E:62:LYS:HE3    | 1.67                     | 0.40              |
| 6:G:164:LYS:NZ   | 32:2:71:A:OP2     | 2.37                     | 0.40              |
| 10:K:56:LYS:HE2  | 10:K:56:LYS:HB2   | 1.74                     | 0.40              |
| 11:L:8:GLN:OE1   | 11:L:8:GLN:N      | 2.54                     | 0.40              |
| 17:S:81:ILE:HD13 | 17:S:81:ILE:HA    | 1.94                     | 0.40              |
| 18:T:128:GLY:HA2 | 18:T:132:LEU:HD23 | 2.02                     | 0.40              |
| 18:T:130:ARG:HE  | 32:2:1510:G:H5'   | 1.86                     | 0.40              |
| 22:X:16:ARG:HE   | 22:X:16:ARG:HB2   | 1.61                     | 0.40              |
| 30:g:204:ALA:HA  | 30:g:211:ILE:HA   | 2.03                     | 0.40              |
| 31:k:505:LYS:NZ  | 31:k:772:SER:OG   | 2.53                     | 0.40              |
| 32:2:1160:U:H5   | 32:2:1161:U:C4    | 2.39                     | 0.40              |
| 2:C:58:LEU:HD23  | 2:C:58:LEU:HA     | 1.80                     | 0.40              |
| 3:D:60:GLY:HA3   | 3:D:64:ARG:HB2    | 2.03                     | 0.40              |
| 3:D:115:ILE:H    | 3:D:115:ILE:HG12  | 1.73                     | 0.40              |
| 5:F:161:ASP:OD1  | 5:F:161:ASP:N     | 2.54                     | 0.40              |
| 8:I:69:SER:OG    | 8:I:70:GLU:OE1    | 2.35                     | 0.40              |
| 9:J:88:GLU:OE1   | 9:J:88:GLU:N      | 2.54                     | 0.40              |
| 15:Q:26:LYS:HD2  | 15:Q:26:LYS:HA    | 1.78                     | 0.40              |
| 30:g:42:LEU:HB2  | 30:g:61:PHE:HB2   | 2.04                     | 0.40              |
| 31:k:637:ASN:O   | 31:k:694:SER:OG   | 2.39                     | 0.40              |
| 32:2:1380:G:H5'' | 32:2:1381:G:N2    | 2.37                     | 0.40              |
| 32:2:1512:A:H61  | 32:2:1516:G:H1'   | 1.86                     | 0.40              |
| 32:2:1806:G:H4'  | 32:2:1807:A:C8    | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 204/206 (99%) | 181 (89%) | 23 (11%) | 0        | 100         | 100 |
| 2   | C     | 215/217 (99%) | 199 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 3   | D     | 220/223 (99%) | 177 (80%) | 41 (19%) | 2 (1%)   | 14          | 45  |
| 4   | E     | 258/260 (99%) | 231 (90%) | 27 (10%) | 0        | 100         | 100 |
| 5   | F     | 203/206 (98%) | 181 (89%) | 22 (11%) | 0        | 100         | 100 |
| 6   | G     | 230/232 (99%) | 214 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 7   | H     | 182/184 (99%) | 170 (93%) | 12 (7%)  | 0        | 100         | 100 |
| 8   | I     | 184/199 (92%) | 165 (90%) | 19 (10%) | 0        | 100         | 100 |
| 9   | J     | 183/185 (99%) | 163 (89%) | 20 (11%) | 0        | 100         | 100 |
| 10  | K     | 92/96 (96%)   | 72 (78%)  | 19 (21%) | 1 (1%)   | 11          | 42  |
| 11  | L     | 138/140 (99%) | 123 (89%) | 15 (11%) | 0        | 100         | 100 |
| 12  | M     | 123/125 (98%) | 99 (80%)  | 24 (20%) | 0        | 100         | 100 |
| 13  | N     | 148/150 (99%) | 134 (90%) | 14 (10%) | 0        | 100         | 100 |
| 14  | P     | 119/127 (94%) | 89 (75%)  | 30 (25%) | 0        | 100         | 100 |
| 15  | Q     | 125/127 (98%) | 115 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 16  | R     | 123/125 (98%) | 112 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 17  | S     | 133/135 (98%) | 108 (81%) | 25 (19%) | 0        | 100         | 100 |
| 18  | T     | 141/143 (99%) | 129 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 19  | U     | 101/103 (98%) | 91 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 20  | V     | 85/87 (98%)   | 75 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 21  | W     | 127/129 (98%) | 112 (88%) | 15 (12%) | 0        | 100         | 100 |
| 22  | X     | 142/144 (99%) | 116 (82%) | 24 (17%) | 2 (1%)   | 9           | 37  |
| 23  | Y     | 132/134 (98%) | 123 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 24  | Z     | 61/63 (97%)   | 52 (85%)  | 9 (15%)  | 0        | 100         | 100 |
| 25  | b     | 79/81 (98%)   | 68 (86%)  | 11 (14%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 26  | c     | 61/63 (97%)     | 55 (90%)   | 6 (10%)   | 0        | 100         | 100 |
| 27  | d     | 35/37 (95%)     | 29 (83%)   | 6 (17%)   | 0        | 100         | 100 |
| 28  | e     | 44/63 (70%)     | 37 (84%)   | 7 (16%)   | 0        | 100         | 100 |
| 29  | f     | 64/71 (90%)     | 47 (73%)   | 17 (27%)  | 0        | 100         | 100 |
| 30  | g     | 315/317 (99%)   | 279 (89%)  | 36 (11%)  | 0        | 100         | 100 |
| 31  | k     | 630/788 (80%)   | 572 (91%)  | 58 (9%)   | 0        | 100         | 100 |
| All | All   | 4897/5160 (95%) | 4318 (88%) | 574 (12%) | 5 (0%)   | 49          | 78  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | X     | 117 | ILE  |
| 3   | D     | 211 | PRO  |
| 10  | K     | 54  | TYR  |
| 3   | D     | 216 | PRO  |
| 22  | X     | 64  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 171/173 (99%)  | 170 (99%)  | 1 (1%)   | 78          | 79  |
| 2   | C     | 176/176 (100%) | 169 (96%)  | 7 (4%)   | 28          | 52  |
| 3   | D     | 182/182 (100%) | 177 (97%)  | 5 (3%)   | 39          | 59  |
| 4   | E     | 221/221 (100%) | 219 (99%)  | 2 (1%)   | 70          | 75  |
| 5   | F     | 173/173 (100%) | 172 (99%)  | 1 (1%)   | 78          | 79  |
| 6   | G     | 198/198 (100%) | 195 (98%)  | 3 (2%)   | 57          | 68  |
| 7   | H     | 165/165 (100%) | 164 (99%)  | 1 (1%)   | 78          | 79  |
| 8   | I     | 150/160 (94%)  | 150 (100%) | 0        | 100         | 100 |
| 9   | J     | 158/158 (100%) | 155 (98%)  | 3 (2%)   | 50          | 65  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 10  | K     | 89/89 (100%)    | 87 (98%)   | 2 (2%)   | 45          | 63  |
| 11  | L     | 125/125 (100%)  | 124 (99%)  | 1 (1%)   | 73          | 76  |
| 12  | M     | 101/101 (100%)  | 100 (99%)  | 1 (1%)   | 68          | 74  |
| 13  | N     | 127/127 (100%)  | 126 (99%)  | 1 (1%)   | 73          | 76  |
| 14  | P     | 105/105 (100%)  | 105 (100%) | 0        | 100         | 100 |
| 15  | Q     | 107/107 (100%)  | 106 (99%)  | 1 (1%)   | 70          | 75  |
| 16  | R     | 113/113 (100%)  | 112 (99%)  | 1 (1%)   | 70          | 75  |
| 17  | S     | 120/120 (100%)  | 119 (99%)  | 1 (1%)   | 73          | 76  |
| 18  | T     | 115/115 (100%)  | 112 (97%)  | 3 (3%)   | 40          | 60  |
| 19  | U     | 96/96 (100%)    | 95 (99%)   | 1 (1%)   | 68          | 74  |
| 20  | V     | 74/74 (100%)    | 73 (99%)   | 1 (1%)   | 59          | 70  |
| 21  | W     | 110/110 (100%)  | 107 (97%)  | 3 (3%)   | 39          | 59  |
| 22  | X     | 119/119 (100%)  | 113 (95%)  | 6 (5%)   | 22          | 48  |
| 23  | Y     | 112/112 (100%)  | 110 (98%)  | 2 (2%)   | 51          | 67  |
| 24  | Z     | 56/56 (100%)    | 56 (100%)  | 0        | 100         | 100 |
| 25  | b     | 70/70 (100%)    | 69 (99%)   | 1 (1%)   | 59          | 70  |
| 26  | c     | 56/56 (100%)    | 56 (100%)  | 0        | 100         | 100 |
| 27  | d     | 33/33 (100%)    | 31 (94%)   | 2 (6%)   | 17          | 44  |
| 28  | e     | 40/54 (74%)     | 38 (95%)   | 2 (5%)   | 22          | 48  |
| 29  | f     | 43/62 (69%)     | 43 (100%)  | 0        | 100         | 100 |
| 30  | g     | 259/261 (99%)   | 258 (100%) | 1 (0%)   | 84          | 81  |
| 31  | k     | 553/703 (79%)   | 549 (99%)  | 4 (1%)   | 76          | 77  |
| All | All   | 4217/4414 (96%) | 4160 (99%) | 57 (1%)  | 57          | 70  |

All (57) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 157 | ASP  |
| 2   | C     | 80  | VAL  |
| 2   | C     | 111 | VAL  |
| 2   | C     | 113 | LEU  |
| 2   | C     | 139 | ILE  |
| 2   | C     | 158 | THR  |
| 2   | C     | 179 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 221 | THR  |
| 3   | D     | 85  | VAL  |
| 3   | D     | 93  | ASP  |
| 3   | D     | 136 | VAL  |
| 3   | D     | 154 | ASP  |
| 3   | D     | 210 | GLU  |
| 4   | E     | 181 | VAL  |
| 4   | E     | 216 | ASN  |
| 5   | F     | 118 | LEU  |
| 6   | G     | 129 | VAL  |
| 6   | G     | 151 | ASP  |
| 6   | G     | 218 | GLU  |
| 7   | H     | 20  | VAL  |
| 9   | J     | 101 | VAL  |
| 9   | J     | 136 | VAL  |
| 9   | J     | 141 | VAL  |
| 10  | K     | 15  | LEU  |
| 10  | K     | 55  | VAL  |
| 11  | L     | 124 | THR  |
| 12  | M     | 86  | VAL  |
| 13  | N     | 60  | VAL  |
| 15  | Q     | 7   | VAL  |
| 16  | R     | 113 | LEU  |
| 17  | S     | 35  | ILE  |
| 18  | T     | 105 | LEU  |
| 18  | T     | 114 | VAL  |
| 18  | T     | 124 | ILE  |
| 19  | U     | 65  | ILE  |
| 20  | V     | 4   | ASP  |
| 21  | W     | 33  | VAL  |
| 21  | W     | 40  | VAL  |
| 21  | W     | 103 | ILE  |
| 22  | X     | 53  | VAL  |
| 22  | X     | 72  | VAL  |
| 22  | X     | 83  | VAL  |
| 22  | X     | 87  | VAL  |
| 22  | X     | 117 | ILE  |
| 22  | X     | 125 | VAL  |
| 23  | Y     | 27  | VAL  |
| 23  | Y     | 70  | VAL  |
| 25  | b     | 65  | THR  |
| 27  | d     | 23  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | d     | 28  | THR  |
| 28  | e     | 39  | LEU  |
| 28  | e     | 48  | THR  |
| 30  | g     | 207 | ASP  |
| 31  | k     | 52  | LEU  |
| 31  | k     | 61  | LEU  |
| 31  | k     | 89  | VAL  |
| 31  | k     | 282 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 92  | HIS  |
| 1   | A     | 193 | GLN  |
| 2   | C     | 59  | HIS  |
| 2   | C     | 82  | ASN  |
| 2   | C     | 209 | ASN  |
| 3   | D     | 162 | GLN  |
| 3   | D     | 165 | ASN  |
| 3   | D     | 174 | HIS  |
| 4   | E     | 57  | ASN  |
| 4   | E     | 69  | HIS  |
| 4   | E     | 98  | ASN  |
| 4   | E     | 209 | HIS  |
| 5   | F     | 122 | ASN  |
| 5   | F     | 169 | ASN  |
| 5   | F     | 224 | ASN  |
| 6   | G     | 13  | GLN  |
| 6   | G     | 56  | ASN  |
| 6   | G     | 59  | GLN  |
| 6   | G     | 189 | HIS  |
| 7   | H     | 22  | GLN  |
| 7   | H     | 74  | GLN  |
| 7   | H     | 108 | GLN  |
| 7   | H     | 147 | ASN  |
| 8   | I     | 20  | GLN  |
| 8   | I     | 111 | GLN  |
| 9   | J     | 48  | GLN  |
| 9   | J     | 112 | GLN  |
| 10  | K     | 17  | GLN  |
| 11  | L     | 92  | HIS  |
| 11  | L     | 127 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | N     | 21  | ASN  |
| 13  | N     | 69  | ASN  |
| 13  | N     | 105 | ASN  |
| 13  | N     | 123 | HIS  |
| 14  | P     | 82  | ASN  |
| 14  | P     | 103 | ASN  |
| 15  | Q     | 83  | GLN  |
| 15  | Q     | 100 | GLN  |
| 15  | Q     | 103 | ASN  |
| 16  | R     | 48  | ASN  |
| 16  | R     | 105 | GLN  |
| 17  | S     | 63  | GLN  |
| 17  | S     | 71  | GLN  |
| 17  | S     | 78  | HIS  |
| 17  | S     | 122 | HIS  |
| 17  | S     | 127 | HIS  |
| 18  | T     | 43  | ASN  |
| 18  | T     | 77  | ASN  |
| 19  | U     | 40  | ASN  |
| 19  | U     | 48  | HIS  |
| 19  | U     | 87  | HIS  |
| 20  | V     | 33  | GLN  |
| 20  | V     | 35  | ASN  |
| 21  | W     | 80  | ASN  |
| 21  | W     | 92  | ASN  |
| 23  | Y     | 77  | ASN  |
| 23  | Y     | 106 | GLN  |
| 23  | Y     | 110 | GLN  |
| 25  | b     | 51  | GLN  |
| 26  | c     | 27  | GLN  |
| 27  | d     | 20  | GLN  |
| 28  | e     | 46  | ASN  |
| 29  | f     | 123 | ASN  |
| 30  | g     | 187 | GLN  |
| 30  | g     | 196 | ASN  |
| 30  | g     | 237 | GLN  |
| 31  | k     | 56  | ASN  |
| 31  | k     | 183 | GLN  |
| 31  | k     | 255 | ASN  |
| 31  | k     | 506 | ASN  |
| 31  | k     | 513 | GLN  |
| 31  | k     | 547 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | k     | 631 | GLN  |
| 31  | k     | 711 | HIS  |
| 31  | k     | 766 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 32  | 2     | 1620/1910 (84%) | 720 (44%)         | 22 (1%)         |

All (720) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2     | 5   | U    |
| 32  | 2     | 9   | U    |
| 32  | 2     | 10  | G    |
| 32  | 2     | 13  | C    |
| 32  | 2     | 19  | A    |
| 32  | 2     | 25  | C    |
| 32  | 2     | 26  | A    |
| 32  | 2     | 27  | U    |
| 32  | 2     | 32  | U    |
| 32  | 2     | 34  | G    |
| 32  | 2     | 40  | A    |
| 32  | 2     | 42  | G    |
| 32  | 2     | 45  | U    |
| 32  | 2     | 46  | A    |
| 32  | 2     | 47  | A    |
| 32  | 2     | 50  | C    |
| 32  | 2     | 55  | A    |
| 32  | 2     | 57  | G    |
| 32  | 2     | 58  | U    |
| 32  | 2     | 59  | C    |
| 32  | 2     | 60  | U    |
| 32  | 2     | 66  | U    |
| 32  | 2     | 72  | A    |
| 32  | 2     | 73  | U    |
| 32  | 2     | 74  | U    |
| 32  | 2     | 75  | U    |
| 32  | 2     | 77  | U    |
| 32  | 2     | 82  | U    |
| 32  | 2     | 84  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2     | 93  | A    |
| 32  | 2     | 96  | G    |
| 32  | 2     | 98  | U    |
| 32  | 2     | 100 | A    |
| 32  | 2     | 101 | U    |
| 32  | 2     | 102 | U    |
| 32  | 2     | 104 | A    |
| 32  | 2     | 108 | A    |
| 32  | 2     | 114 | C    |
| 32  | 2     | 115 | G    |
| 32  | 2     | 116 | U    |
| 32  | 2     | 127 | G    |
| 32  | 2     | 130 | C    |
| 32  | 2     | 131 | C    |
| 32  | 2     | 133 | U    |
| 32  | 2     | 134 | U    |
| 32  | 2     | 137 | U    |
| 32  | 2     | 138 | A    |
| 32  | 2     | 141 | U    |
| 32  | 2     | 148 | A    |
| 32  | 2     | 420 | A    |
| 32  | 2     | 422 | U    |
| 32  | 2     | 441 | U    |
| 32  | 2     | 446 | U    |
| 32  | 2     | 448 | U    |
| 32  | 2     | 449 | C    |
| 32  | 2     | 450 | G    |
| 32  | 2     | 453 | C    |
| 32  | 2     | 454 | C    |
| 32  | 2     | 455 | U    |
| 32  | 2     | 457 | U    |
| 32  | 2     | 458 | G    |
| 32  | 2     | 459 | G    |
| 32  | 2     | 460 | A    |
| 32  | 2     | 461 | A    |
| 32  | 2     | 466 | U    |
| 32  | 2     | 478 | A    |
| 32  | 2     | 479 | U    |
| 32  | 2     | 480 | A    |
| 32  | 2     | 481 | A    |
| 32  | 2     | 482 | A    |
| 32  | 2     | 488 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2     | 490 | U    |
| 32  | 2     | 491 | G    |
| 32  | 2     | 492 | U    |
| 32  | 2     | 493 | C    |
| 32  | 2     | 494 | U    |
| 32  | 2     | 496 | C    |
| 32  | 2     | 498 | G    |
| 32  | 2     | 499 | A    |
| 32  | 2     | 500 | C    |
| 32  | 2     | 503 | U    |
| 32  | 2     | 504 | U    |
| 32  | 2     | 505 | U    |
| 32  | 2     | 513 | C    |
| 32  | 2     | 514 | A    |
| 32  | 2     | 519 | A    |
| 32  | 2     | 520 | A    |
| 32  | 2     | 524 | U    |
| 32  | 2     | 525 | U    |
| 32  | 2     | 526 | C    |
| 32  | 2     | 529 | A    |
| 32  | 2     | 530 | U    |
| 32  | 2     | 534 | A    |
| 32  | 2     | 535 | U    |
| 32  | 2     | 537 | G    |
| 32  | 2     | 539 | C    |
| 32  | 2     | 540 | U    |
| 32  | 2     | 542 | G    |
| 32  | 2     | 543 | U    |
| 32  | 2     | 544 | G    |
| 32  | 2     | 551 | A    |
| 32  | 2     | 558 | A    |
| 32  | 2     | 562 | A    |
| 32  | 2     | 568 | C    |
| 32  | 2     | 571 | C    |
| 32  | 2     | 573 | C    |
| 32  | 2     | 577 | C    |
| 32  | 2     | 579 | A    |
| 32  | 2     | 584 | C    |
| 32  | 2     | 585 | G    |
| 32  | 2     | 587 | U    |
| 32  | 2     | 592 | G    |
| 32  | 2     | 599 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2     | 600 | G    |
| 32  | 2     | 601 | C    |
| 32  | 2     | 604 | A    |
| 32  | 2     | 605 | C    |
| 32  | 2     | 606 | C    |
| 32  | 2     | 615 | A    |
| 32  | 2     | 622 | A    |
| 32  | 2     | 623 | A    |
| 32  | 2     | 624 | C    |
| 32  | 2     | 626 | G    |
| 32  | 2     | 631 | U    |
| 32  | 2     | 635 | G    |
| 32  | 2     | 644 | C    |
| 32  | 2     | 647 | G    |
| 32  | 2     | 656 | C    |
| 32  | 2     | 659 | G    |
| 32  | 2     | 663 | A    |
| 32  | 2     | 664 | A    |
| 32  | 2     | 665 | C    |
| 32  | 2     | 667 | G    |
| 32  | 2     | 674 | C    |
| 32  | 2     | 675 | A    |
| 32  | 2     | 679 | A    |
| 32  | 2     | 680 | A    |
| 32  | 2     | 682 | G    |
| 32  | 2     | 686 | G    |
| 32  | 2     | 687 | C    |
| 32  | 2     | 688 | A    |
| 32  | 2     | 689 | G    |
| 32  | 2     | 693 | G    |
| 32  | 2     | 694 | C    |
| 32  | 2     | 695 | G    |
| 32  | 2     | 698 | C    |
| 32  | 2     | 700 | A    |
| 32  | 2     | 701 | A    |
| 32  | 2     | 702 | U    |
| 32  | 2     | 707 | C    |
| 32  | 2     | 708 | A    |
| 32  | 2     | 711 | C    |
| 32  | 2     | 717 | U    |
| 32  | 2     | 718 | C    |
| 32  | 2     | 720 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2     | 722 | G    |
| 32  | 2     | 730 | G    |
| 32  | 2     | 731 | A    |
| 32  | 2     | 732 | C    |
| 32  | 2     | 738 | A    |
| 32  | 2     | 740 | A    |
| 32  | 2     | 743 | G    |
| 32  | 2     | 744 | A    |
| 32  | 2     | 745 | U    |
| 32  | 2     | 748 | A    |
| 32  | 2     | 749 | G    |
| 32  | 2     | 753 | C    |
| 32  | 2     | 754 | C    |
| 32  | 2     | 755 | A    |
| 32  | 2     | 756 | U    |
| 32  | 2     | 758 | C    |
| 32  | 2     | 759 | G    |
| 32  | 2     | 760 | G    |
| 32  | 2     | 763 | C    |
| 32  | 2     | 765 | U    |
| 32  | 2     | 766 | G    |
| 32  | 2     | 767 | U    |
| 32  | 2     | 769 | A    |
| 32  | 2     | 770 | U    |
| 32  | 2     | 771 | U    |
| 32  | 2     | 773 | G    |
| 32  | 2     | 774 | A    |
| 32  | 2     | 782 | C    |
| 32  | 2     | 783 | A    |
| 32  | 2     | 786 | G    |
| 32  | 2     | 790 | A    |
| 32  | 2     | 797 | A    |
| 32  | 2     | 803 | G    |
| 32  | 2     | 804 | A    |
| 32  | 2     | 805 | A    |
| 32  | 2     | 806 | C    |
| 32  | 2     | 808 | A    |
| 32  | 2     | 814 | G    |
| 32  | 2     | 820 | G    |
| 32  | 2     | 822 | C    |
| 32  | 2     | 823 | U    |
| 32  | 2     | 824 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2     | 825 | G    |
| 32  | 2     | 826 | U    |
| 32  | 2     | 827 | G    |
| 32  | 2     | 828 | C    |
| 32  | 2     | 829 | C    |
| 32  | 2     | 830 | A    |
| 32  | 2     | 831 | G    |
| 32  | 2     | 833 | A    |
| 32  | 2     | 835 | C    |
| 32  | 2     | 836 | C    |
| 32  | 2     | 837 | G    |
| 32  | 2     | 839 | G    |
| 32  | 2     | 840 | G    |
| 32  | 2     | 841 | U    |
| 32  | 2     | 842 | A    |
| 32  | 2     | 843 | A    |
| 32  | 2     | 844 | U    |
| 32  | 2     | 845 | U    |
| 32  | 2     | 848 | A    |
| 32  | 2     | 855 | A    |
| 32  | 2     | 856 | U    |
| 32  | 2     | 857 | A    |
| 32  | 2     | 858 | G    |
| 32  | 2     | 859 | C    |
| 32  | 2     | 869 | A    |
| 32  | 2     | 876 | G    |
| 32  | 2     | 879 | G    |
| 32  | 2     | 880 | U    |
| 32  | 2     | 883 | A    |
| 32  | 2     | 885 | A    |
| 32  | 2     | 886 | A    |
| 32  | 2     | 887 | G    |
| 32  | 2     | 889 | U    |
| 32  | 2     | 890 | C    |
| 32  | 2     | 891 | G    |
| 32  | 2     | 892 | U    |
| 32  | 2     | 893 | A    |
| 32  | 2     | 902 | U    |
| 32  | 2     | 903 | U    |
| 32  | 2     | 904 | G    |
| 32  | 2     | 915 | G    |
| 32  | 2     | 916 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 918  | G    |
| 32  | 2     | 919  | G    |
| 32  | 2     | 921  | C    |
| 32  | 2     | 923  | G    |
| 32  | 2     | 926  | U    |
| 32  | 2     | 927  | U    |
| 32  | 2     | 928  | C    |
| 32  | 2     | 929  | C    |
| 32  | 2     | 930  | A    |
| 32  | 2     | 931  | A    |
| 32  | 2     | 933  | G    |
| 32  | 2     | 937  | C    |
| 32  | 2     | 942  | C    |
| 32  | 2     | 943  | C    |
| 32  | 2     | 944  | U    |
| 32  | 2     | 949  | G    |
| 32  | 2     | 951  | U    |
| 32  | 2     | 952  | A    |
| 32  | 2     | 954  | C    |
| 32  | 2     | 959  | A    |
| 32  | 2     | 960  | G    |
| 32  | 2     | 962  | C    |
| 32  | 2     | 963  | C    |
| 32  | 2     | 964  | U    |
| 32  | 2     | 968  | G    |
| 32  | 2     | 969  | G    |
| 32  | 2     | 972  | C    |
| 32  | 2     | 974  | U    |
| 32  | 2     | 977  | C    |
| 32  | 2     | 980  | A    |
| 32  | 2     | 984  | G    |
| 32  | 2     | 985  | G    |
| 32  | 2     | 986  | A    |
| 32  | 2     | 987  | C    |
| 32  | 2     | 989  | U    |
| 32  | 2     | 997  | G    |
| 32  | 2     | 998  | A    |
| 32  | 2     | 999  | A    |
| 32  | 2     | 1000 | A    |
| 32  | 2     | 1007 | G    |
| 32  | 2     | 1011 | G    |
| 32  | 2     | 1012 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1014 | C    |
| 32  | 2     | 1020 | A    |
| 32  | 2     | 1021 | G    |
| 32  | 2     | 1025 | U    |
| 32  | 2     | 1027 | U    |
| 32  | 2     | 1028 | U    |
| 32  | 2     | 1029 | G    |
| 32  | 2     | 1030 | C    |
| 32  | 2     | 1035 | A    |
| 32  | 2     | 1036 | U    |
| 32  | 2     | 1039 | A    |
| 32  | 2     | 1040 | U    |
| 32  | 2     | 1049 | A    |
| 32  | 2     | 1053 | A    |
| 32  | 2     | 1056 | G    |
| 32  | 2     | 1057 | A    |
| 32  | 2     | 1058 | A    |
| 32  | 2     | 1060 | A    |
| 32  | 2     | 1061 | G    |
| 32  | 2     | 1062 | G    |
| 32  | 2     | 1065 | G    |
| 32  | 2     | 1066 | U    |
| 32  | 2     | 1067 | U    |
| 32  | 2     | 1069 | G    |
| 32  | 2     | 1070 | G    |
| 32  | 2     | 1072 | U    |
| 32  | 2     | 1073 | C    |
| 32  | 2     | 1076 | U    |
| 32  | 2     | 1077 | U    |
| 32  | 2     | 1079 | U    |
| 32  | 2     | 1087 | U    |
| 32  | 2     | 1090 | A    |
| 32  | 2     | 1095 | C    |
| 32  | 2     | 1096 | A    |
| 32  | 2     | 1097 | U    |
| 32  | 2     | 1098 | C    |
| 32  | 2     | 1099 | G    |
| 32  | 2     | 1102 | A    |
| 32  | 2     | 1106 | U    |
| 32  | 2     | 1108 | A    |
| 32  | 2     | 1109 | A    |
| 32  | 2     | 1115 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1118 | G    |
| 32  | 2     | 1122 | G    |
| 32  | 2     | 1131 | C    |
| 32  | 2     | 1132 | U    |
| 32  | 2     | 1133 | A    |
| 32  | 2     | 1134 | C    |
| 32  | 2     | 1135 | U    |
| 32  | 2     | 1142 | G    |
| 32  | 2     | 1144 | A    |
| 32  | 2     | 1149 | C    |
| 32  | 2     | 1151 | A    |
| 32  | 2     | 1159 | U    |
| 32  | 2     | 1160 | U    |
| 32  | 2     | 1162 | C    |
| 32  | 2     | 1167 | A    |
| 32  | 2     | 1168 | U    |
| 32  | 2     | 1169 | C    |
| 32  | 2     | 1173 | C    |
| 32  | 2     | 1176 | U    |
| 32  | 2     | 1179 | A    |
| 32  | 2     | 1182 | A    |
| 32  | 2     | 1186 | C    |
| 32  | 2     | 1194 | G    |
| 32  | 2     | 1202 | G    |
| 32  | 2     | 1203 | G    |
| 32  | 2     | 1204 | U    |
| 32  | 2     | 1205 | G    |
| 32  | 2     | 1209 | U    |
| 32  | 2     | 1210 | U    |
| 32  | 2     | 1213 | A    |
| 32  | 2     | 1214 | A    |
| 32  | 2     | 1215 | U    |
| 32  | 2     | 1217 | A    |
| 32  | 2     | 1218 | C    |
| 32  | 2     | 1225 | G    |
| 32  | 2     | 1228 | A    |
| 32  | 2     | 1232 | U    |
| 32  | 2     | 1234 | C    |
| 32  | 2     | 1235 | G    |
| 32  | 2     | 1244 | A    |
| 32  | 2     | 1248 | C    |
| 32  | 2     | 1252 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1254 | G    |
| 32  | 2     | 1255 | U    |
| 32  | 2     | 1257 | C    |
| 32  | 2     | 1263 | G    |
| 32  | 2     | 1264 | G    |
| 32  | 2     | 1265 | A    |
| 32  | 2     | 1276 | A    |
| 32  | 2     | 1281 | U    |
| 32  | 2     | 1284 | A    |
| 32  | 2     | 1286 | C    |
| 32  | 2     | 1290 | A    |
| 32  | 2     | 1295 | A    |
| 32  | 2     | 1297 | U    |
| 32  | 2     | 1299 | A    |
| 32  | 2     | 1300 | C    |
| 32  | 2     | 1301 | G    |
| 32  | 2     | 1302 | G    |
| 32  | 2     | 1303 | A    |
| 32  | 2     | 1304 | A    |
| 32  | 2     | 1307 | G    |
| 32  | 2     | 1308 | C    |
| 32  | 2     | 1309 | A    |
| 32  | 2     | 1310 | C    |
| 32  | 2     | 1311 | C    |
| 32  | 2     | 1312 | A    |
| 32  | 2     | 1313 | C    |
| 32  | 2     | 1315 | A    |
| 32  | 2     | 1318 | A    |
| 32  | 2     | 1319 | G    |
| 32  | 2     | 1321 | G    |
| 32  | 2     | 1322 | G    |
| 32  | 2     | 1327 | U    |
| 32  | 2     | 1328 | G    |
| 32  | 2     | 1331 | G    |
| 32  | 2     | 1332 | C    |
| 32  | 2     | 1333 | U    |
| 32  | 2     | 1336 | A    |
| 32  | 2     | 1337 | U    |
| 32  | 2     | 1339 | U    |
| 32  | 2     | 1340 | G    |
| 32  | 2     | 1341 | A    |
| 32  | 2     | 1342 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1343 | U    |
| 32  | 2     | 1346 | A    |
| 32  | 2     | 1347 | C    |
| 32  | 2     | 1349 | C    |
| 32  | 2     | 1350 | G    |
| 32  | 2     | 1351 | G    |
| 32  | 2     | 1352 | G    |
| 32  | 2     | 1353 | G    |
| 32  | 2     | 1354 | A    |
| 32  | 2     | 1355 | A    |
| 32  | 2     | 1356 | A    |
| 32  | 2     | 1357 | C    |
| 32  | 2     | 1358 | U    |
| 32  | 2     | 1359 | C    |
| 32  | 2     | 1361 | C    |
| 32  | 2     | 1362 | C    |
| 32  | 2     | 1363 | A    |
| 32  | 2     | 1364 | G    |
| 32  | 2     | 1366 | U    |
| 32  | 2     | 1367 | C    |
| 32  | 2     | 1369 | A    |
| 32  | 2     | 1370 | G    |
| 32  | 2     | 1371 | A    |
| 32  | 2     | 1372 | C    |
| 32  | 2     | 1374 | C    |
| 32  | 2     | 1375 | A    |
| 32  | 2     | 1376 | A    |
| 32  | 2     | 1378 | A    |
| 32  | 2     | 1379 | A    |
| 32  | 2     | 1380 | G    |
| 32  | 2     | 1381 | G    |
| 32  | 2     | 1382 | A    |
| 32  | 2     | 1383 | U    |
| 32  | 2     | 1384 | U    |
| 32  | 2     | 1385 | G    |
| 32  | 2     | 1386 | A    |
| 32  | 2     | 1387 | C    |
| 32  | 2     | 1388 | A    |
| 32  | 2     | 1391 | U    |
| 32  | 2     | 1392 | U    |
| 32  | 2     | 1393 | G    |
| 32  | 2     | 1394 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1396 | A    |
| 32  | 2     | 1397 | G    |
| 32  | 2     | 1398 | C    |
| 32  | 2     | 1399 | U    |
| 32  | 2     | 1400 | C    |
| 32  | 2     | 1403 | U    |
| 32  | 2     | 1404 | C    |
| 32  | 2     | 1405 | U    |
| 32  | 2     | 1406 | U    |
| 32  | 2     | 1408 | A    |
| 32  | 2     | 1409 | U    |
| 32  | 2     | 1410 | U    |
| 32  | 2     | 1411 | U    |
| 32  | 2     | 1412 | U    |
| 32  | 2     | 1413 | G    |
| 32  | 2     | 1414 | U    |
| 32  | 2     | 1415 | G    |
| 32  | 2     | 1417 | G    |
| 32  | 2     | 1418 | U    |
| 32  | 2     | 1419 | G    |
| 32  | 2     | 1420 | G    |
| 32  | 2     | 1421 | U    |
| 32  | 2     | 1422 | G    |
| 32  | 2     | 1423 | G    |
| 32  | 2     | 1425 | G    |
| 32  | 2     | 1426 | C    |
| 32  | 2     | 1427 | A    |
| 32  | 2     | 1429 | G    |
| 32  | 2     | 1431 | C    |
| 32  | 2     | 1432 | C    |
| 32  | 2     | 1437 | U    |
| 32  | 2     | 1438 | U    |
| 32  | 2     | 1439 | A    |
| 32  | 2     | 1440 | G    |
| 32  | 2     | 1445 | U    |
| 32  | 2     | 1446 | G    |
| 32  | 2     | 1450 | U    |
| 32  | 2     | 1454 | U    |
| 32  | 2     | 1455 | U    |
| 32  | 2     | 1458 | C    |
| 32  | 2     | 1459 | U    |
| 32  | 2     | 1466 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1467 | U    |
| 32  | 2     | 1468 | G    |
| 32  | 2     | 1471 | A    |
| 32  | 2     | 1473 | A    |
| 32  | 2     | 1474 | A    |
| 32  | 2     | 1475 | C    |
| 32  | 2     | 1476 | G    |
| 32  | 2     | 1477 | A    |
| 32  | 2     | 1478 | A    |
| 32  | 2     | 1482 | G    |
| 32  | 2     | 1491 | C    |
| 32  | 2     | 1492 | U    |
| 32  | 2     | 1493 | A    |
| 32  | 2     | 1494 | C    |
| 32  | 2     | 1495 | U    |
| 32  | 2     | 1496 | A    |
| 32  | 2     | 1497 | A    |
| 32  | 2     | 1498 | A    |
| 32  | 2     | 1499 | U    |
| 32  | 2     | 1500 | A    |
| 32  | 2     | 1501 | G    |
| 32  | 2     | 1502 | U    |
| 32  | 2     | 1503 | G    |
| 32  | 2     | 1504 | G    |
| 32  | 2     | 1506 | G    |
| 32  | 2     | 1510 | G    |
| 32  | 2     | 1511 | C    |
| 32  | 2     | 1512 | A    |
| 32  | 2     | 1513 | U    |
| 32  | 2     | 1514 | U    |
| 32  | 2     | 1515 | U    |
| 32  | 2     | 1516 | G    |
| 32  | 2     | 1518 | U    |
| 32  | 2     | 1519 | G    |
| 32  | 2     | 1521 | U    |
| 32  | 2     | 1522 | U    |
| 32  | 2     | 1529 | U    |
| 32  | 2     | 1530 | U    |
| 32  | 2     | 1537 | G    |
| 32  | 2     | 1540 | A    |
| 32  | 2     | 1542 | U    |
| 32  | 2     | 1551 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1554 | G    |
| 32  | 2     | 1557 | G    |
| 32  | 2     | 1558 | A    |
| 32  | 2     | 1559 | U    |
| 32  | 2     | 1565 | U    |
| 32  | 2     | 1567 | U    |
| 32  | 2     | 1573 | A    |
| 32  | 2     | 1574 | A    |
| 32  | 2     | 1576 | A    |
| 32  | 2     | 1577 | A    |
| 32  | 2     | 1578 | C    |
| 32  | 2     | 1579 | A    |
| 32  | 2     | 1580 | G    |
| 32  | 2     | 1581 | G    |
| 32  | 2     | 1582 | U    |
| 32  | 2     | 1583 | C    |
| 32  | 2     | 1584 | U    |
| 32  | 2     | 1585 | G    |
| 32  | 2     | 1586 | U    |
| 32  | 2     | 1588 | A    |
| 32  | 2     | 1590 | G    |
| 32  | 2     | 1593 | C    |
| 32  | 2     | 1594 | U    |
| 32  | 2     | 1595 | U    |
| 32  | 2     | 1597 | G    |
| 32  | 2     | 1598 | A    |
| 32  | 2     | 1599 | C    |
| 32  | 2     | 1600 | G    |
| 32  | 2     | 1601 | U    |
| 32  | 2     | 1602 | U    |
| 32  | 2     | 1603 | C    |
| 32  | 2     | 1605 | G    |
| 32  | 2     | 1606 | G    |
| 32  | 2     | 1607 | G    |
| 32  | 2     | 1608 | C    |
| 32  | 2     | 1611 | C    |
| 32  | 2     | 1612 | A    |
| 32  | 2     | 1613 | C    |
| 32  | 2     | 1614 | G    |
| 32  | 2     | 1618 | G    |
| 32  | 2     | 1619 | C    |
| 32  | 2     | 1620 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1621 | A    |
| 32  | 2     | 1623 | A    |
| 32  | 2     | 1625 | U    |
| 32  | 2     | 1626 | G    |
| 32  | 2     | 1630 | G    |
| 32  | 2     | 1631 | A    |
| 32  | 2     | 1634 | C    |
| 32  | 2     | 1636 | G    |
| 32  | 2     | 1638 | G    |
| 32  | 2     | 1642 | C    |
| 32  | 2     | 1643 | U    |
| 32  | 2     | 1644 | A    |
| 32  | 2     | 1646 | C    |
| 32  | 2     | 1648 | U    |
| 32  | 2     | 1649 | U    |
| 32  | 2     | 1650 | G    |
| 32  | 2     | 1651 | G    |
| 32  | 2     | 1652 | C    |
| 32  | 2     | 1653 | C    |
| 32  | 2     | 1656 | G    |
| 32  | 2     | 1662 | U    |
| 32  | 2     | 1666 | U    |
| 32  | 2     | 1667 | A    |
| 32  | 2     | 1668 | A    |
| 32  | 2     | 1669 | U    |
| 32  | 2     | 1670 | C    |
| 32  | 2     | 1672 | U    |
| 32  | 2     | 1673 | G    |
| 32  | 2     | 1675 | G    |
| 32  | 2     | 1676 | A    |
| 32  | 2     | 1681 | C    |
| 32  | 2     | 1687 | U    |
| 32  | 2     | 1688 | G    |
| 32  | 2     | 1689 | C    |
| 32  | 2     | 1690 | U    |
| 32  | 2     | 1692 | G    |
| 32  | 2     | 1693 | G    |
| 32  | 2     | 1694 | G    |
| 32  | 2     | 1695 | A    |
| 32  | 2     | 1696 | U    |
| 32  | 2     | 1697 | A    |
| 32  | 2     | 1698 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1700 | G    |
| 32  | 2     | 1701 | C    |
| 32  | 2     | 1703 | U    |
| 32  | 2     | 1704 | U    |
| 32  | 2     | 1705 | G    |
| 32  | 2     | 1709 | U    |
| 32  | 2     | 1710 | U    |
| 32  | 2     | 1711 | A    |
| 32  | 2     | 1713 | U    |
| 32  | 2     | 1715 | C    |
| 32  | 2     | 1716 | U    |
| 32  | 2     | 1720 | C    |
| 32  | 2     | 1721 | A    |
| 32  | 2     | 1722 | A    |
| 32  | 2     | 1732 | C    |
| 32  | 2     | 1733 | C    |
| 32  | 2     | 1734 | U    |
| 32  | 2     | 1735 | A    |
| 32  | 2     | 1736 | G    |
| 32  | 2     | 1740 | G    |
| 32  | 2     | 1742 | G    |
| 32  | 2     | 1743 | C    |
| 32  | 2     | 1744 | A    |
| 32  | 2     | 1745 | A    |
| 32  | 2     | 1749 | A    |
| 32  | 2     | 1750 | U    |
| 32  | 2     | 1752 | A    |
| 32  | 2     | 1753 | G    |
| 32  | 2     | 1754 | C    |
| 32  | 2     | 1755 | U    |
| 32  | 2     | 1756 | U    |
| 32  | 2     | 1757 | G    |
| 32  | 2     | 1759 | G    |
| 32  | 2     | 1765 | U    |
| 32  | 2     | 1766 | A    |
| 32  | 2     | 1767 | C    |
| 32  | 2     | 1770 | C    |
| 32  | 2     | 1771 | C    |
| 32  | 2     | 1774 | G    |
| 32  | 2     | 1775 | C    |
| 32  | 2     | 1781 | G    |
| 32  | 2     | 1782 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1783 | A    |
| 32  | 2     | 1786 | C    |
| 32  | 2     | 1787 | A    |
| 32  | 2     | 1788 | C    |
| 32  | 2     | 1790 | G    |
| 32  | 2     | 1791 | C    |
| 32  | 2     | 1792 | C    |
| 32  | 2     | 1793 | C    |
| 32  | 2     | 1794 | G    |
| 32  | 2     | 1795 | U    |
| 32  | 2     | 1797 | G    |
| 32  | 2     | 1798 | C    |
| 32  | 2     | 1799 | U    |
| 32  | 2     | 1800 | A    |
| 32  | 2     | 1801 | G    |
| 32  | 2     | 1802 | U    |
| 32  | 2     | 1803 | A    |
| 32  | 2     | 1804 | C    |
| 32  | 2     | 1805 | C    |
| 32  | 2     | 1807 | A    |
| 32  | 2     | 1809 | U    |
| 32  | 2     | 1811 | A    |
| 32  | 2     | 1812 | A    |
| 32  | 2     | 1821 | U    |
| 32  | 2     | 1826 | C    |
| 32  | 2     | 1827 | C    |
| 32  | 2     | 1838 | C    |
| 32  | 2     | 1839 | U    |
| 32  | 2     | 1841 | A    |
| 32  | 2     | 1844 | G    |
| 32  | 2     | 1845 | A    |
| 32  | 2     | 1846 | A    |
| 32  | 2     | 1847 | G    |
| 32  | 2     | 1848 | G    |
| 32  | 2     | 1850 | G    |
| 32  | 2     | 1851 | G    |
| 32  | 2     | 1852 | C    |
| 32  | 2     | 1853 | A    |
| 32  | 2     | 1855 | C    |
| 32  | 2     | 1858 | C    |
| 32  | 2     | 1861 | C    |
| 32  | 2     | 1863 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1864 | A    |
| 32  | 2     | 1865 | G    |
| 32  | 2     | 1867 | G    |
| 32  | 2     | 1869 | G    |
| 32  | 2     | 1882 | A    |
| 32  | 2     | 1884 | A    |
| 32  | 2     | 1888 | G    |
| 32  | 2     | 1891 | C    |
| 32  | 2     | 1893 | U    |
| 32  | 2     | 1894 | U    |
| 32  | 2     | 1895 | U    |
| 32  | 2     | 1896 | A    |
| 32  | 2     | 1897 | G    |
| 32  | 2     | 1900 | G    |
| 32  | 2     | 1901 | A    |
| 32  | 2     | 1905 | A    |
| 32  | 2     | 1906 | A    |
| 32  | 2     | 1907 | A    |
| 32  | 2     | 1909 | G    |

All (22) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 541  | U    |
| 32  | 2     | 826  | U    |
| 32  | 2     | 856  | U    |
| 32  | 2     | 1056 | G    |
| 32  | 2     | 1108 | A    |
| 32  | 2     | 1168 | U    |
| 32  | 2     | 1181 | U    |
| 32  | 2     | 1346 | A    |
| 32  | 2     | 1358 | U    |
| 32  | 2     | 1383 | U    |
| 32  | 2     | 1430 | G    |
| 32  | 2     | 1431 | C    |
| 32  | 2     | 1495 | U    |
| 32  | 2     | 1502 | U    |
| 32  | 2     | 1578 | C    |
| 32  | 2     | 1605 | G    |
| 32  | 2     | 1633 | C    |
| 32  | 2     | 1643 | U    |
| 32  | 2     | 1667 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2     | 1734 | U    |
| 32  | 2     | 1753 | G    |
| 32  | 2     | 1866 | A    |

## 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 32  | 2     | 34               |
| 29  | f     | 3                |
| 14  | P     | 3                |
| 10  | K     | 1                |
| 5   | F     | 1                |
| 3   | D     | 1                |
| 31  | k     | 1                |
| 2   | C     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 2     | 1169:C    | O3'    | 1170:U    | P      | 30.51        |
| 1     | 2     | 921:C     | O3'    | 922:G     | P      | 23.31        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 2     | 1128:U    | O3'    | 1129:A    | P      | 22.80        |
| 1     | 2     | 1588:A    | O3'    | 1589:U    | P      | 17.38        |
| 1     | 2     | 1616:G    | O3'    | 1617:C    | P      | 13.69        |
| 1     | f     | 137:ASP   | C      | 138:ARG   | N      | 12.35        |
| 1     | 2     | 1179:A    | O3'    | 1180:C    | P      | 11.43        |
| 1     | 2     | 1859:A    | O3'    | 1860:U    | P      | 11.20        |
| 1     | 2     | 1164:U    | O3'    | 1165:U    | P      | 10.82        |
| 1     | 2     | 1165:U    | O3'    | 1166:A    | P      | 10.56        |
| 1     | 2     | 1784:C    | O3'    | 1785:A    | P      | 10.46        |
| 1     | 2     | 1182:A    | O3'    | 1183:U    | P      | 10.22        |
| 1     | 2     | 1184:G    | O3'    | 1185:C    | P      | 9.57         |
| 1     | 2     | 1590:G    | O3'    | 1591:C    | P      | 7.83         |
| 1     | 2     | 1609:C    | O3'    | 1610:G    | P      | 7.76         |
| 1     | f     | 136:LYS   | C      | 137:ASP   | N      | 6.90         |
| 1     | 2     | 1586:U    | O3'    | 1587:G    | P      | 6.33         |
| 1     | 2     | 1180:C    | O3'    | 1181:U    | P      | 6.32         |
| 1     | 2     | 1183:U    | O3'    | 1184:G    | P      | 6.23         |
| 1     | 2     | 1858:C    | O3'    | 1859:A    | P      | 6.11         |
| 1     | 2     | 1591:C    | O3'    | 1592:C    | P      | 5.49         |
| 1     | 2     | 1297:U    | O3'    | 1298:G    | P      | 5.36         |
| 1     | 2     | 1163:A    | O3'    | 1164:U    | P      | 4.79         |
| 1     | K     | 26:ASP    | C      | 27:PHE    | N      | 4.75         |
| 1     | 2     | 1783:A    | O3'    | 1784:C    | P      | 4.69         |
| 1     | 2     | 1595:U    | O3'    | 1596:A    | P      | 4.65         |
| 1     | f     | 129:GLY   | C      | 130:VAL   | N      | 4.44         |
| 1     | 2     | 1176:U    | O3'    | 1177:A    | P      | 4.40         |
| 1     | F     | 224:ASN   | C      | 225:ARG   | N      | 4.34         |
| 1     | 2     | 1522:U    | O3'    | 1523:A    | P      | 4.21         |
| 1     | 2     | 1177:A    | O3'    | 1178:A    | P      | 3.95         |
| 1     | P     | 79:HIS    | C      | 80:MET    | N      | 3.90         |
| 1     | 2     | 1205:G    | O3'    | 1206:U    | P      | 3.58         |
| 1     | 2     | 1280:A    | O3'    | 1281:U    | P      | 3.32         |
| 1     | 2     | 1529:U    | O3'    | 1530:U    | P      | 3.32         |
| 1     | D     | 224:ASP   | C      | 225:TYR   | N      | 3.22         |
| 1     | 2     | 1647:C    | O3'    | 1648:U    | P      | 3.20         |
| 1     | 2     | 1193:G    | O3'    | 1194:G    | P      | 3.18         |
| 1     | 2     | 1351:G    | O3'    | 1352:G    | P      | 3.18         |
| 1     | P     | 70:ASN    | C      | 71:GLU    | N      | 3.17         |
| 1     | 2     | 1223:U    | O3'    | 1224:C    | P      | 3.17         |
| 1     | k     | 60:GLN    | C      | 61:LEU    | N      | 3.16         |
| 1     | P     | 108:ARG   | C      | 109:PRO   | N      | 3.14         |
| 1     | 2     | 1587:G    | O3'    | 1588:A    | P      | 3.11         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 60:SER    | C      | 61:LEU    | N      | 1.19         |

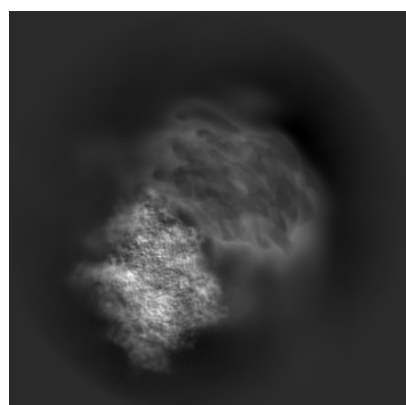
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21644. These allow visual inspection of the internal detail of the map and identification of artifacts.

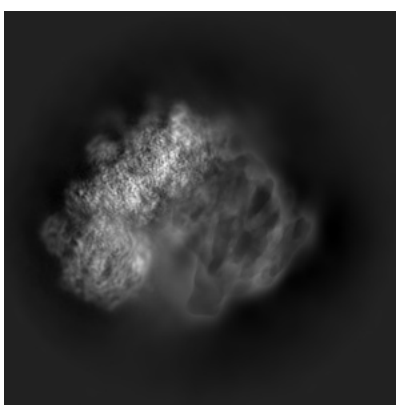
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

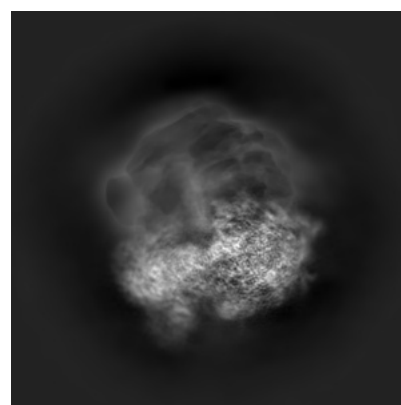
#### 6.1.1 Primary map



X



Y

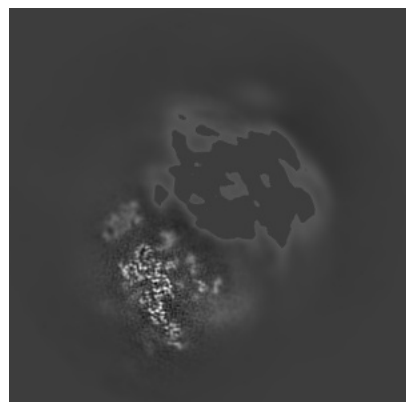


Z

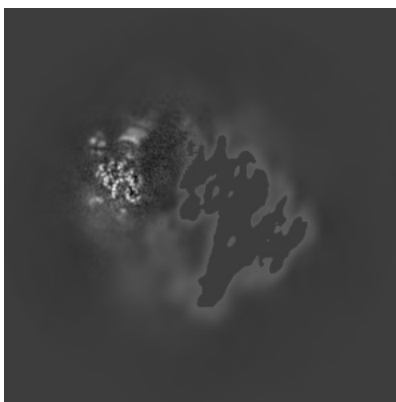
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 192



Y Index: 192

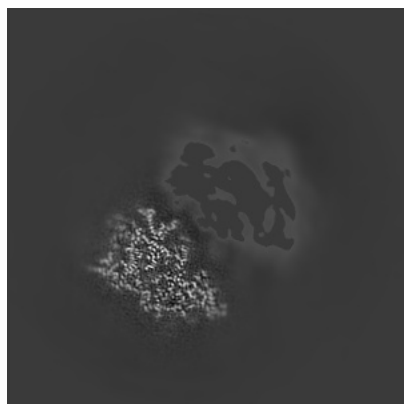


Z Index: 192

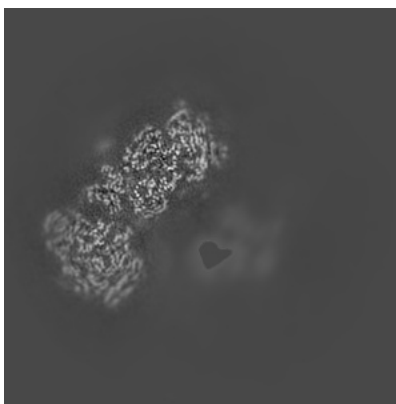
The images above show central slices of the map in three orthogonal directions.

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

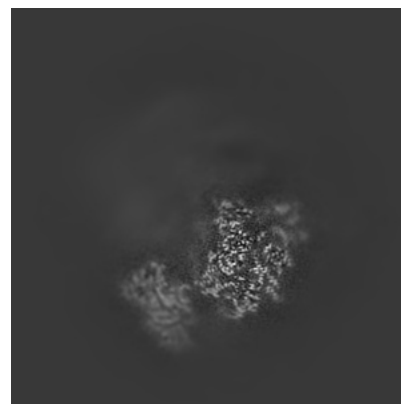
### 6.3.1 Primary map



X Index: 224



Y Index: 131

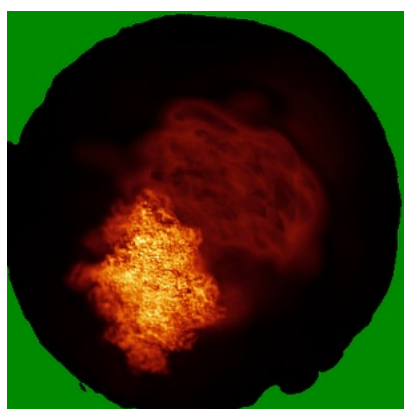


Z Index: 127

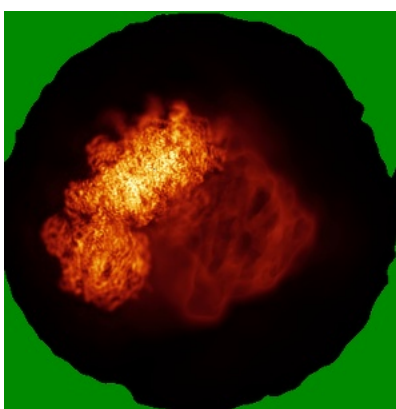
The images above show the largest variance slices of the map in three orthogonal directions.

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

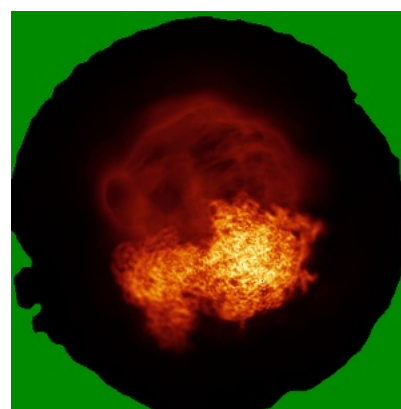
### 6.4.1 Primary map



X



Y

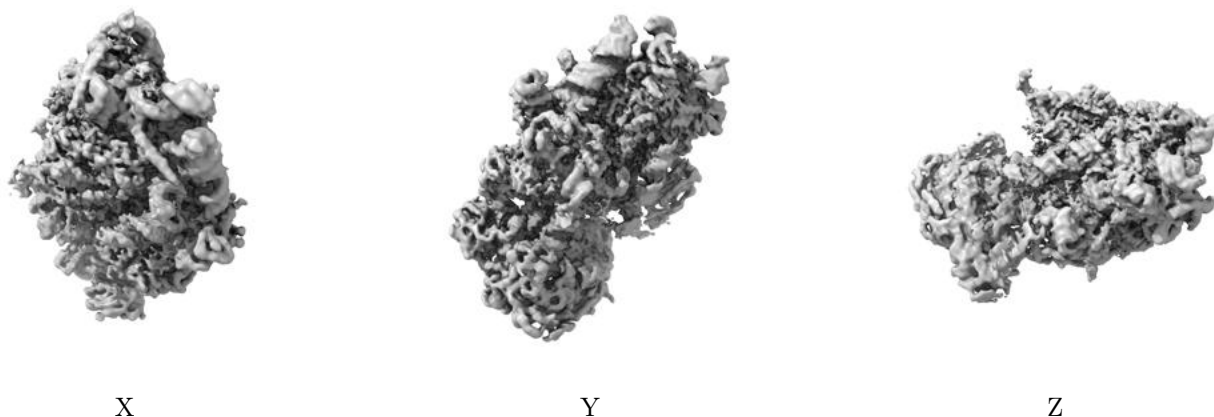


Z

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 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

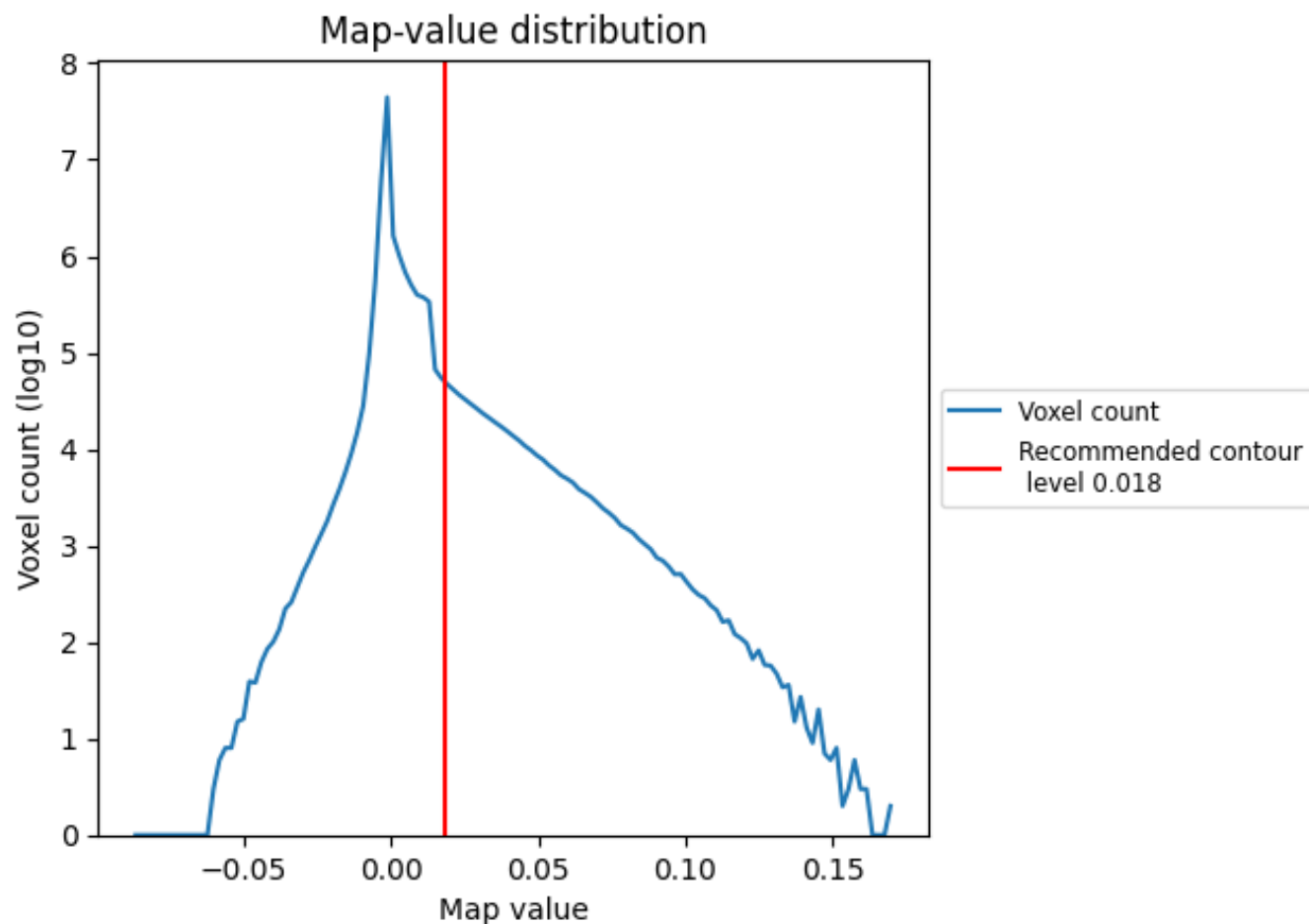
## 6.6 Mask visualisation [i](#)

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.

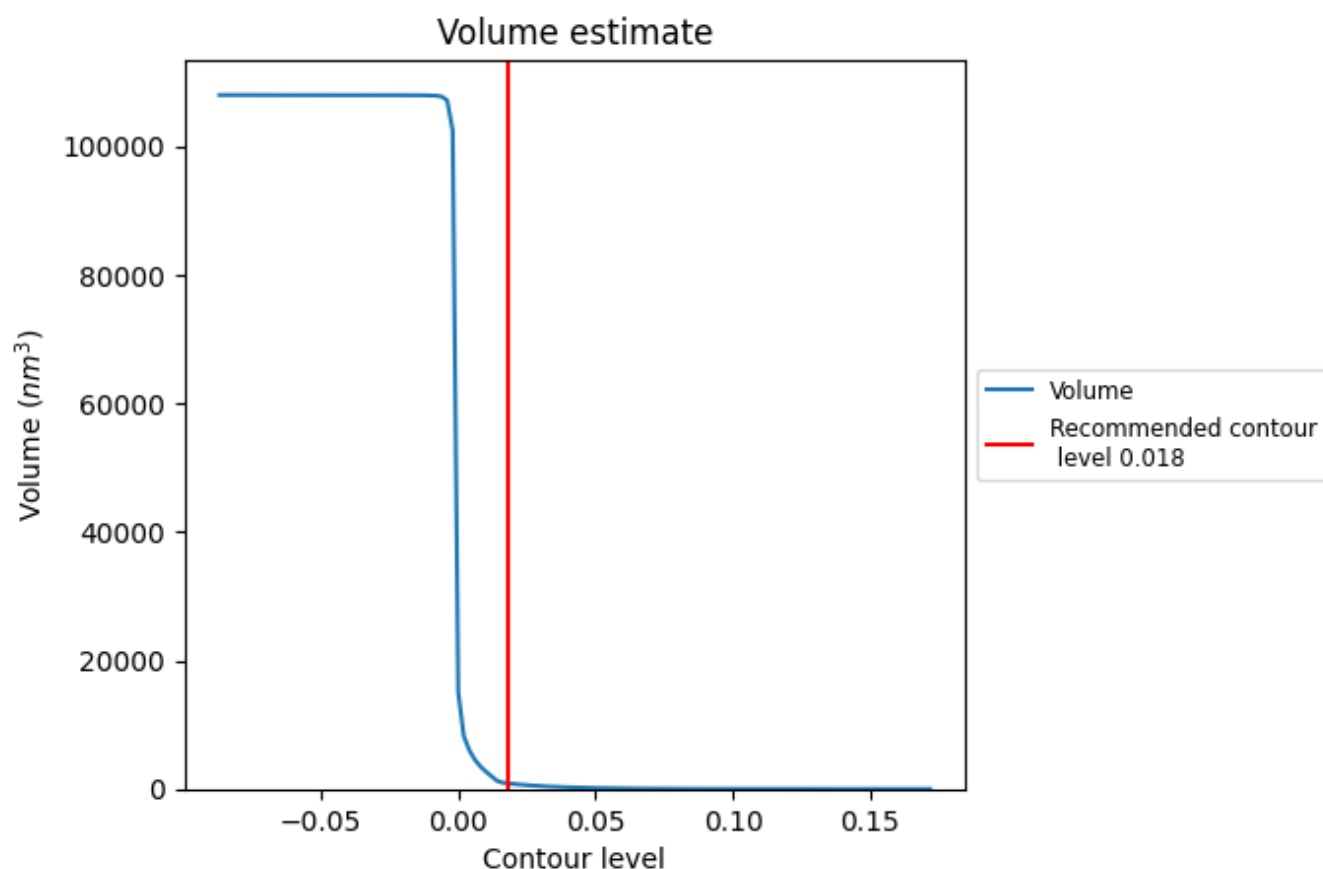
### 7.1 Map-value distribution [i](#)



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.



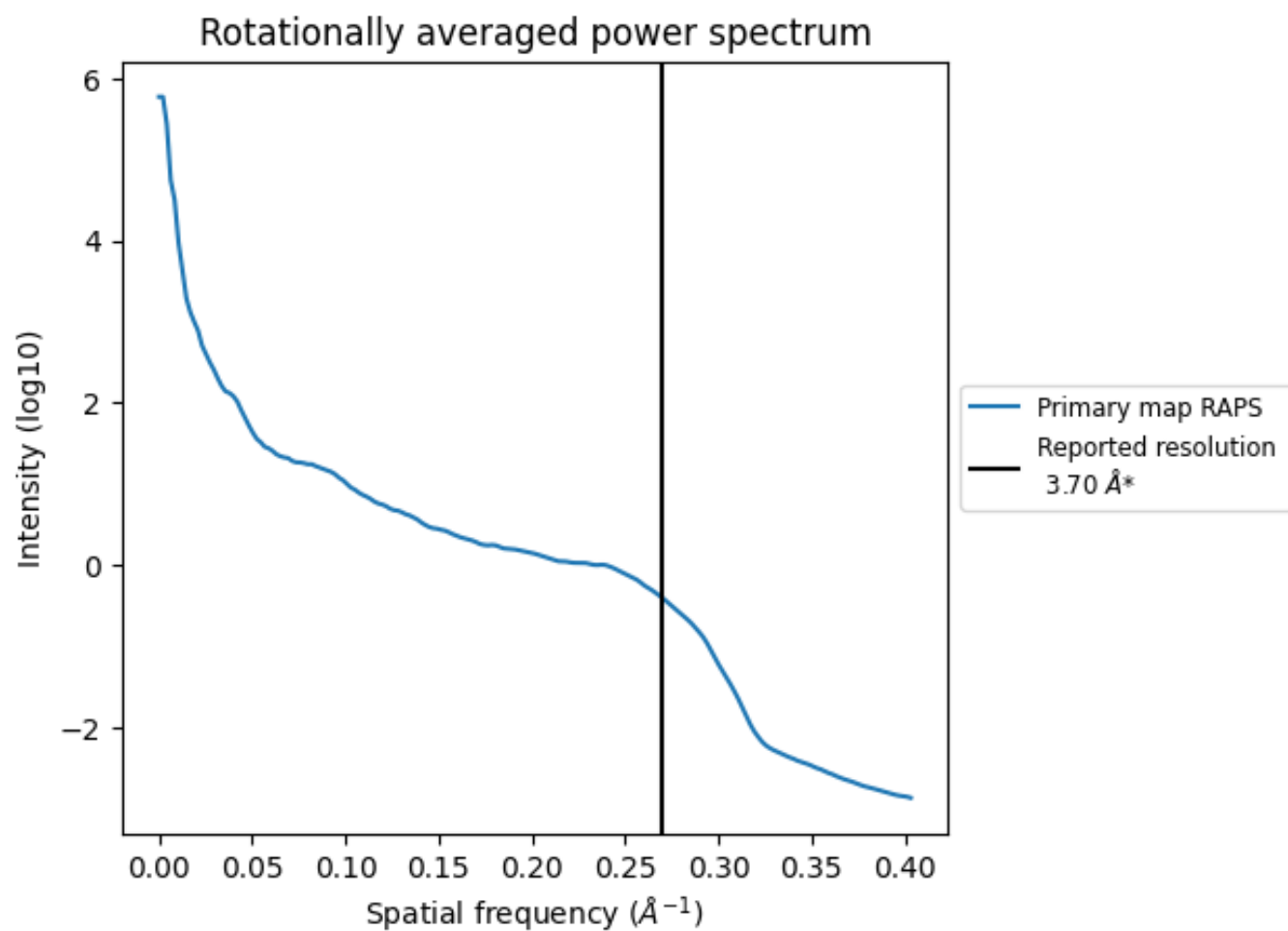
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 881  $\text{nm}^3$ ; this corresponds to an approximate mass of 796 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 0.270 Å<sup>-1</sup>

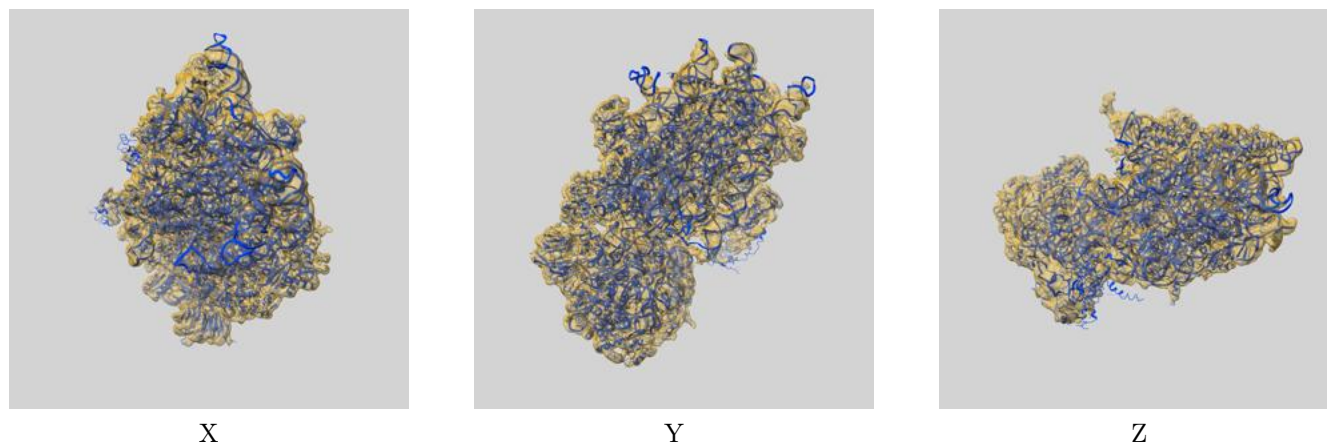
## 8 Fourier-Shell correlation

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

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

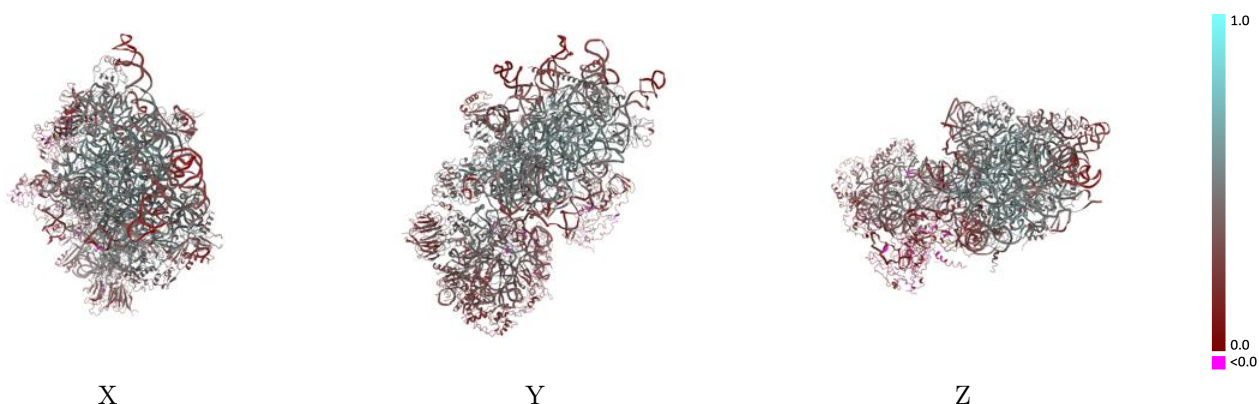
This section contains information regarding the fit between EMDB map EMD-21644 and PDB model 6WDR. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

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



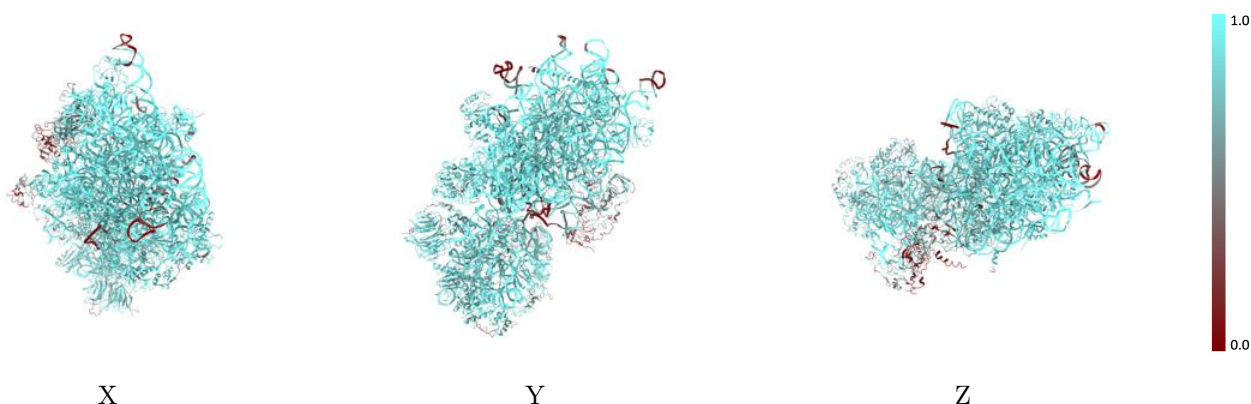
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



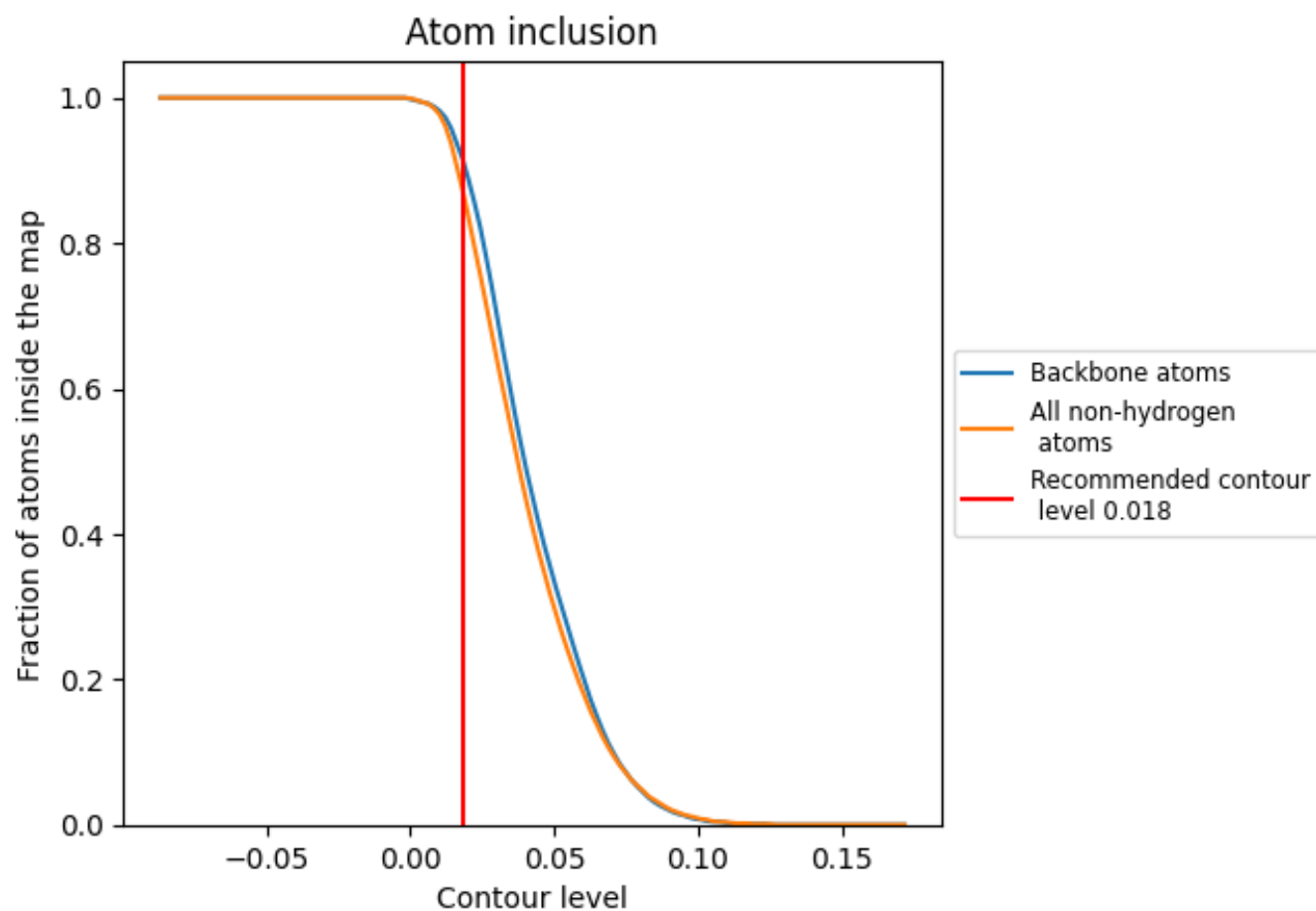
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.018) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8760   |  0.3970   |
| 2     |  0.9390   |  0.4170   |
| A     |  0.9480   |  0.4780   |
| C     |  0.9450   |  0.5100   |
| D     |  0.7440   |  0.2880   |
| E     |  0.9580   |  0.5260   |
| F     |  0.7810   |  0.3070   |
| G     |  0.9140   |  0.4250   |
| H     |  0.8810   |  0.3970   |
| I     |  0.9190   |  0.4800   |
| J     |  0.9490   |  0.4960   |
| K     |  0.8360   |  0.2430   |
| L     |  0.9550   |  0.5420   |
| M     |  0.4310   |  0.1370   |
| N     |  0.9010  |  0.4590  |
| P     |  0.8070 |  0.2300 |
| Q     |  0.8950 |  0.3780 |
| R     |  0.8460 |  0.3910 |
| S     |  0.7420 |  0.2260 |
| T     |  0.8940 |  0.3060 |
| U     |  0.8350 |  0.3810 |
| V     |  0.9350 |  0.5080 |
| W     |  0.9790 |  0.5620 |
| X     |  0.9040 |  0.4970 |
| Y     |  0.9440 |  0.4850 |
| Z     |  0.7460 |  0.2200 |
| b     |  0.9500 |  0.4720 |
| c     |  0.6980 |  0.3250 |
| d     |  0.9280 |  0.4310 |
| e     |  0.6850 |  0.4080 |
| f     |  0.6110 |  0.1540 |
| g     |  0.8470 |  0.3050 |
| k     |  0.5170 |  0.2580 |

