



## Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 12:54 PM JST

PDB ID : 7D80 / pdb\_00007d80  
EMDB ID : EMD-30611  
Title : Molecular model of the cryo-EM structure of 70S ribosome in complex with peptide deformylase, trigger factor, and methionine aminopeptidase  
Authors : Akbar, S.; Bhakta, S.; Sengupta, J.  
Deposited on : 2020-10-06  
Resolution : 4.10 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:

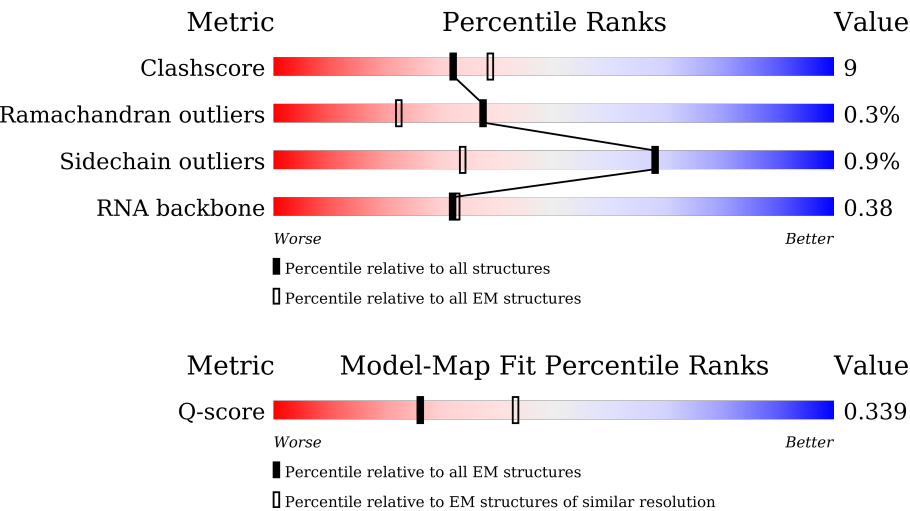
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 4.10 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                       | 6458 ( 3.60 - 4.60 )                                     |

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

| Mol | Chain | Length | Quality of chain                                      |
|-----|-------|--------|-------------------------------------------------------|
| 1   | 0     | 46     | <div><div>78%</div><div>22%</div></div>               |
| 2   | 1     | 65     | <div><div>75%</div><div>18%</div><div>...</div></div> |
| 3   | 2     | 38     | <div><div>61%</div><div>37%</div><div>.</div></div>   |

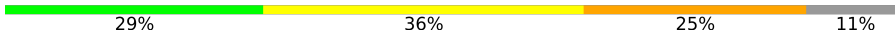
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 3     | 169    |    |
| 5   | 5     | 432    |    |
| 6   | 6     | 57     |    |
| 7   | A     | 2903   |    |
| 8   | B     | 1539   |    |
| 9   | C     | 241    |    |
| 10  | D     | 233    |    |
| 11  | E     | 206    |    |
| 12  | F     | 167    |    |
| 13  | G     | 135    |    |
| 14  | H     | 179    |    |
| 15  | I     | 130    |    |
| 16  | J     | 130    |  |
| 17  | K     | 103    |  |
| 18  | L     | 129    |  |
| 19  | M     | 124    |  |
| 20  | N     | 118    |  |
| 21  | O     | 101    |  |
| 22  | P     | 89     |  |
| 23  | Q     | 82     |  |
| 24  | R     | 84     |  |
| 25  | S     | 75     |  |
| 26  | T     | 92     |  |
| 27  | U     | 87     |  |
| 28  | V     | 71     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | W     | 100    |    |
| 30  | X     | 73     |    |
| 31  | Z     | 76     |    |
| 32  | a     | 118    |    |
| 33  | b     | 273    |    |
| 34  | c     | 209    |    |
| 35  | d     | 201    |    |
| 36  | e     | 179    |    |
| 37  | f     | 177    |    |
| 38  | g     | 149    |    |
| 39  | h     | 142    |    |
| 40  | i     | 142    |   |
| 41  | j     | 123    |  |
| 42  | k     | 144    |  |
| 43  | l     | 136    |  |
| 44  | m     | 127    |  |
| 45  | n     | 117    |  |
| 46  | o     | 115    |  |
| 47  | p     | 118    |  |
| 48  | q     | 103    |  |
| 49  | r     | 110    |  |
| 50  | s     | 104    |  |
| 51  | t     | 94     |  |
| 52  | u     | 85     |  |
| 53  | v     | 78     |  |

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| Mol | Chain | Length | Quality of chain                                                             |
|-----|-------|--------|------------------------------------------------------------------------------|
| 54  | w     | 63     | <div><div></div><div>78%</div><div>22%</div></div>                           |
| 55  | x     | 59     | <div><div></div><div>85%</div><div>14%</div><div></div></div>                |
| 56  | y     | 77     | <div><div></div><div>45%</div><div>39%</div><div>6%</div><div>9%</div></div> |
| 57  | z     | 55     | <div><div></div><div>73%</div><div>18%</div><div>9%</div></div>              |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 150808 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 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 0     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |
|     |       |          |       |     |    |    |   |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 2   | 1     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |
|     |       |          |       |     |     |    |   |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |
|     |       |          |       |     |    |    |   |         |       |

- Molecule 4 is a protein called Peptide deformylase.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 3     | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 844 | 241 | 255 | 6 |         |       |
|     |       |          |       |     |     |     |   |         |       |

- Molecule 5 is a protein called Trigger factor.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | 5     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3386  | 2119 | 582 | 674 | 11 |         |       |
|     |       |          |       |      |     |     |    |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | 6     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |
|     |       |          |       |     |    |    |   |         |       |

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 7   | A     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62317 | 27801 | 11467 | 20147 | 2902 |         |       |

- Molecule 8 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 8   | B     | 1539     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33015 | 14725 | 6052 | 10699 | 1539 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | C     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | D     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | E     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | F     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S6, fully modified isoform.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | G     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | H     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | I     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | J     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | K     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | L     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | M     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | N     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | O     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | P     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 437 | 143 | 129 | 1 |         |       |

- Molecule 23 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Q     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 24 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | R     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 25  | S     | 55       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |       |

- Molecule 26 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | T     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |       |

- Molecule 27 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | U     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 28 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | V     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | W     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 484 | 142 | 136 | 2 |         |       |

- Molecule 30 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 30  | X     | 65       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1392  | 621 | 258 | 449 | 64 |         |       |

- Molecule 31 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 31  | Z     | 66       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1406  | 629 | 255 | 457 | 65 |         |       |

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 32  | a     | 118      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2529  | 1126 | 464 | 821 | 118 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33  | b     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | c     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | d     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | e     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | f     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | g     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 233 | 62 | 63 | 1 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | h     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | i     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | j     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | k     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | l     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | m     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 45  | n     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | o     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 47  | p     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | q     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | r     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | s     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | t     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | u     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 569   | 353 | 113 | 102 | 1 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | v     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | w     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | x     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 56 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 56  | y     | 70       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1496  | 665 | 267 | 494 | 70 |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 57  | z     | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |       |

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

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

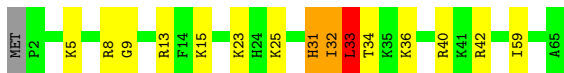
- Molecule 1: 50S ribosomal protein L34

Chain 0:  78% 22%



- Molecule 2: 50S ribosomal protein L35

Chain 1:  75% 18% . . .



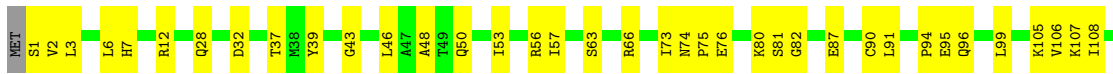
- Molecule 3: 50S ribosomal protein L36

Chain 2:  61% 37% .



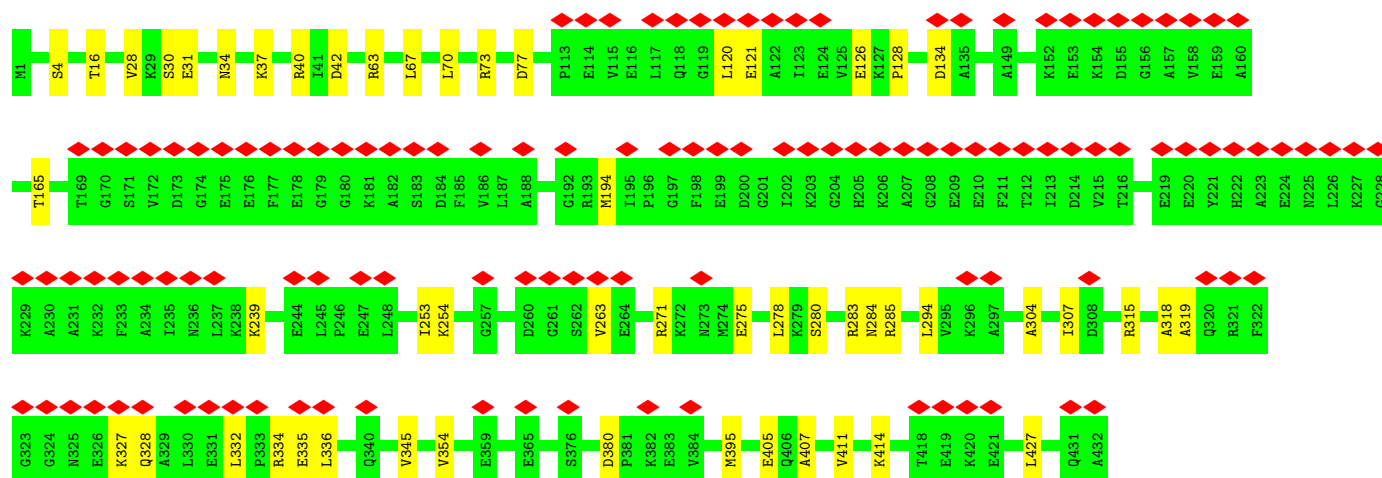
- Molecule 4: Peptide deformylase

Chain 3:  71% 28% .



- Molecule 5: Trigger factor

Chain 5:  28% 88% 12%



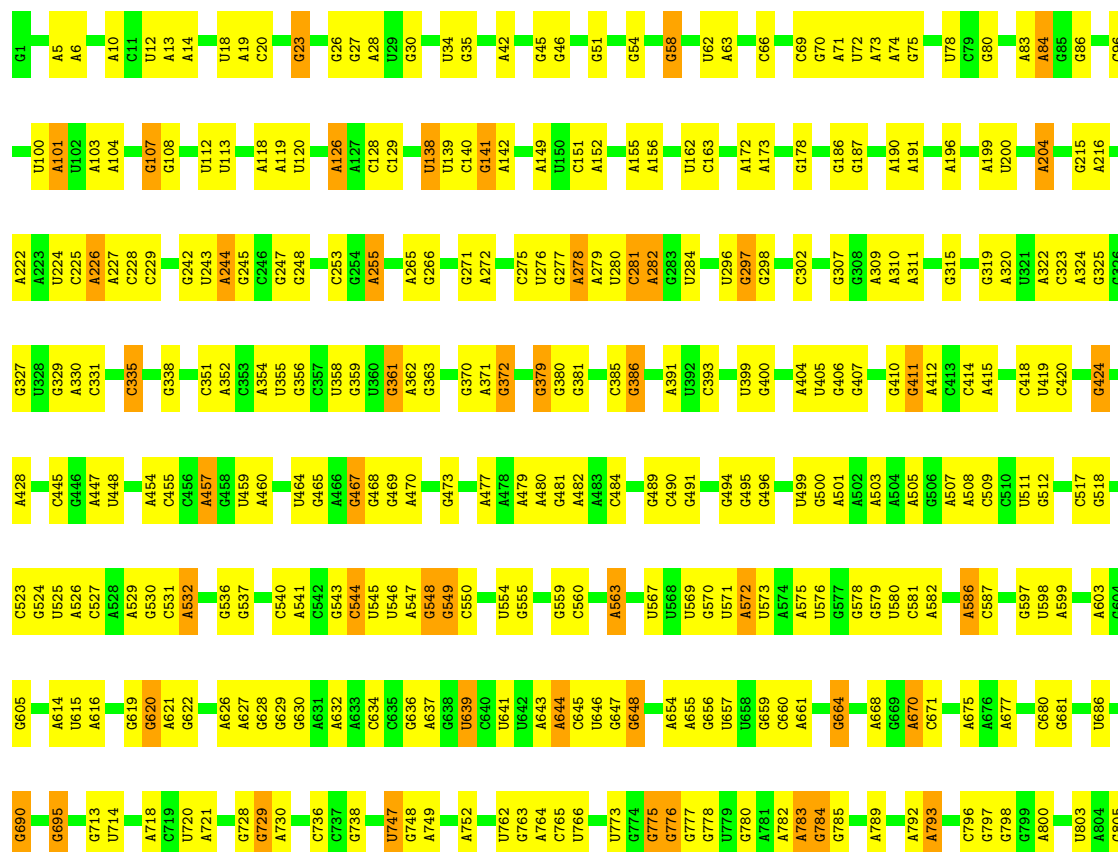
- Molecule 6: 50S ribosomal protein L32

Chain 6: 84% 14% .



- Molecule 7: 23S ribosomal RNA

Chain A: 56% 37% 7%



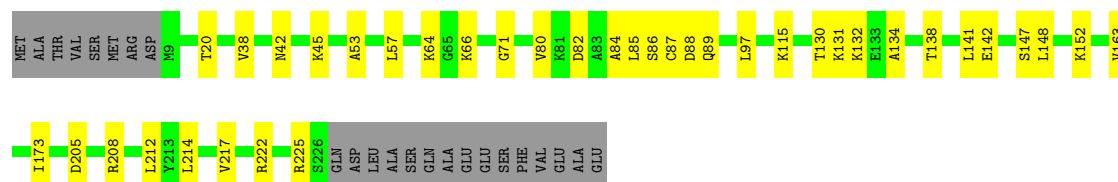
|       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|
| A2114 | A2033 | A1953 | G1817 | G1730 | A1632 | G1537 | A1433 | G1349 | G1256 | C1161 | A1077 | G989  | G907 | C806 |
| G2115 | U2034 | G1954 | U1818 | G1731 | A1635 | G1540 | A1434 | C1349 | C1257 | G1162 | U1078 | A990  | C908 | U807 |
| G2116 | G2035 | U1955 | A1819 | U1636 | U1636 | G1541 | C1437 | U1352 | U1258 | G1163 | A1080 | C992  | A909 | U811 |
| A2117 | C2036 | U1956 | C1822 | A1637 | A1637 | G1542 | C1437 | U1352 | U1258 | C1164 | U1081 | G993  | A910 | C812 |
| U2118 |       |       |       |       |       | G1543 | C1451 | G1355 | U1263 | G1165 | G1087 | C994  | A911 | C812 |
| A2119 | U2039 | A1960 | U1825 | G1738 | A1641 | G1544 | G1452 | G1356 | A1264 | G1167 | A1088 | C995  | A913 | A819 |
| G2120 | G2040 | U1963 | G1826 | G1743 | G1642 | A1544 | A1453 | G1357 | A1265 | C1168 | A1089 | A996  | U913 | A820 |
| U2121 | A2042 | G1964 | U1827 |       |       |       | C1454 | C1358 | G1266 | A1169 | U1091 | U999  | G914 |      |
| G2123 | C2043 | G1965 | G1828 | G1748 | C1646 | G1545 | G1455 | G1359 | C1270 | G1170 | A1090 | U999  | A917 | U827 |
| G2124 | A1966 | A1966 | A1829 | A1749 | U1647 | C1561 | G1456 | A1359 | A1272 | G1171 | U1097 | G1002 | C921 | A829 |
| G2125 | G2049 | C1967 | C1830 | G1750 | U1648 | U1562 | U1457 | G1360 | A1273 | C1172 | A1098 | U1004 | C922 | G830 |
| A2126 |       |       | G1831 |       | G1649 |       | U1458 | C1362 | U1273 | U1173 | U1097 | G1003 | G923 | G831 |
| G2127 | A2052 | A1970 | C1832 | G1753 | A1650 | A1566 | C1459 | G1363 | C1278 | U1174 | A1098 | C1005 | G924 | U832 |
| G2128 | G2053 | U1971 | C1833 | G1756 | G1651 | G1567 | U1460 | G1364 | C1279 | G1175 | G1099 | U1009 | U929 | A833 |
| C2129 | A2054 | G1972 | U1834 | G1757 | A1652 | G1568 | C1461 | G1365 | G1283 | U1176 | U1101 | C1009 | U929 | G834 |
| G2130 | C2055 | U1757 | G1835 | A1757 | G1653 | A1569 | U1466 | A1366 | G1284 | C1177 | A1102 | U1012 | U832 | G841 |
| U2131 | G2056 | G1980 | G1845 | U1758 | C1658 | C1577 | U1466 | A1367 | A1285 | C1178 | A1103 | U1012 | U832 | G841 |
| U2132 |       | A1981 | G1846 | C1761 |       | U1578 | G1471 | G1368 | A1286 | U1180 | A1104 | C1013 | C935 | A845 |
| G2133 | A2059 | U1982 | A1847 |       | G1666 | U1578 | G1471 | G1369 | A1287 | U1181 | U1105 | A1021 | U846 | U847 |
| A2134 | A2060 | G1983 | A1848 | C1764 | G1667 | C1581 | G1478 | G1370 | U1287 | U1182 | G1106 | G1022 | A941 | U847 |
| G2135 | G2061 | G1984 | G1849 | U1764 | A1668 | C1582 | C1480 | C1371 | U1287 | U1183 | G1110 | G1022 | A941 | U847 |
| G2136 | A2062 | C1985 | U1850 | G1769 | A1669 | U1583 | U1481 | U1372 | U1294 | U1184 | G1110 | U1023 | G942 | G858 |
| U2137 | C2063 |       | G1851 | G1770 |       | C1584 | U1481 | C1376 | U1295 | U1185 | G1112 | G1026 | A943 | G859 |
| G2140 | C2064 | G1989 | U1855 |       | G1674 | C1585 | U1482 | C1376 | G1296 | G1186 |       |       |      |      |
| G2141 | C2065 | U1991 | U1855 | A1773 | C1675 |       | U1500 | G1389 | C1297 | G1187 |       |       |      |      |
| G2144 | U2068 | G1992 | U1864 | U1774 | A1676 | A1590 | A1490 | U1379 | U1298 | G1188 | G1115 | C946  | A947 | A863 |
| C2145 | G2069 | U1993 | U1865 | U1775 | A1677 | A1591 | G1491 | G1380 | G1299 | U1189 | G1116 | G1031 | G949 | G864 |
| A2146 | A2070 | G1994 | G1876 | U1776 | A1678 | C1592 | G1492 | G1380 | G1300 | G1190 | U1119 | U1033 | C949 | C865 |
| U2147 | C2072 | U1995 | C1869 | U1777 | A1679 | G1595 | C1493 | A1383 | A1301 | G1191 | G1120 | G1037 | G953 | A866 |
|       |       | C1996 | C1870 | U1778 | U1683 | A1596 | A1494 | C1386 | A1302 | G1195 | G1121 | G1038 | G954 | C873 |
| G2152 | U2075 | A1997 | A1871 | U1779 | G1684 | A1597 | A1496 | C1387 | A1304 | G1196 | G1122 | U1039 | U955 | A877 |
|       |       | C1999 | G1872 | U1781 | U1684 | A1598 | A1496 | G1388 | A1305 | A1204 | U1130 | A1040 | G956 | G878 |
| G2156 | U2079 | C2000 | G1873 | U1782 | A1690 | U1598 | G1500 | G1389 | G1309 | C1208 | G1125 | G1045 | C957 | G879 |
| G2157 |       | A1783 | U1882 | A1783 | U1602 | U1602 | A1501 | A1392 | G1310 | U1209 | A1126 | A1046 | C961 | G880 |
| A2158 | G2087 | A1784 | G1904 | A1784 | A1603 | A1604 | A1502 | A1392 | G1311 | G1210 |       | A1047 | G962 | G881 |
| G2159 | A2088 | G1791 | C1905 | A1792 | C1604 |       | A1503 | A1395 | U1316 | C1211 | A1129 | G1056 | U963 | G882 |
| C2160 | C2089 | G1792 | G1906 | G1792 | A1607 | C1607 | A1508 | U1396 | U1316 | G1212 | U1130 | C964  | C964 | G883 |
| G2162 | A2090 | G1907 | C1907 |       | A1608 | A1609 | A1509 | U1397 | U1316 | G1212 | U1131 | A1057 | C965 | G884 |
| A2163 | G2093 | U2011 | A1913 | U1796 | A1701 | A1609 | G1510 | C1398 | A1321 | U1217 | U1132 | U1060 | C968 | C885 |
| C2164 | A2094 | G2012 | C1914 | G1797 | G1702 | G1610 | G1511 | G1401 | G1324 | U1218 | A1133 | U1061 | G969 | A886 |
| C2165 | A2095 | A2013 | G1914 | U1798 | G1703 | C1611 | G1512 | U1402 | U1325 | G1219 | A1134 | G1062 | U970 | U887 |
| U2166 | C2096 |       | A1919 | G1799 | G1704 | A1616 | G1513 | A1403 | U1326 | G1223 | G1136 | G1063 | G971 | C888 |
| U2167 | A2097 | U2016 | A1919 | G1800 | A1705 | A1617 | G1514 | A1403 | A1327 | G1237 | G1137 | C1064 | A972 | C889 |
| G2168 | U2098 | U2017 | A1801 | A1801 | A1705 | C1617 | A1515 | U1411 | A1328 | A1237 | U1065 | U1066 | A973 | C890 |
| A2169 | U2099 |       | U1926 | A1802 | C1708 | A1618 | G1619 | U1412 | U1329 | G1238 | G1139 | U1067 | G974 | G891 |
| A2170 | G2100 | C2021 | G1929 | C1806 | U1709 | G1619 | U1523 | A1413 | C1330 |       |       | A1067 | A975 | A892 |
| A2171 | A2101 | U2022 | G1930 | G1807 | G1710 | G1622 | G1524 | G1416 | G1337 | C1243 | A1142 | G1068 | G976 | C893 |
| U2172 | G2102 | C2023 | G1930 | G1807 | A1711 |       | G1527 | G1416 | G1338 | A1247 | A1143 | A1069 | U995 | U895 |
| A2173 |       | G2024 | A1936 | A1808 |       | C1625 | G1527 | G1416 | U1339 | A1247 | A1144 | A1070 | A980 | A896 |
| C2174 | G2107 | C2025 | U1936 | A1809 | U1714 | A1626 | G1529 | G1421 | U1340 | G1248 | C1145 | A1071 | C987 | A981 |
| C2175 | U2109 | G2026 | G1811 | G1811 | U1716 | G1627 | G1533 | U1340 | U1340 | G1248 | C1146 | C1072 | C982 | C998 |
| G2110 | G2110 | G2027 | U1944 | G1811 | A1717 | G1628 | C1533 | G1428 | G1341 | G1252 | A1147 | A1073 | A883 | A899 |
| G2111 | U2111 | A2030 | G1945 | G1814 | G1718 | U1629 | U1534 | C1428 | G1341 | G1252 | A1147 | A1073 | A883 | A899 |
| U2182 | G2112 | A2031 | U1946 | G1815 | G1718 | U1629 | U1534 | C1428 | G1341 | G1252 | A1147 | A1073 | A883 | A899 |
| A2183 | U2113 | G2032 | A1952 | C1816 | U1729 | G1631 | C1536 | G1432 | G1343 | A1254 | G1157 | C1075 | C985 | G904 |



| Response   | Percentage |
|------------|------------|
| Yes        | 49%        |
| No         | 41%        |
| Don't know | 9%         |



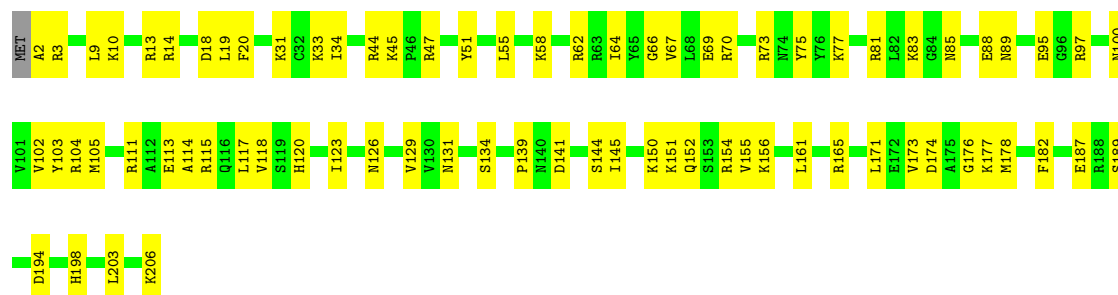




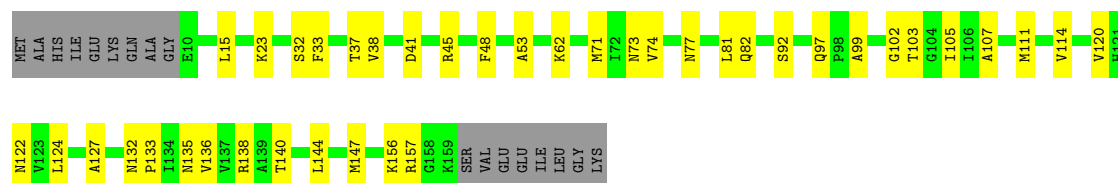
• Molecule 10: 30S ribosomal protein S3



• Molecule 11: 30S ribosomal protein S4



• Molecule 12: 30S ribosomal protein S5



• Molecule 13: 30S ribosomal protein S6, fully modified isoform



ASP  
ASP  
PHE  
ALA  
ASN  
GLU  
THR  
ALA  
ASP  
ASP  
ALA  
GLU  
ALA  
GLY  
ASP  
SER  
SER  
GLU  
GLU  
GLU  
GLU

• Molecule 14: 30S ribosomal protein S7

Chain H: 60% 24% 16%

MET P2 R3 R4 R5 V6 I7 P16 E21 A24 K25 F26 V27 N28 K31 K35 V43 L47 A51 S57 E58 A65 N68 V69 R70 P71 K76 R79 V89 R96 N97 A108 R111 G112 D113 K114 S115 M116 A117 L118 R119 L120 A121

N122 E123 D126 A127 A128 E129 N130 D140 R143 A152 HIS TYR ARG TRP LEU SER LEU ARG SER PHE SER HIS GLN ALA GLY ALA SER SER LYS GLN PRO ALA LEU GLY TYR LEU ASN

• Molecule 15: 30S ribosomal protein S8

Chain I: 66% 33% .

MET S2 M3 Q4 D5 P6 I7 A8 D9 M10 L11 I14 A15 M16 M27 P28 S29 S30 K31 L32 K33 V34 K41 F45 F49 L59 K64 K67 G68 K69 A70 V71 S74 I75 Q76 R77 R84 K87 R88 A102 V103 V104 S105 D113 R117

E124 I125 I126 C127 Y128 V129 A130

• Molecule 16: 30S ribosomal protein S9

Chain J: 65% 32% ..

MET ALA GLU M4 Q5 Y6 T9 R12 R13 K18 V19 K22 P23 Q24 P25 Q26 K27 L28 V29 I30 R45 R49 L52 E53 L54 V55 D56 M57 V58 E59 K60 L61 D62 L63 L64 I65 T66 G74 T83 T84 R85 E89 Y90 D91 R95 L98 G102

R106 D107 K120 A121 R122 R123 P125 Q126 F127 S128 K129 R130

• Molecule 17: 30S ribosomal protein S10

Chain K: 68% 26% . 5%

MET GLN ASN GLN R5 I6 R7 A12 F13 L14 H15 I18 P41 L42 P43 T44 R45 K46 E47 S54 P55 H56 V57 N58 R62 D63 Q64 Y65 E66 T69 H70 L71 L72 T80 T83 V84 D85 M88 R89 L102 GLY

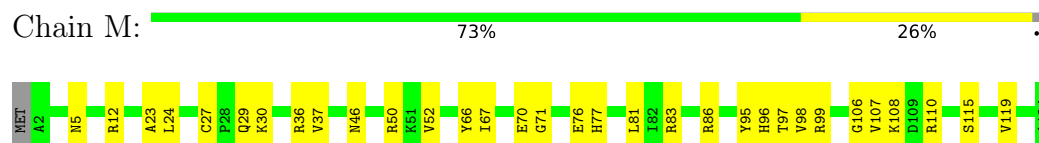
• Molecule 18: 30S ribosomal protein S11

Chain L: 69% 22% 9%

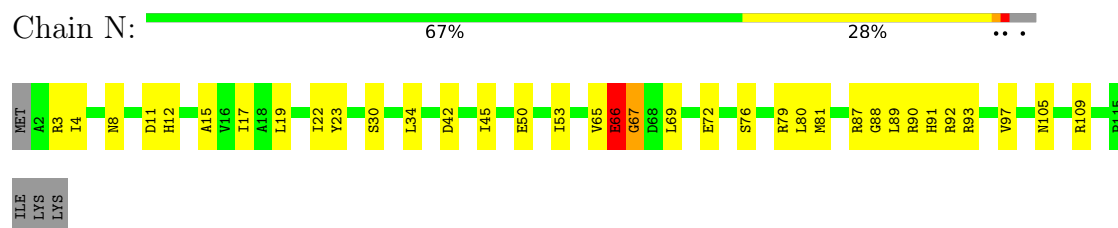
MET ALA LYS ALA PRO ILE ARG ARG ARG LYS ARG VAL R13 S17 V20 A21 H22 I23 V32 T33 N40 W44 R53 G54 S55 S58 E76 I79 E83 W84 W85 V86 K87 R93 N101 R106 I107 D112 V113 P117 R122 K126 R127

R128 V129

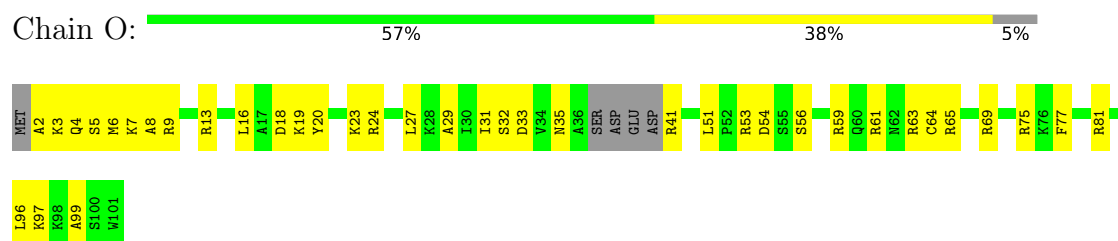
• Molecule 19: 30S ribosomal protein S12



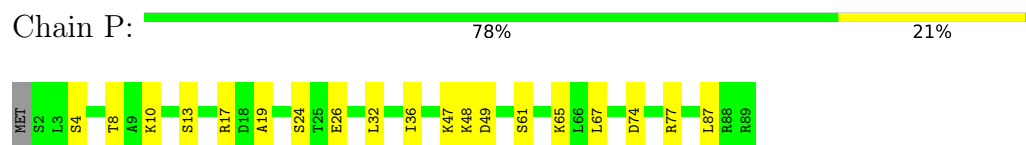
- Molecule 20: 30S ribosomal protein S13



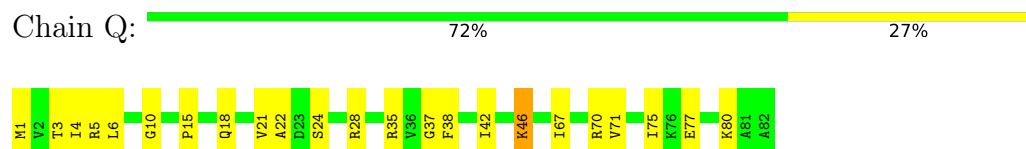
- Molecule 21: 30S ribosomal protein S14



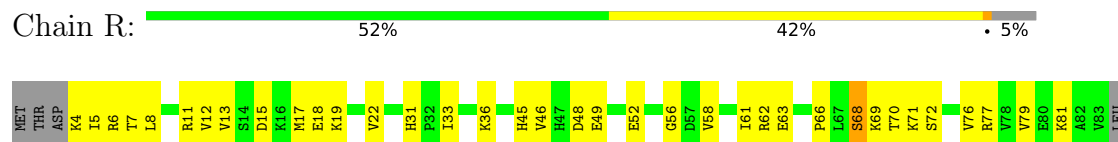
- Molecule 22: 30S ribosomal protein S15



- Molecule 23: 30S ribosomal protein S16

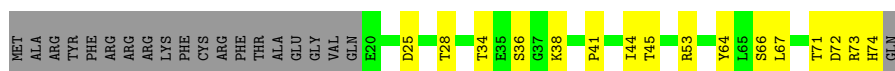


- Molecule 24: 30S ribosomal protein S17

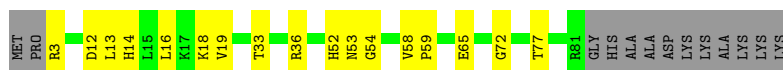


- Molecule 25: 30S ribosomal protein S18





- Molecule 26: 30S ribosomal protein S19



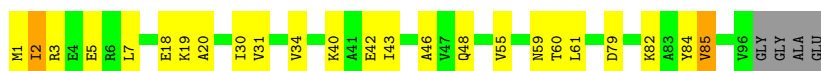
- Molecule 27: 30S ribosomal protein S20



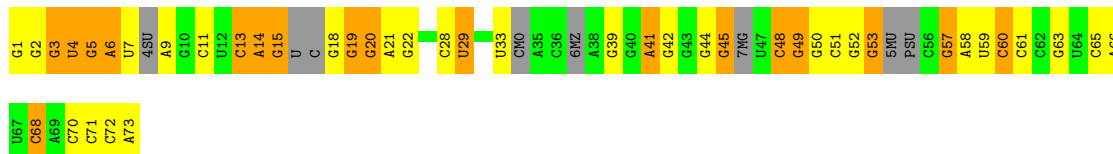
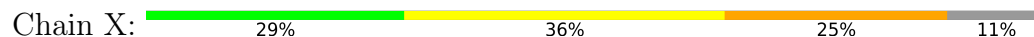
- Molecule 28: 30S ribosomal protein S21



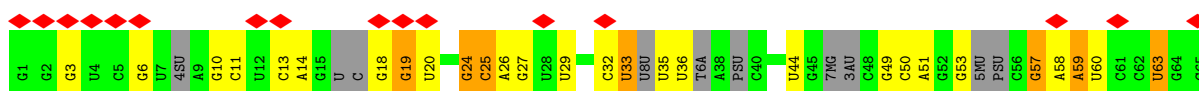
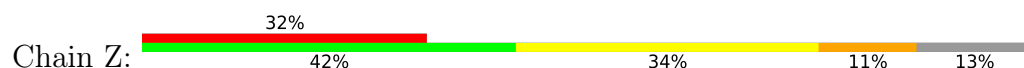
- Molecule 29: 50S ribosomal protein L23

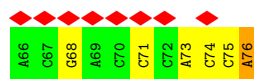


- Molecule 30: E-site tRNA



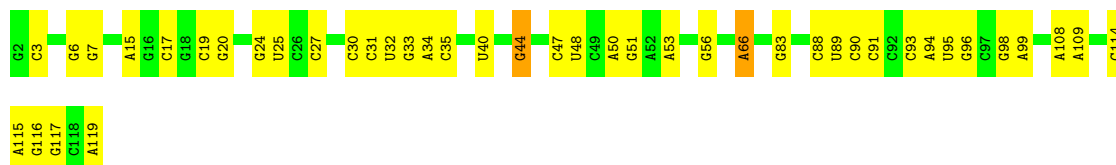
- Molecule 31: A-site tRNA





• Molecule 32: 5S ribosomal RNA

Chain a: 64% 35%



• Molecule 33: 50S ribosomal protein L2

Chain b: 71% 27%



• Molecule 34: 50S ribosomal protein L3

Chain c: 78% 21%



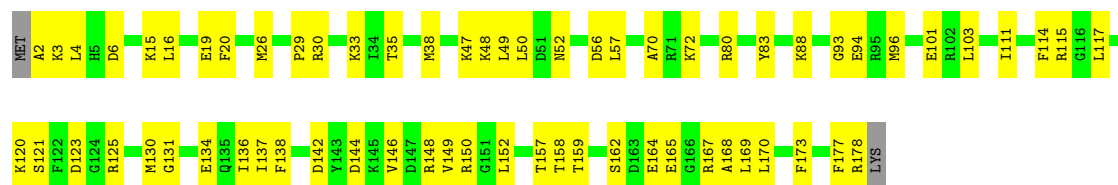
• Molecule 35: 50S ribosomal protein L4

Chain d: 84% 16%



• Molecule 36: 50S ribosomal protein L5

Chain e: 63% 36%



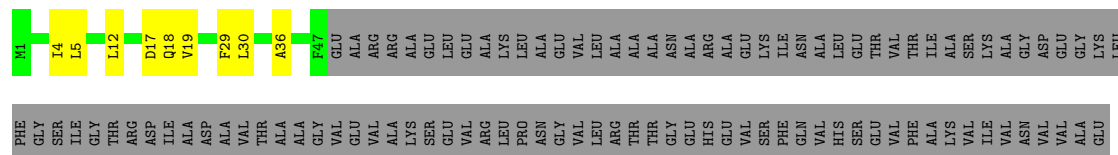
- Molecule 37: 50S ribosomal protein L6

Chain f: 81% 17% ..



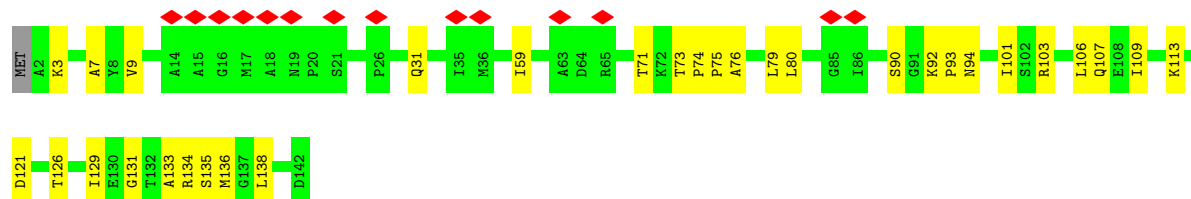
- Molecule 38: 50S ribosomal protein L9

Chain g: 26% 6% 68%



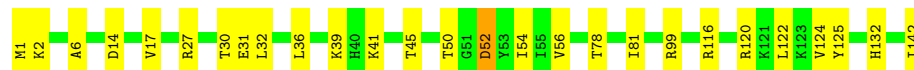
- Molecule 39: 50S ribosomal protein L11

Chain h: 10% 77% 22%



- Molecule 40: 50S ribosomal protein L13

Chain i: 81% 18%



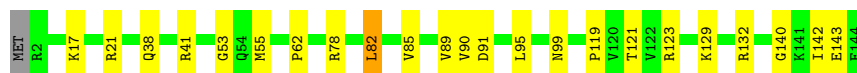
- Molecule 41: 50S ribosomal protein L14

Chain j: 72% 27%



- Molecule 42: 50S ribosomal protein L15

Chain k:  83% 15% ..



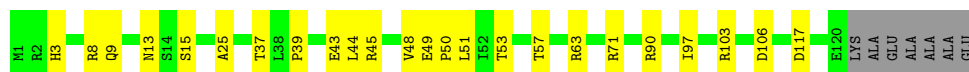
- Molecule 43: 50S ribosomal protein L16

Chain l:  81% 18% .



- Molecule 44: 50S ribosomal protein L17

Chain m:  76% 19% 6%



- Molecule 45: 50S ribosomal protein L18

Chain n:  83% 16% .



- Molecule 46: 50S ribosomal protein L19

Chain o:  77% 23% .



- Molecule 47: 50S ribosomal protein L20

Chain p:  78% 21% .



- Molecule 48: 50S ribosomal protein L21

Chain q:  83% 17%



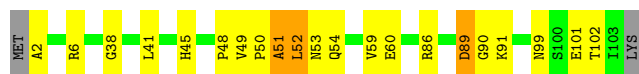
- Molecule 49: 50S ribosomal protein L22

Chain r:  81% 18%



- Molecule 50: 50S ribosomal protein L24

Chain s:  78% 17%



- Molecule 51: 50S ribosomal protein L25

Chain t:  86% 13%



- Molecule 52: 50S ribosomal protein L27

Chain u:  81% 7% 12%



- Molecule 53: 50S ribosomal protein L28

Chain v:  74% 24%



- Molecule 54: 50S ribosomal protein L29

Chain w:  78% 22%



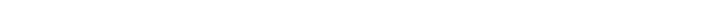
- Molecule 55: 50S ribosomal protein L30

Chain x:  85% 14%



- Molecule 56: P-site tRNA

|    |    |    |    |     |    |     |     |     |     |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|----|-----|----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| G1 | G2 | A3 | G7 | A5U | A9 | G10 | G13 | U16 | G17 | G17A | G18 | U19 | U20 | A21 | G22 | A26 | U29 | G30 | U33 | Q30 | U35 | U35 | C36 | 2NA | C38 | G39 | G45 | 7MG | U47 | C48 | G49 | C50 | G51 | G52 | G53 | SKU | PSU | C56 | G57 | G64 | PSU | C66 | C67 | G68 | U69 | U70 | C71 | C72 | G73 | C74 | C75 | A76 |
|----|----|----|----|-----|----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Chain z:  73% 18% 9%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 54875                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 32.57                                   | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.093                                   | Depositor |
| Minimum map value                    | -0.024                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.005                                   | Depositor |
| Map size (Å)                         | 441.6, 441.6, 441.6                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.38, 1.38, 1.38                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | 0     | 0.79         | 0/380       | 0.76        | 0/498          |
| 2   | 1     | 0.66         | 0/513       | 0.86        | 1/676 (0.1%)   |
| 3   | 2     | 0.57         | 0/303       | 0.66        | 0/397          |
| 4   | 3     | 0.25         | 0/1361      | 0.58        | 0/1830         |
| 5   | 5     | 0.21         | 0/3426      | 0.52        | 0/4605         |
| 6   | 6     | 0.66         | 0/450       | 0.76        | 0/599          |
| 7   | A     | 0.72         | 0/69796     | 0.52        | 0/108888       |
| 8   | B     | 0.36         | 0/36966     | 0.40        | 1/57666 (0.0%) |
| 9   | C     | 0.32         | 0/1735      | 0.57        | 0/2338         |
| 10  | D     | 0.27         | 0/1651      | 0.57        | 0/2225         |
| 11  | E     | 0.27         | 0/1665      | 0.61        | 0/2227         |
| 12  | F     | 0.36         | 0/1118      | 0.71        | 2/1504 (0.1%)  |
| 13  | G     | 0.29         | 0/835       | 0.66        | 0/1128         |
| 14  | H     | 0.24         | 0/1195      | 0.54        | 0/1602         |
| 15  | I     | 0.33         | 0/989       | 0.55        | 0/1326         |
| 16  | J     | 0.24         | 0/1034      | 0.60        | 0/1375         |
| 17  | K     | 0.26         | 0/796       | 0.64        | 0/1077         |
| 18  | L     | 0.31         | 0/893       | 0.60        | 0/1205         |
| 19  | M     | 0.35         | 0/969       | 0.65        | 0/1300         |
| 20  | N     | 0.25         | 0/892       | 0.62        | 1/1193 (0.1%)  |
| 21  | O     | 0.25         | 0/785       | 0.58        | 0/1043         |
| 22  | P     | 0.34         | 0/718       | 0.61        | 0/959          |
| 23  | Q     | 0.30         | 0/659       | 0.59        | 0/884          |
| 24  | R     | 0.33         | 0/657       | 0.66        | 0/881          |
| 25  | S     | 0.30         | 0/462       | 0.64        | 2/621 (0.3%)   |
| 26  | T     | 0.23         | 0/652       | 0.50        | 0/877          |
| 27  | U     | 0.31         | 0/671       | 0.61        | 0/888          |
| 28  | V     | 0.35         | 0/430       | 0.87        | 0/570          |
| 29  | W     | 0.63         | 0/771       | 0.76        | 0/1031         |
| 30  | X     | 0.20         | 0/1551      | 0.38        | 0/2404         |
| 31  | Z     | 0.23         | 0/1565      | 0.37        | 0/2421         |
| 32  | a     | 0.51         | 0/2828      | 0.40        | 0/4410         |
| 33  | b     | 0.70         | 0/2121      | 0.72        | 0/2852         |
| 34  | c     | 0.67         | 0/1586      | 0.69        | 0/2134         |

| Mol | Chain | Bond lengths |          | Bond angles |                  |
|-----|-------|--------------|----------|-------------|------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5          |
| 35  | d     | 0.69         | 0/1571   | 0.65        | 0/2113           |
| 36  | e     | 0.31         | 0/1434   | 0.56        | 0/1926           |
| 37  | f     | 0.43         | 0/1343   | 0.56        | 0/1816           |
| 38  | g     | 0.41         | 0/364    | 0.74        | 0/490            |
| 39  | h     | 0.28         | 0/1046   | 0.65        | 1/1410 (0.1%)    |
| 40  | i     | 0.71         | 0/1152   | 0.68        | 2/1551 (0.1%)    |
| 41  | j     | 0.65         | 0/947    | 0.77        | 0/1268           |
| 42  | k     | 0.66         | 0/1054   | 0.82        | 0/1403           |
| 43  | l     | 0.63         | 0/1093   | 0.73        | 0/1460           |
| 44  | m     | 0.71         | 0/973    | 0.86        | 0/1301           |
| 45  | n     | 0.45         | 0/902    | 0.58        | 0/1209           |
| 46  | o     | 0.61         | 0/929    | 0.69        | 0/1242           |
| 47  | p     | 0.78         | 0/960    | 0.71        | 0/1278           |
| 48  | q     | 0.64         | 0/829    | 0.68        | 0/1107           |
| 49  | r     | 0.71         | 0/864    | 0.70        | 0/1156           |
| 50  | s     | 0.56         | 0/787    | 0.69        | 0/1051           |
| 51  | t     | 0.53         | 0/766    | 0.54        | 0/1025           |
| 52  | u     | 0.63         | 0/576    | 0.61        | 0/762            |
| 53  | v     | 0.67         | 0/635    | 0.66        | 0/848            |
| 54  | w     | 0.56         | 0/510    | 0.65        | 0/677            |
| 55  | x     | 0.65         | 0/453    | 0.71        | 0/605            |
| 56  | y     | 0.21         | 0/1664   | 0.35        | 0/2577           |
| 57  | z     | 0.41         | 0/416    | 0.57        | 0/554            |
| All | All   | 0.57         | 0/163691 | 0.53        | 10/244463 (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 |
|-----|-------|---------------------|---------------------|
| 2   | 1     | 0                   | 1                   |
| 3   | 2     | 0                   | 1                   |
| 9   | C     | 0                   | 1                   |
| 11  | E     | 0                   | 2                   |
| 12  | F     | 0                   | 2                   |
| 13  | G     | 0                   | 1                   |
| 16  | J     | 0                   | 2                   |
| 17  | K     | 0                   | 1                   |
| 19  | M     | 0                   | 1                   |
| 20  | N     | 0                   | 1                   |
| 23  | Q     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 24  | R     | 0                   | 2                   |
| 28  | V     | 0                   | 2                   |
| 29  | W     | 0                   | 1                   |
| 34  | c     | 0                   | 1                   |
| 37  | f     | 0                   | 2                   |
| 41  | j     | 0                   | 1                   |
| 42  | k     | 0                   | 1                   |
| 43  | l     | 0                   | 1                   |
| 50  | s     | 0                   | 3                   |
| All | All   | 0                   | 28                  |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | S     | 67  | LEU  | CA-C-N      | 7.08  | 138.87      | 122.31   |
| 25  | S     | 67  | LEU  | C-N-CA      | 7.08  | 138.87      | 122.31   |
| 39  | h     | 109 | ILE  | N-CA-C      | -6.89 | 105.78      | 111.91   |
| 2   | 1     | 32  | ILE  | N-CA-C      | 6.32  | 122.49      | 109.34   |
| 12  | F     | 77  | ASN  | CA-C-N      | 5.89  | 132.78      | 121.54   |
| 12  | F     | 77  | ASN  | C-N-CA      | 5.89  | 132.78      | 121.54   |
| 8   | B     | 702 | A    | C4'-C3'-O3' | 5.55  | 121.33      | 113.00   |
| 20  | N     | 67  | GLY  | N-CA-C      | 5.23  | 125.58      | 113.18   |
| 40  | i     | 99  | ARG  | CA-C-N      | -5.18 | 117.89      | 122.97   |
| 40  | i     | 99  | ARG  | C-N-CA      | -5.18 | 117.89      | 122.97   |

There are no chirality outliers.

All (28) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | 1     | 31  | HIS  | Peptide |
| 3   | 2     | 20  | ASP  | Peptide |
| 9   | C     | 84  | ALA  | Peptide |
| 11  | E     | 173 | VAL  | Peptide |
| 11  | E     | 20  | PHE  | Peptide |
| 12  | F     | 102 | GLY  | Peptide |
| 12  | F     | 105 | ILE  | Peptide |
| 13  | G     | 53  | LYS  | Peptide |
| 16  | J     | 55  | VAL  | Peptide |
| 16  | J     | 60  | LYS  | Peptide |
| 17  | K     | 57  | VAL  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 19  | M     | 24  | LEU  | Peptide |
| 20  | N     | 66  | GLU  | Peptide |
| 23  | Q     | 46  | LYS  | Peptide |
| 24  | R     | 68  | SER  | Peptide |
| 24  | R     | 70  | THR  | Peptide |
| 28  | V     | 34  | ARG  | Peptide |
| 28  | V     | 9   | ASN  | Peptide |
| 29  | W     | 2   | ILE  | Peptide |
| 34  | c     | 151 | THR  | Peptide |
| 37  | f     | 46  | ALA  | Peptide |
| 37  | f     | 47  | ASP  | Peptide |
| 41  | j     | 92  | GLU  | Peptide |
| 42  | k     | 53  | GLY  | Peptide |
| 43  | l     | 58  | LYS  | Peptide |
| 50  | s     | 52  | LEU  | Peptide |
| 50  | s     | 6   | ARG  | Peptide |
| 50  | s     | 89  | ASP  | 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   | 0     | 377   | 0        | 418      | 7       | 0            |
| 2   | 1     | 504   | 0        | 572      | 13      | 0            |
| 3   | 2     | 302   | 0        | 343      | 13      | 0            |
| 4   | 3     | 1346  | 0        | 1394     | 31      | 0            |
| 5   | 5     | 3386  | 0        | 3403     | 34      | 0            |
| 6   | 6     | 444   | 0        | 458      | 7       | 0            |
| 7   | A     | 62317 | 0        | 31343    | 644     | 0            |
| 8   | B     | 33015 | 0        | 16617    | 383     | 0            |
| 9   | C     | 1704  | 0        | 1732     | 26      | 0            |
| 10  | D     | 1624  | 0        | 1696     | 34      | 0            |
| 11  | E     | 1643  | 0        | 1707     | 59      | 0            |
| 12  | F     | 1105  | 0        | 1148     | 29      | 0            |
| 13  | G     | 817   | 0        | 808      | 18      | 0            |
| 14  | H     | 1181  | 0        | 1238     | 34      | 0            |
| 15  | I     | 979   | 0        | 1031     | 33      | 0            |
| 16  | J     | 1022  | 0        | 1070     | 33      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 17  | K     | 786    | 0        | 828      | 22      | 0            |
| 18  | L     | 877    | 0        | 887      | 22      | 0            |
| 19  | M     | 955    | 0        | 1016     | 23      | 0            |
| 20  | N     | 883    | 0        | 941      | 26      | 0            |
| 21  | O     | 774    | 0        | 824      | 33      | 0            |
| 22  | P     | 710    | 0        | 728      | 13      | 0            |
| 23  | Q     | 649    | 0        | 666      | 18      | 0            |
| 24  | R     | 648    | 0        | 691      | 25      | 0            |
| 25  | S     | 455    | 0        | 478      | 15      | 0            |
| 26  | T     | 637    | 0        | 665      | 13      | 0            |
| 27  | U     | 665    | 0        | 714      | 17      | 0            |
| 28  | V     | 425    | 0        | 449      | 9       | 0            |
| 29  | W     | 764    | 0        | 829      | 19      | 0            |
| 30  | X     | 1392   | 0        | 714      | 24      | 0            |
| 31  | Z     | 1406   | 0        | 722      | 25      | 0            |
| 32  | a     | 2529   | 0        | 1281     | 17      | 0            |
| 33  | b     | 2082   | 0        | 2154     | 50      | 0            |
| 34  | c     | 1565   | 0        | 1616     | 33      | 0            |
| 35  | d     | 1552   | 0        | 1619     | 21      | 0            |
| 36  | e     | 1410   | 0        | 1444     | 47      | 0            |
| 37  | f     | 1323   | 0        | 1371     | 18      | 0            |
| 38  | g     | 359    | 0        | 381      | 6       | 0            |
| 39  | h     | 1032   | 0        | 1085     | 22      | 0            |
| 40  | i     | 1129   | 0        | 1162     | 18      | 0            |
| 41  | j     | 938    | 0        | 1012     | 22      | 0            |
| 42  | k     | 1045   | 0        | 1117     | 18      | 0            |
| 43  | l     | 1074   | 0        | 1157     | 16      | 0            |
| 44  | m     | 960    | 0        | 1000     | 18      | 0            |
| 45  | n     | 892    | 0        | 923      | 16      | 0            |
| 46  | o     | 917    | 0        | 962      | 21      | 0            |
| 47  | p     | 947    | 0        | 1019     | 19      | 0            |
| 48  | q     | 816    | 0        | 839      | 14      | 0            |
| 49  | r     | 857    | 0        | 922      | 14      | 0            |
| 50  | s     | 779    | 0        | 831      | 12      | 0            |
| 51  | t     | 753    | 0        | 780      | 10      | 0            |
| 52  | u     | 569    | 0        | 581      | 3       | 0            |
| 53  | v     | 625    | 0        | 652      | 14      | 0            |
| 54  | w     | 509    | 0        | 543      | 13      | 0            |
| 55  | x     | 449    | 0        | 488      | 5       | 0            |
| 56  | y     | 1496   | 0        | 764      | 14      | 0            |
| 57  | z     | 409    | 0        | 440      | 7       | 0            |
| All | All   | 150808 | 0        | 102273   | 1872    | 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 (1872) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 7:A:2506:U:O2'  | 7:A:2507:C:O4'   | 1.56                     | 1.19              |
| 8:B:98:A:H2'    | 8:B:99:C:C6      | 1.85                     | 1.11              |
| 7:A:2572:A:N6   | 34:c:150:GLN:OE1 | 1.93                     | 1.02              |
| 7:A:2508:G:OP1  | 31:Z:76:A:O5'    | 1.82                     | 0.95              |
| 7:A:2507:C:O2'  | 31:Z:76:A:C1'    | 2.14                     | 0.95              |
| 8:B:98:A:H2'    | 8:B:99:C:C5      | 2.00                     | 0.95              |
| 7:A:2711:A:N6   | 7:A:2714:G:N7    | 2.14                     | 0.95              |
| 7:A:1358:G:N2   | 7:A:1372:U:OP2   | 2.02                     | 0.93              |
| 7:A:576:U:O2'   | 7:A:2502:G:C6    | 2.22                     | 0.92              |
| 7:A:2267:A:N6   | 7:A:2272:U:H3    | 1.66                     | 0.92              |
| 7:A:2711:A:C6   | 7:A:2714:G:C8    | 2.59                     | 0.91              |
| 7:A:2060:A:C5   | 7:A:2502:G:N2    | 2.40                     | 0.90              |
| 7:A:2267:A:H61  | 7:A:2272:U:H3    | 0.99                     | 0.90              |
| 7:A:2507:C:O2'  | 31:Z:76:A:H1'    | 1.70                     | 0.89              |
| 7:A:1846:G:O2'  | 8:B:702:A:C2     | 2.24                     | 0.89              |
| 7:A:2722:G:N7   | 7:A:2723:C:C4    | 2.42                     | 0.87              |
| 7:A:2507:C:HO2' | 31:Z:76:A:C1'    | 1.87                     | 0.87              |
| 7:A:2711:A:N6   | 7:A:2714:G:C8    | 2.42                     | 0.87              |
| 7:A:2453:A:C2   | 7:A:2504:U:N3    | 2.43                     | 0.87              |
| 7:A:2508:G:C6   | 7:A:2582:G:O6    | 2.28                     | 0.86              |
| 7:A:2576:G:H21  | 7:A:2576:G:P     | 1.98                     | 0.86              |
| 7:A:963:U:O2'   | 7:A:2250:G:C6    | 2.34                     | 0.81              |
| 8:B:98:A:C2'    | 8:B:99:C:C6      | 2.63                     | 0.80              |
| 7:A:576:U:O2'   | 7:A:2502:G:C5    | 2.36                     | 0.79              |
| 7:A:2722:G:C8   | 7:A:2723:C:C4    | 2.70                     | 0.79              |
| 7:A:1846:G:O2'  | 8:B:702:A:H2     | 1.60                     | 0.79              |
| 7:A:2576:G:OP2  | 7:A:2576:G:N2    | 2.15                     | 0.79              |
| 7:A:2060:A:C6   | 7:A:2502:G:N2    | 2.51                     | 0.78              |
| 7:A:2689:U:OP2  | 7:A:2719:G:N2    | 2.15                     | 0.78              |
| 7:A:284:U:H3    | 7:A:356:G:H1     | 1.33                     | 0.77              |
| 8:B:84:U:H3     | 8:B:88:U:HO2'    | 1.33                     | 0.76              |
| 7:A:2572:A:N7   | 34:c:150:GLN:HB2 | 2.01                     | 0.75              |
| 8:B:203:G:H1    | 8:B:215:C:H42    | 1.33                     | 0.75              |
| 7:A:783:A:H2'   | 7:A:784:G:H4'    | 1.68                     | 0.74              |
| 7:A:2297:A:N7   | 7:A:2320:U:N3    | 2.35                     | 0.74              |
| 7:A:2720:U:H5'' | 46:o:53:ARG:HH22 | 1.52                     | 0.74              |
| 7:A:2060:A:C5   | 7:A:2502:G:C2    | 2.75                     | 0.74              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:2576:G:O2'   | 7:A:2579:C:OP2    | 2.05                     | 0.74              |
| 7:A:2508:G:OP1   | 31:Z:76:A:P       | 2.46                     | 0.73              |
| 7:A:1847:A:H4'   | 8:B:702:A:H1'     | 1.71                     | 0.72              |
| 7:A:1814:G:C8    | 7:A:1815:A:C8     | 2.78                     | 0.72              |
| 7:A:2516:A:N6    | 7:A:2517:C:H42    | 1.88                     | 0.72              |
| 7:A:2008:C:H2'   | 7:A:2009:A:H8     | 1.55                     | 0.71              |
| 8:B:1305:G:H22   | 8:B:1331:G:H1'    | 1.55                     | 0.71              |
| 7:A:1368:G:H2'   | 7:A:1369:G:C8     | 2.26                     | 0.71              |
| 7:A:2060:A:C6    | 7:A:2502:G:C2     | 2.79                     | 0.71              |
| 7:A:1358:G:C8    | 7:A:1371:G:O6     | 2.44                     | 0.71              |
| 7:A:1270:C:H5''  | 7:A:1271:G:H5'    | 1.73                     | 0.70              |
| 7:A:2276:G:H2'   | 7:A:2277:G:H8     | 1.56                     | 0.70              |
| 7:A:1529:G:H1    | 7:A:1542:U:H3     | 1.39                     | 0.70              |
| 7:A:1849:G:H2'   | 7:A:1850:G:H8     | 1.56                     | 0.70              |
| 7:A:2297:A:N3    | 7:A:2297:A:H2'    | 2.06                     | 0.70              |
| 7:A:2267:A:H3'   | 7:A:2267:A:N3     | 2.07                     | 0.69              |
| 7:A:2500:U:O2    | 7:A:2504:U:C5     | 2.44                     | 0.69              |
| 7:A:2506:U:O2'   | 7:A:2507:C:C1'    | 2.40                     | 0.69              |
| 7:A:2087:G:H2'   | 7:A:2088:A:H8     | 1.58                     | 0.69              |
| 7:A:1770:G:C6    | 7:A:1983:G:C6     | 2.81                     | 0.69              |
| 31:Z:10:G:H1     | 31:Z:25:C:H42     | 1.41                     | 0.68              |
| 7:A:571:U:N3     | 7:A:2030:A:N1     | 2.41                     | 0.68              |
| 7:A:2064:C:C5    | 7:A:2065:C:N4     | 2.62                     | 0.68              |
| 7:A:2267:A:N6    | 7:A:2272:U:C2     | 2.60                     | 0.68              |
| 7:A:2507:C:O2'   | 31:Z:76:A:O4'     | 2.10                     | 0.68              |
| 8:B:1264:U:H3    | 8:B:1271:A:H61    | 1.39                     | 0.68              |
| 46:o:60:THR:HG22 | 46:o:73:VAL:HG12  | 1.74                     | 0.68              |
| 7:A:2711:A:C6    | 7:A:2714:G:N9     | 2.62                     | 0.68              |
| 7:A:2097:A:H61   | 7:A:2192:U:H3     | 1.42                     | 0.68              |
| 7:A:2711:A:N6    | 7:A:2714:G:C5     | 2.61                     | 0.68              |
| 7:A:2087:G:H2'   | 7:A:2088:A:C8     | 2.29                     | 0.67              |
| 8:B:196:A:H2'    | 8:B:197:A:H2'     | 1.75                     | 0.67              |
| 7:A:956:G:N7     | 43:l:14:LYS:NZ    | 2.42                     | 0.67              |
| 7:A:2723:C:O5'   | 7:A:2723:C:H6     | 1.78                     | 0.67              |
| 7:A:2722:G:C5    | 7:A:2723:C:N3     | 2.63                     | 0.67              |
| 7:A:2453:A:H2    | 7:A:2504:U:N3     | 1.89                     | 0.67              |
| 8:B:460:A:N6     | 8:B:472:U:O4      | 2.27                     | 0.67              |
| 31:Z:18:G:N2     | 31:Z:57:G:N7      | 2.44                     | 0.66              |
| 14:H:114:LYS:H   | 14:H:118:LEU:HD23 | 1.60                     | 0.66              |
| 7:A:1482:G:H1'   | 7:A:1509:A:H61    | 1.61                     | 0.66              |
| 7:A:1846:G:HO2'  | 8:B:702:A:H2      | 0.80                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:B:1373:G:H4'    | 14:H:31:MET:HE1  | 1.78                     | 0.66              |
| 39:h:80:LEU:HD13  | 39:h:133:ALA:HB2 | 1.77                     | 0.66              |
| 7:A:381:G:OP1     | 53:v:18:ARG:NH1  | 2.28                     | 0.66              |
| 53:v:19:SER:OG    | 53:v:20:HIS:N    | 2.29                     | 0.65              |
| 6:6:2:ALA:HA      | 7:A:2056:G:N2    | 2.11                     | 0.65              |
| 7:A:2711:A:C6     | 7:A:2714:G:C4    | 2.84                     | 0.65              |
| 7:A:1368:G:H2'    | 7:A:1369:G:H8    | 1.61                     | 0.65              |
| 5:5:120:LEU:HD23  | 5:5:294:LEU:HD13 | 1.76                     | 0.65              |
| 7:A:2250:G:H8     | 7:A:2250:G:OP2   | 1.79                     | 0.65              |
| 7:A:2305:U:H5''   | 36:e:131:GLY:HA3 | 1.79                     | 0.65              |
| 8:B:1033:G:N7     | 8:B:1035:A:N6    | 2.45                     | 0.65              |
| 34:c:32:ASN:ND2   | 34:c:52:THR:OG1  | 2.30                     | 0.65              |
| 41:j:37:ASP:N     | 41:j:37:ASP:OD1  | 2.28                     | 0.65              |
| 7:A:18:U:O2'      | 7:A:554:U:OP1    | 2.14                     | 0.64              |
| 37:f:88:GLN:HE21  | 37:f:163:ARG:HD2 | 1.61                     | 0.64              |
| 7:A:2500:U:O2     | 7:A:2504:U:C4    | 2.51                     | 0.64              |
| 8:B:1004:A:H1'    | 8:B:1035:A:H61   | 1.62                     | 0.64              |
| 8:B:448:A:N6      | 8:B:486:U:O2     | 2.30                     | 0.64              |
| 7:A:627:A:OP1     | 42:k:78:ARG:NH1  | 2.30                     | 0.64              |
| 34:c:199:SER:OG   | 34:c:200:ASP:N   | 2.30                     | 0.64              |
| 12:F:45:ARG:H     | 12:F:73:ASN:HA   | 1.61                     | 0.64              |
| 7:A:2643:G:N2     | 7:A:2772:C:O2    | 2.31                     | 0.64              |
| 8:B:101:A:N6      | 8:B:102:G:C6     | 2.66                     | 0.64              |
| 7:A:2722:G:N7     | 7:A:2723:C:N3    | 2.46                     | 0.63              |
| 4:3:127:ALA:O     | 4:3:131:GLN:NE2  | 2.32                     | 0.63              |
| 7:A:2746:U:H2'    | 7:A:2747:G:H8    | 1.63                     | 0.63              |
| 9:C:86:SER:OG     | 9:C:222:ARG:NH2  | 2.32                     | 0.63              |
| 33:b:141:VAL:HG11 | 33:b:190:ALA:HB1 | 1.80                     | 0.63              |
| 7:A:883:G:H1      | 7:A:894:U:H1'    | 1.63                     | 0.63              |
| 7:A:2008:C:H2'    | 7:A:2009:A:C8    | 2.33                     | 0.63              |
| 39:h:133:ALA:HA   | 39:h:136:MET:HB3 | 1.80                     | 0.63              |
| 7:A:2711:A:N1     | 7:A:2714:G:C4    | 2.67                     | 0.63              |
| 8:B:468:A:OP2     | 8:B:470:C:N4     | 2.31                     | 0.63              |
| 8:B:756:C:O2      | 15:I:4:GLN:NE2   | 2.31                     | 0.63              |
| 7:A:1172:C:N4     | 7:A:1177:G:O6    | 2.32                     | 0.63              |
| 8:B:182:A:OP2     | 8:B:193:C:N4     | 2.31                     | 0.63              |
| 39:h:133:ALA:HB1  | 39:h:138:LEU:HB3 | 1.81                     | 0.63              |
| 7:A:1500:G:H2'    | 7:A:1501:G:H8    | 1.64                     | 0.62              |
| 7:A:1361:G:HO2'   | 7:A:2215:C:HO2'  | 1.44                     | 0.62              |
| 8:B:197:A:O2'     | 8:B:220:G:N2     | 2.32                     | 0.62              |
| 5:5:40:ARG:HH22   | 7:A:1337:G:H1'   | 1.64                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:1026:G:OP2    | 8:B:1028:C:N4     | 2.32                     | 0.62              |
| 5:5:73:ARG:NH1    | 5:5:77:ASP:OD2    | 2.32                     | 0.62              |
| 7:A:2087:G:N2     | 7:A:2233:U:O2     | 2.33                     | 0.62              |
| 8:B:406:G:N2      | 8:B:436:C:N3      | 2.47                     | 0.62              |
| 39:h:76:ALA:HA    | 39:h:79:LEU:HB3   | 1.81                     | 0.62              |
| 4:3:143:MET:HB3   | 4:3:151:GLN:HE21  | 1.63                     | 0.62              |
| 7:A:559:G:N3      | 47:p:56:GLN:NE2   | 2.48                     | 0.62              |
| 7:A:963:U:O2'     | 7:A:2250:G:N1     | 2.33                     | 0.62              |
| 8:B:291:U:H2'     | 8:B:292:G:H8      | 1.64                     | 0.62              |
| 7:A:1849:G:H8     | 7:A:1849:G:O5'    | 1.81                     | 0.62              |
| 7:A:2008:C:N4     | 7:A:2009:A:H62    | 1.97                     | 0.62              |
| 7:A:1077:A:H4'    | 39:h:94:ASN:HB2   | 1.81                     | 0.62              |
| 12:F:97:GLN:HB3   | 12:F:124:LEU:HB2  | 1.81                     | 0.62              |
| 33:b:17:VAL:HG22  | 33:b:204:VAL:HG22 | 1.81                     | 0.62              |
| 8:B:587:G:OP1     | 15:I:84:ARG:NH2   | 2.33                     | 0.62              |
| 7:A:2516:A:N6     | 7:A:2517:C:N4     | 2.46                     | 0.62              |
| 8:B:99:C:O5'      | 8:B:99:C:H6       | 1.83                     | 0.62              |
| 36:e:148:ARG:HH11 | 36:e:150:ARG:HG2  | 1.64                     | 0.61              |
| 8:B:352:C:O2      | 8:B:356:A:N6      | 2.33                     | 0.61              |
| 50:s:50:PRO:HA    | 50:s:54:GLN:HE22  | 1.65                     | 0.61              |
| 2:1:42:ARG:NH2    | 7:A:2349:G:OP2    | 2.34                     | 0.61              |
| 7:A:2079:U:O2     | 7:A:2242:G:N2     | 2.34                     | 0.61              |
| 7:A:2118:U:N3     | 7:A:2145:C:N3     | 2.48                     | 0.61              |
| 8:B:908:A:H2'     | 8:B:909:A:H8      | 1.66                     | 0.61              |
| 8:B:1114:C:H42    | 8:B:1186:G:H1     | 1.48                     | 0.61              |
| 4:3:50:GLN:NE2    | 4:3:90:CYS:SG     | 2.73                     | 0.61              |
| 7:A:1009:A:OP2    | 40:i:39:LYS:NZ    | 2.32                     | 0.61              |
| 7:A:2646:C:O5'    | 7:A:2646:C:H6     | 1.83                     | 0.61              |
| 8:B:1266:G:N2     | 8:B:1269:A:OP2    | 2.34                     | 0.61              |
| 12:F:107:ALA:HB1  | 12:F:111:MET:HE3  | 1.81                     | 0.61              |
| 26:T:36:ARG:NH1   | 26:T:52:HIS:O     | 2.34                     | 0.61              |
| 7:A:320:A:N3      | 35:d:163:ASN:ND2  | 2.48                     | 0.61              |
| 7:A:999:U:O2      | 7:A:1157:G:N2     | 2.34                     | 0.61              |
| 19:M:50:ARG:NH2   | 19:M:67:ILE:O     | 2.33                     | 0.61              |
| 31:Z:11:C:H42     | 31:Z:24:G:H1      | 1.49                     | 0.61              |
| 19:M:70:GLU:H     | 19:M:107:VAL:HG11 | 1.65                     | 0.61              |
| 7:A:864:G:OP2     | 43:l:22:GLN:NE2   | 2.33                     | 0.61              |
| 7:A:1266:G:H22    | 7:A:2012:G:H2'    | 1.65                     | 0.61              |
| 8:B:823:C:HO2'    | 15:I:2:SER:N      | 1.98                     | 0.61              |
| 10:D:22:TRP:HB3   | 10:D:59:ARG:H     | 1.66                     | 0.61              |
| 3:2:27:CYS:HG     | 3:2:33:HIS:HD1    | 1.47                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:B:1298:U:O2    | 8:B:1299:A:N6    | 2.34                     | 0.61              |
| 23:Q:5:ARG:HH12  | 23:Q:22:ALA:HB3  | 1.66                     | 0.61              |
| 49:r:13:SER:OG   | 49:r:14:ALA:N    | 2.32                     | 0.61              |
| 7:A:993:G:OP1    | 47:p:50:ARG:NH2  | 2.32                     | 0.60              |
| 7:A:1796:U:H2'   | 7:A:1797:G:H8    | 1.66                     | 0.60              |
| 8:B:101:A:C5     | 8:B:102:G:C5     | 2.89                     | 0.60              |
| 8:B:340:U:O2     | 8:B:350:G:N2     | 2.34                     | 0.60              |
| 17:K:15:HIS:HA   | 17:K:18:ILE:HG22 | 1.83                     | 0.60              |
| 7:A:2336:A:H61   | 52:u:43:THR:HG21 | 1.66                     | 0.60              |
| 30:X:15:G:N2     | 30:X:48:C:O2'    | 2.34                     | 0.60              |
| 45:n:31:THR:O    | 45:n:102:ARG:NH1 | 2.34                     | 0.60              |
| 7:A:2582:G:H2'   | 31:Z:76:A:H61    | 1.65                     | 0.60              |
| 8:B:105:G:N2     | 8:B:379:C:O2'    | 2.35                     | 0.60              |
| 8:B:546:A:OP2    | 11:E:62:ARG:NH2  | 2.34                     | 0.60              |
| 8:B:606:G:N2     | 8:B:632:U:OP1    | 2.31                     | 0.60              |
| 7:A:1056:G:H5'   | 7:A:1057:A:H5'   | 1.82                     | 0.60              |
| 7:A:1364:G:N7    | 53:v:2:SER:OG    | 2.33                     | 0.60              |
| 7:A:1798:U:OP2   | 33:b:271:ARG:NH2 | 2.34                     | 0.60              |
| 8:B:201:G:N2     | 8:B:469:C:O2'    | 2.34                     | 0.60              |
| 29:W:3:ARG:O     | 29:W:3:ARG:NE    | 2.34                     | 0.60              |
| 7:A:1252:G:H1    | 47:p:37:GLN:HE21 | 1.48                     | 0.60              |
| 7:A:2267:A:N6    | 7:A:2272:U:N3    | 2.32                     | 0.60              |
| 26:T:53:ASN:HB2  | 26:T:77:THR:HA   | 1.82                     | 0.60              |
| 6:6:13:ARG:NH1   | 7:A:1263:U:OP1   | 2.35                     | 0.60              |
| 7:A:2130:U:O2'   | 7:A:2159:G:N2    | 2.35                     | 0.60              |
| 8:B:898:G:N2     | 8:B:901:A:OP2    | 2.34                     | 0.60              |
| 8:B:1162:C:H42   | 8:B:1174:G:H1    | 1.49                     | 0.60              |
| 9:C:42:ASN:HD22  | 9:C:45:LYS:HB2   | 1.66                     | 0.60              |
| 30:X:60:C:H5'    | 30:X:61:C:H5     | 1.66                     | 0.60              |
| 7:A:2233:U:H2'   | 7:A:2234:G:H8    | 1.67                     | 0.60              |
| 52:u:37:ILE:HG22 | 52:u:38:VAL:HG23 | 1.84                     | 0.60              |
| 7:A:1358:G:C8    | 7:A:1371:G:C6    | 2.89                     | 0.59              |
| 8:B:80:A:N6      | 8:B:90:C:O2      | 2.35                     | 0.59              |
| 18:L:23:ILE:HG22 | 18:L:32:VAL:HG13 | 1.84                     | 0.59              |
| 7:A:2722:G:N7    | 7:A:2723:C:N4    | 2.49                     | 0.59              |
| 8:B:140:U:O2'    | 8:B:223:A:N6     | 2.35                     | 0.59              |
| 6:6:2:ALA:N      | 7:A:2612:C:HO2'  | 2.00                     | 0.59              |
| 7:A:2506:U:O2'   | 7:A:2507:C:C4'   | 2.51                     | 0.59              |
| 8:B:913:A:OP2    | 19:M:86:ARG:NH2  | 2.36                     | 0.59              |
| 8:B:1014:A:H4'   | 26:T:14:HIS:HB2  | 1.85                     | 0.59              |
| 21:O:20:TYR:HA   | 21:O:24:ARG:HH21 | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:G:44:ARG:O     | 13:G:56:LYS:NZ    | 2.35                     | 0.59              |
| 15:I:15:ARG:NH1   | 15:I:75:ILE:O     | 2.35                     | 0.59              |
| 8:B:880:C:OP1     | 19:M:5:ASN:ND2    | 2.35                     | 0.59              |
| 8:B:1125:U:H4'    | 17:K:7:ARG:HH12   | 1.67                     | 0.59              |
| 40:i:31:GLU:HG2   | 40:i:142:ILE:HG12 | 1.84                     | 0.59              |
| 7:A:58:G:N3       | 7:A:70:G:N2       | 2.50                     | 0.59              |
| 7:A:1283:G:N2     | 7:A:1286:A:OP2    | 2.36                     | 0.59              |
| 7:A:2070:A:H2'    | 7:A:2071:A:C8     | 2.37                     | 0.59              |
| 33:b:71:LYS:O     | 33:b:118:SER:OG   | 2.20                     | 0.59              |
| 7:A:1357:C:H2'    | 7:A:1358:G:H5'    | 1.83                     | 0.59              |
| 7:A:2711:A:C6     | 7:A:2714:G:C5     | 2.91                     | 0.59              |
| 10:D:30:ALA:O     | 21:O:65:ARG:NH1   | 2.32                     | 0.59              |
| 15:I:49:PHE:HB2   | 15:I:59:LEU:HD11  | 1.84                     | 0.59              |
| 37:f:11:VAL:HB    | 37:f:48:ASN:HB2   | 1.84                     | 0.59              |
| 7:A:1708:C:H42    | 7:A:1750:G:H1     | 1.49                     | 0.59              |
| 39:h:103:ARG:NH1  | 39:h:107:GLN:OE1  | 2.36                     | 0.59              |
| 8:B:519:C:N4      | 8:B:529:G:O2'     | 2.35                     | 0.59              |
| 21:O:31:ILE:O     | 21:O:35:ASN:ND2   | 2.36                     | 0.59              |
| 30:X:1:G:H22      | 30:X:72:C:H2'     | 1.66                     | 0.59              |
| 2:1:8:ARG:NH1     | 7:A:243:U:OP2     | 2.36                     | 0.58              |
| 18:L:23:ILE:HD11  | 18:L:86:VAL:HG22  | 1.83                     | 0.58              |
| 18:L:86:VAL:HG11  | 18:L:93:ARG:HG3   | 1.83                     | 0.58              |
| 27:U:59:ASP:OD1   | 27:U:69:LYS:NZ    | 2.35                     | 0.58              |
| 7:A:587:C:OP2     | 42:k:21:ARG:NH2   | 2.35                     | 0.58              |
| 7:A:2507:C:O3'    | 31:Z:76:A:C4'     | 2.51                     | 0.58              |
| 8:B:182:A:N6      | 8:B:223:A:O2'     | 2.36                     | 0.58              |
| 7:A:2052:A:H2'    | 7:A:2053:G:H8     | 1.66                     | 0.58              |
| 8:B:101:A:N7      | 8:B:102:G:N7      | 2.51                     | 0.58              |
| 8:B:108:G:OP2     | 8:B:325:A:N6      | 2.36                     | 0.58              |
| 30:X:20:G:OP2     | 30:X:60:C:N4      | 2.34                     | 0.58              |
| 35:d:125:SER:O    | 35:d:137:LYS:NZ   | 2.36                     | 0.58              |
| 54:w:16:THR:HA    | 54:w:19:LEU:HB2   | 1.84                     | 0.58              |
| 5:5:63:ARG:NH1    | 5:5:63:ARG:O      | 2.37                     | 0.58              |
| 6:6:13:ARG:NH2    | 7:A:517:C:OP1     | 2.37                     | 0.58              |
| 7:A:296:U:H2'     | 7:A:297:G:H8      | 1.67                     | 0.58              |
| 7:A:2848:G:O2'    | 7:A:2867:G:N2     | 2.36                     | 0.58              |
| 8:B:324:G:N2      | 8:B:327:A:OP2     | 2.36                     | 0.58              |
| 8:B:450:G:N2      | 8:B:482:A:N1      | 2.51                     | 0.58              |
| 29:W:7:LEU:HD12   | 29:W:46:ALA:HA    | 1.86                     | 0.58              |
| 33:b:140:THR:HG22 | 33:b:163:GLN:HG2  | 1.85                     | 0.58              |
| 7:A:747:U:O2'     | 49:r:92:ARG:NH2   | 2.37                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:H:143:ARG:NH1 | 30:X:42:G:OP1     | 2.37                     | 0.58              |
| 16:J:28:ILE:HG23 | 16:J:63:LEU:HD23  | 1.84                     | 0.58              |
| 5:5:30:SER:O     | 5:5:34:ASN:ND2    | 2.37                     | 0.58              |
| 7:A:2657:A:H62   | 7:A:2664:G:H21    | 1.50                     | 0.58              |
| 8:B:1305:G:N1    | 8:B:1331:G:N3     | 2.51                     | 0.58              |
| 40:i:36:LEU:HD11 | 40:i:122:LEU:HD13 | 1.84                     | 0.58              |
| 41:j:8:LEU:HD23  | 41:j:84:CYS:HB3   | 1.85                     | 0.58              |
| 50:s:86:ARG:NH1  | 50:s:102:THR:OG1  | 2.36                     | 0.58              |
| 8:B:60:A:N1      | 8:B:107:G:O2'     | 2.31                     | 0.58              |
| 8:B:408:A:H61    | 8:B:434:U:H3      | 1.50                     | 0.58              |
| 21:O:20:TYR:HB3  | 21:O:51:LEU:HD13  | 1.86                     | 0.58              |
| 26:T:36:ARG:NH2  | 26:T:72:GLY:O     | 2.35                     | 0.58              |
| 49:r:11:ARG:HH21 | 49:r:98:LYS:HD2   | 1.68                     | 0.58              |
| 7:A:659:G:N2     | 35:d:30:GLN:OE1   | 2.36                     | 0.58              |
| 8:B:614:C:OP2    | 11:E:81:ARG:NH1   | 2.36                     | 0.58              |
| 11:E:62:ARG:HH21 | 11:E:69:GLU:H     | 1.52                     | 0.58              |
| 35:d:22:ASP:N    | 35:d:22:ASP:OD1   | 2.35                     | 0.58              |
| 32:a:30:C:OP1    | 45:n:3:LYS:NZ     | 2.36                     | 0.58              |
| 7:A:532:A:N7     | 7:A:2021:C:O2'    | 2.36                     | 0.58              |
| 7:A:660:C:H2'    | 7:A:661:A:H8      | 1.69                     | 0.58              |
| 7:A:2266:A:H5'   | 7:A:2267:A:C8     | 2.39                     | 0.58              |
| 7:A:2507:C:HO2'  | 31:Z:76:A:H1'     | 1.56                     | 0.58              |
| 8:B:1271:A:H5'   | 8:B:1314:C:H5''   | 1.86                     | 0.58              |
| 10:D:19:ASN:HB3  | 10:D:40:ARG:HH22  | 1.68                     | 0.58              |
| 11:E:2:ALA:N     | 11:E:66:GLY:O     | 2.37                     | 0.58              |
| 7:A:1451:C:H42   | 7:A:1459:G:H1     | 1.52                     | 0.57              |
| 7:A:2351:G:N2    | 7:A:2367:G:O6     | 2.37                     | 0.57              |
| 8:B:196:A:OP1    | 27:U:64:LYS:NZ    | 2.36                     | 0.57              |
| 6:6:38:HIS:HB3   | 6:6:44:THR:HG22   | 1.86                     | 0.57              |
| 7:A:1173:U:O2    | 7:A:1176:U:N3     | 2.37                     | 0.57              |
| 20:N:3:ARG:HH22  | 36:e:142:ASP:HB2  | 1.69                     | 0.57              |
| 36:e:15:LYS:NZ   | 36:e:19:GLU:OE2   | 2.37                     | 0.57              |
| 7:A:1219:U:OP2   | 47:p:19:LYS:NZ    | 2.36                     | 0.57              |
| 7:A:2248:C:H42   | 7:A:2256:G:H1     | 1.50                     | 0.57              |
| 56:y:9:A:N3      | 56:y:21:A:N6      | 2.52                     | 0.57              |
| 5:5:28:VAL:HG22  | 5:5:63:ARG:HD3    | 1.86                     | 0.57              |
| 7:A:1481:U:H3    | 7:A:1510:G:H1     | 1.53                     | 0.57              |
| 8:B:1088:G:H21   | 8:B:1167:A:H62    | 1.52                     | 0.57              |
| 8:B:1250:A:H61   | 8:B:1354:U:H1'    | 1.70                     | 0.57              |
| 33:b:135:ILE:O   | 33:b:167:ARG:NH1  | 2.37                     | 0.57              |
| 7:A:2508:G:P     | 31:Z:76:A:O5'     | 2.61                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:2578:G:N2    | 7:A:2579:C:O2     | 2.37                     | 0.57              |
| 8:B:937:A:N6     | 8:B:1345:U:O4     | 2.38                     | 0.57              |
| 11:E:103:TYR:HB3 | 11:E:111:ARG:HH11 | 1.69                     | 0.57              |
| 47:p:46:ALA:O    | 47:p:50:ARG:NH1   | 2.36                     | 0.57              |
| 4:3:73:ILE:HG23  | 4:3:111:LEU:HB2   | 1.85                     | 0.57              |
| 7:A:1817:G:OP1   | 33:b:87:ARG:NH2   | 2.37                     | 0.57              |
| 7:A:2117:A:H61   | 7:A:2170:A:H61    | 1.53                     | 0.57              |
| 8:B:142:G:O2'    | 8:B:195:A:N6      | 2.37                     | 0.57              |
| 8:B:181:A:N6     | 8:B:195:A:OP2     | 2.38                     | 0.57              |
| 31:Z:19:G:OP1    | 31:Z:59:A:N6      | 2.37                     | 0.57              |
| 42:k:85:VAL:HG11 | 42:k:90:VAL:HG22  | 1.85                     | 0.57              |
| 7:A:1368:G:N3    | 7:A:1369:G:N7     | 2.53                     | 0.57              |
| 8:B:376:G:H1     | 8:B:387:U:H3      | 1.52                     | 0.57              |
| 8:B:974:A:OP1    | 21:O:69:ARG:NH2   | 2.36                     | 0.57              |
| 8:B:976:G:N1     | 8:B:1362:A:O2'    | 2.37                     | 0.57              |
| 8:B:1145:A:H2    | 8:B:1147:C:H41    | 1.52                     | 0.57              |
| 7:A:355:U:H2'    | 7:A:356:G:H8      | 1.68                     | 0.57              |
| 7:A:1070:A:H2'   | 7:A:1097:U:H4'    | 1.87                     | 0.57              |
| 8:B:401:C:N4     | 8:B:548:G:OP1     | 2.38                     | 0.57              |
| 8:B:522:C:H1'    | 8:B:536:C:H5''    | 1.87                     | 0.57              |
| 49:r:59:GLU:HB2  | 49:r:66:ILE:HD11  | 1.86                     | 0.57              |
| 1:O:24:THR:OG1   | 1:O:27:GLY:N      | 2.34                     | 0.57              |
| 7:A:1364:G:OP2   | 53:v:2:SER:N      | 2.37                     | 0.57              |
| 7:A:2711:A:C5    | 7:A:2714:G:C8     | 2.92                     | 0.57              |
| 9:C:86:SER:H     | 9:C:89:GLN:HE21   | 1.51                     | 0.57              |
| 46:o:90:GLY:O    | 46:o:113:ARG:NH1  | 2.35                     | 0.57              |
| 48:q:7:SER:OG    | 48:q:8:GLY:N      | 2.37                     | 0.57              |
| 49:r:14:ALA:O    | 49:r:18:ARG:NH1   | 2.38                     | 0.57              |
| 7:A:2144:G:O2'   | 7:A:2147:A:N6     | 2.38                     | 0.56              |
| 8:B:544:G:OP2    | 11:E:14:ARG:NH2   | 2.38                     | 0.56              |
| 13:G:63:ASN:ND2  | 13:G:96:VAL:O     | 2.38                     | 0.56              |
| 30:X:49:G:H22    | 30:X:66:A:H1'     | 1.69                     | 0.56              |
| 7:A:302:C:H42    | 7:A:315:G:H1      | 1.53                     | 0.56              |
| 8:B:707:U:OP1    | 18:L:87:LYS:NZ    | 2.37                     | 0.56              |
| 14:H:71:PRO:O    | 14:H:96:ARG:NH1   | 2.38                     | 0.56              |
| 29:W:3:ARG:HH11  | 29:W:5:GLU:HA     | 1.69                     | 0.56              |
| 39:h:9:VAL:H     | 39:h:59:ILE:HD13  | 1.70                     | 0.56              |
| 7:A:84:A:H62     | 7:A:101:A:H2      | 1.53                     | 0.56              |
| 7:A:563:A:OP2    | 48:q:79:ARG:NH1   | 2.37                     | 0.56              |
| 7:A:1057:A:N6    | 7:A:1087:G:OP2    | 2.38                     | 0.56              |
| 7:A:1779:U:OP2   | 7:A:1784:A:N6     | 2.38                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:A:2711:A:C8     | 7:A:2714:G:O4'   | 2.58                     | 0.56              |
| 8:B:520:A:H61     | 8:B:533:A:H61    | 1.53                     | 0.56              |
| 8:B:1126:U:OP1    | 17:K:7:ARG:NH2   | 2.39                     | 0.56              |
| 8:B:1166:G:O2'    | 8:B:1169:A:N6    | 2.38                     | 0.56              |
| 8:B:1220:G:N2     | 26:T:54:GLY:O    | 2.35                     | 0.56              |
| 33:b:246:THR:HG23 | 33:b:248:TRP:H   | 1.70                     | 0.56              |
| 6:6:16:ARG:NH1    | 7:A:1264:A:OP1   | 2.39                     | 0.56              |
| 7:A:576:U:H4'     | 7:A:2502:G:N7    | 2.21                     | 0.56              |
| 7:A:668:A:H2'     | 7:A:670:A:H62    | 1.70                     | 0.56              |
| 7:A:1597:A:H5''   | 7:A:1598:A:H5'   | 1.86                     | 0.56              |
| 8:B:160:A:H2'     | 8:B:161:A:H8     | 1.69                     | 0.56              |
| 10:D:47:LEU:HD11  | 10:D:76:VAL:HG12 | 1.88                     | 0.56              |
| 32:a:98:G:H1      | 51:t:14:LYS:HB3  | 1.71                     | 0.56              |
| 37:f:10:VAL:HG23  | 37:f:49:THR:HG22 | 1.87                     | 0.56              |
| 45:n:64:TYR:O     | 45:n:67:ASN:ND2  | 2.38                     | 0.56              |
| 53:v:60:ASP:OD1   | 53:v:60:ASP:N    | 2.38                     | 0.56              |
| 8:B:599:C:H2'     | 8:B:600:A:H8     | 1.69                     | 0.56              |
| 8:B:1012:A:H61    | 8:B:1017:U:H3    | 1.53                     | 0.56              |
| 15:I:11:LEU:HD22  | 15:I:75:ILE:HD11 | 1.88                     | 0.56              |
| 16:J:123:ARG:NH1  | 16:J:124:ARG:O   | 2.38                     | 0.56              |
| 40:i:41:LYS:NZ    | 40:i:50:THR:O    | 2.38                     | 0.56              |
| 7:A:570:G:C4      | 7:A:2030:A:N7    | 2.74                     | 0.56              |
| 7:A:571:U:C4      | 7:A:2030:A:C6    | 2.94                     | 0.56              |
| 7:A:1668:A:H4'    | 7:A:1669:A:H5'   | 1.87                     | 0.56              |
| 7:A:2584:U:H2'    | 7:A:2585:U:H2'   | 1.88                     | 0.56              |
| 7:A:2722:G:H3'    | 7:A:2723:C:C6    | 2.41                     | 0.56              |
| 8:B:101:A:N6      | 8:B:102:G:N1     | 2.54                     | 0.56              |
| 10:D:35:SER:HA    | 10:D:38:LYS:HB2  | 1.87                     | 0.56              |
| 10:D:63:SER:HA    | 10:D:97:VAL:HG11 | 1.88                     | 0.56              |
| 51:t:45:ASP:N     | 51:t:45:ASP:OD1  | 2.37                     | 0.56              |
| 8:B:66:A:H1'      | 8:B:173:U:H2'    | 1.88                     | 0.56              |
| 8:B:674:G:H2'     | 8:B:675:A:H8     | 1.69                     | 0.56              |
| 8:B:1223:C:H5''   | 8:B:1224:U:H5''  | 1.86                     | 0.56              |
| 11:E:85:ASN:ND2   | 11:E:88:GLU:OE2  | 2.38                     | 0.56              |
| 23:Q:1:MET:HE3    | 23:Q:24:SER:HB2  | 1.88                     | 0.56              |
| 7:A:2646:C:N4     | 7:A:2675:A:C2    | 2.74                     | 0.56              |
| 7:A:2683:C:O2     | 41:j:70:ARG:NH2  | 2.38                     | 0.56              |
| 8:B:126:G:OP1     | 8:B:633:G:N2     | 2.38                     | 0.56              |
| 8:B:684:U:O2'     | 18:L:40:ASN:O    | 2.21                     | 0.56              |
| 11:E:85:ASN:O     | 11:E:89:ASN:ND2  | 2.39                     | 0.56              |
| 13:G:91:ARG:NH1   | 13:G:92:THR:O    | 2.39                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 56:y:9:A:O2'      | 56:y:10:G:N7     | 2.36                     | 0.56              |
| 5:5:126:GLU:HG2   | 5:5:128:PRO:HD3  | 1.88                     | 0.56              |
| 7:A:626:A:H2'     | 42:k:78:ARG:HH22 | 1.69                     | 0.56              |
| 7:A:948:C:H2'     | 7:A:949:G:H8     | 1.70                     | 0.56              |
| 8:B:586:C:OP1     | 24:R:36:LYS:NZ   | 2.39                     | 0.56              |
| 8:B:976:G:H1      | 8:B:1362:A:HO2'  | 1.51                     | 0.56              |
| 10:D:64:ILE:HG23  | 10:D:99:ALA:HA   | 1.88                     | 0.56              |
| 17:K:54:SER:O     | 21:O:81:ARG:NH1  | 2.38                     | 0.56              |
| 32:a:93:C:H2'     | 32:a:94:A:H8     | 1.71                     | 0.56              |
| 2:1:25:LYS:HB3    | 42:k:62:PRO:HG2  | 1.88                     | 0.56              |
| 4:3:48:ALA:HB2    | 4:3:57:ILE:HG22  | 1.87                     | 0.56              |
| 7:A:1412:U:H2'    | 7:A:1413:A:H8    | 1.71                     | 0.56              |
| 8:B:407:U:OP1     | 11:E:3:ARG:NH2   | 2.38                     | 0.56              |
| 21:O:16:LEU:HA    | 21:O:19:LYS:HB3  | 1.88                     | 0.56              |
| 36:e:2:ALA:N      | 36:e:94:GLU:OE2  | 2.39                     | 0.56              |
| 36:e:29:PRO:HG2   | 36:e:165:GLU:HB3 | 1.86                     | 0.56              |
| 1:0:3:ARG:O       | 1:0:6:GLN:NE2    | 2.39                     | 0.55              |
| 7:A:2561:U:O3'    | 41:j:40:LYS:NZ   | 2.38                     | 0.55              |
| 7:A:2633:G:N2     | 7:A:2786:U:O2    | 2.39                     | 0.55              |
| 8:B:434:U:H2'     | 8:B:435:A:H8     | 1.71                     | 0.55              |
| 40:i:41:LYS:NZ    | 40:i:52:ASP:OD1  | 2.38                     | 0.55              |
| 7:A:571:U:C4      | 7:A:2030:A:N6    | 2.73                     | 0.55              |
| 8:B:437:U:O2'     | 11:E:120:HIS:ND1 | 2.39                     | 0.55              |
| 34:c:142:VAL:HG13 | 34:c:144:GLY:H   | 1.72                     | 0.55              |
| 43:l:40:ARG:HD3   | 43:l:93:VAL:HG21 | 1.86                     | 0.55              |
| 5:5:278:LEU:HD21  | 5:5:427:LEU:HD21 | 1.89                     | 0.55              |
| 7:A:247:G:OP1     | 7:A:386:G:O2'    | 2.24                     | 0.55              |
| 7:A:2516:A:C6     | 7:A:2517:C:N4    | 2.74                     | 0.55              |
| 8:B:902:G:H2'     | 8:B:903:G:H8     | 1.70                     | 0.55              |
| 8:B:1045:C:H2'    | 8:B:1046:A:H8    | 1.70                     | 0.55              |
| 7:A:1666:G:O2'    | 41:j:6:THR:OG1   | 2.25                     | 0.55              |
| 12:F:156:LYS:O    | 15:I:64:LYS:NZ   | 2.39                     | 0.55              |
| 50:s:99:ASN:ND2   | 50:s:101:GLU:OE2 | 2.40                     | 0.55              |
| 2:1:8:ARG:NH2     | 7:A:244:A:OP2    | 2.39                     | 0.55              |
| 7:A:629:G:N3      | 7:A:639:U:O2'    | 2.40                     | 0.55              |
| 7:A:2126:A:N6     | 7:A:2171:A:OP2   | 2.40                     | 0.55              |
| 8:B:546:A:OP1     | 11:E:70:ARG:N    | 2.38                     | 0.55              |
| 8:B:585:G:H21     | 8:B:879:C:H1'    | 1.72                     | 0.55              |
| 8:B:1078:U:O2     | 12:F:135:ASN:ND2 | 2.37                     | 0.55              |
| 8:B:1439:G:H1     | 8:B:1462:C:H42   | 1.54                     | 0.55              |
| 20:N:88:GLY:HA2   | 20:N:91:HIS:HD2  | 1.72                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:c:108:ASP:HB3 | 34:c:174:SER:H    | 1.72                     | 0.55              |
| 47:p:26:GLY:O    | 47:p:30:ARG:NH1   | 2.40                     | 0.55              |
| 2:l:23:LYS:NZ    | 7:A:630:G:OP2     | 2.38                     | 0.55              |
| 7:A:885:C:O2'    | 7:A:891:G:N2      | 2.38                     | 0.55              |
| 7:A:2171:A:H3'   | 7:A:2173:A:H62    | 1.72                     | 0.55              |
| 8:B:208:U:O2     | 8:B:210:C:O2'     | 2.24                     | 0.55              |
| 11:E:105:MET:HE2 | 11:E:171:LEU:HD22 | 1.89                     | 0.55              |
| 13:G:21:MET:HA   | 13:G:24:ARG:HE    | 1.71                     | 0.55              |
| 35:d:80:SER:O    | 35:d:80:SER:OG    | 2.24                     | 0.55              |
| 54:w:16:THR:O    | 54:w:20:ASN:ND2   | 2.33                     | 0.55              |
| 5:5:275:GLU:HA   | 5:5:278:LEU:HD12  | 1.87                     | 0.55              |
| 7:A:1753:G:OP1   | 46:o:93:ARG:NH1   | 2.40                     | 0.55              |
| 19:M:71:GLY:O    | 19:M:99:ARG:NH1   | 2.40                     | 0.55              |
| 8:B:75:G:H22     | 8:B:93:U:H3       | 1.54                     | 0.55              |
| 8:B:428:G:OP2    | 11:E:10:LYS:NZ    | 2.40                     | 0.55              |
| 30:X:4:U:O4      | 30:X:6:A:N6       | 2.39                     | 0.55              |
| 34:c:8:LYS:NZ    | 34:c:195:GLY:O    | 2.36                     | 0.55              |
| 41:j:76:VAL:H    | 46:o:73:VAL:HG22  | 1.71                     | 0.55              |
| 42:k:91:ASP:OD1  | 42:k:91:ASP:N     | 2.36                     | 0.55              |
| 5:5:134:ASP:OD1  | 5:5:271:ARG:NH1   | 2.40                     | 0.55              |
| 7:A:2484:G:OP1   | 43:l:44:ARG:NH2   | 2.37                     | 0.55              |
| 8:B:35:G:N3      | 19:M:115:SER:OG   | 2.40                     | 0.55              |
| 8:B:140:U:O4     | 8:B:221:C:N4      | 2.40                     | 0.55              |
| 8:B:1342:C:H2'   | 8:B:1343:G:H8     | 1.71                     | 0.55              |
| 8:B:1532:U:O4    | 28:V:47:ARG:NH1   | 2.40                     | 0.55              |
| 11:E:44:ARG:NH1  | 11:E:45:LYS:O     | 2.40                     | 0.55              |
| 16:J:12:ARG:HG3  | 16:J:13:LYS:HG2   | 1.88                     | 0.55              |
| 56:y:10:G:H22    | 56:y:26:A:H1'     | 1.72                     | 0.55              |
| 7:A:2002:G:OP2   | 44:m:9:GLN:NE2    | 2.40                     | 0.55              |
| 15:I:2:SER:OG    | 15:I:3:MET:N      | 2.41                     | 0.55              |
| 18:L:13:ARG:N    | 18:L:76:GLU:O     | 2.40                     | 0.55              |
| 19:M:27:CYS:SG   | 19:M:30:LYS:NZ    | 2.70                     | 0.55              |
| 22:P:26:GLU:OE2  | 22:P:77:ARG:NE    | 2.40                     | 0.55              |
| 36:e:49:LEU:HA   | 36:e:52:ASN:HB2   | 1.89                     | 0.55              |
| 37:f:17:VAL:HG12 | 37:f:26:ILE:HG12  | 1.89                     | 0.55              |
| 7:A:325:G:O6     | 7:A:338:G:N2      | 2.40                     | 0.54              |
| 7:A:1658:C:OP1   | 34:c:140:HIS:NE2  | 2.40                     | 0.54              |
| 7:A:2849:U:O4    | 46:o:21:ARG:NH1   | 2.40                     | 0.54              |
| 8:B:151:A:OP2    | 8:B:169:C:N4      | 2.40                     | 0.54              |
| 12:F:32:SER:OG   | 12:F:33:PHE:N     | 2.38                     | 0.54              |
| 13:G:2:ARG:NH2   | 13:G:92:THR:OG1   | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:X:28:C:N4     | 30:X:42:G:O6     | 2.40                     | 0.54              |
| 43:l:19:GLY:O    | 43:l:38:ARG:NH1  | 2.40                     | 0.54              |
| 7:A:605:G:N3     | 7:A:657:U:O2'    | 2.38                     | 0.54              |
| 7:A:1088:A:N6    | 39:h:131:GLY:O   | 2.40                     | 0.54              |
| 8:B:663:A:O3'    | 25:S:53:ARG:NH2  | 2.40                     | 0.54              |
| 8:B:1359:C:H4'   | 8:B:1362:A:H62   | 1.72                     | 0.54              |
| 48:q:15:SER:OG   | 48:q:16:GLU:N    | 2.38                     | 0.54              |
| 7:A:370:G:O2'    | 7:A:424:G:OP1    | 2.26                     | 0.54              |
| 33:b:6:CYS:SG    | 33:b:18:LYS:NZ   | 2.70                     | 0.54              |
| 7:A:83:A:OP1     | 50:s:2:ALA:N     | 2.40                     | 0.54              |
| 7:A:2258:C:O2'   | 7:A:2427:C:OP2   | 2.20                     | 0.54              |
| 24:R:68:SER:OG   | 24:R:69:LYS:N    | 2.41                     | 0.54              |
| 45:n:31:THR:OG1  | 45:n:34:HIS:O    | 2.26                     | 0.54              |
| 7:A:2522:U:O2'   | 7:A:2647:U:OP1   | 2.21                     | 0.54              |
| 7:A:2875:C:HO2'  | 46:o:2:SER:N     | 2.04                     | 0.54              |
| 8:B:980:C:O2'    | 21:O:13:ARG:NH2  | 2.40                     | 0.54              |
| 9:C:131:LYS:HA   | 9:C:134:ALA:HB3  | 1.88                     | 0.54              |
| 45:n:67:ASN:OD1  | 45:n:70:ALA:N    | 2.40                     | 0.54              |
| 57:z:17:THR:OG1  | 57:z:18:GLY:N    | 2.38                     | 0.54              |
| 7:A:141:G:N1     | 29:W:1:MET:SD    | 2.72                     | 0.54              |
| 7:A:1368:G:C2    | 7:A:1369:G:C5    | 2.95                     | 0.54              |
| 8:B:18:C:OP1     | 12:F:132:ASN:ND2 | 2.40                     | 0.54              |
| 8:B:73:C:O2'     | 8:B:75:G:N7      | 2.36                     | 0.54              |
| 14:H:16:PRO:O    | 16:J:45:ARG:NH2  | 2.41                     | 0.54              |
| 34:c:124:ARG:NH1 | 34:c:161:MET:O   | 2.40                     | 0.54              |
| 43:l:1:MET:SD    | 43:l:1:MET:N     | 2.75                     | 0.54              |
| 7:A:1129:A:N6    | 7:A:2491:U:OP1   | 2.40                     | 0.54              |
| 7:A:1792:G:O2'   | 7:A:1830:C:OP1   | 2.26                     | 0.54              |
| 8:B:974:A:H4'    | 8:B:975:A:H3'    | 1.89                     | 0.54              |
| 8:B:1249:C:N4    | 8:B:1288:A:OP2   | 2.38                     | 0.54              |
| 14:H:113:ASP:HB2 | 14:H:119:ARG:HB3 | 1.90                     | 0.54              |
| 20:N:8:ASN:HD21  | 20:N:22:ILE:HD12 | 1.73                     | 0.54              |
| 33:b:160:THR:OG1 | 33:b:161:TYR:N   | 2.41                     | 0.54              |
| 44:m:117:ASP:OD1 | 44:m:117:ASP:N   | 2.33                     | 0.54              |
| 56:y:18:G:N1     | 56:y:57:G:OP2    | 2.41                     | 0.54              |
| 7:A:636:G:OP1    | 42:k:129:LYS:NZ  | 2.41                     | 0.54              |
| 7:A:2507:C:O3'   | 31:Z:76:A:H4'    | 2.08                     | 0.54              |
| 7:A:30:G:N1      | 7:A:511:U:O2     | 2.39                     | 0.54              |
| 7:A:151:C:H2'    | 7:A:152:A:H8     | 1.73                     | 0.54              |
| 7:A:379:G:O2'    | 7:A:2232:C:OP1   | 2.26                     | 0.54              |
| 7:A:776:G:N2     | 7:A:2072:C:OP1   | 2.36                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:140:U:N3      | 8:B:141:G:O6      | 2.40                     | 0.54              |
| 8:B:318:G:H1      | 8:B:335:C:H42     | 1.56                     | 0.54              |
| 8:B:419:C:N4      | 8:B:424:G:O6      | 2.41                     | 0.54              |
| 9:C:82:ASP:OD1    | 9:C:82:ASP:N      | 2.40                     | 0.54              |
| 15:I:64:LYS:HB3   | 15:I:71:VAL:HG11  | 1.90                     | 0.54              |
| 15:I:87:LYS:NZ    | 15:I:88:ARG:O     | 2.41                     | 0.54              |
| 17:K:85:ASP:OD1   | 17:K:85:ASP:N     | 2.41                     | 0.54              |
| 20:N:50:GLU:HA    | 20:N:53:ILE:HB    | 1.90                     | 0.54              |
| 50:s:48:PRO:HB2   | 50:s:54:GLN:HB3   | 1.90                     | 0.54              |
| 7:A:242:G:N2      | 7:A:255:A:OP2     | 2.40                     | 0.54              |
| 7:A:572:A:OP2     | 48:q:79:ARG:NH2   | 2.41                     | 0.54              |
| 7:A:2635:A:O2'    | 34:c:49:GLN:NE2   | 2.41                     | 0.54              |
| 8:B:1237:C:O2'    | 8:B:1300:G:N2     | 2.33                     | 0.54              |
| 14:H:57:SER:OG    | 14:H:58:GLU:N     | 2.41                     | 0.54              |
| 3:2:20:ASP:O      | 3:2:22:VAL:N      | 2.41                     | 0.53              |
| 7:A:2529:G:OP2    | 37:f:172:LYS:NZ   | 2.33                     | 0.53              |
| 7:A:2857:G:N2     | 7:A:2860:A:OP2    | 2.41                     | 0.53              |
| 8:B:1320:C:O2     | 26:T:36:ARG:NH2   | 2.37                     | 0.53              |
| 20:N:76:SER:O     | 20:N:80:LEU:N     | 2.37                     | 0.53              |
| 29:W:79:ASP:OD1   | 29:W:79:ASP:N     | 2.41                     | 0.53              |
| 7:A:319:G:OP2     | 35:d:132:LYS:NZ   | 2.40                     | 0.53              |
| 7:A:2060:A:N7     | 7:A:2502:G:N2     | 2.55                     | 0.53              |
| 7:A:2840:C:H5''   | 44:m:53:THR:HG21  | 1.91                     | 0.53              |
| 8:B:1011:C:O2     | 8:B:1018:G:N2     | 2.42                     | 0.53              |
| 7:A:880:G:OP2     | 7:A:892:A:N6      | 2.42                     | 0.53              |
| 8:B:673:A:O3'     | 13:G:86:ARG:NH2   | 2.41                     | 0.53              |
| 16:J:9:THR:HB     | 16:J:85:ARG:HH11  | 1.74                     | 0.53              |
| 21:O:4:GLN:O      | 21:O:8:ALA:N      | 2.39                     | 0.53              |
| 36:e:111:ILE:HD13 | 36:e:137:ILE:HD13 | 1.90                     | 0.53              |
| 52:u:40:GLN:OE1   | 52:u:44:LYS:N     | 2.42                     | 0.53              |
| 4:3:95:GLU:O      | 4:3:96:GLN:NE2    | 2.42                     | 0.53              |
| 7:A:690:G:O2'     | 7:A:780:G:OP1     | 2.23                     | 0.53              |
| 7:A:1358:G:H2'    | 7:A:1359:A:OP2    | 2.09                     | 0.53              |
| 8:B:402:G:O2'     | 8:B:620:C:N4      | 2.42                     | 0.53              |
| 10:D:191:THR:HG23 | 10:D:193:TYR:H    | 1.73                     | 0.53              |
| 3:2:1:MET:HE2     | 3:2:36:ARG:HB2    | 1.91                     | 0.53              |
| 5:5:253:ILE:HD11  | 5:5:263:VAL:HG22  | 1.91                     | 0.53              |
| 7:A:414:C:N4      | 7:A:2409:G:O6     | 2.38                     | 0.53              |
| 9:C:20:THR:HB     | 9:C:38:VAL:HG22   | 1.90                     | 0.53              |
| 21:O:65:ARG:NH2   | 21:O:77:PHE:O     | 2.42                     | 0.53              |
| 29:W:20:ALA:HA    | 29:W:31:VAL:HG21  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:3:ARG:NH1    | 7:A:752:A:OP1     | 2.38                     | 0.53              |
| 5:5:304:ALA:HA   | 5:5:307:ILE:HG22  | 1.90                     | 0.53              |
| 7:A:20:C:OP1     | 47:p:22:LYS:NZ    | 2.42                     | 0.53              |
| 7:A:1065:U:OP2   | 39:h:92:LYS:NZ    | 2.41                     | 0.53              |
| 8:B:582:C:OP2    | 8:B:758:C:N4      | 2.32                     | 0.53              |
| 28:V:40:LYS:O    | 28:V:44:GLU:N     | 2.36                     | 0.53              |
| 7:A:833:A:H2'    | 7:A:834:G:H8      | 1.73                     | 0.53              |
| 7:A:963:U:O2'    | 7:A:2250:G:O6     | 2.24                     | 0.53              |
| 10:D:120:ILE:HA  | 10:D:123:GLN:HE21 | 1.72                     | 0.53              |
| 19:M:36:ARG:NH1  | 19:M:37:VAL:O     | 2.42                     | 0.53              |
| 24:R:31:HIS:HD2  | 24:R:33:ILE:H     | 1.57                     | 0.53              |
| 1:0:33:ARG:NH2   | 7:A:467:G:OP1     | 2.41                     | 0.53              |
| 7:A:578:G:OP1    | 7:A:1255:U:O2'    | 2.25                     | 0.53              |
| 7:A:1683:U:H2'   | 7:A:1684:G:H8     | 1.74                     | 0.53              |
| 7:A:2124:G:H1    | 7:A:2175:C:H1'    | 1.73                     | 0.53              |
| 8:B:1178:G:N2    | 8:B:1181:G:OP2    | 2.34                     | 0.53              |
| 37:f:27:LYS:NZ   | 37:f:28:GLY:O     | 2.41                     | 0.53              |
| 7:A:2461:A:H1'   | 7:A:2492:U:H3     | 1.73                     | 0.53              |
| 7:A:2720:U:OP1   | 46:o:53:ARG:NH2   | 2.41                     | 0.53              |
| 8:B:811:C:O2'    | 8:B:901:A:N1      | 2.42                     | 0.53              |
| 9:C:89:GLN:HE22  | 9:C:222:ARG:HH22  | 1.57                     | 0.53              |
| 14:H:113:ASP:OD2 | 14:H:122:ASN:ND2  | 2.42                     | 0.53              |
| 43:l:69:PRO:HA   | 43:l:94:ALA:HB2   | 1.90                     | 0.53              |
| 7:A:544:C:N4     | 7:A:547:A:O2'     | 2.42                     | 0.53              |
| 7:A:1091:G:H22   | 7:A:1100:C:H42    | 1.56                     | 0.53              |
| 7:A:2746:U:C5    | 7:A:2747:G:N7     | 2.77                     | 0.53              |
| 7:A:2782:G:N2    | 7:A:2783:U:C2     | 2.77                     | 0.53              |
| 8:B:504:C:H42    | 8:B:541:G:H1      | 1.57                     | 0.53              |
| 8:B:944:G:N1     | 8:B:1338:G:OP2    | 2.42                     | 0.53              |
| 14:H:28:ASN:ND2  | 14:H:31:MET:SD    | 2.76                     | 0.53              |
| 23:Q:35:ARG:HH22 | 23:Q:38:PHE:HD2   | 1.56                     | 0.53              |
| 30:X:48:C:H5''   | 30:X:49:G:H5''    | 1.90                     | 0.53              |
| 44:m:15:SER:O    | 44:m:15:SER:OG    | 2.27                     | 0.53              |
| 47:p:83:LEU:HD22 | 47:p:88:VAL:HB    | 1.90                     | 0.53              |
| 7:A:1392:A:N6    | 29:W:18:GLU:OE1   | 2.41                     | 0.52              |
| 7:A:2482:A:O3'   | 31:Z:63:U:O2'     | 2.27                     | 0.52              |
| 8:B:651:C:N4     | 8:B:753:A:OP2     | 2.41                     | 0.52              |
| 8:B:953:G:O6     | 8:B:1228:C:N4     | 2.41                     | 0.52              |
| 9:C:87:CYS:H     | 9:C:89:GLN:HE21   | 1.55                     | 0.52              |
| 46:o:52:ASN:N    | 46:o:52:ASN:OD1   | 2.41                     | 0.52              |
| 46:o:63:LYS:HE3  | 46:o:65:SER:HB3   | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:1064:C:H2'    | 7:A:1066:U:H4'    | 1.90                     | 0.52              |
| 7:A:243:U:H2'     | 7:A:244:A:H8      | 1.74                     | 0.52              |
| 7:A:576:U:O2'     | 7:A:2502:G:O6     | 2.25                     | 0.52              |
| 7:A:1031:G:N3     | 7:A:1124:G:N2     | 2.57                     | 0.52              |
| 7:A:1782:U:O2     | 7:A:2608:G:O2'    | 2.26                     | 0.52              |
| 17:K:66:GLU:OE2   | 21:O:97:LYS:NZ    | 2.42                     | 0.52              |
| 3:2:6:SER:HB2     | 7:A:1031:G:H4'    | 1.92                     | 0.52              |
| 5:5:126:GLU:OE2   | 5:5:285:ARG:NH1   | 2.42                     | 0.52              |
| 7:A:922:C:H2'     | 7:A:923:G:H8      | 1.73                     | 0.52              |
| 7:A:1403:A:HO2'   | 7:A:1471:G:HO2'   | 1.52                     | 0.52              |
| 7:A:2304:G:H4'    | 36:e:130:MET:HA   | 1.91                     | 0.52              |
| 8:B:981:U:H1'     | 21:O:61:ARG:HE    | 1.73                     | 0.52              |
| 15:I:76:GLN:HG3   | 15:I:128:TYR:HB2  | 1.90                     | 0.52              |
| 36:e:148:ARG:HB3  | 36:e:150:ARG:HG3  | 1.90                     | 0.52              |
| 54:w:21:LEU:HA    | 54:w:25:GLN:HB3   | 1.91                     | 0.52              |
| 7:A:381:G:H1      | 7:A:393:C:H42     | 1.57                     | 0.52              |
| 7:A:1536:C:O2     | 7:A:1537:G:N2     | 2.43                     | 0.52              |
| 7:A:2291:U:OP1    | 7:A:2380:C:O2'    | 2.28                     | 0.52              |
| 7:A:2297:A:N3     | 7:A:2297:A:C2'    | 2.73                     | 0.52              |
| 8:B:585:G:O2'     | 8:B:879:C:OP1     | 2.25                     | 0.52              |
| 8:B:1116:U:H3     | 8:B:1184:G:H1     | 1.57                     | 0.52              |
| 8:B:1295:U:O2'    | 20:N:42:ASP:OD2   | 2.28                     | 0.52              |
| 11:E:58:LYS:HE3   | 11:E:203:LEU:HD23 | 1.92                     | 0.52              |
| 11:E:150:LYS:O    | 11:E:152:GLN:NE2  | 2.43                     | 0.52              |
| 16:J:30:ILE:HA    | 16:J:65:ILE:HB    | 1.91                     | 0.52              |
| 21:O:64:CYS:SG    | 21:O:65:ARG:N     | 2.82                     | 0.52              |
| 39:h:126:THR:HA   | 39:h:129:ILE:HG22 | 1.91                     | 0.52              |
| 41:j:13:ASN:OD1   | 41:j:98:ARG:N     | 2.40                     | 0.52              |
| 7:A:18:U:H2'      | 7:A:19:A:C8       | 2.45                     | 0.52              |
| 7:A:1119:U:OP1    | 51:t:83:LYS:NZ    | 2.42                     | 0.52              |
| 7:A:1649:G:N1     | 7:A:2009:A:C6     | 2.78                     | 0.52              |
| 7:A:1796:U:H2'    | 7:A:1797:G:C8     | 2.45                     | 0.52              |
| 7:A:2375:G:N2     | 7:A:2378:A:OP2    | 2.38                     | 0.52              |
| 7:A:2688:G:N1     | 7:A:2720:U:OP2    | 2.42                     | 0.52              |
| 8:B:446:G:H21     | 8:B:488:C:H41     | 1.56                     | 0.52              |
| 11:E:100:ASN:HD21 | 11:E:104:ARG:HE   | 1.57                     | 0.52              |
| 23:Q:4:ILE:HG12   | 23:Q:21:VAL:HG12  | 1.91                     | 0.52              |
| 39:h:90:SER:HB2   | 39:h:93:PRO:HA    | 1.92                     | 0.52              |
| 5:5:334:ARG:NH1   | 5:5:335:GLU:OE2   | 2.42                     | 0.52              |
| 7:A:1223:G:OP2    | 48:q:90:ARG:NH1   | 2.40                     | 0.52              |
| 7:A:1865:U:OP1    | 7:A:2409:G:N2     | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:B:885:G:H1     | 8:B:912:C:H42    | 1.57                     | 0.52              |
| 18:L:20:VAL:HG12 | 18:L:83:GLU:HB2  | 1.92                     | 0.52              |
| 2:1:9:GLY:O      | 2:1:13:ARG:NH2   | 2.43                     | 0.52              |
| 4:3:6:LEU:HD11   | 4:3:12:ARG:HH21  | 1.74                     | 0.52              |
| 4:3:80:LYS:HA    | 4:3:106:VAL:HG12 | 1.92                     | 0.52              |
| 7:A:1718:G:O6    | 7:A:1743:G:N2    | 2.42                     | 0.52              |
| 8:B:335:C:H2'    | 8:B:336:A:H8     | 1.75                     | 0.52              |
| 8:B:842:U:O2'    | 8:B:845:A:OP2    | 2.26                     | 0.52              |
| 8:B:1049:U:OP1   | 21:O:2:ALA:N     | 2.43                     | 0.52              |
| 8:B:1314:C:N4    | 26:T:3:ARG:O     | 2.43                     | 0.52              |
| 10:D:28:GLU:O    | 10:D:32:ASN:ND2  | 2.42                     | 0.52              |
| 21:O:35:ASN:HD22 | 21:O:41:ARG:HH22 | 1.58                     | 0.52              |
| 55:x:3:LYS:NZ    | 55:x:40:ASP:OD2  | 2.36                     | 0.52              |
| 7:A:1952:A:OP1   | 41:j:44:LYS:NZ   | 2.39                     | 0.52              |
| 8:B:1106:G:O2'   | 10:D:169:ARG:NH1 | 2.43                     | 0.52              |
| 11:E:44:ARG:HH12 | 11:E:47:ARG:HB2  | 1.74                     | 0.52              |
| 33:b:10:SER:O    | 33:b:10:SER:OG   | 2.26                     | 0.52              |
| 7:A:280:U:O4     | 7:A:361:G:N2     | 2.43                     | 0.52              |
| 7:A:445:C:OP1    | 47:p:2:ALA:N     | 2.43                     | 0.52              |
| 7:A:1653:G:OP1   | 7:A:2822:G:N1    | 2.31                     | 0.52              |
| 7:A:2163:A:O3'   | 7:A:2170:A:O2'   | 2.27                     | 0.52              |
| 7:A:2591:C:H42   | 7:A:2603:G:H1    | 1.57                     | 0.52              |
| 33:b:5:LYS:HD2   | 33:b:17:VAL:HG12 | 1.92                     | 0.52              |
| 33:b:180:GLU:OE2 | 33:b:270:ARG:NH1 | 2.43                     | 0.52              |
| 36:e:48:LYS:O    | 36:e:52:ASN:ND2  | 2.39                     | 0.52              |
| 5:5:165:THR:HB   | 5:5:239:LYS:HG3  | 1.92                     | 0.51              |
| 7:A:540:C:H2'    | 7:A:541:A:H8     | 1.75                     | 0.51              |
| 7:A:576:U:H4'    | 7:A:2502:G:C8    | 2.45                     | 0.51              |
| 7:A:1904:G:N2    | 7:A:1905:C:O2    | 2.43                     | 0.51              |
| 7:A:2576:G:N3    | 7:A:2576:G:C5'   | 2.73                     | 0.51              |
| 8:B:428:G:O2'    | 11:E:33:LYS:NZ   | 2.43                     | 0.51              |
| 8:B:1372:U:OP2   | 16:J:13:LYS:NZ   | 2.42                     | 0.51              |
| 14:H:65:ALA:HB2  | 14:H:128:ALA:HA  | 1.92                     | 0.51              |
| 7:A:1395:A:N6    | 7:A:1398:C:O2    | 2.42                     | 0.51              |
| 7:A:1814:G:C5    | 7:A:1815:A:N7    | 2.79                     | 0.51              |
| 7:A:2295:C:OP1   | 45:n:10:ARG:NH2  | 2.44                     | 0.51              |
| 7:A:2343:U:O2'   | 7:A:2373:G:O2'   | 2.28                     | 0.51              |
| 7:A:2649:C:H42   | 7:A:2671:G:H1    | 1.59                     | 0.51              |
| 8:B:1058:G:H22   | 17:K:55:PRO:HG3  | 1.75                     | 0.51              |
| 11:E:194:ASP:OD1 | 11:E:194:ASP:N   | 2.44                     | 0.51              |
| 11:E:198:HIS:HE2 | 12:F:103:THR:HG1 | 1.52                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:J:91:ASP:OD1   | 16:J:91:ASP:N     | 2.43                     | 0.51              |
| 7:A:2447:G:N2     | 7:A:2450:A:OP2    | 2.32                     | 0.51              |
| 8:B:559:A:H4'     | 8:B:560:A:H3'     | 1.93                     | 0.51              |
| 8:B:1302:C:N4     | 20:N:42:ASP:OD1   | 2.41                     | 0.51              |
| 10:D:138:VAL:HA   | 10:D:149:ILE:HD11 | 1.91                     | 0.51              |
| 15:I:5:ASP:OD2    | 15:I:77:ARG:NE    | 2.42                     | 0.51              |
| 17:K:41:PRO:O     | 17:K:72:ARG:NH1   | 2.43                     | 0.51              |
| 24:R:52:GLU:O     | 24:R:81:LYS:NZ    | 2.44                     | 0.51              |
| 47:p:81:ASN:OD1   | 47:p:85:LYS:NZ    | 2.37                     | 0.51              |
| 7:A:410:G:N2      | 7:A:418:C:O2      | 2.44                     | 0.51              |
| 8:B:571:U:O4      | 8:B:864:A:N6      | 2.44                     | 0.51              |
| 8:B:948:C:H2'     | 8:B:949:A:H8      | 1.75                     | 0.51              |
| 8:B:977:A:O2'     | 8:B:981:U:N3      | 2.36                     | 0.51              |
| 8:B:1218:C:H2'    | 8:B:1219:A:H8     | 1.75                     | 0.51              |
| 8:B:1348:U:H2'    | 8:B:1349:A:H8     | 1.76                     | 0.51              |
| 12:F:82:GLN:N     | 12:F:147:MET:SD   | 2.79                     | 0.51              |
| 15:I:15:ARG:HH11  | 15:I:75:ILE:HG23  | 1.73                     | 0.51              |
| 39:h:101:ILE:HG12 | 39:h:138:LEU:HD11 | 1.92                     | 0.51              |
| 1:0:31:LEU:HD22   | 1:0:42:LEU:HD23   | 1.92                     | 0.51              |
| 7:A:2127:G:H22    | 7:A:2161:C:H2'    | 1.75                     | 0.51              |
| 8:B:137:U:H2'     | 8:B:138:G:H8      | 1.76                     | 0.51              |
| 11:E:144:SER:OG   | 11:E:145:ILE:N    | 2.43                     | 0.51              |
| 15:I:113:ASP:O    | 15:I:117:ARG:NH1  | 2.43                     | 0.51              |
| 16:J:52:LEU:HB3   | 16:J:57:MET:HG2   | 1.91                     | 0.51              |
| 7:A:385:C:H42     | 7:A:411:G:H1      | 1.58                     | 0.51              |
| 7:A:776:G:N7      | 7:A:793:A:O2'     | 2.42                     | 0.51              |
| 7:A:2798:U:H4'    | 7:A:2799:A:H5'    | 1.93                     | 0.51              |
| 8:B:127:G:O2'     | 24:R:6:ARG:NH2    | 2.43                     | 0.51              |
| 8:B:254:G:N2      | 24:R:18:GLU:OE1   | 2.42                     | 0.51              |
| 8:B:456:A:N6      | 8:B:476:U:O4      | 2.44                     | 0.51              |
| 8:B:1242:G:N2     | 8:B:1296:C:O2'    | 2.44                     | 0.51              |
| 14:H:76:LYS:HE2   | 14:H:89:VAL:HG11  | 1.93                     | 0.51              |
| 21:O:16:LEU:HD12  | 21:O:54:ASP:HB2   | 1.92                     | 0.51              |
| 35:d:7:ASP:OD1    | 35:d:7:ASP:N      | 2.41                     | 0.51              |
| 39:h:74:PRO:HD2   | 39:h:113:LYS:HE3  | 1.93                     | 0.51              |
| 5:5:315:ARG:HA    | 5:5:318:ALA:HB3   | 1.93                     | 0.51              |
| 7:A:690:G:N2      | 7:A:773:U:O2      | 2.43                     | 0.51              |
| 34:c:18:ASP:OD1   | 34:c:18:ASP:N     | 2.37                     | 0.51              |
| 7:A:775:G:OP1     | 7:A:777:G:O2'     | 2.24                     | 0.51              |
| 8:B:28:A:O2'      | 8:B:296:U:OP1     | 2.22                     | 0.51              |
| 8:B:738:C:OP1     | 13:G:2:ARG:NE     | 2.44                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:B:932:C:H5''   | 14:H:5:ARG:HH12   | 1.76                     | 0.51              |
| 8:B:1345:U:OP1   | 16:J:122:ARG:NH1  | 2.44                     | 0.51              |
| 38:g:5:LEU:HD12  | 38:g:17:ASP:HB2   | 1.93                     | 0.51              |
| 7:A:807:U:OP2    | 42:k:41:ARG:NH1   | 2.43                     | 0.51              |
| 8:B:54:C:H2'     | 8:B:352:C:H41     | 1.75                     | 0.51              |
| 8:B:1445:U:H3    | 8:B:1457:G:H1     | 1.57                     | 0.51              |
| 36:e:170:LEU:HG  | 36:e:173:PHE:HB2  | 1.92                     | 0.51              |
| 7:A:2065:C:O2    | 7:A:2446:G:N2     | 2.43                     | 0.51              |
| 7:A:2112:G:N2    | 30:X:19:G:O4'     | 2.44                     | 0.51              |
| 7:A:2131:U:H5'   | 7:A:2158:A:H62    | 1.76                     | 0.51              |
| 7:A:2564:A:OP1   | 7:A:2648:G:O2'    | 2.24                     | 0.51              |
| 8:B:1193:G:OP1   | 10:D:167:TRP:NE1  | 2.39                     | 0.51              |
| 8:B:1372:U:OP1   | 16:J:74:GLY:N     | 2.38                     | 0.51              |
| 11:E:19:LEU:HA   | 11:E:64:ILE:HG12  | 1.91                     | 0.51              |
| 14:H:113:ASP:O   | 14:H:119:ARG:NH2  | 2.44                     | 0.51              |
| 16:J:120:LYS:HB2 | 16:J:123:ARG:HB3  | 1.92                     | 0.51              |
| 19:M:29:GLN:HG2  | 19:M:81:LEU:HD23  | 1.93                     | 0.51              |
| 34:c:103:ASP:N   | 34:c:103:ASP:OD1  | 2.42                     | 0.51              |
| 3:2:19:ARG:NE    | 7:A:2756:U:OP2    | 2.44                     | 0.50              |
| 4:3:46:LEU:HD21  | 4:3:91:LEU:HD23   | 1.93                     | 0.50              |
| 7:A:2285:C:OP2   | 57:z:6:ARG:NH1    | 2.39                     | 0.50              |
| 7:A:2403:C:C4    | 7:A:2415:G:N1     | 2.79                     | 0.50              |
| 8:B:1250:A:N1    | 8:B:1353:G:N2     | 2.50                     | 0.50              |
| 10:D:24:ALA:HB1  | 10:D:28:GLU:HG2   | 1.94                     | 0.50              |
| 32:a:27:C:OP1    | 45:n:34:HIS:NE2   | 2.40                     | 0.50              |
| 50:s:38:GLY:HA2  | 50:s:41:LEU:HD21  | 1.92                     | 0.50              |
| 7:A:18:U:H6      | 7:A:18:U:H3'      | 1.77                     | 0.50              |
| 7:A:2041:U:H2'   | 7:A:2042:A:H8     | 1.77                     | 0.50              |
| 7:A:2368:C:H2'   | 7:A:2369:A:H8     | 1.77                     | 0.50              |
| 8:B:933:G:O6     | 14:H:3:ARG:NH2    | 2.44                     | 0.50              |
| 18:L:33:THR:HG22 | 18:L:44:TRP:HB3   | 1.92                     | 0.50              |
| 19:M:106:GLY:HA3 | 19:M:119:VAL:HG22 | 1.91                     | 0.50              |
| 22:P:24:SER:OG   | 22:P:26:GLU:OE1   | 2.28                     | 0.50              |
| 4:3:56:ARG:NH2   | 4:3:74:ASN:OD1    | 2.41                     | 0.50              |
| 7:A:680:C:N3     | 7:A:798:G:N2      | 2.60                     | 0.50              |
| 7:A:2658:C:OP1   | 37:f:158:LYS:NZ   | 2.44                     | 0.50              |
| 8:B:613:C:OP2    | 11:E:81:ARG:NE    | 2.44                     | 0.50              |
| 8:B:1097:C:O2'   | 8:B:1169:A:O2'    | 2.28                     | 0.50              |
| 8:B:1128:C:O2'   | 8:B:1147:C:N3     | 2.39                     | 0.50              |
| 21:O:33:ASP:H    | 21:O:35:ASN:HD21  | 1.57                     | 0.50              |
| 26:T:16:LEU:HA   | 26:T:19:VAL:HG12  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:2579:C:H3'    | 7:A:2579:C:H6     | 1.76                     | 0.50              |
| 11:E:161:LEU:O    | 11:E:165:ARG:N    | 2.43                     | 0.50              |
| 32:a:114:C:H2'    | 32:a:115:A:H8     | 1.77                     | 0.50              |
| 33:b:146:MET:HE3  | 33:b:154:LEU:HD11 | 1.93                     | 0.50              |
| 36:e:33:LYS:HE2   | 36:e:157:THR:HG21 | 1.92                     | 0.50              |
| 51:t:41:GLU:N     | 51:t:41:GLU:OE1   | 2.44                     | 0.50              |
| 53:v:39:TRP:HB2   | 53:v:46:PHE:HE1   | 1.75                     | 0.50              |
| 5:5:411:VAL:HA    | 5:5:414:LYS:HE2   | 1.93                     | 0.50              |
| 8:B:632:U:H5''    | 8:B:633:G:H8      | 1.75                     | 0.50              |
| 11:E:73:ARG:O     | 11:E:77:LYS:NZ    | 2.38                     | 0.50              |
| 16:J:26:GLY:HA3   | 16:J:58:VAL:HA    | 1.94                     | 0.50              |
| 39:h:7:ALA:HB3    | 39:h:31:GLN:HE21  | 1.76                     | 0.50              |
| 53:v:35:SER:O     | 53:v:35:SER:OG    | 2.26                     | 0.50              |
| 57:z:10:LYS:HB3   | 57:z:52:ALA:HB3   | 1.94                     | 0.50              |
| 7:A:1146:C:H2'    | 7:A:1147:A:H8     | 1.77                     | 0.50              |
| 7:A:1296:G:OP1    | 7:A:2709:G:O2'    | 2.26                     | 0.50              |
| 7:A:2796:U:H3     | 7:A:2799:A:H61    | 1.59                     | 0.50              |
| 8:B:589:U:H5''    | 15:I:30:SER:HB2   | 1.93                     | 0.50              |
| 8:B:928:G:O2'     | 8:B:1533:C:OP1    | 2.27                     | 0.50              |
| 8:B:1078:U:O2'    | 12:F:138:ARG:NH1  | 2.45                     | 0.50              |
| 8:B:1237:C:N4     | 8:B:1336:C:O2     | 2.44                     | 0.50              |
| 11:E:118:VAL:HG22 | 11:E:123:ILE:HD12 | 1.93                     | 0.50              |
| 32:a:48:U:H4'     | 45:n:100:HIS:HD2  | 1.76                     | 0.50              |
| 7:A:1069:A:O2'    | 7:A:1073:A:OP2    | 2.29                     | 0.50              |
| 7:A:1357:C:C2'    | 7:A:1358:G:H5'    | 2.41                     | 0.50              |
| 7:A:1432:G:O6     | 7:A:1561:C:N4     | 2.43                     | 0.50              |
| 7:A:1834:U:O2     | 7:A:1972:G:N2     | 2.44                     | 0.50              |
| 7:A:2292:U:H2'    | 7:A:2293:G:H8     | 1.77                     | 0.50              |
| 8:B:410:G:N7      | 8:B:429:U:O2'     | 2.37                     | 0.50              |
| 8:B:1251:A:N3     | 8:B:1369:C:O2'    | 2.42                     | 0.50              |
| 29:W:3:ARG:O      | 29:W:5:GLU:N      | 2.45                     | 0.50              |
| 30:X:5:G:N1       | 30:X:68:C:N3      | 2.58                     | 0.50              |
| 41:j:59:LYS:NZ    | 41:j:89:ASN:O     | 2.45                     | 0.50              |
| 41:j:77:ILE:HG12  | 46:o:72:ARG:HD2   | 1.94                     | 0.50              |
| 7:A:13:A:C2       | 7:A:526:A:C5      | 2.99                     | 0.50              |
| 7:A:13:A:C6       | 7:A:525:U:C2      | 3.00                     | 0.50              |
| 8:B:54:C:N4       | 8:B:353:A:OP2     | 2.43                     | 0.50              |
| 8:B:74:A:C5       | 8:B:75:G:H1'      | 2.47                     | 0.50              |
| 8:B:874:G:N2      | 15:I:16:ASN:OD1   | 2.44                     | 0.50              |
| 12:F:99:ALA:HB3   | 12:F:122:ASN:HB3  | 1.92                     | 0.50              |
| 30:X:53:G:N2      | 30:X:57:G:OP1     | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:c:129:THR:OG1  | 34:c:140:HIS:O    | 2.28                     | 0.50              |
| 56:y:7:G:N2       | 56:y:67:C:O2      | 2.45                     | 0.50              |
| 7:A:2017:U:O2     | 7:A:2017:U:H2'    | 2.11                     | 0.49              |
| 8:B:689:C:OP2     | 18:L:53:ARG:NH2   | 2.45                     | 0.49              |
| 8:B:1310:G:OP2    | 20:N:87:ARG:NH2   | 2.45                     | 0.49              |
| 9:C:138:THR:HA    | 9:C:141:LEU:HB2   | 1.94                     | 0.49              |
| 19:M:23:ALA:HB2   | 19:M:95:TYR:HE1   | 1.75                     | 0.49              |
| 22:P:13:SER:HA    | 22:P:19:ALA:HA    | 1.94                     | 0.49              |
| 25:S:71:THR:O     | 25:S:74:HIS:NE2   | 2.45                     | 0.49              |
| 34:c:131:ASP:O    | 34:c:136:ASN:ND2  | 2.45                     | 0.49              |
| 35:d:150:THR:OG1  | 35:d:151:GLY:N    | 2.46                     | 0.49              |
| 36:e:121:SER:O    | 36:e:121:SER:OG   | 2.28                     | 0.49              |
| 37:f:104:ASN:ND2  | 37:f:114:ASP:OD1  | 2.44                     | 0.49              |
| 7:A:372:G:OP2     | 53:v:61:LYS:NZ    | 2.45                     | 0.49              |
| 7:A:1999:C:O2     | 7:A:2687:U:O2'    | 2.27                     | 0.49              |
| 7:A:2117:A:N6     | 7:A:2166:U:O2     | 2.44                     | 0.49              |
| 8:B:41:G:N3       | 8:B:402:G:N1      | 2.58                     | 0.49              |
| 8:B:1308:U:OP1    | 20:N:97:VAL:N     | 2.41                     | 0.49              |
| 12:F:114:VAL:HG11 | 12:F:140:THR:HG21 | 1.94                     | 0.49              |
| 18:L:126:LYS:O    | 28:V:34:ARG:NE    | 2.29                     | 0.49              |
| 23:Q:35:ARG:NH2   | 23:Q:37:GLY:O     | 2.45                     | 0.49              |
| 49:r:80:PRO:O     | 49:r:100:THR:OG1  | 2.27                     | 0.49              |
| 2:l:31:HIS:O      | 2:l:33:LEU:N      | 2.41                     | 0.49              |
| 7:A:307:G:N2      | 7:A:310:A:OP2     | 2.43                     | 0.49              |
| 7:A:457:A:H61     | 7:A:470:A:H5''    | 1.77                     | 0.49              |
| 7:A:1849:G:H2'    | 7:A:1850:G:C8     | 2.42                     | 0.49              |
| 7:A:2072:C:O2     | 7:A:2440:C:N4     | 2.45                     | 0.49              |
| 7:A:2303:G:O2'    | 36:e:121:SER:O    | 2.28                     | 0.49              |
| 8:B:1238:A:H2'    | 8:B:1239:A:H8     | 1.75                     | 0.49              |
| 10:D:19:ASN:O     | 10:D:40:ARG:NH2   | 2.44                     | 0.49              |
| 24:R:11:ARG:HH21  | 24:R:56:GLY:HA3   | 1.76                     | 0.49              |
| 43:l:50:ARG:HG3   | 43:l:65:ILE:HD11  | 1.93                     | 0.49              |
| 54:w:3:ALA:O      | 54:w:7:ARG:NH2    | 2.46                     | 0.49              |
| 7:A:1102:C:H2'    | 7:A:1103:A:C8     | 2.47                     | 0.49              |
| 8:B:252:U:O4      | 8:B:253:A:N6      | 2.46                     | 0.49              |
| 8:B:470:C:H2'     | 8:B:471:U:H4'     | 1.94                     | 0.49              |
| 10:D:11:ARG:NH2   | 10:D:177:THR:O    | 2.45                     | 0.49              |
| 15:I:8:ALA:HB2    | 15:I:77:ARG:HD3   | 1.94                     | 0.49              |
| 40:i:14:ASP:OD1   | 40:i:14:ASP:N     | 2.34                     | 0.49              |
| 51:t:2:PHE:O      | 51:t:62:THR:OG1   | 2.30                     | 0.49              |
| 7:A:2313:C:H2'    | 7:A:2314:A:H8     | 1.77                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:2711:A:C5    | 7:A:2714:G:O4'    | 2.66                     | 0.49              |
| 11:E:67:VAL:HG11 | 11:E:75:TYR:HE2   | 1.77                     | 0.49              |
| 15:I:30:SER:OG   | 15:I:31:LYS:N     | 2.45                     | 0.49              |
| 44:m:57:THR:O    | 44:m:57:THR:OG1   | 2.29                     | 0.49              |
| 5:5:67:LEU:HD23  | 5:5:70:LEU:HD23   | 1.93                     | 0.49              |
| 7:A:224:U:O4     | 7:A:419:U:O2'     | 2.30                     | 0.49              |
| 7:A:2267:A:N3    | 7:A:2267:A:C3'    | 2.74                     | 0.49              |
| 7:A:2446:G:H4'   | 7:A:2448:A:N7     | 2.28                     | 0.49              |
| 8:B:98:A:H8      | 8:B:99:C:C5       | 2.31                     | 0.49              |
| 17:K:71:LEU:O    | 17:K:72:ARG:NH1   | 2.39                     | 0.49              |
| 23:Q:3:THR:OG1   | 23:Q:24:SER:OG    | 2.31                     | 0.49              |
| 25:S:34:THR:HG23 | 25:S:36:SER:H     | 1.77                     | 0.49              |
| 35:d:21:ARG:O    | 35:d:114:ARG:NH2  | 2.34                     | 0.49              |
| 36:e:38:MET:HG3  | 36:e:57:LEU:HD11  | 1.95                     | 0.49              |
| 49:r:47:VAL:HG12 | 49:r:103:ILE:HG21 | 1.93                     | 0.49              |
| 5:5:121:GLU:HG2  | 5:5:414:LYS:HB2   | 1.94                     | 0.49              |
| 7:A:495:G:H21    | 49:r:61:ASN:HD21  | 1.59                     | 0.49              |
| 7:A:571:U:C4     | 7:A:2030:A:N1     | 2.80                     | 0.49              |
| 7:A:598:U:H2'    | 7:A:599:A:H8      | 1.77                     | 0.49              |
| 7:A:1143:A:OP1   | 40:i:27:ARG:NH2   | 2.40                     | 0.49              |
| 7:A:1748:C:H2'   | 7:A:1749:A:H8     | 1.78                     | 0.49              |
| 7:A:2009:A:H2'   | 7:A:2010:G:H8     | 1.77                     | 0.49              |
| 7:A:2133:G:N2    | 7:A:2158:A:O5'    | 2.44                     | 0.49              |
| 8:B:677:U:H3     | 8:B:713:G:H22     | 1.61                     | 0.49              |
| 8:B:978:A:N7     | 8:B:1318:A:N6     | 2.60                     | 0.49              |
| 11:E:174:ASP:OD1 | 11:E:174:ASP:N    | 2.45                     | 0.49              |
| 16:J:106:ARG:NH1 | 16:J:107:ASP:O    | 2.45                     | 0.49              |
| 32:a:66:A:O4'    | 32:a:108:A:N6     | 2.46                     | 0.49              |
| 36:e:70:ALA:N    | 36:e:83:TYR:O     | 2.46                     | 0.49              |
| 46:o:55:LEU:HA   | 46:o:77:HIS:HD2   | 1.76                     | 0.49              |
| 3:2:3:VAL:HG21   | 7:A:2539:C:H5'    | 1.95                     | 0.49              |
| 4:3:81:SER:OG    | 4:3:82:GLY:N      | 2.45                     | 0.49              |
| 7:A:27:G:N2      | 7:A:512:G:H1'     | 2.28                     | 0.49              |
| 7:A:729:G:N2     | 33:b:11:PRO:O     | 2.45                     | 0.49              |
| 7:A:1458:U:H4'   | 7:A:1459:G:H5'    | 1.95                     | 0.49              |
| 7:A:2128:G:O6    | 7:A:2160:C:N4     | 2.46                     | 0.49              |
| 7:A:1652:A:OP1   | 44:m:8:ARG:NH2    | 2.46                     | 0.49              |
| 7:A:1945:G:N2    | 7:A:1963:U:O4     | 2.46                     | 0.49              |
| 7:A:2026:U:H2'   | 7:A:2027:G:H8     | 1.78                     | 0.49              |
| 8:B:1445:U:O2    | 8:B:1457:G:N2     | 2.35                     | 0.49              |
| 13:G:51:ILE:HD13 | 13:G:86:ARG:HH21  | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:Q:75:ILE:HD11 | 23:Q:80:LYS:HE2  | 1.94                     | 0.49              |
| 7:A:500:G:N1     | 7:A:503:A:OP2    | 2.42                     | 0.49              |
| 7:A:780:G:N1     | 33:b:229:ASP:OD2 | 2.42                     | 0.49              |
| 7:A:1130:U:OP2   | 7:A:2570:G:N2    | 2.41                     | 0.49              |
| 7:A:1826:G:OP2   | 33:b:222:GLY:N   | 2.46                     | 0.49              |
| 8:B:1074:G:O2'   | 8:B:1101:A:N1    | 2.36                     | 0.49              |
| 12:F:15:LEU:HA   | 12:F:37:THR:HG22 | 1.94                     | 0.49              |
| 31:Z:27:G:H22    | 31:Z:44:U:H3     | 1.61                     | 0.49              |
| 48:q:55:ASP:N    | 48:q:55:ASP:OD1  | 2.36                     | 0.49              |
| 56:y:38:C:H3'    | 56:y:39:G:H8     | 1.77                     | 0.49              |
| 7:A:1607:C:N4    | 7:A:1622:G:OP2   | 2.42                     | 0.48              |
| 7:A:2252:G:N2    | 56:y:75:C:N3     | 2.61                     | 0.48              |
| 8:B:729:A:H2'    | 8:B:730:G:H8     | 1.79                     | 0.48              |
| 17:K:45:ARG:NH1  | 17:K:47:GLU:OE2  | 2.38                     | 0.48              |
| 20:N:23:TYR:HD2  | 20:N:66:GLU:HA   | 1.78                     | 0.48              |
| 39:h:121:ASP:N   | 39:h:121:ASP:OD1 | 2.45                     | 0.48              |
| 41:j:60:ALA:HB1  | 41:j:84:CYS:HB2  | 1.95                     | 0.48              |
| 7:A:537:G:N2     | 7:A:555:G:N3     | 2.61                     | 0.48              |
| 7:A:1368:G:C2    | 7:A:1369:G:N7    | 2.81                     | 0.48              |
| 8:B:667:G:N2     | 22:P:49:ASP:OD2  | 2.45                     | 0.48              |
| 8:B:1009:U:H3    | 8:B:1020:G:H1    | 1.61                     | 0.48              |
| 14:H:126:ASP:OD1 | 14:H:126:ASP:N   | 2.44                     | 0.48              |
| 24:R:4:LYS:NZ    | 24:R:5:ILE:O     | 2.44                     | 0.48              |
| 27:U:76:LYS:O    | 27:U:80:THR:OG1  | 2.24                     | 0.48              |
| 33:b:114:ASP:OD1 | 33:b:114:ASP:N   | 2.44                     | 0.48              |
| 47:p:110:VAL:O   | 47:p:114:LYS:N   | 2.46                     | 0.48              |
| 7:A:548:G:O2'    | 7:A:549:G:N7     | 2.43                     | 0.48              |
| 7:A:2087:G:C2    | 7:A:2088:A:C5    | 3.00                     | 0.48              |
| 7:A:2298:A:H5''  | 36:e:72:LYS:HZ1  | 1.78                     | 0.48              |
| 7:A:2581:G:H1    | 7:A:2610:C:HO2'  | 1.59                     | 0.48              |
| 12:F:136:VAL:O   | 12:F:140:THR:N   | 2.46                     | 0.48              |
| 14:H:70:ARG:HE   | 14:H:97:ASN:HB3  | 1.78                     | 0.48              |
| 17:K:80:THR:O    | 17:K:83:THR:OG1  | 2.30                     | 0.48              |
| 27:U:31:PHE:O    | 27:U:34:LYS:NZ   | 2.44                     | 0.48              |
| 31:Z:58:A:O2'    | 31:Z:60:U:OP2    | 2.30                     | 0.48              |
| 3:2:23:ILE:HB    | 3:2:38:GLY:HA3   | 1.95                     | 0.48              |
| 5:5:280:SER:O    | 5:5:284:ASN:N    | 2.46                     | 0.48              |
| 7:A:414:C:H2'    | 7:A:415:A:H8     | 1.78                     | 0.48              |
| 7:A:1171:G:N1    | 7:A:1179:G:O6    | 2.46                     | 0.48              |
| 7:A:1190:G:H2'   | 7:A:1191:G:H8    | 1.78                     | 0.48              |
| 7:A:2167:U:N3    | 7:A:2170:A:N7    | 2.60                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:2831:G:OP2   | 34:c:59:ARG:NH1   | 2.41                     | 0.48              |
| 8:B:1073:U:OP1   | 12:F:62:LYS:NZ    | 2.46                     | 0.48              |
| 11:E:126:ASN:ND2 | 11:E:141:ASP:OD1  | 2.46                     | 0.48              |
| 25:S:44:ILE:HG23 | 25:S:45:THR:HG23  | 1.96                     | 0.48              |
| 53:v:72:ARG:NH1  | 53:v:78:TYR:OH    | 2.44                     | 0.48              |
| 56:y:74:C:N3     | 56:y:75:C:N4      | 2.61                     | 0.48              |
| 7:A:2588:G:O6    | 7:A:2607:G:N1     | 2.46                     | 0.48              |
| 7:A:2827:C:H2'   | 7:A:2828:G:H8     | 1.78                     | 0.48              |
| 8:B:231:U:H2'    | 8:B:232:G:H8      | 1.78                     | 0.48              |
| 9:C:85:LEU:HA    | 9:C:89:GLN:HG3    | 1.96                     | 0.48              |
| 19:M:110:ARG:HD2 | 19:M:119:VAL:HB   | 1.95                     | 0.48              |
| 22:P:61:SER:O    | 22:P:65:LYS:NZ    | 2.43                     | 0.48              |
| 7:A:391:A:O2'    | 7:A:410:G:OP1     | 2.30                     | 0.48              |
| 7:A:548:G:H4'    | 7:A:549:G:C4      | 2.48                     | 0.48              |
| 7:A:644:A:H61    | 7:A:2349:G:H21    | 1.61                     | 0.48              |
| 7:A:1061:U:O2'   | 7:A:1064:C:N4     | 2.45                     | 0.48              |
| 7:A:1806:C:O2    | 33:b:44:ASN:ND2   | 2.46                     | 0.48              |
| 7:A:2315:G:OP1   | 36:e:33:LYS:NZ    | 2.45                     | 0.48              |
| 7:A:2589:A:H2'   | 7:A:2590:A:C8     | 2.49                     | 0.48              |
| 7:A:2641:G:H5''  | 40:i:78:THR:HB    | 1.94                     | 0.48              |
| 8:B:461:A:H2'    | 8:B:462:G:H8      | 1.79                     | 0.48              |
| 8:B:942:G:H21    | 16:J:126:GLN:HE22 | 1.61                     | 0.48              |
| 8:B:949:A:N7     | 20:N:105:ASN:ND2  | 2.61                     | 0.48              |
| 8:B:1288:A:N3    | 8:B:1352:C:O2'    | 2.45                     | 0.48              |
| 17:K:85:ASP:O    | 17:K:89:ARG:NH1   | 2.37                     | 0.48              |
| 30:X:29:U:H3     | 30:X:41:A:H61     | 1.60                     | 0.48              |
| 7:A:833:A:H2'    | 7:A:834:G:C8      | 2.48                     | 0.48              |
| 7:A:1358:G:C2    | 7:A:1372:U:OP2    | 2.65                     | 0.48              |
| 7:A:2353:G:N2    | 7:A:2354:C:O2     | 2.46                     | 0.48              |
| 7:A:2855:C:H2'   | 7:A:2856:A:H8     | 1.78                     | 0.48              |
| 8:B:1243:C:H2'   | 8:B:1244:G:H8     | 1.77                     | 0.48              |
| 11:E:151:LYS:HE3 | 11:E:178:MET:HE3  | 1.95                     | 0.48              |
| 32:a:34:A:N6     | 32:a:44:G:O2'     | 2.47                     | 0.48              |
| 5:5:34:ASN:HA    | 5:5:37:LYS:HE3    | 1.95                     | 0.48              |
| 7:A:970:U:O2     | 7:A:984:A:O2'     | 2.29                     | 0.48              |
| 7:A:1176:U:H2'   | 7:A:1177:G:C5     | 2.49                     | 0.48              |
| 7:A:2008:C:N4    | 7:A:2009:A:N6     | 2.60                     | 0.48              |
| 8:B:434:U:H2'    | 8:B:435:A:C8      | 2.49                     | 0.48              |
| 9:C:71:GLY:HA3   | 9:C:80:VAL:HG21   | 1.94                     | 0.48              |
| 9:C:147:SER:OG   | 9:C:148:LEU:N     | 2.47                     | 0.48              |
| 10:D:113:ALA:HA  | 10:D:116:VAL:HG12 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:H:111:ARG:NH1 | 14:H:123:GLU:OE1  | 2.47                     | 0.48              |
| 29:W:19:LYS:NZ   | 29:W:84:TYR:OH    | 2.46                     | 0.48              |
| 30:X:13:C:N3     | 30:X:14:A:N6      | 2.61                     | 0.48              |
| 45:n:72:ALA:HB2  | 45:n:105:ALA:HB1  | 1.94                     | 0.48              |
| 4:3:43:GLY:HA3   | 4:3:91:LEU:HD22   | 1.95                     | 0.48              |
| 7:A:1105:U:H2'   | 7:A:1106:G:C8     | 2.48                     | 0.48              |
| 7:A:2500:U:C2    | 7:A:2504:U:C4     | 3.01                     | 0.48              |
| 11:E:58:LYS:NZ   | 11:E:69:GLU:OE2   | 2.42                     | 0.48              |
| 33:b:227:PRO:HG3 | 33:b:234:GLY:HA3  | 1.95                     | 0.48              |
| 3:2:24:ARG:NH1   | 7:A:2742:G:OP2    | 2.43                     | 0.48              |
| 7:A:482:A:H4'    | 50:s:45:HIS:CD2   | 2.48                     | 0.48              |
| 7:A:1326:U:HO2'  | 7:A:2010:G:HO2'   | 1.59                     | 0.48              |
| 7:A:2591:C:N4    | 7:A:2592:G:O6     | 2.46                     | 0.48              |
| 8:B:103:U:H2'    | 8:B:172:A:H61     | 1.79                     | 0.48              |
| 8:B:408:A:O4'    | 11:E:154:ARG:NH2  | 2.47                     | 0.48              |
| 8:B:1034:G:OP2   | 8:B:1036:A:N6     | 2.47                     | 0.48              |
| 33:b:16:VAL:HB   | 33:b:206:GLY:HA3  | 1.96                     | 0.48              |
| 42:k:132:ARG:HG3 | 42:k:142:ILE:HD12 | 1.96                     | 0.48              |
| 56:y:1:G:H22     | 56:y:73:G:H21     | 1.61                     | 0.48              |
| 3:2:3:VAL:HG12   | 3:2:36:ARG:HB3    | 1.96                     | 0.47              |
| 4:3:50:GLN:HE22  | 4:3:90:CYS:HG     | 1.60                     | 0.47              |
| 5:5:307:ILE:HG13 | 5:5:345:VAL:HG21  | 1.95                     | 0.47              |
| 7:A:680:C:H2'    | 7:A:681:G:H8      | 1.78                     | 0.47              |
| 7:A:1358:G:C2'   | 7:A:1359:A:OP2    | 2.61                     | 0.47              |
| 7:A:2746:U:C4    | 7:A:2747:G:N7     | 2.82                     | 0.47              |
| 8:B:2:A:N1       | 8:B:627:G:N2      | 2.62                     | 0.47              |
| 8:B:1179:A:OP1   | 16:J:95:ARG:NH2   | 2.47                     | 0.47              |
| 42:k:95:LEU:O    | 42:k:99:ASN:N     | 2.47                     | 0.47              |
| 7:A:883:G:N2     | 7:A:894:U:O2'     | 2.47                     | 0.47              |
| 7:A:1136:G:H2'   | 7:A:1137:G:H8     | 1.79                     | 0.47              |
| 7:A:2354:C:H2'   | 7:A:2355:G:H8     | 1.79                     | 0.47              |
| 10:D:12:LEU:HA   | 10:D:16:LYS:HB2   | 1.96                     | 0.47              |
| 24:R:58:VAL:HB   | 24:R:79:VAL:HG23  | 1.95                     | 0.47              |
| 28:V:34:ARG:HB3  | 28:V:35:ARG:HG2   | 1.95                     | 0.47              |
| 30:X:11:C:H42    | 30:X:45:G:H21     | 1.62                     | 0.47              |
| 33:b:252:THR:OG1 | 33:b:253:LYS:N    | 2.45                     | 0.47              |
| 34:c:181:ASP:OD2 | 34:c:184:ARG:NH2  | 2.47                     | 0.47              |
| 53:v:5:CYS:HB2   | 53:v:52:SER:HB3   | 1.96                     | 0.47              |
| 5:5:327:LYS:NZ   | 50:s:60:GLU:OE1   | 2.47                     | 0.47              |
| 7:A:1864:U:OP1   | 7:A:2410:G:O2'    | 2.30                     | 0.47              |
| 7:A:2049:G:N2    | 7:A:2619:C:O2     | 2.36                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:2101:A:N6     | 7:A:2102:G:O6     | 2.48                     | 0.47              |
| 7:A:2313:C:H5''   | 36:e:88:LYS:HD3   | 1.95                     | 0.47              |
| 8:B:924:C:N4      | 8:B:925:G:O6      | 2.47                     | 0.47              |
| 10:D:73:PRO:HG3   | 10:D:105:GLU:HB2  | 1.96                     | 0.47              |
| 27:U:35:VAL:HG11  | 27:U:79:LEU:HD21  | 1.96                     | 0.47              |
| 30:X:5:G:O6       | 30:X:68:C:N4      | 2.41                     | 0.47              |
| 34:c:181:ASP:HB3  | 34:c:186:LEU:HB2  | 1.97                     | 0.47              |
| 55:x:6:LYS:HG2    | 55:x:37:GLU:HB3   | 1.95                     | 0.47              |
| 55:x:9:GLN:HG2    | 55:x:32:ILE:HA    | 1.96                     | 0.47              |
| 1:O:37:LYS:NZ     | 7:A:468:G:OP2     | 2.48                     | 0.47              |
| 7:A:2060:A:N6     | 7:A:2502:G:N2     | 2.62                     | 0.47              |
| 7:A:2898:U:H2'    | 7:A:2899:A:C8     | 2.49                     | 0.47              |
| 8:B:517:G:N2      | 8:B:530:G:OP1     | 2.42                     | 0.47              |
| 8:B:693:G:OP1     | 18:L:127:ARG:NH1  | 2.44                     | 0.47              |
| 8:B:1083:U:O2'    | 8:B:1102:A:OP2    | 2.32                     | 0.47              |
| 8:B:1158:C:O2'    | 9:C:132:LYS:NZ    | 2.37                     | 0.47              |
| 10:D:113:ALA:HB3  | 10:D:185:ASN:HB2  | 1.97                     | 0.47              |
| 10:D:118:ASP:HA   | 10:D:121:THR:HG22 | 1.95                     | 0.47              |
| 20:N:22:ILE:HG13  | 20:N:66:GLU:HG3   | 1.96                     | 0.47              |
| 33:b:141:VAL:O    | 33:b:162:VAL:N    | 2.48                     | 0.47              |
| 44:m:45:ARG:HD3   | 44:m:97:ILE:HD11  | 1.96                     | 0.47              |
| 7:A:1039:A:H61    | 7:A:1116:G:H1     | 1.63                     | 0.47              |
| 7:A:1776:G:N2     | 7:A:1777:U:O2     | 2.47                     | 0.47              |
| 8:B:543:U:OP1     | 11:E:14:ARG:NH2   | 2.48                     | 0.47              |
| 8:B:714:G:N2      | 8:B:777:A:N3      | 2.63                     | 0.47              |
| 8:B:1111:A:N6     | 10:D:176:HIS:O    | 2.47                     | 0.47              |
| 11:E:105:MET:HG2  | 11:E:171:LEU:HB3  | 1.96                     | 0.47              |
| 14:H:2:PRO:HA     | 14:H:5:ARG:HB2    | 1.97                     | 0.47              |
| 27:U:15:GLU:HA    | 27:U:18:ARG:HB3   | 1.96                     | 0.47              |
| 34:c:109:VAL:HG11 | 34:c:193:VAL:HG23 | 1.95                     | 0.47              |
| 36:e:117:LEU:H    | 36:e:177:PHE:N    | 2.13                     | 0.47              |
| 3:2:1:MET:N       | 7:A:2526:G:N3     | 2.62                     | 0.47              |
| 7:A:598:U:H2'     | 7:A:599:A:C8      | 2.50                     | 0.47              |
| 7:A:970:U:H2'     | 7:A:971:G:H8      | 1.78                     | 0.47              |
| 7:A:1079:C:O2'    | 39:h:134:ARG:NH1  | 2.48                     | 0.47              |
| 7:A:2056:G:O6     | 7:A:2612:C:N3     | 2.47                     | 0.47              |
| 7:A:2134:A:N6     | 7:A:2157:G:O2'    | 2.46                     | 0.47              |
| 7:A:2722:G:C5     | 7:A:2723:C:C2     | 3.03                     | 0.47              |
| 8:B:141:G:N2      | 8:B:222:C:O2'     | 2.47                     | 0.47              |
| 8:B:625:U:H2'     | 8:B:626:G:H8      | 1.79                     | 0.47              |
| 11:E:69:GLU:O     | 11:E:73:ARG:NH1   | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:W:30:ILE:HG13  | 29:W:85:VAL:HG13  | 1.97                     | 0.47              |
| 7:A:690:G:H21     | 33:b:43:ARG:HH21  | 1.61                     | 0.47              |
| 7:A:877:A:H2'     | 7:A:878:A:C8      | 2.50                     | 0.47              |
| 7:A:895:U:H2'     | 7:A:899:A:H61     | 1.80                     | 0.47              |
| 7:A:1073:A:OP1    | 7:A:1075:C:N4     | 2.42                     | 0.47              |
| 7:A:1649:G:N1     | 7:A:2009:A:N6     | 2.63                     | 0.47              |
| 7:A:2370:G:O2'    | 57:z:44:ARG:NH1   | 2.47                     | 0.47              |
| 7:A:2575:C:OP1    | 34:c:149:ASN:ND2  | 2.48                     | 0.47              |
| 7:A:2674:G:H4'    | 41:j:30:ARG:HD2   | 1.96                     | 0.47              |
| 8:B:164:G:H2'     | 8:B:165:G:H8      | 1.80                     | 0.47              |
| 8:B:436:C:H4'     | 11:E:154:ARG:HG2  | 1.97                     | 0.47              |
| 8:B:477:C:N3      | 8:B:478:A:N6      | 2.62                     | 0.47              |
| 8:B:564:C:OP1     | 19:M:12:ARG:NH1   | 2.48                     | 0.47              |
| 8:B:971:G:O2'     | 8:B:1365:G:O2'    | 2.31                     | 0.47              |
| 12:F:74:VAL:HG21  | 12:F:144:LEU:HB3  | 1.95                     | 0.47              |
| 14:H:51:ALA:HB2   | 14:H:58:GLU:HG3   | 1.96                     | 0.47              |
| 23:Q:18:GLN:HB3   | 23:Q:35:ARG:HH21  | 1.80                     | 0.47              |
| 26:T:13:LEU:HD12  | 26:T:16:LEU:HB3   | 1.96                     | 0.47              |
| 28:V:18:ARG:HA    | 28:V:21:ARG:HD3   | 1.96                     | 0.47              |
| 35:d:143:LEU:HD13 | 35:d:146:VAL:HG11 | 1.97                     | 0.47              |
| 36:e:47:LYS:HA    | 36:e:50:LEU:HD12  | 1.96                     | 0.47              |
| 38:g:30:LEU:HD22  | 38:g:36:ALA:HB2   | 1.97                     | 0.47              |
| 51:t:90:ASP:N     | 51:t:90:ASP:OD1   | 2.46                     | 0.47              |
| 57:z:34:LEU:N     | 57:z:51:GLU:OE1   | 2.45                     | 0.47              |
| 7:A:69:C:HO2'     | 7:A:73:A:HO2'     | 1.56                     | 0.47              |
| 7:A:581:C:H2'     | 7:A:582:A:C8      | 2.50                     | 0.47              |
| 7:A:2068:U:H3     | 7:A:2430:A:H62    | 1.62                     | 0.47              |
| 7:A:2189:U:H2'    | 7:A:2190:G:H8     | 1.80                     | 0.47              |
| 7:A:2746:U:C2     | 7:A:2747:G:C8     | 3.02                     | 0.47              |
| 13:G:86:ARG:NH1   | 25:S:64:TYR:O     | 2.48                     | 0.47              |
| 20:N:91:HIS:CE1   | 20:N:97:VAL:HG21  | 2.50                     | 0.47              |
| 23:Q:18:GLN:HA    | 23:Q:38:PHE:HA    | 1.97                     | 0.47              |
| 28:V:41:PRO:HA    | 28:V:45:ARG:HB2   | 1.97                     | 0.47              |
| 31:Z:53:G:OP1     | 43:l:55:ARG:NH2   | 2.48                     | 0.47              |
| 33:b:98:ASP:OD1   | 33:b:98:ASP:N     | 2.41                     | 0.47              |
| 34:c:108:ASP:OD1  | 34:c:108:ASP:N    | 2.48                     | 0.47              |
| 4:3:48:ALA:HB1    | 4:3:53:ILE:HG23   | 1.97                     | 0.47              |
| 7:A:459:U:H2'     | 7:A:460:A:H8      | 1.80                     | 0.47              |
| 7:A:1266:G:N2     | 7:A:2012:G:H2'    | 2.28                     | 0.47              |
| 7:A:2267:A:N3     | 7:A:2267:A:C2'    | 2.77                     | 0.47              |
| 8:B:101:A:C8      | 8:B:102:G:N7      | 2.82                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:B:779:C:O2'    | 18:L:122:ARG:NE  | 2.32                     | 0.47              |
| 8:B:1166:G:N1    | 8:B:1169:A:OP2   | 2.46                     | 0.47              |
| 11:E:187:GLU:OE1 | 11:E:189:SER:OG  | 2.32                     | 0.47              |
| 21:O:5:SER:O     | 21:O:9:ARG:N     | 2.47                     | 0.47              |
| 33:b:161:TYR:HD2 | 33:b:194:GLU:HG2 | 1.80                     | 0.47              |
| 36:e:6:ASP:N     | 36:e:6:ASP:OD1   | 2.46                     | 0.47              |
| 46:o:24:ASP:OD1  | 46:o:90:GLY:N    | 2.41                     | 0.47              |
| 7:A:190:A:N6     | 7:A:191:A:N1     | 2.63                     | 0.47              |
| 7:A:1496:A:N3    | 7:A:1577:C:O2'   | 2.48                     | 0.47              |
| 7:A:2314:A:H5'   | 36:e:35:THR:HG21 | 1.96                     | 0.47              |
| 8:B:104:G:O2'    | 8:B:105:G:O4'    | 2.33                     | 0.47              |
| 8:B:369:G:OP2    | 8:B:388:G:N1     | 2.37                     | 0.47              |
| 8:B:619:U:N3     | 11:E:131:ASN:OD1 | 2.43                     | 0.47              |
| 9:C:138:THR:O    | 9:C:142:GLU:N    | 2.46                     | 0.47              |
| 12:F:111:MET:HE1 | 12:F:127:ALA:HB2 | 1.96                     | 0.47              |
| 16:J:24:GLY:N    | 16:J:60:LYS:O    | 2.47                     | 0.47              |
| 29:W:48:GLN:HG3  | 29:W:55:VAL:HG12 | 1.96                     | 0.47              |
| 37:f:56:ASP:OD1  | 37:f:56:ASP:N    | 2.48                     | 0.47              |
| 44:m:106:ASP:OD1 | 44:m:106:ASP:N   | 2.45                     | 0.47              |
| 4:3:135:ASP:HA   | 4:3:138:VAL:HG12 | 1.97                     | 0.46              |
| 7:A:974:G:OP1    | 7:A:1187:G:O2'   | 2.31                     | 0.46              |
| 7:A:1184:U:OP2   | 55:x:31:ARG:NH2  | 2.47                     | 0.46              |
| 8:B:138:G:H1     | 8:B:225:C:H42    | 1.62                     | 0.46              |
| 8:B:390:U:O3'    | 23:Q:28:ARG:NH1  | 2.48                     | 0.46              |
| 10:D:88:ARG:HG2  | 10:D:99:ALA:HB3  | 1.96                     | 0.46              |
| 19:M:52:VAL:HG12 | 19:M:66:TYR:HA   | 1.96                     | 0.46              |
| 29:W:34:VAL:HG11 | 29:W:43:ILE:HD12 | 1.97                     | 0.46              |
| 38:g:12:LEU:HD13 | 38:g:19:VAL:HG21 | 1.96                     | 0.46              |
| 4:3:153:ARG:NH1  | 49:r:52:GLU:OE2  | 2.48                     | 0.46              |
| 7:A:1667:G:H21   | 7:A:1994:C:H42   | 1.62                     | 0.46              |
| 7:A:2508:G:OP1   | 31:Z:76:A:OP1    | 2.32                     | 0.46              |
| 8:B:411:A:H5''   | 11:E:31:LYS:HD3  | 1.97                     | 0.46              |
| 8:B:801:U:H2'    | 8:B:802:A:C8     | 2.50                     | 0.46              |
| 8:B:861:G:O6     | 8:B:869:G:N2     | 2.49                     | 0.46              |
| 24:R:46:VAL:HG21 | 24:R:61:ILE:HD12 | 1.96                     | 0.46              |
| 31:Z:19:G:O6     | 31:Z:57:G:N2     | 2.48                     | 0.46              |
| 7:A:954:G:OP2    | 43:l:16:ARG:NH1  | 2.48                     | 0.46              |
| 7:A:1301:A:H62   | 7:A:1641:A:H61   | 1.64                     | 0.46              |
| 7:A:1583:A:H4'   | 7:A:1584:U:H5    | 1.79                     | 0.46              |
| 8:B:517:G:N1     | 8:B:533:A:OP1    | 2.39                     | 0.46              |
| 8:B:1218:C:H2'   | 8:B:1219:A:C8    | 2.51                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:B:1273:C:H2'   | 8:B:1274:A:H8     | 1.80                     | 0.46              |
| 8:B:1536:C:N3    | 8:B:1538:C:N4     | 2.64                     | 0.46              |
| 15:I:11:LEU:HD23 | 15:I:14:ILE:HD12  | 1.97                     | 0.46              |
| 25:S:71:THR:HG22 | 25:S:73:ARG:H     | 1.80                     | 0.46              |
| 27:U:43:ASP:OD1  | 27:U:46:ALA:N     | 2.45                     | 0.46              |
| 43:l:54:THR:HG22 | 43:l:63:ILE:HD12  | 1.97                     | 0.46              |
| 49:r:66:ILE:HA   | 49:r:69:LEU:HD12  | 1.98                     | 0.46              |
| 54:w:21:LEU:O    | 54:w:26:PHE:N     | 2.49                     | 0.46              |
| 4:3:75:PRO:HB2   | 4:3:108:ILE:HD11  | 1.97                     | 0.46              |
| 5:5:31:GLU:HA    | 5:5:34:ASN:HD21   | 1.80                     | 0.46              |
| 7:A:281:C:H2'    | 7:A:282:A:H8      | 1.80                     | 0.46              |
| 7:A:980:A:N6     | 7:A:981:A:N1      | 2.63                     | 0.46              |
| 8:B:49:U:H3      | 8:B:362:G:H1'     | 1.80                     | 0.46              |
| 8:B:413:G:O3'    | 8:B:428:G:N2      | 2.48                     | 0.46              |
| 19:M:76:GLU:O    | 19:M:77:HIS:ND1   | 2.48                     | 0.46              |
| 27:U:7:ALA:O     | 27:U:11:ALA:N     | 2.49                     | 0.46              |
| 34:c:121:THR:O   | 34:c:121:THR:OG1  | 2.29                     | 0.46              |
| 35:d:130:LYS:HB2 | 35:d:133:LEU:HD13 | 1.97                     | 0.46              |
| 7:A:327:G:H1     | 7:A:335:C:H42     | 1.64                     | 0.46              |
| 7:A:1454:C:OP1   | 44:m:63:ARG:NH2   | 2.48                     | 0.46              |
| 7:A:2060:A:C4    | 7:A:2502:G:N3     | 2.84                     | 0.46              |
| 8:B:18:C:H1'     | 8:B:1079:G:H21    | 1.80                     | 0.46              |
| 9:C:214:LEU:HA   | 9:C:217:VAL:HG12  | 1.98                     | 0.46              |
| 13:G:10:VAL:HB   | 13:G:58:HIS:HB3   | 1.97                     | 0.46              |
| 14:H:119:ARG:HA  | 14:H:122:ASN:HB2  | 1.98                     | 0.46              |
| 45:n:15:ARG:NH2  | 45:n:95:SER:OG    | 2.48                     | 0.46              |
| 54:w:13:GLU:HA   | 54:w:16:THR:HG22  | 1.96                     | 0.46              |
| 7:A:12:U:O5'     | 7:A:12:U:H6       | 1.99                     | 0.46              |
| 7:A:2403:C:C4    | 7:A:2415:G:C2     | 3.03                     | 0.46              |
| 9:C:130:THR:HG23 | 9:C:132:LYS:H     | 1.80                     | 0.46              |
| 24:R:13:VAL:HB   | 24:R:22:VAL:HG23  | 1.98                     | 0.46              |
| 33:b:66:ASP:OD2  | 33:b:102:ARG:NH1  | 2.48                     | 0.46              |
| 42:k:119:PRO:HB3 | 42:k:140:GLY:H    | 1.81                     | 0.46              |
| 5:5:319:ALA:HA   | 5:5:328:GLN:HE22  | 1.81                     | 0.46              |
| 7:A:586:A:O2'    | 7:A:671:C:O2      | 2.34                     | 0.46              |
| 7:A:1590:A:H2'   | 7:A:1591:A:C8     | 2.51                     | 0.46              |
| 7:A:2039:U:H2'   | 7:A:2040:G:C8     | 2.51                     | 0.46              |
| 7:A:2403:C:N4    | 7:A:2415:G:N1     | 2.64                     | 0.46              |
| 7:A:2786:U:H5'   | 34:c:70:LYS:HD3   | 1.97                     | 0.46              |
| 8:B:891:U:H2'    | 8:B:892:A:H8      | 1.81                     | 0.46              |
| 9:C:66:LYS:HG3   | 9:C:88:ASP:HB2    | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 35:d:176:ASP:N   | 35:d:176:ASP:OD1 | 2.49                     | 0.46              |
| 36:e:158:THR:OG1 | 36:e:159:THR:N   | 2.49                     | 0.46              |
| 7:A:400:G:O6     | 53:v:57:ARG:NH1  | 2.48                     | 0.46              |
| 7:A:460:A:H62    | 7:A:469:G:H21    | 1.62                     | 0.46              |
| 7:A:619:G:OP2    | 7:A:620:G:N2     | 2.48                     | 0.46              |
| 7:A:953:G:H2'    | 7:A:954:G:H8     | 1.80                     | 0.46              |
| 7:A:2824:C:N4    | 7:A:2825:G:N7    | 2.64                     | 0.46              |
| 8:B:303:A:HO2'   | 8:B:555:U:HO2'   | 1.62                     | 0.46              |
| 8:B:1391:U:H2'   | 8:B:1392:G:C8    | 2.50                     | 0.46              |
| 10:D:157:LEU:O   | 10:D:164:ARG:NH2 | 2.49                     | 0.46              |
| 18:L:112:ASP:HB3 | 28:V:4:ILE:HG13  | 1.97                     | 0.46              |
| 20:N:89:LEU:O    | 20:N:93:ARG:NE   | 2.48                     | 0.46              |
| 24:R:7:THR:OG1   | 24:R:8:LEU:N     | 2.49                     | 0.46              |
| 50:s:89:ASP:N    | 50:s:89:ASP:OD1  | 2.48                     | 0.46              |
| 7:A:2507:C:H4'   | 31:Z:76:A:H4'    | 1.97                     | 0.46              |
| 8:B:198:G:H1     | 8:B:219:U:H2'    | 1.81                     | 0.46              |
| 8:B:685:G:N2     | 8:B:704:A:OP2    | 2.37                     | 0.46              |
| 8:B:757:U:O2'    | 8:B:879:C:O2     | 2.27                     | 0.46              |
| 8:B:801:U:H2'    | 8:B:802:A:H8     | 1.81                     | 0.46              |
| 8:B:992:U:N3     | 8:B:1043:G:N7    | 2.64                     | 0.46              |
| 17:K:56:HIS:HD2  | 17:K:57:VAL:HG12 | 1.81                     | 0.46              |
| 3:2:2:LYS:HE2    | 3:2:2:LYS:HB3    | 1.82                     | 0.46              |
| 7:A:664:G:OP1    | 42:k:17:LYS:NZ   | 2.40                     | 0.46              |
| 7:A:1388:G:H2'   | 7:A:1389:G:H8    | 1.81                     | 0.46              |
| 7:A:2559:C:H2'   | 7:A:2560:A:H8    | 1.81                     | 0.46              |
| 7:A:2722:G:C8    | 7:A:2723:C:C5    | 3.04                     | 0.46              |
| 8:B:101:A:N7     | 8:B:102:G:C5     | 2.84                     | 0.46              |
| 8:B:123:U:O2'    | 8:B:290:C:O2     | 2.30                     | 0.46              |
| 8:B:769:G:H4'    | 8:B:1513:A:H4'   | 1.97                     | 0.46              |
| 10:D:189:ALA:HB3 | 10:D:196:ILE:HB  | 1.98                     | 0.46              |
| 21:O:54:ASP:HA   | 21:O:59:ARG:HD3  | 1.98                     | 0.46              |
| 33:b:129:THR:HB  | 33:b:191:THR:HB  | 1.98                     | 0.46              |
| 41:j:9:ASN:OD1   | 41:j:18:ARG:NH1  | 2.48                     | 0.46              |
| 41:j:42:THR:O    | 41:j:42:THR:OG1  | 2.33                     | 0.46              |
| 44:m:13:ASN:OD1  | 44:m:13:ASN:N    | 2.40                     | 0.46              |
| 2:1:34:THR:OG1   | 57:z:22:THR:O    | 2.34                     | 0.45              |
| 5:5:283:ARG:NE   | 5:5:405:GLU:OE1  | 2.44                     | 0.45              |
| 7:A:2529:G:H4'   | 37:f:175:LYS:HG3 | 1.97                     | 0.45              |
| 7:A:2691:C:C4    | 7:A:2719:G:N2    | 2.84                     | 0.45              |
| 7:A:2841:C:H2'   | 7:A:2842:G:H8    | 1.82                     | 0.45              |
| 8:B:108:G:N2     | 8:B:326:G:O6     | 2.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:G:48:ALA:N     | 25:S:66:SER:OG    | 2.49                     | 0.45              |
| 16:J:61:LEU:HD11  | 16:J:63:LEU:HD13  | 1.97                     | 0.45              |
| 33:b:2:ALA:N      | 33:b:199:GLU:OE2  | 2.49                     | 0.45              |
| 36:e:123:ASP:O    | 36:e:125:ARG:NH1  | 2.48                     | 0.45              |
| 7:A:629:G:N2      | 7:A:639:U:O3'     | 2.40                     | 0.45              |
| 7:A:1342:A:O2'    | 7:A:1344:U:OP2    | 2.26                     | 0.45              |
| 8:B:63:C:H42      | 8:B:104:G:H22     | 1.65                     | 0.45              |
| 8:B:875:U:O2      | 15:I:16:ASN:ND2   | 2.45                     | 0.45              |
| 8:B:1083:U:O3'    | 8:B:1086:U:N3     | 2.49                     | 0.45              |
| 8:B:1381:U:O2'    | 14:H:79:ARG:NH1   | 2.49                     | 0.45              |
| 16:J:128:SER:OG   | 16:J:129:LYS:N    | 2.49                     | 0.45              |
| 17:K:13:PHE:HE1   | 17:K:69:THR:HG22  | 1.81                     | 0.45              |
| 18:L:21:ALA:HB3   | 18:L:84:VAL:HG12  | 1.97                     | 0.45              |
| 23:Q:3:THR:N      | 23:Q:22:ALA:O     | 2.45                     | 0.45              |
| 35:d:97:ASN:ND2   | 35:d:100:MET:SD   | 2.90                     | 0.45              |
| 36:e:136:ILE:HD13 | 36:e:146:VAL:HG11 | 1.98                     | 0.45              |
| 4:3:135:ASP:HB2   | 4:3:140:LYS:HB2   | 1.98                     | 0.45              |
| 7:A:580:U:H2'     | 7:A:581:C:H6      | 1.80                     | 0.45              |
| 7:A:1341:G:H21    | 29:W:59:ASN:HD22  | 1.64                     | 0.45              |
| 7:A:1421:G:H21    | 7:A:1494:A:H61    | 1.65                     | 0.45              |
| 7:A:1595:C:H2'    | 7:A:1596:A:H8     | 1.81                     | 0.45              |
| 9:C:64:LYS:HE2    | 9:C:225:ARG:HB2   | 1.98                     | 0.45              |
| 14:H:27:VAL:HG12  | 14:H:43:VAL:HG11  | 1.97                     | 0.45              |
| 35:d:118:LEU:HD12 | 35:d:186:VAL:HB   | 1.98                     | 0.45              |
| 40:i:6:ALA:H      | 40:i:45:THR:HG21  | 1.81                     | 0.45              |
| 40:i:32:LEU:HD22  | 40:i:54:ILE:HG21  | 1.98                     | 0.45              |
| 7:A:820:A:C2      | 7:A:943:A:H4'     | 2.52                     | 0.45              |
| 7:A:1807:G:O2'    | 7:A:1809:A:N6     | 2.38                     | 0.45              |
| 8:B:318:G:H2'     | 8:B:319:G:H8      | 1.81                     | 0.45              |
| 8:B:1316:G:N1     | 8:B:1319:A:OP2    | 2.49                     | 0.45              |
| 14:H:21:GLU:O     | 14:H:25:LYS:N     | 2.44                     | 0.45              |
| 29:W:61:LEU:HD21  | 29:W:82:LYS:HE3   | 1.98                     | 0.45              |
| 45:n:99:TYR:OH    | 45:n:111:ARG:NH1  | 2.49                     | 0.45              |
| 47:p:66:ASN:OD1   | 47:p:70:ARG:NH1   | 2.49                     | 0.45              |
| 7:A:355:U:H2'     | 7:A:356:G:C8      | 2.50                     | 0.45              |
| 7:A:1846:G:N2     | 7:A:1848:A:H61    | 2.13                     | 0.45              |
| 8:B:65:A:H5'      | 8:B:200:G:H4'     | 1.98                     | 0.45              |
| 8:B:408:A:H5'     | 11:E:113:GLU:HB2  | 1.99                     | 0.45              |
| 8:B:585:G:N1      | 8:B:757:U:O2      | 2.49                     | 0.45              |
| 8:B:1374:A:H2'    | 8:B:1375:A:H8     | 1.82                     | 0.45              |
| 11:E:151:LYS:HA   | 11:E:155:VAL:HG23 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:N:15:ALA:HB1  | 20:N:34:LEU:HD11 | 1.98                     | 0.45              |
| 21:O:53:ARG:O    | 21:O:56:SER:OG   | 2.31                     | 0.45              |
| 56:y:17(A):G:O2' | 56:y:19:U:OP2    | 2.35                     | 0.45              |
| 3:2:6:SER:O      | 3:2:6:SER:OG     | 2.29                     | 0.45              |
| 5:5:332:LEU:HB3  | 5:5:336:LEU:HD22 | 1.98                     | 0.45              |
| 7:A:523:C:H2'    | 7:A:524:G:H8     | 1.81                     | 0.45              |
| 7:A:897:C:OP2    | 7:A:899:A:N6     | 2.38                     | 0.45              |
| 8:B:1343:G:H4'   | 16:J:124:ARG:HB3 | 1.98                     | 0.45              |
| 9:C:53:ALA:O     | 9:C:57:LEU:N     | 2.42                     | 0.45              |
| 14:H:108:ALA:HA  | 14:H:111:ARG:HD2 | 1.98                     | 0.45              |
| 19:M:37:VAL:N    | 19:M:76:GLU:OE2  | 2.49                     | 0.45              |
| 26:T:18:LYS:HD2  | 26:T:33:THR:HB   | 1.98                     | 0.45              |
| 1:O:45:SER:OG    | 7:A:126:A:OP1    | 2.32                     | 0.45              |
| 7:A:621:A:OP2    | 42:k:99:ASN:ND2  | 2.49                     | 0.45              |
| 7:A:1217:U:OP2   | 47:p:15:LYS:NZ   | 2.40                     | 0.45              |
| 7:A:2588:G:C6    | 7:A:2607:G:C2    | 3.05                     | 0.45              |
| 7:A:2655:G:O2'   | 7:A:2664:G:O6    | 2.30                     | 0.45              |
| 27:U:35:VAL:HG21 | 27:U:54:MET:HG2  | 1.99                     | 0.45              |
| 33:b:73:GLY:O    | 33:b:117:GLN:NE2 | 2.50                     | 0.45              |
| 4:3:135:ASP:OD1  | 4:3:135:ASP:N    | 2.35                     | 0.45              |
| 5:5:42:ASP:O     | 7:A:1337:G:O2'   | 2.23                     | 0.45              |
| 7:A:1089:A:O2'   | 7:A:1091:G:N7    | 2.41                     | 0.45              |
| 7:A:2678:C:H2'   | 7:A:2679:A:H8    | 1.81                     | 0.45              |
| 8:B:79:G:N2      | 8:B:90:C:O2      | 2.50                     | 0.45              |
| 8:B:680:C:H42    | 8:B:710:G:H1     | 1.63                     | 0.45              |
| 8:B:1069:C:O2'   | 8:B:1192:C:O2    | 2.34                     | 0.45              |
| 8:B:1234:C:O2'   | 8:B:1364:U:O2    | 2.30                     | 0.45              |
| 15:I:67:GLN:HB2  | 15:I:69:LYS:HG3  | 1.99                     | 0.45              |
| 22:P:48:LYS:HE2  | 22:P:48:LYS:HB2  | 1.84                     | 0.45              |
| 33:b:145:GLU:HB2 | 33:b:188:CYS:HB2 | 1.99                     | 0.45              |
| 39:h:3:LYS:HD3   | 39:h:3:LYS:HA    | 1.75                     | 0.45              |
| 40:i:116:ARG:O   | 40:i:120:ARG:NH2 | 2.50                     | 0.45              |
| 7:A:141:G:H22    | 29:W:1:MET:HE1   | 1.82                     | 0.45              |
| 7:A:172:A:H2'    | 7:A:173:A:C8     | 2.52                     | 0.45              |
| 7:A:351:C:H2'    | 7:A:352:A:C8     | 2.52                     | 0.45              |
| 7:A:2055:C:H5'   | 7:A:2056:G:OP1   | 2.17                     | 0.45              |
| 7:A:2446:G:O2'   | 7:A:2448:A:C8    | 2.70                     | 0.45              |
| 8:B:1386:G:H2'   | 8:B:1387:G:H8    | 1.82                     | 0.45              |
| 15:I:74:SER:H    | 15:I:130:ALA:HB2 | 1.82                     | 0.45              |
| 21:O:18:ASP:O    | 21:O:23:LYS:NZ   | 2.47                     | 0.45              |
| 41:j:17:ARG:HD3  | 41:j:17:ARG:HA   | 1.72                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:358:U:H2'    | 7:A:359:G:H8      | 1.81                     | 0.45              |
| 7:A:695:G:OP1    | 7:A:1380:G:O2'    | 2.34                     | 0.45              |
| 7:A:2315:G:H1'   | 36:e:125:ARG:HH21 | 1.82                     | 0.45              |
| 8:B:453:G:N7     | 8:B:479:U:N3      | 2.65                     | 0.45              |
| 8:B:1391:U:H2'   | 8:B:1392:G:H8     | 1.82                     | 0.45              |
| 16:J:4:ASN:OD1   | 16:J:4:ASN:N      | 2.49                     | 0.45              |
| 19:M:83:ARG:HB2  | 19:M:98:VAL:HG22  | 1.99                     | 0.45              |
| 22:P:67:LEU:HD21 | 22:P:87:LEU:HD23  | 1.99                     | 0.45              |
| 34:c:25:THR:HG21 | 34:c:193:VAL:HG11 | 1.98                     | 0.45              |
| 45:n:3:LYS:HE3   | 45:n:3:LYS:HB2    | 1.85                     | 0.45              |
| 49:r:69:LEU:HD22 | 49:r:107:VAL:HG22 | 1.98                     | 0.45              |
| 5:5:354:VAL:HB   | 5:5:407:ALA:HB1   | 2.00                     | 0.44              |
| 5:5:380:ASP:OD1  | 5:5:380:ASP:N     | 2.49                     | 0.44              |
| 7:A:138:U:H5'    | 29:W:1:MET:HG2    | 2.00                     | 0.44              |
| 7:A:641:U:O2     | 7:A:648:G:N2      | 2.50                     | 0.44              |
| 7:A:923:G:H2'    | 7:A:924:G:H8      | 1.82                     | 0.44              |
| 7:A:1063:G:N2    | 7:A:1075:C:O2'    | 2.45                     | 0.44              |
| 7:A:2562:U:H4'   | 41:j:25:LEU:HD22  | 1.99                     | 0.44              |
| 7:A:2711:A:C5    | 7:A:2714:G:N9     | 2.85                     | 0.44              |
| 7:A:2735:G:H2'   | 7:A:2736:A:H8     | 1.81                     | 0.44              |
| 8:B:41:G:N2      | 8:B:42:G:N7       | 2.59                     | 0.44              |
| 14:H:47:LEU:HG   | 14:H:58:GLU:HG2   | 1.99                     | 0.44              |
| 37:f:5:ALA:HB2   | 37:f:66:GLY:HA2   | 1.99                     | 0.44              |
| 45:n:34:HIS:ND1  | 45:n:53:THR:O     | 2.50                     | 0.44              |
| 48:q:48:LYS:HB3  | 48:q:48:LYS:HE3   | 1.84                     | 0.44              |
| 5:5:194:MET:HE2  | 5:5:194:MET:HB3   | 1.90                     | 0.44              |
| 7:A:1069:A:O2'   | 7:A:1097:U:OP1    | 2.29                     | 0.44              |
| 7:A:1386:C:H2'   | 7:A:1387:A:C8     | 2.52                     | 0.44              |
| 7:A:2400:G:N2    | 7:A:2401:U:O2     | 2.50                     | 0.44              |
| 8:B:410:G:H2'    | 8:B:429:U:C4      | 2.52                     | 0.44              |
| 23:Q:70:ARG:HA   | 23:Q:70:ARG:HD2   | 1.83                     | 0.44              |
| 44:m:90:ARG:HA   | 44:m:90:ARG:HD3   | 1.83                     | 0.44              |
| 50:s:49:VAL:HG22 | 50:s:51:ALA:H     | 1.81                     | 0.44              |
| 4:3:87:GLU:HA    | 4:3:99:LEU:HA     | 2.00                     | 0.44              |
| 7:A:23:G:C2      | 7:A:518:G:C2      | 3.06                     | 0.44              |
| 7:A:1287:A:O4'   | 44:m:103:ARG:NH1  | 2.50                     | 0.44              |
| 7:A:2438:U:O2'   | 7:A:2440:C:OP1    | 2.34                     | 0.44              |
| 7:A:2793:C:H42   | 7:A:2803:G:H1     | 1.64                     | 0.44              |
| 8:B:37:U:H2'     | 8:B:38:G:H8       | 1.83                     | 0.44              |
| 8:B:617:G:H1     | 8:B:623:C:H42     | 1.65                     | 0.44              |
| 8:B:1232:U:H5''  | 16:J:126:GLN:HB3  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:E:151:LYS:HB3 | 11:E:156:LYS:HG3 | 1.99                     | 0.44              |
| 27:U:5:LYS:HB3   | 27:U:8:LYS:HB2   | 2.00                     | 0.44              |
| 40:i:125:TYR:OH  | 40:i:132:HIS:NE2 | 2.49                     | 0.44              |
| 41:j:42:THR:HG22 | 41:j:57:VAL:HG12 | 2.00                     | 0.44              |
| 50:s:52:LEU:HD12 | 50:s:53:ASN:H    | 1.82                     | 0.44              |
| 3:2:26:ILE:HD13  | 3:2:26:ILE:HA    | 1.88                     | 0.44              |
| 7:A:190:A:H5''   | 7:A:204:A:H61    | 1.83                     | 0.44              |
| 7:A:873:C:O2'    | 43:l:64:TRP:NE1  | 2.43                     | 0.44              |
| 7:A:2112:G:N2    | 30:X:19:G:OP2    | 2.50                     | 0.44              |
| 7:A:2508:G:H1'   | 7:A:2582:G:H22   | 1.81                     | 0.44              |
| 7:A:2515:C:H42   | 7:A:2569:G:H1    | 1.64                     | 0.44              |
| 7:A:2516:A:C5    | 7:A:2517:C:N4    | 2.86                     | 0.44              |
| 8:B:81:A:H61     | 8:B:88:U:H3      | 1.66                     | 0.44              |
| 8:B:446:G:H21    | 8:B:488:C:N4     | 2.16                     | 0.44              |
| 13:G:3:HIS:HB3   | 13:G:95:ALA:HB2  | 1.99                     | 0.44              |
| 41:j:21:CYS:HB2  | 41:j:39:ILE:HD12 | 2.00                     | 0.44              |
| 7:A:1527:G:N1    | 7:A:1544:A:OP2   | 2.48                     | 0.44              |
| 7:A:1748:C:H2'   | 7:A:1749:A:C8    | 2.52                     | 0.44              |
| 7:A:2543:G:C6    | 7:A:2544:G:C6    | 3.06                     | 0.44              |
| 8:B:501:C:H1'    | 8:B:549:C:H1'    | 1.99                     | 0.44              |
| 30:X:7:U:H3'     | 30:X:13:C:H5     | 1.82                     | 0.44              |
| 30:X:51:C:H2'    | 30:X:52:G:H8     | 1.82                     | 0.44              |
| 33:b:8:PRO:HB3   | 33:b:14:ARG:HG3  | 2.00                     | 0.44              |
| 33:b:74:ILE:HA   | 33:b:75:PRO:HD3  | 1.88                     | 0.44              |
| 34:c:39:ASP:OD1  | 34:c:39:ASP:N    | 2.51                     | 0.44              |
| 47:p:24:TYR:O    | 47:p:29:SER:OG   | 2.30                     | 0.44              |
| 7:A:2446:G:O2'   | 7:A:2448:A:H8    | 2.01                     | 0.44              |
| 7:A:2516:A:C5    | 7:A:2517:C:C4    | 3.05                     | 0.44              |
| 8:B:363:A:N6     | 19:M:27:CYS:SG   | 2.90                     | 0.44              |
| 8:B:1342:C:H2'   | 8:B:1343:G:C8    | 2.50                     | 0.44              |
| 8:B:1384:C:H2'   | 8:B:1385:G:C8    | 2.53                     | 0.44              |
| 36:e:93:GLY:H    | 36:e:96:MET:HE2  | 1.82                     | 0.44              |
| 47:p:50:ARG:HH22 | 48:q:74:ILE:HG13 | 1.83                     | 0.44              |
| 55:x:27:LEU:HA   | 55:x:27:LEU:HD23 | 1.83                     | 0.44              |
| 7:A:1316:U:O2    | 7:A:1337:G:N2    | 2.51                     | 0.44              |
| 7:A:1339:G:N2    | 7:A:1603:A:N3    | 2.66                     | 0.44              |
| 7:A:1432:G:N2    | 7:A:1562:U:O2    | 2.51                     | 0.44              |
| 7:A:2089:C:H2'   | 7:A:2090:A:H8    | 1.82                     | 0.44              |
| 7:A:2292:U:H2'   | 7:A:2293:G:C8    | 2.53                     | 0.44              |
| 7:A:2722:G:H3'   | 7:A:2723:C:C5    | 2.52                     | 0.44              |
| 8:B:1175:G:H2'   | 8:B:1176:A:H8    | 1.82                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:B:1512:U:H2'   | 8:B:1513:A:H8     | 1.83                     | 0.44              |
| 12:F:38:VAL:HA   | 12:F:48:PHE:HA    | 1.98                     | 0.44              |
| 17:K:88:MET:SD   | 17:K:89:ARG:NH1   | 2.82                     | 0.44              |
| 20:N:12:HIS:H    | 20:N:45:ILE:HB    | 1.83                     | 0.44              |
| 37:f:159:GLY:O   | 37:f:163:ARG:NH1  | 2.50                     | 0.44              |
| 42:k:82:LEU:HD22 | 42:k:90:VAL:HG21  | 1.99                     | 0.44              |
| 43:l:54:THR:HA   | 43:l:57:VAL:HG12  | 2.00                     | 0.44              |
| 4:3:39:TYR:HB3   | 4:3:66:ARG:HH11   | 1.82                     | 0.44              |
| 7:A:954:G:N1     | 7:A:964:C:N3      | 2.65                     | 0.44              |
| 7:A:1749:A:H2'   | 7:A:1750:G:H8     | 1.82                     | 0.44              |
| 8:B:302:G:N2     | 8:B:556:C:O2'     | 2.51                     | 0.44              |
| 8:B:522:C:H42    | 8:B:528:C:H42     | 1.64                     | 0.44              |
| 8:B:644:U:H2'    | 8:B:645:G:H8      | 1.82                     | 0.44              |
| 8:B:880:C:H2'    | 8:B:881:G:H8      | 1.82                     | 0.44              |
| 8:B:1025:U:O2'   | 8:B:1033:G:O6     | 2.35                     | 0.44              |
| 8:B:1150:A:H4'   | 17:K:43:PRO:HG3   | 2.00                     | 0.44              |
| 8:B:1513:A:H2'   | 8:B:1514:G:H8     | 1.83                     | 0.44              |
| 13:G:64:VAL:HG12 | 13:G:66:ALA:HB2   | 2.00                     | 0.44              |
| 15:I:7:ILE:HG21  | 15:I:126:ILE:HD11 | 1.99                     | 0.44              |
| 20:N:19:LEU:HB2  | 20:N:30:SER:HB2   | 1.99                     | 0.44              |
| 33:b:53:HIS:O    | 33:b:217:ARG:N    | 2.47                     | 0.44              |
| 33:b:111:LYS:HE2 | 33:b:111:LYS:HB2  | 1.86                     | 0.44              |
| 36:e:142:ASP:OD1 | 36:e:142:ASP:N    | 2.46                     | 0.44              |
| 56:y:64:G:N2     | 56:y:66:C:OP1     | 2.49                     | 0.44              |
| 4:3:107:LYS:NZ   | 4:3:121:GLU:OE1   | 2.47                     | 0.44              |
| 7:A:992:C:H2'    | 7:A:993:G:C8      | 2.53                     | 0.44              |
| 7:A:994:C:H1'    | 48:q:10:LYS:HE2   | 1.98                     | 0.44              |
| 7:A:1636:U:H2'   | 7:A:1637:A:H8     | 1.83                     | 0.44              |
| 8:B:182:A:H8     | 8:B:193:C:H42     | 1.65                     | 0.44              |
| 8:B:552:U:O4     | 8:B:553:A:N6      | 2.51                     | 0.44              |
| 8:B:751:U:OP1    | 22:P:17:ARG:NH2   | 2.41                     | 0.44              |
| 32:a:6:G:H2'     | 32:a:7:G:H8       | 1.82                     | 0.44              |
| 36:e:26:MET:O    | 36:e:30:ARG:NH1   | 2.50                     | 0.44              |
| 42:k:55:MET:HB3  | 42:k:55:MET:HE2   | 1.69                     | 0.44              |
| 42:k:123:ARG:NH1 | 42:k:143:GLU:OE2  | 2.51                     | 0.44              |
| 44:m:25:ALA:HB1  | 44:m:48:VAL:HG13  | 1.99                     | 0.44              |
| 53:v:39:TRP:NE1  | 53:v:41:GLU:OE2   | 2.40                     | 0.44              |
| 7:A:277:G:H2'    | 7:A:361:G:C6      | 2.53                     | 0.43              |
| 7:A:2070:A:C2    | 7:A:2071:A:C5     | 3.05                     | 0.43              |
| 7:A:2471:A:N6    | 7:A:2476:A:O2'    | 2.51                     | 0.43              |
| 7:A:2499:C:N4    | 7:A:2500:U:O4     | 2.50                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:A:2508:G:C4    | 7:A:2582:G:N1    | 2.82                     | 0.43              |
| 8:B:120:A:O2'    | 8:B:122:G:N7     | 2.49                     | 0.43              |
| 8:B:530:G:H5''   | 8:B:531:U:H5''   | 1.99                     | 0.43              |
| 8:B:586:C:P      | 24:R:36:LYS:HZ1  | 2.41                     | 0.43              |
| 11:E:151:LYS:NZ  | 11:E:176:GLY:O   | 2.34                     | 0.43              |
| 4:3:63:SER:HA    | 5:5:395:MET:HE1  | 2.01                     | 0.43              |
| 8:B:140:U:H2'    | 8:B:141:G:C8     | 2.53                     | 0.43              |
| 23:Q:46:LYS:HB3  | 23:Q:46:LYS:HE2  | 1.77                     | 0.43              |
| 23:Q:77:GLU:OE1  | 23:Q:77:GLU:N    | 2.52                     | 0.43              |
| 24:R:22:VAL:HG12 | 24:R:45:HIS:HA   | 1.99                     | 0.43              |
| 27:U:10:ARG:HG3  | 27:U:13:GLN:HE21 | 1.81                     | 0.43              |
| 29:W:2:ILE:HG12  | 29:W:42:GLU:HG2  | 1.99                     | 0.43              |
| 48:q:61:ALA:HB2  | 48:q:98:ILE:HD13 | 1.99                     | 0.43              |
| 7:A:26:G:H8      | 7:A:26:G:O5'     | 2.01                     | 0.43              |
| 7:A:467:G:O2'    | 7:A:796:C:O2'    | 2.25                     | 0.43              |
| 7:A:1161:C:H2'   | 7:A:1162:G:H8    | 1.83                     | 0.43              |
| 7:A:1170:C:H42   | 7:A:1178:C:N4    | 2.16                     | 0.43              |
| 7:A:1297:C:OP1   | 7:A:2710:C:H4'   | 2.18                     | 0.43              |
| 7:A:1980:G:O2'   | 7:A:1982:U:OP2   | 2.33                     | 0.43              |
| 7:A:2711:A:C5    | 7:A:2714:G:C1'   | 3.01                     | 0.43              |
| 8:B:859:G:OP2    | 8:B:869:G:N1     | 2.43                     | 0.43              |
| 24:R:76:VAL:HG12 | 24:R:77:ARG:H    | 1.83                     | 0.43              |
| 33:b:259:SER:O   | 33:b:259:SER:OG  | 2.26                     | 0.43              |
| 35:d:171:ASP:OD1 | 35:d:171:ASP:N   | 2.46                     | 0.43              |
| 2:1:36:LYS:HB3   | 2:1:40:ARG:HD3   | 1.99                     | 0.43              |
| 7:A:5:A:H2'      | 7:A:6:A:C8       | 2.54                     | 0.43              |
| 7:A:499:U:H3     | 7:A:503:A:H62    | 1.66                     | 0.43              |
| 7:A:1062:G:N2    | 39:h:135:SER:O   | 2.45                     | 0.43              |
| 7:A:1845:G:OP1   | 33:b:256:LYS:NZ  | 2.41                     | 0.43              |
| 7:A:2578:G:C5    | 34:c:145:SER:HB3 | 2.52                     | 0.43              |
| 13:G:49:TYR:CZ   | 25:S:66:SER:HB2  | 2.53                     | 0.43              |
| 14:H:21:GLU:HA   | 14:H:24:ALA:HB3  | 2.01                     | 0.43              |
| 15:I:41:LYS:HB3  | 15:I:41:LYS:HE2  | 1.82                     | 0.43              |
| 19:M:50:ARG:HD2  | 19:M:50:ARG:HA   | 1.75                     | 0.43              |
| 23:Q:10:GLY:HA3  | 23:Q:15:PRO:HA   | 2.00                     | 0.43              |
| 48:q:14:VAL:HG12 | 48:q:20:VAL:HG11 | 2.01                     | 0.43              |
| 7:A:1168:G:N3    | 7:A:1182:G:N1    | 2.66                     | 0.43              |
| 7:A:1411:U:N3    | 7:A:1592:C:O2    | 2.51                     | 0.43              |
| 7:A:1676:A:N6    | 7:A:1677:A:N1    | 2.67                     | 0.43              |
| 7:A:2740:A:N6    | 7:A:2741:A:N1    | 2.65                     | 0.43              |
| 8:B:676:A:H1'    | 18:L:117:PRO:HB3 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:B:825:A:O2'    | 15:I:9:ASP:OD2   | 2.29                     | 0.43              |
| 8:B:835:U:H3     | 8:B:851:G:H1     | 1.66                     | 0.43              |
| 16:J:49:ARG:O    | 16:J:53:GLU:N    | 2.50                     | 0.43              |
| 20:N:81:MET:HE3  | 20:N:92:ARG:HG3  | 1.99                     | 0.43              |
| 24:R:15:ASP:O    | 24:R:17:MET:N    | 2.52                     | 0.43              |
| 24:R:19:LYS:NZ   | 24:R:48:ASP:O    | 2.46                     | 0.43              |
| 24:R:31:HIS:CD2  | 24:R:33:ILE:H    | 2.36                     | 0.43              |
| 29:W:40:LYS:HB3  | 29:W:60:THR:HG21 | 1.99                     | 0.43              |
| 54:w:9:LYS:HA    | 54:w:9:LYS:HD2   | 1.85                     | 0.43              |
| 7:A:720:U:H2'    | 7:A:721:A:H8     | 1.82                     | 0.43              |
| 7:A:1814:G:C4    | 7:A:1815:A:N7    | 2.86                     | 0.43              |
| 8:B:861:G:H1     | 8:B:868:C:H42    | 1.66                     | 0.43              |
| 9:C:64:LYS:HD3   | 9:C:64:LYS:HA    | 1.91                     | 0.43              |
| 12:F:157:ARG:HB2 | 15:I:45:PHE:HE1  | 1.83                     | 0.43              |
| 16:J:52:LEU:HD22 | 16:J:57:MET:HB3  | 2.01                     | 0.43              |
| 23:Q:42:ILE:H    | 23:Q:42:ILE:HG13 | 1.70                     | 0.43              |
| 26:T:12:ASP:O    | 26:T:16:LEU:N    | 2.51                     | 0.43              |
| 44:m:25:ALA:HB2  | 44:m:44:LEU:HD11 | 2.00                     | 0.43              |
| 5:5:254:LYS:HE2  | 5:5:254:LYS:HB3  | 1.82                     | 0.43              |
| 6:6:4:GLN:HA     | 7:A:2615:U:C2    | 2.53                     | 0.43              |
| 7:A:1627:G:H2'   | 7:A:1628:G:H8    | 1.83                     | 0.43              |
| 7:A:1846:G:C2'   | 8:B:702:A:H2     | 2.31                     | 0.43              |
| 8:B:223:A:N6     | 8:B:224:U:O2     | 2.52                     | 0.43              |
| 8:B:1090:U:HO2'  | 8:B:1171:A:HO2'  | 1.64                     | 0.43              |
| 8:B:1367:C:OP1   | 17:K:62:ARG:NH2  | 2.52                     | 0.43              |
| 10:D:49:LYS:HD2  | 10:D:49:LYS:HA   | 1.82                     | 0.43              |
| 12:F:41:ASP:N    | 12:F:41:ASP:OD1  | 2.52                     | 0.43              |
| 20:N:53:ILE:HD13 | 20:N:53:ILE:HA   | 1.90                     | 0.43              |
| 21:O:33:ASP:O    | 21:O:35:ASN:ND2  | 2.51                     | 0.43              |
| 22:P:32:LEU:O    | 22:P:36:ILE:N    | 2.40                     | 0.43              |
| 48:q:24:LYS:HB3  | 48:q:24:LYS:HE2  | 1.84                     | 0.43              |
| 7:A:1278:C:H2'   | 7:A:1279:G:H8    | 1.84                     | 0.43              |
| 7:A:1368:G:C2    | 7:A:1369:G:C6    | 3.07                     | 0.43              |
| 7:A:1368:G:N1    | 7:A:1369:G:O6    | 2.52                     | 0.43              |
| 7:A:1649:G:H1    | 7:A:2009:A:N6    | 2.17                     | 0.43              |
| 7:A:2453:A:C2    | 7:A:2504:U:C4    | 3.06                     | 0.43              |
| 8:B:375:U:H4'    | 23:Q:6:LEU:HD12  | 1.99                     | 0.43              |
| 8:B:607:A:H2'    | 8:B:608:A:C8     | 2.53                     | 0.43              |
| 11:E:3:ARG:HG3   | 11:E:115:ARG:NH2 | 2.33                     | 0.43              |
| 15:I:10:MET:HG3  | 15:I:27:MET:HE2  | 2.01                     | 0.43              |
| 16:J:6:TYR:CG    | 16:J:89:GLU:HB2  | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:d:131:THR:HG22 | 35:d:160:ALA:HA   | 2.00                     | 0.43              |
| 36:e:30:ARG:H     | 36:e:159:THR:HG22 | 1.82                     | 0.43              |
| 40:i:81:ILE:HD12  | 40:i:81:ILE:HA    | 1.81                     | 0.43              |
| 51:t:31:TYR:HB3   | 51:t:37:PRO:HB3   | 2.00                     | 0.43              |
| 8:B:981:U:H5''    | 21:O:63:ARG:HH21  | 1.84                     | 0.43              |
| 8:B:1300:G:N2     | 8:B:1301:U:O4     | 2.38                     | 0.43              |
| 12:F:53:ALA:HB2   | 12:F:62:LYS:HD3   | 2.00                     | 0.43              |
| 15:I:28:PRO:O     | 15:I:33:LYS:NZ    | 2.42                     | 0.43              |
| 19:M:67:ILE:HD13  | 19:M:97:THR:HG21  | 2.00                     | 0.43              |
| 20:N:11:ASP:N     | 20:N:11:ASP:OD1   | 2.51                     | 0.43              |
| 20:N:79:ARG:NH2   | 26:T:65:GLU:O     | 2.51                     | 0.43              |
| 20:N:91:HIS:HA    | 20:N:109:ARG:HH22 | 1.84                     | 0.43              |
| 36:e:80:ARG:HD3   | 36:e:80:ARG:HA    | 1.70                     | 0.43              |
| 39:h:101:ILE:HD11 | 39:h:106:LEU:HD21 | 2.01                     | 0.43              |
| 2:1:5:LYS:NZ      | 7:A:253:C:OP2     | 2.33                     | 0.43              |
| 7:A:806:C:O2      | 7:A:2444:G:O2'    | 2.31                     | 0.43              |
| 7:A:1604:C:O2'    | 7:A:1610:A:N1     | 2.49                     | 0.43              |
| 7:A:2543:G:C6     | 7:A:2544:G:C5     | 3.07                     | 0.43              |
| 7:A:2617:U:H2'    | 7:A:2618:G:H8     | 1.83                     | 0.43              |
| 7:A:2711:A:C4     | 7:A:2714:G:C1'    | 3.02                     | 0.43              |
| 7:A:2839:G:H4'    | 44:m:49:GLU:HB3   | 2.00                     | 0.43              |
| 8:B:459:A:H61     | 8:B:473:U:H3      | 1.67                     | 0.43              |
| 8:B:1404:C:H42    | 8:B:1497:G:H1     | 1.66                     | 0.43              |
| 11:E:97:ARG:HA    | 11:E:134:SER:HA   | 2.01                     | 0.43              |
| 11:E:102:VAL:HG23 | 11:E:114:ALA:HB1  | 2.01                     | 0.43              |
| 20:N:69:LEU:HD12  | 20:N:72:GLU:HB3   | 2.01                     | 0.43              |
| 32:a:50:A:OP1     | 45:n:68:LYS:N     | 2.52                     | 0.43              |
| 33:b:167:ARG:HG3  | 33:b:172:VAL:HG22 | 2.01                     | 0.43              |
| 7:A:1984:G:N2     | 7:A:1985:C:O2     | 2.52                     | 0.42              |
| 7:A:2345:G:O2'    | 7:A:2381:A:N3     | 2.43                     | 0.42              |
| 8:B:231:U:H2'     | 8:B:232:G:C8      | 2.54                     | 0.42              |
| 8:B:664:G:H22     | 8:B:741:G:H1      | 1.67                     | 0.42              |
| 8:B:720:C:H5'     | 25:S:41:PRO:HB3   | 2.01                     | 0.42              |
| 9:C:205:ASP:OD1   | 9:C:205:ASP:N     | 2.47                     | 0.42              |
| 10:D:139:GLN:O    | 10:D:143:ARG:N    | 2.41                     | 0.42              |
| 11:E:177:LYS:HD3  | 11:E:177:LYS:HA   | 1.80                     | 0.42              |
| 11:E:206:LYS:HB3  | 11:E:206:LYS:HE2  | 1.81                     | 0.42              |
| 14:H:35:LYS:HD2   | 14:H:35:LYS:HA    | 1.64                     | 0.42              |
| 15:I:102:ALA:N    | 15:I:113:ASP:OD1  | 2.52                     | 0.42              |
| 16:J:19:VAL:HG11  | 16:J:83:ILE:HA    | 2.01                     | 0.42              |
| 16:J:98:LEU:O     | 16:J:102:GLY:N    | 2.51                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 33:b:62:TYR:HE1   | 33:b:87:ARG:HH22 | 1.67                     | 0.42              |
| 36:e:16:LEU:HD22  | 36:e:20:PHE:HE2  | 1.84                     | 0.42              |
| 51:t:51:GLN:OE1   | 51:t:57:TYR:OH   | 2.32                     | 0.42              |
| 53:v:6:GLN:OE1    | 53:v:50:ARG:N    | 2.44                     | 0.42              |
| 2:1:31:HIS:HA     | 7:A:2420:C:H5    | 1.84                     | 0.42              |
| 4:3:1:SER:OG      | 4:3:2:VAL:N      | 2.50                     | 0.42              |
| 7:A:1992:G:N2     | 7:A:1996:C:O2    | 2.52                     | 0.42              |
| 8:B:41:G:N2       | 8:B:43:C:N3      | 2.67                     | 0.42              |
| 8:B:1124:G:O2'    | 8:B:1145:A:N6    | 2.49                     | 0.42              |
| 8:B:1221:G:OP1    | 8:B:1321:U:N3    | 2.52                     | 0.42              |
| 8:B:1259:C:O2'    | 8:B:1283:U:O2    | 2.33                     | 0.42              |
| 10:D:47:LEU:HD12  | 10:D:47:LEU:HA   | 1.75                     | 0.42              |
| 15:I:34:VAL:HG12  | 15:I:59:LEU:HD13 | 2.01                     | 0.42              |
| 21:O:75:ARG:HD3   | 21:O:75:ARG:HA   | 1.88                     | 0.42              |
| 22:P:4:SER:O      | 22:P:8:THR:OG1   | 2.33                     | 0.42              |
| 26:T:58:VAL:HA    | 26:T:59:PRO:HD3  | 1.86                     | 0.42              |
| 31:Z:53:G:N2      | 31:Z:57:G:OP1    | 2.52                     | 0.42              |
| 50:s:91:LYS:HB2   | 50:s:91:LYS:HE3  | 1.78                     | 0.42              |
| 7:A:1369:G:N3     | 7:A:1810:A:H2    | 2.17                     | 0.42              |
| 7:A:2636:C:O2'    | 34:c:45:TYR:OH   | 2.34                     | 0.42              |
| 7:A:2848:G:N7     | 46:o:95:ALA:HB2  | 2.34                     | 0.42              |
| 8:B:1237:C:H42    | 8:B:1337:G:H1    | 1.68                     | 0.42              |
| 11:E:198:HIS:CE1  | 12:F:103:THR:HG1 | 2.38                     | 0.42              |
| 15:I:74:SER:O     | 15:I:130:ALA:N   | 2.53                     | 0.42              |
| 17:K:65:TYR:HB3   | 21:O:96:LEU:HD11 | 2.00                     | 0.42              |
| 18:L:106:ARG:HH12 | 28:V:8:GLU:HG3   | 1.85                     | 0.42              |
| 19:M:83:ARG:HE    | 19:M:96:HIS:HB2  | 1.84                     | 0.42              |
| 24:R:12:VAL:HB    | 24:R:56:GLY:H    | 1.84                     | 0.42              |
| 27:U:45:ALA:O     | 27:U:49:LYS:N    | 2.49                     | 0.42              |
| 32:a:40:U:N3      | 32:a:44:G:OP2    | 2.36                     | 0.42              |
| 36:e:117:LEU:HB3  | 36:e:177:PHE:H   | 1.84                     | 0.42              |
| 7:A:579:G:C8      | 7:A:2017:U:O4    | 2.73                     | 0.42              |
| 7:A:2075:U:O2'    | 7:A:2596:U:N3    | 2.53                     | 0.42              |
| 7:A:2544:G:H2'    | 7:A:2545:G:H8    | 1.84                     | 0.42              |
| 8:B:220:G:H2'     | 8:B:221:C:O4'    | 2.20                     | 0.42              |
| 8:B:300:A:O2'     | 8:B:564:C:N3     | 2.52                     | 0.42              |
| 8:B:1005:A:H3'    | 8:B:1006:G:C8    | 2.54                     | 0.42              |
| 8:B:1065:U:H5''   | 8:B:1190:G:H22   | 1.85                     | 0.42              |
| 8:B:1401:G:O6     | 8:B:1504:G:N2    | 2.51                     | 0.42              |
| 33:b:196:GLY:O    | 33:b:198:ALA:N   | 2.52                     | 0.42              |
| 39:h:74:PRO:HA    | 39:h:75:PRO:HD3  | 1.82                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:p:91:ASP:OD1   | 47:p:91:ASP:N     | 2.45                     | 0.42              |
| 7:A:411:G:OP2     | 7:A:2406:A:O2'    | 2.28                     | 0.42              |
| 7:A:641:U:O2'     | 7:A:2350:C:OP1    | 2.36                     | 0.42              |
| 7:A:1636:U:H2'    | 7:A:1637:A:C8     | 2.55                     | 0.42              |
| 7:A:2463:C:H42    | 7:A:2487:G:H1     | 1.68                     | 0.42              |
| 7:A:2683:C:OP1    | 46:o:51:ARG:NH2   | 2.40                     | 0.42              |
| 8:B:186:C:H5''    | 27:U:77:ALA:HB2   | 2.01                     | 0.42              |
| 8:B:1441:A:H3'    | 8:B:1442:G:H8     | 1.85                     | 0.42              |
| 10:D:5:VAL:HG11   | 10:D:10:ILE:HD12  | 2.00                     | 0.42              |
| 10:D:22:TRP:HD1   | 10:D:58:GLU:HA    | 1.85                     | 0.42              |
| 11:E:117:LEU:HD21 | 11:E:155:VAL:HG11 | 2.02                     | 0.42              |
| 12:F:97:GLN:N     | 12:F:124:LEU:O    | 2.52                     | 0.42              |
| 36:e:4:LEU:HD12   | 36:e:101:GLU:HB3  | 2.02                     | 0.42              |
| 41:j:111:LYS:HE3  | 41:j:111:LYS:HB2  | 1.80                     | 0.42              |
| 49:r:74:ILE:HD12  | 49:r:105:VAL:HG22 | 2.01                     | 0.42              |
| 4:3:81:SER:N      | 4:3:105:LYS:O     | 2.51                     | 0.42              |
| 7:A:1625:C:N4     | 7:A:1626:A:N1     | 2.67                     | 0.42              |
| 7:A:1995:U:N3     | 7:A:1996:C:N3     | 2.68                     | 0.42              |
| 7:A:2016:U:H2'    | 7:A:2017:U:C6     | 2.54                     | 0.42              |
| 8:B:1078:U:H1'    | 12:F:135:ASN:HD21 | 1.85                     | 0.42              |
| 8:B:1115:U:H3     | 8:B:1185:G:H1     | 1.67                     | 0.42              |
| 8:B:1244:G:H1     | 8:B:1293:C:H42    | 1.67                     | 0.42              |
| 11:E:10:LYS:HA    | 11:E:13:ARG:HB2   | 2.01                     | 0.42              |
| 30:X:2:G:H2'      | 30:X:3:G:C8       | 2.55                     | 0.42              |
| 35:d:153:LEU:HD11 | 35:d:158:PHE:HB2  | 2.02                     | 0.42              |
| 40:i:56:VAL:HB    | 40:i:124:VAL:HG22 | 2.02                     | 0.42              |
| 48:q:4:VAL:HG23   | 48:q:39:LEU:HB2   | 2.01                     | 0.42              |
| 54:w:15:ASN:OD1   | 54:w:16:THR:N     | 2.50                     | 0.42              |
| 7:A:859:G:N2      | 7:A:917:A:OP2     | 2.33                     | 0.42              |
| 7:A:1999:C:H5''   | 7:A:2723:C:O2'    | 2.19                     | 0.42              |
| 8:B:108:G:P       | 8:B:326:G:H22     | 2.42                     | 0.42              |
| 8:B:121:U:H3'     | 8:B:122:G:H8      | 1.83                     | 0.42              |
| 8:B:193:C:N3      | 8:B:194:C:N4      | 2.67                     | 0.42              |
| 8:B:632:U:H5''    | 8:B:633:G:C8      | 2.54                     | 0.42              |
| 8:B:977:A:OP1     | 21:O:61:ARG:NH2   | 2.53                     | 0.42              |
| 8:B:1343:G:H5''   | 16:J:124:ARG:HH21 | 1.85                     | 0.42              |
| 12:F:92:SER:OG    | 12:F:135:ASN:O    | 2.24                     | 0.42              |
| 13:G:19:PRO:HA    | 13:G:22:ILE:HB    | 2.01                     | 0.42              |
| 16:J:45:ARG:HD3   | 16:J:45:ARG:H     | 1.84                     | 0.42              |
| 34:c:33:ARG:NH2   | 34:c:74:GLU:O     | 2.53                     | 0.42              |
| 36:e:144:ASP:N    | 36:e:144:ASP:OD1  | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:o:87:LYS:HA    | 46:o:87:LYS:HD3   | 1.69                     | 0.42              |
| 51:t:71:LYS:HA    | 51:t:71:LYS:HD2   | 1.92                     | 0.42              |
| 4:3:107:LYS:HD2   | 4:3:107:LYS:HA    | 1.75                     | 0.42              |
| 7:A:35:G:O2'      | 7:A:454:A:O4'     | 2.36                     | 0.42              |
| 7:A:882:G:H2'     | 7:A:883:G:C8      | 2.54                     | 0.42              |
| 7:A:1165:A:H2'    | 7:A:1166:G:H8     | 1.85                     | 0.42              |
| 8:B:11:G:H1       | 8:B:23:C:H42      | 1.67                     | 0.42              |
| 8:B:65:A:OP1      | 8:B:382:A:N6      | 2.52                     | 0.42              |
| 8:B:1354:U:H2'    | 8:B:1355:G:H8     | 1.84                     | 0.42              |
| 27:U:21:ASN:O     | 27:U:25:ARG:N     | 2.43                     | 0.42              |
| 30:X:18:G:H21     | 30:X:53:G:H21     | 1.66                     | 0.42              |
| 32:a:19:C:H2'     | 32:a:20:G:H8      | 1.84                     | 0.42              |
| 36:e:3:LYS:HD3    | 36:e:3:LYS:HA     | 1.76                     | 0.42              |
| 48:q:29:THR:O     | 48:q:29:THR:OG1   | 2.35                     | 0.42              |
| 4:3:32:ASP:OD1    | 4:3:32:ASP:N      | 2.46                     | 0.42              |
| 7:A:626:A:H2'     | 42:k:78:ARG:HH12  | 1.84                     | 0.42              |
| 7:A:2192:U:H2'    | 7:A:2193:G:C8     | 2.55                     | 0.42              |
| 8:B:464:U:C2      | 8:B:466:A:H5''    | 2.55                     | 0.42              |
| 10:D:108:LYS:HE2  | 10:D:144:LEU:HD13 | 2.02                     | 0.42              |
| 14:H:116:MET:HE3  | 14:H:120:LEU:HG   | 2.02                     | 0.42              |
| 17:K:64:GLN:O     | 21:O:99:ALA:N     | 2.48                     | 0.42              |
| 21:O:3:LYS:HB3    | 21:O:6:MET:HG2    | 2.02                     | 0.42              |
| 32:a:33:G:H2'     | 32:a:34:A:H8      | 1.83                     | 0.42              |
| 35:d:180:LEU:HD23 | 35:d:180:LEU:HA   | 1.84                     | 0.42              |
| 39:h:73:THR:HA    | 39:h:113:LYS:HG3  | 2.02                     | 0.42              |
| 46:o:92:VAL:HG11  | 46:o:97:LEU:HD11  | 2.02                     | 0.42              |
| 7:A:965:C:HO2'    | 7:A:2272:U:HO2'   | 1.66                     | 0.42              |
| 7:A:1062:G:N2     | 39:h:93:PRO:HG2   | 2.35                     | 0.42              |
| 7:A:1595:C:H2'    | 7:A:1596:A:C8     | 2.54                     | 0.42              |
| 7:A:1651:G:H4'    | 44:m:39:PRO:HG2   | 2.02                     | 0.42              |
| 8:B:735:C:H2'     | 8:B:736:C:H6      | 1.85                     | 0.42              |
| 8:B:757:U:OP1     | 8:B:822:U:O2'     | 2.37                     | 0.42              |
| 8:B:950:U:H2'     | 8:B:951:G:H8      | 1.83                     | 0.42              |
| 8:B:1317:C:C2     | 21:O:53:ARG:HD3   | 2.54                     | 0.42              |
| 11:E:95:GLU:HG3   | 11:E:104:ARG:HE   | 1.85                     | 0.42              |
| 24:R:62:ARG:NH1   | 24:R:63:GLU:O     | 2.53                     | 0.42              |
| 25:S:25:ASP:HB3   | 25:S:28:THR:HB    | 2.01                     | 0.42              |
| 33:b:7:LYS:HE3    | 33:b:7:LYS:HB3    | 1.86                     | 0.42              |
| 34:c:156:PHE:CG   | 40:i:81:ILE:HG12  | 2.55                     | 0.42              |
| 38:g:5:LEU:HA     | 38:g:5:LEU:HD23   | 1.87                     | 0.42              |
| 57:z:33:LYS:HD2   | 57:z:51:GLU:HB2   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:A:1919:A:N1     | 8:B:1495:U:O2'   | 2.45                     | 0.41              |
| 7:A:2198:A:C4     | 38:g:29:PHE:HB2  | 2.54                     | 0.41              |
| 7:A:2351:G:H2'    | 7:A:2365:G:H22   | 1.84                     | 0.41              |
| 7:A:2559:C:H2'    | 7:A:2560:A:C8    | 2.55                     | 0.41              |
| 7:A:2676:C:H2'    | 7:A:2677:G:H8    | 1.85                     | 0.41              |
| 8:B:101:A:C6      | 8:B:102:G:C5     | 3.08                     | 0.41              |
| 8:B:711:G:H2'     | 8:B:712:A:C8     | 2.55                     | 0.41              |
| 11:E:51:TYR:O     | 11:E:55:LEU:N    | 2.45                     | 0.41              |
| 25:S:34:THR:HG22  | 25:S:38:LYS:H    | 1.84                     | 0.41              |
| 30:X:49:G:H2'     | 30:X:50:G:H8     | 1.84                     | 0.41              |
| 7:A:186:G:H2'     | 7:A:187:G:H8     | 1.85                     | 0.41              |
| 7:A:1710:G:H2'    | 7:A:1711:A:C8    | 2.54                     | 0.41              |
| 8:B:98:A:C8       | 8:B:99:C:C5      | 3.08                     | 0.41              |
| 9:C:115:LYS:NZ    | 9:C:152:LYS:O    | 2.43                     | 0.41              |
| 11:E:9:LEU:HD13   | 11:E:34:ILE:HD11 | 2.02                     | 0.41              |
| 11:E:139:PRO:HA   | 11:E:182:PHE:HB2 | 2.03                     | 0.41              |
| 15:I:105:SER:HB3  | 15:I:124:GLU:HG3 | 2.02                     | 0.41              |
| 16:J:9:THR:H      | 16:J:85:ARG:HD2  | 1.84                     | 0.41              |
| 24:R:72:SER:O     | 24:R:72:SER:OG   | 2.31                     | 0.41              |
| 27:U:67:ILE:HG13  | 27:U:71:LYS:HD3  | 2.00                     | 0.41              |
| 30:X:1:G:H2'      | 30:X:2:G:C5      | 2.55                     | 0.41              |
| 51:t:34:LYS:HA    | 51:t:34:LYS:HD2  | 1.87                     | 0.41              |
| 7:A:832:U:OP1     | 42:k:38:GLN:N    | 2.50                     | 0.41              |
| 7:A:1037:G:H22    | 7:A:1119:U:H1'   | 1.85                     | 0.41              |
| 8:B:303:A:O2'     | 8:B:555:U:O2'    | 2.35                     | 0.41              |
| 8:B:1288:A:N6     | 8:B:1371:G:O2'   | 2.43                     | 0.41              |
| 8:B:1522:U:H2'    | 8:B:1523:G:H8    | 1.85                     | 0.41              |
| 14:H:140:ASP:HA   | 14:H:143:ARG:HG3 | 2.01                     | 0.41              |
| 21:O:24:ARG:HA    | 21:O:27:LEU:HB2  | 2.02                     | 0.41              |
| 33:b:142:HIS:ND1  | 33:b:193:GLY:O   | 2.53                     | 0.41              |
| 37:f:23:VAL:HB    | 37:f:36:THR:HG23 | 2.01                     | 0.41              |
| 37:f:95:ARG:HD3   | 37:f:95:ARG:HA   | 1.91                     | 0.41              |
| 46:o:100:LEU:HD23 | 46:o:100:LEU:HA  | 1.89                     | 0.41              |
| 56:y:67:C:H2'     | 56:y:68:G:H8     | 1.85                     | 0.41              |
| 7:A:1491:G:O2'    | 33:b:100:GLU:OE1 | 2.38                     | 0.41              |
| 7:A:1832:C:N4     | 7:A:1833:C:N3    | 2.69                     | 0.41              |
| 7:A:2035:G:H5''   | 7:A:2036:C:H5    | 1.84                     | 0.41              |
| 8:B:264:C:O2'     | 24:R:66:PRO:O    | 2.32                     | 0.41              |
| 8:B:916:U:H2'     | 8:B:917:G:H8     | 1.85                     | 0.41              |
| 8:B:978:A:OP1     | 8:B:1361:G:N1    | 2.53                     | 0.41              |
| 8:B:1025:U:H5''   | 8:B:1026:G:C8    | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:1086:U:O2'    | 8:B:1087:G:O4'    | 2.38                     | 0.41              |
| 8:B:1297:G:C2     | 14:H:114:LYS:HB3  | 2.56                     | 0.41              |
| 13:G:40:GLU:HB3   | 13:G:42:TRP:NE1   | 2.35                     | 0.41              |
| 16:J:22:LYS:HB3   | 16:J:62:ASP:HB2   | 2.03                     | 0.41              |
| 32:a:116:G:H2'    | 32:a:117:G:C8     | 2.55                     | 0.41              |
| 34:c:142:VAL:HG22 | 34:c:143:PRO:HD2  | 2.01                     | 0.41              |
| 36:e:38:MET:HE2   | 36:e:38:MET:HB3   | 1.91                     | 0.41              |
| 40:i:142:ILE:HD12 | 40:i:142:ILE:HA   | 1.90                     | 0.41              |
| 54:w:21:LEU:HA    | 54:w:21:LEU:HD23  | 1.82                     | 0.41              |
| 7:A:72:U:O4       | 54:w:58:ASN:ND2   | 2.53                     | 0.41              |
| 7:A:447:A:OP1     | 47:p:5:LYS:NZ     | 2.54                     | 0.41              |
| 7:A:882:G:H2'     | 7:A:883:G:H8      | 1.85                     | 0.41              |
| 7:A:1278:C:H2'    | 7:A:1279:G:C8     | 2.55                     | 0.41              |
| 7:A:1305:C:N4     | 7:A:1607:C:OP1    | 2.53                     | 0.41              |
| 7:A:2297:A:C5     | 7:A:2320:U:C2     | 3.08                     | 0.41              |
| 7:A:2332:C:O2'    | 7:A:2335:A:N3     | 2.45                     | 0.41              |
| 7:A:2398:U:H2'    | 7:A:2399:G:H8     | 1.84                     | 0.41              |
| 8:B:449:G:H2'     | 8:B:450:G:C8      | 2.55                     | 0.41              |
| 8:B:946:A:H2'     | 8:B:947:G:C8      | 2.55                     | 0.41              |
| 10:D:31:ASP:OD1   | 10:D:31:ASP:N     | 2.49                     | 0.41              |
| 16:J:18:ARG:HE    | 16:J:66:THR:HG22  | 1.86                     | 0.41              |
| 18:L:101:ASN:HB3  | 18:L:107:ILE:HD12 | 2.03                     | 0.41              |
| 22:P:10:LYS:O     | 22:P:13:SER:OG    | 2.31                     | 0.41              |
| 22:P:74:ASP:OD2   | 22:P:77:ARG:NH1   | 2.54                     | 0.41              |
| 33:b:175:ARG:HD3  | 33:b:181:MET:HE2  | 2.02                     | 0.41              |
| 33:b:195:VAL:H    | 33:b:195:VAL:HG12 | 1.68                     | 0.41              |
| 36:e:115:ARG:HB2  | 36:e:178:ARG:HD3  | 2.03                     | 0.41              |
| 7:A:28:A:O2'      | 7:A:582:A:O2'     | 2.31                     | 0.41              |
| 7:A:86:G:O2'      | 7:A:104:A:O2'     | 2.33                     | 0.41              |
| 7:A:1508:A:O2'    | 7:A:1509:A:O4'    | 2.30                     | 0.41              |
| 7:A:2128:G:N1     | 7:A:2161:C:O2'    | 2.49                     | 0.41              |
| 8:B:186:C:N4      | 8:B:187:G:O6      | 2.53                     | 0.41              |
| 8:B:527:G:O6      | 19:M:46:ASN:ND2   | 2.54                     | 0.41              |
| 8:B:1071:C:H2'    | 8:B:1072:G:H8     | 1.86                     | 0.41              |
| 17:K:7:ARG:H      | 17:K:102:LEU:HA   | 1.85                     | 0.41              |
| 17:K:57:VAL:HG22  | 17:K:58:ASN:H     | 1.85                     | 0.41              |
| 18:L:55:SER:O     | 18:L:58:SER:OG    | 2.37                     | 0.41              |
| 36:e:103:LEU:HD12 | 36:e:138:PHE:HZ   | 1.85                     | 0.41              |
| 45:n:30:ARG:HD3   | 45:n:102:ARG:HE   | 1.86                     | 0.41              |
| 53:v:32:ASN:HD22  | 53:v:53:ALA:HB2   | 1.85                     | 0.41              |
| 2:1:15:LYS:HB2    | 2:1:23:LYS:HE2    | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:1171:G:O6     | 7:A:1178:C:N4     | 2.44                     | 0.41              |
| 7:A:1395:A:O2'    | 7:A:1396:U:H5''   | 2.21                     | 0.41              |
| 7:A:1480:C:H42    | 7:A:1511:G:H1     | 1.69                     | 0.41              |
| 7:A:1769:U:H2'    | 7:A:1770:G:C8     | 2.55                     | 0.41              |
| 7:A:2548:U:O2     | 41:j:23:LYS:NZ    | 2.48                     | 0.41              |
| 7:A:2818:U:H2'    | 7:A:2819:G:C8     | 2.56                     | 0.41              |
| 8:B:191:G:H2'     | 8:B:192:A:H8      | 1.86                     | 0.41              |
| 8:B:253:A:OP1     | 24:R:69:LYS:NZ    | 2.47                     | 0.41              |
| 8:B:1284:C:H3'    | 8:B:1285:A:H8     | 1.84                     | 0.41              |
| 11:E:18:ASP:OD1   | 11:E:18:ASP:N     | 2.54                     | 0.41              |
| 12:F:71:MET:HE2   | 12:F:71:MET:HB3   | 1.96                     | 0.41              |
| 12:F:133:PRO:HA   | 12:F:136:VAL:HG22 | 2.03                     | 0.41              |
| 13:G:47:LEU:HD12  | 25:S:66:SER:HB3   | 2.01                     | 0.41              |
| 18:L:113:VAL:HA   | 25:S:73:ARG:HD2   | 2.03                     | 0.41              |
| 22:P:47:LYS:HA    | 22:P:47:LYS:HD3   | 1.86                     | 0.41              |
| 32:a:44:G:N3      | 32:a:47:C:N4      | 2.58                     | 0.41              |
| 35:d:148:ILE:HB   | 35:d:169:VAL:HG22 | 2.03                     | 0.41              |
| 37:f:123:ALA:HA   | 37:f:133:LEU:HA   | 2.03                     | 0.41              |
| 4:3:28:GLN:NE2    | 4:3:113:ARG:O     | 2.54                     | 0.41              |
| 7:A:778:G:H5'     | 33:b:48:ARG:HH11  | 1.85                     | 0.41              |
| 7:A:909:A:N6      | 7:A:912:C:O2      | 2.53                     | 0.41              |
| 7:A:1358:G:N7     | 7:A:1371:G:C6     | 2.89                     | 0.41              |
| 7:A:1369:G:N2     | 7:A:1370:C:C2     | 2.89                     | 0.41              |
| 7:A:1666:G:O6     | 7:A:1667:G:N2     | 2.54                     | 0.41              |
| 8:B:389:A:N6      | 8:B:390:U:O2      | 2.54                     | 0.41              |
| 8:B:398:U:H2'     | 8:B:399:G:C8      | 2.55                     | 0.41              |
| 8:B:1113:C:H42    | 8:B:1187:G:H1     | 1.68                     | 0.41              |
| 9:C:97:LEU:HD23   | 9:C:97:LEU:HA     | 1.92                     | 0.41              |
| 10:D:54:ARG:HE    | 10:D:54:ARG:HB3   | 1.68                     | 0.41              |
| 11:E:77:LYS:HA    | 11:E:77:LYS:HD3   | 1.87                     | 0.41              |
| 18:L:17:SER:HA    | 18:L:79:ILE:HA    | 2.02                     | 0.41              |
| 18:L:113:VAL:HG23 | 25:S:73:ARG:HD2   | 2.01                     | 0.41              |
| 30:X:9:A:H1'      | 30:X:45:G:H2'     | 2.02                     | 0.41              |
| 34:c:33:ARG:NH1   | 34:c:53:GLY:O     | 2.46                     | 0.41              |
| 34:c:159:LYS:HA   | 34:c:159:LYS:HD2  | 1.87                     | 0.41              |
| 35:d:48:THR:HG22  | 35:d:86:ALA:HB2   | 2.02                     | 0.41              |
| 41:j:69:VAL:HG11  | 41:j:104:THR:HG21 | 2.01                     | 0.41              |
| 43:l:74:THR:OG1   | 43:l:75:GLU:N     | 2.54                     | 0.41              |
| 43:l:132:THR:OG1  | 43:l:133:LYS:N    | 2.54                     | 0.41              |
| 4:3:7:HIS:HD2     | 4:3:94:PRO:HD3    | 1.86                     | 0.41              |
| 7:A:571:U:N3      | 7:A:2030:A:C6     | 2.88                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:675:A:OP1    | 35:d:58:LYS:NZ    | 2.47                     | 0.41              |
| 7:A:762:U:N3     | 7:A:1431:A:OP1    | 2.54                     | 0.41              |
| 7:A:866:A:N6     | 7:A:914:G:N7      | 2.69                     | 0.41              |
| 7:A:2116:G:O4'   | 7:A:2165:C:N4     | 2.38                     | 0.41              |
| 7:A:2265:U:H3'   | 7:A:2266:A:H8     | 1.85                     | 0.41              |
| 7:A:2403:C:N3    | 7:A:2415:G:C2     | 2.89                     | 0.41              |
| 7:A:2811:G:N2    | 7:A:2889:C:O2     | 2.41                     | 0.41              |
| 8:B:729:A:H2'    | 8:B:730:G:C8      | 2.56                     | 0.41              |
| 8:B:1081:A:H5'   | 12:F:23:LYS:HG3   | 2.03                     | 0.41              |
| 8:B:1116:U:H2'   | 8:B:1117:A:C8     | 2.55                     | 0.41              |
| 8:B:1141:C:H1'   | 8:B:1142:G:H5'    | 2.03                     | 0.41              |
| 9:C:87:CYS:H     | 9:C:89:GLN:NE2    | 2.18                     | 0.41              |
| 9:C:208:ARG:HH12 | 9:C:212:LEU:HD13  | 1.86                     | 0.41              |
| 17:K:12:ALA:HB3  | 17:K:18:ILE:HD12  | 2.03                     | 0.41              |
| 27:U:35:VAL:HG12 | 27:U:39:ILE:HD11  | 2.02                     | 0.41              |
| 27:U:36:TYR:HA   | 27:U:39:ILE:HD12  | 2.03                     | 0.41              |
| 36:e:134:GLU:HB3 | 36:e:149:VAL:HG22 | 2.02                     | 0.41              |
| 38:g:4:ILE:HD13  | 38:g:18:GLN:HG2   | 2.02                     | 0.41              |
| 47:p:41:LYS:HA   | 47:p:41:LYS:HD2   | 1.86                     | 0.41              |
| 54:w:56:LEU:HD23 | 54:w:56:LEU:HA    | 1.87                     | 0.41              |
| 4:3:3:LEU:HD23   | 4:3:37:THR:HG21   | 2.03                     | 0.41              |
| 7:A:107:G:H2'    | 7:A:108:G:H8      | 1.86                     | 0.41              |
| 7:A:2156:G:C5    | 7:A:2157:G:H1'    | 2.56                     | 0.41              |
| 7:A:2354:C:H2'   | 7:A:2355:G:C8     | 2.56                     | 0.41              |
| 7:A:2744:G:H21   | 37:f:143:GLN:HE22 | 1.68                     | 0.41              |
| 8:B:643:C:H5'    | 15:I:32:LEU:HD13  | 2.02                     | 0.41              |
| 8:B:839:C:O2     | 8:B:847:G:N2      | 2.48                     | 0.41              |
| 8:B:1116:U:H2'   | 8:B:1117:A:H8     | 1.86                     | 0.41              |
| 14:H:68:ASN:HB3  | 14:H:130:ASN:HB3  | 2.03                     | 0.41              |
| 18:L:21:ALA:N    | 18:L:83:GLU:O     | 2.54                     | 0.41              |
| 24:R:19:LYS:HZ3  | 24:R:49:GLU:HA    | 1.86                     | 0.41              |
| 31:Z:53:G:H5'    | 43:l:59:ARG:HH12  | 1.86                     | 0.41              |
| 36:e:120:LYS:HA  | 36:e:167:ARG:HH21 | 1.86                     | 0.41              |
| 49:r:4:ILE:HA    | 49:r:106:VAL:HG12 | 2.03                     | 0.41              |
| 4:3:56:ARG:NH2   | 4:3:76:GLU:OE2    | 2.45                     | 0.40              |
| 7:A:277:G:H1'    | 7:A:278:A:C6      | 2.56                     | 0.40              |
| 7:A:1188:U:H2'   | 7:A:1189:A:H8     | 1.86                     | 0.40              |
| 7:A:1769:U:H2'   | 7:A:1770:G:H8     | 1.86                     | 0.40              |
| 7:A:2577:A:O5'   | 7:A:2577:A:H8     | 2.04                     | 0.40              |
| 8:B:652:U:O4     | 8:B:752:G:O2'     | 2.36                     | 0.40              |
| 8:B:894:G:H2'    | 8:B:895:G:H8      | 1.85                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:1071:C:H2'    | 8:B:1072:G:C8     | 2.55                     | 0.40              |
| 9:C:163:VAL:HG11  | 9:C:173:ILE:HD11  | 2.03                     | 0.40              |
| 19:M:108:LYS:HA   | 19:M:108:LYS:HD3  | 1.94                     | 0.40              |
| 20:N:90:ARG:HA    | 20:N:93:ARG:HE    | 1.87                     | 0.40              |
| 31:Z:33:U:H1'     | 31:Z:35:U:H5''    | 2.03                     | 0.40              |
| 33:b:117:GLN:N    | 33:b:128:ASN:OD1  | 2.50                     | 0.40              |
| 33:b:161:TYR:CD2  | 33:b:194:GLU:HG2  | 2.56                     | 0.40              |
| 33:b:171:TYR:HD1  | 33:b:171:TYR:HA   | 1.73                     | 0.40              |
| 36:e:111:ILE:HG23 | 36:e:114:PHE:HB2  | 2.02                     | 0.40              |
| 40:i:1:MET:HE3    | 40:i:1:MET:HB3    | 1.74                     | 0.40              |
| 40:i:2:LYS:HB2    | 40:i:2:LYS:HE3    | 1.93                     | 0.40              |
| 46:o:71:GLU:OE2   | 46:o:101:ARG:NE   | 2.52                     | 0.40              |
| 49:r:3:THR:O      | 49:r:3:THR:OG1    | 2.32                     | 0.40              |
| 7:A:2579:C:C3'    | 7:A:2579:C:C6     | 3.04                     | 0.40              |
| 7:A:2836:U:H2'    | 7:A:2837:A:H8     | 1.87                     | 0.40              |
| 8:B:2:A:O2'       | 11:E:83:LYS:NZ    | 2.41                     | 0.40              |
| 8:B:327:A:O2'     | 8:B:329:A:O4'     | 2.40                     | 0.40              |
| 8:B:1253:G:H2'    | 8:B:1254:A:C8     | 2.56                     | 0.40              |
| 13:G:62:MET:HB3   | 13:G:64:VAL:HG23  | 2.02                     | 0.40              |
| 14:H:31:MET:HB2   | 14:H:31:MET:HE3   | 1.85                     | 0.40              |
| 21:O:29:ALA:HA    | 21:O:32:SER:HB3   | 2.02                     | 0.40              |
| 36:e:164:GLU:O    | 36:e:168:ALA:N    | 2.48                     | 0.40              |
| 37:f:126:PRO:HD3  | 37:f:132:VAL:HG12 | 2.03                     | 0.40              |
| 46:o:28:VAL:HG23  | 46:o:84:ILE:HG12  | 2.04                     | 0.40              |
| 54:w:4:LYS:HA     | 54:w:7:ARG:HH21   | 1.86                     | 0.40              |
| 54:w:15:ASN:O     | 54:w:19:LEU:N     | 2.53                     | 0.40              |
| 7:A:281:C:H2'     | 7:A:282:A:C8      | 2.56                     | 0.40              |
| 7:A:1091:G:N2     | 7:A:1099:G:O6     | 2.54                     | 0.40              |
| 7:A:1478:G:H1     | 7:A:1513:U:H3     | 1.69                     | 0.40              |
| 7:A:2252:G:N2     | 56:y:74:C:O2      | 2.43                     | 0.40              |
| 7:A:2425:A:H4'    | 7:A:2426:A:H5''   | 2.03                     | 0.40              |
| 8:B:522:C:H42     | 8:B:528:C:N4      | 2.20                     | 0.40              |
| 8:B:686:U:O2'     | 8:B:703:G:N2      | 2.52                     | 0.40              |
| 8:B:702:A:H8      | 8:B:702:A:C5'     | 2.34                     | 0.40              |
| 25:S:72:ASP:OD1   | 25:S:72:ASP:N     | 2.51                     | 0.40              |
| 28:V:40:LYS:HA    | 28:V:40:LYS:HD2   | 1.78                     | 0.40              |
| 34:c:8:LYS:HB2    | 34:c:201:LEU:HD11 | 2.03                     | 0.40              |
| 34:c:83:ARG:HD2   | 34:c:83:ARG:HA    | 1.88                     | 0.40              |
| 36:e:56:ASP:OD1   | 36:e:57:LEU:N     | 2.55                     | 0.40              |
| 56:y:29:U:H2'     | 56:y:30:G:H8      | 1.86                     | 0.40              |
| 2:1:59:ILE:HD12   | 2:1:59:ILE:HA     | 1.91                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:5:4:SER:OG     | 5:5:16:THR:O      | 2.35                     | 0.40              |
| 7:A:155:A:H2'    | 7:A:156:A:C8      | 2.57                     | 0.40              |
| 7:A:226:A:N6     | 7:A:227:A:N1      | 2.69                     | 0.40              |
| 7:A:863:A:H2'    | 7:A:864:G:H8      | 1.87                     | 0.40              |
| 7:A:1164:C:H2'   | 7:A:1165:A:H8     | 1.85                     | 0.40              |
| 8:B:397:A:O2'    | 8:B:399:G:OP2     | 2.33                     | 0.40              |
| 8:B:1377:A:C5    | 14:H:7:ILE:HD13   | 2.56                     | 0.40              |
| 14:H:117:ALA:O   | 14:H:121:ALA:N    | 2.48                     | 0.40              |
| 20:N:80:LEU:HB3  | 20:N:88:GLY:HA3   | 2.04                     | 0.40              |
| 23:Q:67:ILE:HG23 | 23:Q:71:VAL:HB    | 2.03                     | 0.40              |
| 32:a:95:U:H2'    | 32:a:96:G:C8      | 2.57                     | 0.40              |
| 36:e:162:SER:OG  | 36:e:165:GLU:OE1  | 2.26                     | 0.40              |
| 37:f:137:ASP:OD2 | 37:f:140:VAL:N    | 2.43                     | 0.40              |
| 44:m:8:ARG:HD2   | 44:m:43:GLU:HB2   | 2.03                     | 0.40              |
| 44:m:50:PRO:O    | 44:m:53:THR:OG1   | 2.35                     | 0.40              |
| 46:o:30:VAL:HG11 | 46:o:72:ARG:HH21  | 1.87                     | 0.40              |
| 7:A:1310:G:O6    | 7:A:1311:G:N2     | 2.54                     | 0.40              |
| 7:A:1340:U:OP1   | 29:W:84:TYR:OH    | 2.31                     | 0.40              |
| 7:A:1814:G:N7    | 7:A:1815:A:C8     | 2.89                     | 0.40              |
| 8:B:1346:A:OP1   | 16:J:122:ARG:NH1  | 2.43                     | 0.40              |
| 10:D:155:GLY:HA2 | 10:D:163:ALA:HB1  | 2.02                     | 0.40              |
| 12:F:81:LEU:HD12 | 12:F:120:VAL:HG11 | 2.03                     | 0.40              |
| 20:N:4:ILE:HD12  | 20:N:4:ILE:HA     | 1.97                     | 0.40              |
| 21:O:4:GLN:HA    | 21:O:7:LYS:HB2    | 2.04                     | 0.40              |
| 21:O:9:ARG:O     | 21:O:13:ARG:NH1   | 2.55                     | 0.40              |
| 24:R:17:MET:HE1  | 24:R:45:HIS:CE1   | 2.57                     | 0.40              |
| 32:a:33:G:H2'    | 32:a:34:A:C8      | 2.56                     | 0.40              |
| 33:b:142:HIS:CE1 | 33:b:191:THR:HG23 | 2.56                     | 0.40              |
| 41:j:47:ILE:HA   | 41:j:48:PRO:HD3   | 1.96                     | 0.40              |
| 45:n:35:ILE:N    | 45:n:53:THR:OG1   | 2.52                     | 0.40              |
| 47:p:95:LEU:HD23 | 47:p:95:LEU:HA    | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | 0     | 44/46 (96%)    | 41 (93%)  | 3 (7%)   | 0        | 100         | 100 |
| 2   | 1     | 62/65 (95%)    | 51 (82%)  | 9 (14%)  | 2 (3%)   | 3           | 24  |
| 3   | 2     | 36/38 (95%)    | 30 (83%)  | 5 (14%)  | 1 (3%)   | 4           | 27  |
| 4   | 3     | 166/169 (98%)  | 145 (87%) | 21 (13%) | 0        | 100         | 100 |
| 5   | 5     | 430/432 (100%) | 387 (90%) | 43 (10%) | 0        | 100         | 100 |
| 6   | 6     | 54/57 (95%)    | 45 (83%)  | 8 (15%)  | 1 (2%)   | 6           | 34  |
| 9   | C     | 216/241 (90%)  | 178 (82%) | 38 (18%) | 0        | 100         | 100 |
| 10  | D     | 204/233 (88%)  | 176 (86%) | 28 (14%) | 0        | 100         | 100 |
| 11  | E     | 203/206 (98%)  | 179 (88%) | 24 (12%) | 0        | 100         | 100 |
| 12  | F     | 148/167 (89%)  | 114 (77%) | 34 (23%) | 0        | 100         | 100 |
| 13  | G     | 98/135 (73%)   | 84 (86%)  | 14 (14%) | 0        | 100         | 100 |
| 14  | H     | 149/179 (83%)  | 138 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 15  | I     | 127/130 (98%)  | 119 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 16  | J     | 125/130 (96%)  | 111 (89%) | 14 (11%) | 0        | 100         | 100 |
| 17  | K     | 96/103 (93%)   | 84 (88%)  | 12 (12%) | 0        | 100         | 100 |
| 18  | L     | 115/129 (89%)  | 92 (80%)  | 23 (20%) | 0        | 100         | 100 |
| 19  | M     | 121/124 (98%)  | 95 (78%)  | 26 (22%) | 0        | 100         | 100 |
| 20  | N     | 112/118 (95%)  | 97 (87%)  | 13 (12%) | 2 (2%)   | 6           | 35  |
| 21  | O     | 92/101 (91%)   | 81 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 22  | P     | 86/89 (97%)    | 78 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 23  | Q     | 80/82 (98%)    | 66 (82%)  | 14 (18%) | 0        | 100         | 100 |
| 24  | R     | 78/84 (93%)    | 58 (74%)  | 19 (24%) | 1 (1%)   | 9           | 41  |
| 25  | S     | 53/75 (71%)    | 51 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 26  | T     | 77/92 (84%)    | 69 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 27  | U     | 83/87 (95%)    | 78 (94%)  | 4 (5%)   | 1 (1%)   | 10          | 42  |
| 28  | V     | 49/71 (69%)    | 37 (76%)  | 12 (24%) | 0        | 100         | 100 |
| 29  | W     | 94/100 (94%)   | 80 (85%)  | 14 (15%) | 0        | 100         | 100 |
| 33  | b     | 269/273 (98%)  | 230 (86%) | 39 (14%) | 0        | 100         | 100 |
| 34  | c     | 207/209 (99%)  | 187 (90%) | 18 (9%)  | 2 (1%)   | 12          | 46  |
| 35  | d     | 199/201 (99%)  | 185 (93%) | 14 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 36  | e     | 175/179 (98%)   | 153 (87%)  | 22 (13%)  | 0        | 100         | 100 |
| 37  | f     | 174/177 (98%)   | 159 (91%)  | 13 (8%)   | 2 (1%)   | 11          | 44  |
| 38  | g     | 45/149 (30%)    | 34 (76%)   | 11 (24%)  | 0        | 100         | 100 |
| 39  | h     | 139/142 (98%)   | 115 (83%)  | 24 (17%)  | 0        | 100         | 100 |
| 40  | i     | 140/142 (99%)   | 126 (90%)  | 14 (10%)  | 0        | 100         | 100 |
| 41  | j     | 120/123 (98%)   | 89 (74%)   | 30 (25%)  | 1 (1%)   | 16          | 52  |
| 42  | k     | 141/144 (98%)   | 121 (86%)  | 19 (14%)  | 1 (1%)   | 18          | 55  |
| 43  | l     | 134/136 (98%)   | 118 (88%)  | 13 (10%)  | 3 (2%)   | 5           | 31  |
| 44  | m     | 118/127 (93%)   | 99 (84%)   | 17 (14%)  | 2 (2%)   | 7           | 36  |
| 45  | n     | 114/117 (97%)   | 103 (90%)  | 11 (10%)  | 0        | 100         | 100 |
| 46  | o     | 112/115 (97%)   | 97 (87%)   | 15 (13%)  | 0        | 100         | 100 |
| 47  | p     | 115/118 (98%)   | 109 (95%)  | 6 (5%)    | 0        | 100         | 100 |
| 48  | q     | 101/103 (98%)   | 85 (84%)   | 16 (16%)  | 0        | 100         | 100 |
| 49  | r     | 108/110 (98%)   | 99 (92%)   | 9 (8%)    | 0        | 100         | 100 |
| 50  | s     | 100/104 (96%)   | 81 (81%)   | 17 (17%)  | 2 (2%)   | 6           | 33  |
| 51  | t     | 92/94 (98%)     | 87 (95%)   | 5 (5%)    | 0        | 100         | 100 |
| 52  | u     | 73/85 (86%)     | 62 (85%)   | 11 (15%)  | 0        | 100         | 100 |
| 53  | v     | 75/78 (96%)     | 64 (85%)   | 11 (15%)  | 0        | 100         | 100 |
| 54  | w     | 61/63 (97%)     | 54 (88%)   | 7 (12%)   | 0        | 100         | 100 |
| 55  | x     | 56/59 (95%)     | 51 (91%)   | 5 (9%)    | 0        | 100         | 100 |
| 57  | z     | 48/55 (87%)     | 42 (88%)   | 6 (12%)   | 0        | 100         | 100 |
| All | All   | 6114/6586 (93%) | 5314 (87%) | 779 (13%) | 21 (0%)  | 37          | 70  |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 32  | ILE  |
| 20  | N     | 67  | GLY  |
| 37  | f     | 48  | ASN  |
| 2   | 1     | 33  | LEU  |
| 3   | 2     | 21  | GLY  |
| 6   | 6     | 55  | ILE  |
| 24  | R     | 71  | LYS  |
| 27  | U     | 69  | LYS  |
| 37  | f     | 47  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | k     | 82  | LEU  |
| 43  | l     | 59  | ARG  |
| 50  | s     | 90  | GLY  |
| 34  | c     | 152 | PRO  |
| 20  | N     | 66  | GLU  |
| 34  | c     | 149 | ASN  |
| 43  | l     | 70  | ASP  |
| 44  | m     | 3   | HIS  |
| 44  | m     | 71  | ARG  |
| 41  | j     | 93  | GLN  |
| 43  | l     | 69  | PRO  |
| 50  | s     | 51  | ALA  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 0     | 38/38 (100%)   | 37 (97%)   | 1 (3%)   | 40          | 61  |
| 2   | 1     | 51/52 (98%)    | 50 (98%)   | 1 (2%)   | 48          | 66  |
| 3   | 2     | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 148/149 (99%)  | 148 (100%) | 0        | 100         | 100 |
| 5   | 5     | 359/359 (100%) | 359 (100%) | 0        | 100         | 100 |
| 6   | 6     | 47/48 (98%)    | 46 (98%)   | 1 (2%)   | 47          | 65  |
| 9   | C     | 180/199 (90%)  | 180 (100%) | 0        | 100         | 100 |
| 10  | D     | 170/190 (90%)  | 166 (98%)  | 4 (2%)   | 43          | 63  |
| 11  | E     | 172/173 (99%)  | 171 (99%)  | 1 (1%)   | 78          | 80  |
| 12  | F     | 113/126 (90%)  | 113 (100%) | 0        | 100         | 100 |
| 13  | G     | 87/116 (75%)   | 86 (99%)   | 1 (1%)   | 65          | 74  |
| 14  | H     | 124/147 (84%)  | 124 (100%) | 0        | 100         | 100 |
| 15  | I     | 104/105 (99%)  | 103 (99%)  | 1 (1%)   | 68          | 76  |
| 16  | J     | 105/107 (98%)  | 105 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 17  | K     | 86/90 (96%)    | 85 (99%)   | 1 (1%)   | 63          | 73  |
| 18  | L     | 90/99 (91%)    | 90 (100%)  | 0        | 100         | 100 |
| 19  | M     | 103/104 (99%)  | 103 (100%) | 0        | 100         | 100 |
| 20  | N     | 92/96 (96%)    | 90 (98%)   | 2 (2%)   | 45          | 64  |
| 21  | O     | 79/84 (94%)    | 79 (100%)  | 0        | 100         | 100 |
| 22  | P     | 75/77 (97%)    | 75 (100%)  | 0        | 100         | 100 |
| 23  | Q     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 24  | R     | 74/78 (95%)    | 74 (100%)  | 0        | 100         | 100 |
| 25  | S     | 48/65 (74%)    | 48 (100%)  | 0        | 100         | 100 |
| 26  | T     | 70/79 (89%)    | 70 (100%)  | 0        | 100         | 100 |
| 27  | U     | 65/66 (98%)    | 64 (98%)   | 1 (2%)   | 57          | 70  |
| 28  | V     | 44/61 (72%)    | 43 (98%)   | 1 (2%)   | 44          | 64  |
| 29  | W     | 83/84 (99%)    | 82 (99%)   | 1 (1%)   | 63          | 73  |
| 33  | b     | 216/218 (99%)  | 210 (97%)  | 6 (3%)   | 38          | 59  |
| 34  | c     | 164/164 (100%) | 160 (98%)  | 4 (2%)   | 43          | 63  |
| 35  | d     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 36  | e     | 148/150 (99%)  | 146 (99%)  | 2 (1%)   | 59          | 71  |
| 37  | f     | 137/138 (99%)  | 136 (99%)  | 1 (1%)   | 76          | 79  |
| 38  | g     | 38/114 (33%)   | 38 (100%)  | 0        | 100         | 100 |
| 39  | h     | 109/110 (99%)  | 108 (99%)  | 1 (1%)   | 70          | 76  |
| 40  | i     | 116/116 (100%) | 113 (97%)  | 3 (3%)   | 40          | 61  |
| 41  | j     | 103/104 (99%)  | 101 (98%)  | 2 (2%)   | 50          | 67  |
| 42  | k     | 102/103 (99%)  | 100 (98%)  | 2 (2%)   | 48          | 66  |
| 43  | l     | 109/109 (100%) | 108 (99%)  | 1 (1%)   | 70          | 76  |
| 44  | m     | 100/103 (97%)  | 98 (98%)   | 2 (2%)   | 48          | 66  |
| 45  | n     | 86/87 (99%)    | 86 (100%)  | 0        | 100         | 100 |
| 46  | o     | 99/100 (99%)   | 99 (100%)  | 0        | 100         | 100 |
| 47  | p     | 89/90 (99%)    | 88 (99%)   | 1 (1%)   | 65          | 74  |
| 48  | q     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 49  | r     | 93/93 (100%)   | 92 (99%)   | 1 (1%)   | 65          | 74  |
| 50  | s     | 83/85 (98%)    | 82 (99%)   | 1 (1%)   | 63          | 73  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 51  | t     | 78/78 (100%)    | 77 (99%)   | 1 (1%)   | 61          | 72  |
| 52  | u     | 56/63 (89%)     | 55 (98%)   | 1 (2%)   | 51          | 67  |
| 53  | v     | 67/68 (98%)     | 67 (100%)  | 0        | 100         | 100 |
| 54  | w     | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| 55  | x     | 48/49 (98%)     | 48 (100%)  | 0        | 100         | 100 |
| 57  | z     | 45/49 (92%)     | 45 (100%)  | 0        | 100         | 100 |
| All | All   | 5096/5386 (95%) | 5051 (99%) | 45 (1%)  | 68          | 76  |

All (45) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 44  | VAL  |
| 2   | 1     | 33  | LEU  |
| 6   | 6     | 25  | VAL  |
| 10  | D     | 15  | VAL  |
| 10  | D     | 19  | ASN  |
| 10  | D     | 144 | LEU  |
| 10  | D     | 149 | ILE  |
| 11  | E     | 129 | VAL  |
| 13  | G     | 18  | VAL  |
| 15  | I     | 104 | VAL  |
| 17  | K     | 14  | ASP  |
| 20  | N     | 17  | ILE  |
| 20  | N     | 65  | VAL  |
| 27  | U     | 39  | ILE  |
| 28  | V     | 32  | VAL  |
| 29  | W     | 85  | VAL  |
| 33  | b     | 19  | VAL  |
| 33  | b     | 65  | VAL  |
| 33  | b     | 114 | ASP  |
| 33  | b     | 171 | TYR  |
| 33  | b     | 221 | ARG  |
| 33  | b     | 257 | THR  |
| 34  | c     | 133 | THR  |
| 34  | c     | 142 | VAL  |
| 34  | c     | 197 | THR  |
| 34  | c     | 203 | VAL  |
| 36  | e     | 152 | LEU  |
| 36  | e     | 169 | LEU  |
| 37  | f     | 98  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | h     | 71  | THR  |
| 40  | i     | 17  | VAL  |
| 40  | i     | 30  | THR  |
| 40  | i     | 52  | ASP  |
| 41  | j     | 10  | VAL  |
| 41  | j     | 61  | VAL  |
| 42  | k     | 89  | VAL  |
| 42  | k     | 121 | THR  |
| 43  | l     | 89  | VAL  |
| 44  | m     | 37  | THR  |
| 44  | m     | 51  | LEU  |
| 47  | p     | 34  | VAL  |
| 49  | r     | 74  | ILE  |
| 50  | s     | 59  | VAL  |
| 51  | t     | 90  | ASP  |
| 52  | u     | 71  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 13  | ASN  |
| 2   | 1     | 28  | ASN  |
| 3   | 2     | 13  | ASN  |
| 3   | 2     | 37  | GLN  |
| 4   | 3     | 7   | HIS  |
| 5   | 5     | 2   | GLN  |
| 5   | 5     | 34  | ASN  |
| 5   | 5     | 236 | ASN  |
| 5   | 5     | 298 | ASN  |
| 5   | 5     | 328 | GLN  |
| 5   | 5     | 358 | ASN  |
| 5   | 5     | 400 | ASN  |
| 5   | 5     | 406 | GLN  |
| 9   | C     | 42  | ASN  |
| 9   | C     | 89  | GLN  |
| 9   | C     | 177 | ASN  |
| 10  | D     | 19  | ASN  |
| 10  | D     | 123 | GLN  |
| 11  | E     | 74  | ASN  |
| 12  | F     | 148 | ASN  |
| 13  | G     | 3   | HIS  |
| 15  | I     | 18  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | I     | 67  | GLN  |
| 16  | J     | 4   | ASN  |
| 16  | J     | 25  | ASN  |
| 16  | J     | 75  | GLN  |
| 17  | K     | 56  | HIS  |
| 18  | L     | 119 | ASN  |
| 19  | M     | 59  | ASN  |
| 19  | M     | 96  | HIS  |
| 21  | O     | 4   | GLN  |
| 21  | O     | 35  | ASN  |
| 21  | O     | 62  | ASN  |
| 22  | P     | 37  | ASN  |
| 22  | P     | 62  | GLN  |
| 23  | Q     | 63  | GLN  |
| 23  | Q     | 79  | ASN  |
| 24  | R     | 31  | HIS  |
| 26  | T     | 69  | HIS  |
| 27  | U     | 70  | ASN  |
| 27  | U     | 82  | GLN  |
| 28  | V     | 9   | ASN  |
| 29  | W     | 70  | HIS  |
| 29  | W     | 91  | GLN  |
| 29  | W     | 92  | ASN  |
| 34  | c     | 32  | ASN  |
| 34  | c     | 49  | GLN  |
| 35  | d     | 9   | GLN  |
| 35  | d     | 136 | GLN  |
| 35  | d     | 165 | HIS  |
| 36  | e     | 37  | ASN  |
| 36  | e     | 63  | GLN  |
| 37  | f     | 22  | GLN  |
| 37  | f     | 45  | HIS  |
| 37  | f     | 88  | GLN  |
| 37  | f     | 104 | ASN  |
| 37  | f     | 116 | GLN  |
| 37  | f     | 143 | GLN  |
| 38  | g     | 2   | GLN  |
| 39  | h     | 31  | GLN  |
| 40  | i     | 47  | HIS  |
| 40  | i     | 86  | GLN  |
| 40  | i     | 130 | HIS  |
| 41  | j     | 3   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | j     | 93  | GLN  |
| 42  | k     | 35  | HIS  |
| 43  | l     | 22  | GLN  |
| 44  | m     | 3   | HIS  |
| 44  | m     | 11  | ASN  |
| 44  | m     | 73  | ASN  |
| 45  | n     | 38  | GLN  |
| 45  | n     | 43  | ASN  |
| 46  | o     | 77  | HIS  |
| 47  | p     | 37  | GLN  |
| 47  | p     | 71  | GLN  |
| 49  | r     | 7   | HIS  |
| 50  | s     | 54  | GLN  |
| 50  | s     | 69  | ASN  |
| 51  | t     | 5   | ASN  |
| 51  | t     | 49  | ASN  |
| 54  | w     | 27  | ASN  |
| 54  | w     | 31  | GLN  |
| 54  | w     | 38  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 30  | X     | 58/73 (79%)     | 30 (51%)          | 0               |
| 31  | Z     | 58/76 (76%)     | 24 (41%)          | 1 (1%)          |
| 32  | a     | 117/118 (99%)   | 21 (17%)          | 0               |
| 56  | y     | 63/77 (81%)     | 19 (30%)          | 0               |
| 7   | A     | 2902/2903 (99%) | 740 (25%)         | 13 (0%)         |
| 8   | B     | 1538/1539 (99%) | 427 (27%)         | 3 (0%)          |
| All | All   | 4736/4786 (98%) | 1261 (26%)        | 17 (0%)         |

All (1261) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 10  | A    |
| 7   | A     | 14  | A    |
| 7   | A     | 23  | G    |
| 7   | A     | 34  | U    |
| 7   | A     | 42  | A    |
| 7   | A     | 45  | G    |
| 7   | A     | 46  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 51  | G    |
| 7   | A     | 54  | G    |
| 7   | A     | 58  | G    |
| 7   | A     | 62  | U    |
| 7   | A     | 63  | A    |
| 7   | A     | 66  | C    |
| 7   | A     | 71  | A    |
| 7   | A     | 74  | A    |
| 7   | A     | 75  | G    |
| 7   | A     | 78  | U    |
| 7   | A     | 80  | G    |
| 7   | A     | 84  | A    |
| 7   | A     | 96  | C    |
| 7   | A     | 100 | U    |
| 7   | A     | 101 | A    |
| 7   | A     | 103 | A    |
| 7   | A     | 107 | G    |
| 7   | A     | 112 | U    |
| 7   | A     | 113 | U    |
| 7   | A     | 118 | A    |
| 7   | A     | 119 | A    |
| 7   | A     | 120 | U    |
| 7   | A     | 126 | A    |
| 7   | A     | 128 | C    |
| 7   | A     | 129 | C    |
| 7   | A     | 138 | U    |
| 7   | A     | 139 | U    |
| 7   | A     | 140 | C    |
| 7   | A     | 141 | G    |
| 7   | A     | 142 | A    |
| 7   | A     | 149 | A    |
| 7   | A     | 162 | U    |
| 7   | A     | 163 | C    |
| 7   | A     | 178 | G    |
| 7   | A     | 196 | A    |
| 7   | A     | 199 | A    |
| 7   | A     | 200 | U    |
| 7   | A     | 204 | A    |
| 7   | A     | 215 | G    |
| 7   | A     | 216 | A    |
| 7   | A     | 222 | A    |
| 7   | A     | 225 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 226 | A    |
| 7   | A     | 228 | C    |
| 7   | A     | 229 | C    |
| 7   | A     | 245 | G    |
| 7   | A     | 248 | G    |
| 7   | A     | 255 | A    |
| 7   | A     | 265 | A    |
| 7   | A     | 266 | G    |
| 7   | A     | 271 | G    |
| 7   | A     | 272 | A    |
| 7   | A     | 275 | C    |
| 7   | A     | 276 | U    |
| 7   | A     | 278 | A    |
| 7   | A     | 279 | A    |
| 7   | A     | 281 | C    |
| 7   | A     | 282 | A    |
| 7   | A     | 298 | G    |
| 7   | A     | 309 | A    |
| 7   | A     | 311 | A    |
| 7   | A     | 322 | A    |
| 7   | A     | 323 | C    |
| 7   | A     | 324 | A    |
| 7   | A     | 329 | G    |
| 7   | A     | 330 | A    |
| 7   | A     | 331 | C    |
| 7   | A     | 335 | C    |
| 7   | A     | 354 | A    |
| 7   | A     | 361 | G    |
| 7   | A     | 362 | A    |
| 7   | A     | 363 | G    |
| 7   | A     | 371 | A    |
| 7   | A     | 372 | G    |
| 7   | A     | 379 | G    |
| 7   | A     | 380 | G    |
| 7   | A     | 386 | G    |
| 7   | A     | 399 | U    |
| 7   | A     | 404 | A    |
| 7   | A     | 405 | U    |
| 7   | A     | 406 | G    |
| 7   | A     | 407 | G    |
| 7   | A     | 411 | G    |
| 7   | A     | 412 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 420 | C    |
| 7   | A     | 424 | G    |
| 7   | A     | 428 | A    |
| 7   | A     | 448 | U    |
| 7   | A     | 455 | C    |
| 7   | A     | 457 | A    |
| 7   | A     | 464 | U    |
| 7   | A     | 465 | G    |
| 7   | A     | 467 | G    |
| 7   | A     | 473 | G    |
| 7   | A     | 477 | A    |
| 7   | A     | 479 | A    |
| 7   | A     | 480 | A    |
| 7   | A     | 481 | G    |
| 7   | A     | 484 | C    |
| 7   | A     | 489 | G    |
| 7   | A     | 490 | C    |
| 7   | A     | 491 | G    |
| 7   | A     | 494 | G    |
| 7   | A     | 496 | G    |
| 7   | A     | 501 | A    |
| 7   | A     | 505 | A    |
| 7   | A     | 507 | A    |
| 7   | A     | 508 | A    |
| 7   | A     | 509 | C    |
| 7   | A     | 527 | C    |
| 7   | A     | 529 | A    |
| 7   | A     | 530 | G    |
| 7   | A     | 531 | C    |
| 7   | A     | 532 | A    |
| 7   | A     | 536 | G    |
| 7   | A     | 543 | G    |
| 7   | A     | 544 | C    |
| 7   | A     | 545 | U    |
| 7   | A     | 546 | U    |
| 7   | A     | 548 | G    |
| 7   | A     | 549 | G    |
| 7   | A     | 550 | C    |
| 7   | A     | 560 | C    |
| 7   | A     | 563 | A    |
| 7   | A     | 567 | U    |
| 7   | A     | 569 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 572 | A    |
| 7   | A     | 573 | U    |
| 7   | A     | 575 | A    |
| 7   | A     | 586 | A    |
| 7   | A     | 597 | G    |
| 7   | A     | 603 | A    |
| 7   | A     | 614 | A    |
| 7   | A     | 615 | U    |
| 7   | A     | 616 | A    |
| 7   | A     | 620 | G    |
| 7   | A     | 622 | G    |
| 7   | A     | 628 | G    |
| 7   | A     | 632 | A    |
| 7   | A     | 634 | C    |
| 7   | A     | 637 | A    |
| 7   | A     | 639 | U    |
| 7   | A     | 643 | A    |
| 7   | A     | 644 | A    |
| 7   | A     | 645 | C    |
| 7   | A     | 646 | U    |
| 7   | A     | 647 | G    |
| 7   | A     | 648 | G    |
| 7   | A     | 654 | A    |
| 7   | A     | 655 | A    |
| 7   | A     | 656 | G    |
| 7   | A     | 664 | G    |
| 7   | A     | 670 | A    |
| 7   | A     | 677 | A    |
| 7   | A     | 686 | U    |
| 7   | A     | 690 | G    |
| 7   | A     | 695 | G    |
| 7   | A     | 713 | G    |
| 7   | A     | 714 | U    |
| 7   | A     | 718 | A    |
| 7   | A     | 728 | G    |
| 7   | A     | 729 | G    |
| 7   | A     | 730 | A    |
| 7   | A     | 736 | C    |
| 7   | A     | 738 | G    |
| 7   | A     | 747 | U    |
| 7   | A     | 748 | G    |
| 7   | A     | 749 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 763 | G    |
| 7   | A     | 764 | A    |
| 7   | A     | 765 | C    |
| 7   | A     | 766 | U    |
| 7   | A     | 775 | G    |
| 7   | A     | 776 | G    |
| 7   | A     | 782 | A    |
| 7   | A     | 783 | A    |
| 7   | A     | 784 | G    |
| 7   | A     | 785 | G    |
| 7   | A     | 789 | A    |
| 7   | A     | 792 | A    |
| 7   | A     | 793 | A    |
| 7   | A     | 797 | G    |
| 7   | A     | 800 | A    |
| 7   | A     | 803 | U    |
| 7   | A     | 805 | G    |
| 7   | A     | 811 | U    |
| 7   | A     | 812 | C    |
| 7   | A     | 819 | A    |
| 7   | A     | 827 | U    |
| 7   | A     | 828 | U    |
| 7   | A     | 830 | G    |
| 7   | A     | 841 | G    |
| 7   | A     | 845 | A    |
| 7   | A     | 846 | U    |
| 7   | A     | 847 | U    |
| 7   | A     | 858 | G    |
| 7   | A     | 859 | G    |
| 7   | A     | 866 | A    |
| 7   | A     | 873 | C    |
| 7   | A     | 878 | A    |
| 7   | A     | 885 | C    |
| 7   | A     | 887 | U    |
| 7   | A     | 888 | C    |
| 7   | A     | 890 | C    |
| 7   | A     | 891 | G    |
| 7   | A     | 894 | U    |
| 7   | A     | 896 | A    |
| 7   | A     | 898 | C    |
| 7   | A     | 899 | A    |
| 7   | A     | 904 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 907  | G    |
| 7   | A     | 910  | A    |
| 7   | A     | 914  | G    |
| 7   | A     | 921  | C    |
| 7   | A     | 929  | U    |
| 7   | A     | 932  | U    |
| 7   | A     | 935  | C    |
| 7   | A     | 941  | A    |
| 7   | A     | 946  | C    |
| 7   | A     | 947  | A    |
| 7   | A     | 957  | C    |
| 7   | A     | 961  | C    |
| 7   | A     | 968  | C    |
| 7   | A     | 973  | A    |
| 7   | A     | 974  | G    |
| 7   | A     | 975  | A    |
| 7   | A     | 976  | G    |
| 7   | A     | 981  | A    |
| 7   | A     | 983  | A    |
| 7   | A     | 985  | C    |
| 7   | A     | 989  | G    |
| 7   | A     | 990  | A    |
| 7   | A     | 995  | C    |
| 7   | A     | 996  | A    |
| 7   | A     | 1002 | G    |
| 7   | A     | 1003 | G    |
| 7   | A     | 1005 | C    |
| 7   | A     | 1012 | U    |
| 7   | A     | 1013 | C    |
| 7   | A     | 1021 | A    |
| 7   | A     | 1022 | G    |
| 7   | A     | 1023 | U    |
| 7   | A     | 1026 | G    |
| 7   | A     | 1032 | A    |
| 7   | A     | 1033 | U    |
| 7   | A     | 1040 | A    |
| 7   | A     | 1045 | C    |
| 7   | A     | 1046 | A    |
| 7   | A     | 1047 | G    |
| 7   | A     | 1056 | G    |
| 7   | A     | 1060 | U    |
| 7   | A     | 1061 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1062 | G    |
| 7   | A     | 1063 | G    |
| 7   | A     | 1064 | C    |
| 7   | A     | 1065 | U    |
| 7   | A     | 1066 | U    |
| 7   | A     | 1067 | A    |
| 7   | A     | 1068 | G    |
| 7   | A     | 1070 | A    |
| 7   | A     | 1071 | G    |
| 7   | A     | 1072 | C    |
| 7   | A     | 1073 | A    |
| 7   | A     | 1074 | G    |
| 7   | A     | 1075 | C    |
| 7   | A     | 1076 | C    |
| 7   | A     | 1079 | C    |
| 7   | A     | 1080 | A    |
| 7   | A     | 1081 | U    |
| 7   | A     | 1087 | G    |
| 7   | A     | 1088 | A    |
| 7   | A     | 1089 | A    |
| 7   | A     | 1091 | G    |
| 7   | A     | 1097 | U    |
| 7   | A     | 1098 | A    |
| 7   | A     | 1100 | C    |
| 7   | A     | 1102 | C    |
| 7   | A     | 1110 | G    |
| 7   | A     | 1112 | G    |
| 7   | A     | 1115 | G    |
| 7   | A     | 1121 | C    |
| 7   | A     | 1122 | G    |
| 7   | A     | 1126 | A    |
| 7   | A     | 1130 | U    |
| 7   | A     | 1131 | G    |
| 7   | A     | 1132 | U    |
| 7   | A     | 1134 | A    |
| 7   | A     | 1135 | C    |
| 7   | A     | 1139 | G    |
| 7   | A     | 1142 | A    |
| 7   | A     | 1143 | A    |
| 7   | A     | 1145 | C    |
| 7   | A     | 1169 | A    |
| 7   | A     | 1170 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1173 | U    |
| 7   | A     | 1174 | U    |
| 7   | A     | 1175 | A    |
| 7   | A     | 1176 | U    |
| 7   | A     | 1178 | C    |
| 7   | A     | 1179 | G    |
| 7   | A     | 1180 | U    |
| 7   | A     | 1182 | G    |
| 7   | A     | 1186 | G    |
| 7   | A     | 1190 | G    |
| 7   | A     | 1195 | G    |
| 7   | A     | 1204 | A    |
| 7   | A     | 1208 | C    |
| 7   | A     | 1210 | G    |
| 7   | A     | 1211 | C    |
| 7   | A     | 1212 | G    |
| 7   | A     | 1219 | U    |
| 7   | A     | 1237 | A    |
| 7   | A     | 1238 | G    |
| 7   | A     | 1243 | C    |
| 7   | A     | 1247 | A    |
| 7   | A     | 1248 | G    |
| 7   | A     | 1252 | G    |
| 7   | A     | 1253 | A    |
| 7   | A     | 1256 | G    |
| 7   | A     | 1257 | C    |
| 7   | A     | 1258 | U    |
| 7   | A     | 1265 | A    |
| 7   | A     | 1266 | G    |
| 7   | A     | 1271 | G    |
| 7   | A     | 1272 | A    |
| 7   | A     | 1273 | U    |
| 7   | A     | 1284 | A    |
| 7   | A     | 1294 | U    |
| 7   | A     | 1297 | C    |
| 7   | A     | 1299 | G    |
| 7   | A     | 1300 | G    |
| 7   | A     | 1301 | A    |
| 7   | A     | 1302 | A    |
| 7   | A     | 1304 | A    |
| 7   | A     | 1305 | C    |
| 7   | A     | 1309 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1310 | G    |
| 7   | A     | 1321 | A    |
| 7   | A     | 1324 | G    |
| 7   | A     | 1325 | U    |
| 7   | A     | 1328 | A    |
| 7   | A     | 1329 | U    |
| 7   | A     | 1330 | C    |
| 7   | A     | 1338 | G    |
| 7   | A     | 1341 | G    |
| 7   | A     | 1349 | C    |
| 7   | A     | 1352 | U    |
| 7   | A     | 1355 | G    |
| 7   | A     | 1359 | A    |
| 7   | A     | 1362 | C    |
| 7   | A     | 1365 | A    |
| 7   | A     | 1366 | A    |
| 7   | A     | 1368 | G    |
| 7   | A     | 1375 | U    |
| 7   | A     | 1376 | C    |
| 7   | A     | 1379 | U    |
| 7   | A     | 1383 | A    |
| 7   | A     | 1386 | C    |
| 7   | A     | 1387 | A    |
| 7   | A     | 1392 | A    |
| 7   | A     | 1395 | A    |
| 7   | A     | 1401 | G    |
| 7   | A     | 1403 | A    |
| 7   | A     | 1416 | G    |
| 7   | A     | 1428 | C    |
| 7   | A     | 1432 | G    |
| 7   | A     | 1433 | A    |
| 7   | A     | 1434 | A    |
| 7   | A     | 1437 | C    |
| 7   | A     | 1451 | C    |
| 7   | A     | 1452 | G    |
| 7   | A     | 1453 | A    |
| 7   | A     | 1454 | C    |
| 7   | A     | 1455 | G    |
| 7   | A     | 1456 | G    |
| 7   | A     | 1458 | U    |
| 7   | A     | 1460 | U    |
| 7   | A     | 1461 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1466 | U    |
| 7   | A     | 1478 | G    |
| 7   | A     | 1482 | G    |
| 7   | A     | 1490 | A    |
| 7   | A     | 1493 | C    |
| 7   | A     | 1503 | A    |
| 7   | A     | 1510 | G    |
| 7   | A     | 1515 | A    |
| 7   | A     | 1523 | U    |
| 7   | A     | 1524 | G    |
| 7   | A     | 1529 | G    |
| 7   | A     | 1533 | C    |
| 7   | A     | 1535 | A    |
| 7   | A     | 1536 | C    |
| 7   | A     | 1537 | G    |
| 7   | A     | 1540 | G    |
| 7   | A     | 1558 | C    |
| 7   | A     | 1566 | A    |
| 7   | A     | 1568 | G    |
| 7   | A     | 1569 | A    |
| 7   | A     | 1578 | U    |
| 7   | A     | 1581 | G    |
| 7   | A     | 1583 | A    |
| 7   | A     | 1584 | U    |
| 7   | A     | 1585 | C    |
| 7   | A     | 1602 | U    |
| 7   | A     | 1607 | C    |
| 7   | A     | 1608 | A    |
| 7   | A     | 1610 | A    |
| 7   | A     | 1611 | C    |
| 7   | A     | 1616 | A    |
| 7   | A     | 1617 | C    |
| 7   | A     | 1619 | G    |
| 7   | A     | 1630 | A    |
| 7   | A     | 1632 | A    |
| 7   | A     | 1635 | A    |
| 7   | A     | 1642 | G    |
| 7   | A     | 1646 | C    |
| 7   | A     | 1647 | U    |
| 7   | A     | 1648 | U    |
| 7   | A     | 1667 | G    |
| 7   | A     | 1668 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1669 | A    |
| 7   | A     | 1674 | G    |
| 7   | A     | 1677 | A    |
| 7   | A     | 1679 | A    |
| 7   | A     | 1690 | A    |
| 7   | A     | 1693 | U    |
| 7   | A     | 1694 | C    |
| 7   | A     | 1698 | A    |
| 7   | A     | 1701 | A    |
| 7   | A     | 1703 | G    |
| 7   | A     | 1705 | A    |
| 7   | A     | 1714 | U    |
| 7   | A     | 1715 | G    |
| 7   | A     | 1716 | U    |
| 7   | A     | 1729 | U    |
| 7   | A     | 1731 | G    |
| 7   | A     | 1732 | C    |
| 7   | A     | 1733 | G    |
| 7   | A     | 1738 | G    |
| 7   | A     | 1756 | G    |
| 7   | A     | 1757 | A    |
| 7   | A     | 1758 | U    |
| 7   | A     | 1761 | C    |
| 7   | A     | 1764 | C    |
| 7   | A     | 1773 | A    |
| 7   | A     | 1774 | C    |
| 7   | A     | 1775 | U    |
| 7   | A     | 1781 | U    |
| 7   | A     | 1791 | A    |
| 7   | A     | 1800 | C    |
| 7   | A     | 1801 | A    |
| 7   | A     | 1802 | A    |
| 7   | A     | 1808 | A    |
| 7   | A     | 1809 | A    |
| 7   | A     | 1811 | G    |
| 7   | A     | 1815 | A    |
| 7   | A     | 1816 | C    |
| 7   | A     | 1819 | A    |
| 7   | A     | 1822 | C    |
| 7   | A     | 1825 | U    |
| 7   | A     | 1826 | G    |
| 7   | A     | 1827 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1829 | A    |
| 7   | A     | 1833 | C    |
| 7   | A     | 1834 | U    |
| 7   | A     | 1835 | G    |
| 7   | A     | 1847 | A    |
| 7   | A     | 1855 | U    |
| 7   | A     | 1869 | G    |
| 7   | A     | 1870 | C    |
| 7   | A     | 1871 | A    |
| 7   | A     | 1872 | A    |
| 7   | A     | 1873 | G    |
| 7   | A     | 1882 | U    |
| 7   | A     | 1905 | C    |
| 7   | A     | 1906 | G    |
| 7   | A     | 1907 | G    |
| 7   | A     | 1913 | A    |
| 7   | A     | 1914 | C    |
| 7   | A     | 1919 | A    |
| 7   | A     | 1926 | U    |
| 7   | A     | 1929 | G    |
| 7   | A     | 1930 | G    |
| 7   | A     | 1936 | A    |
| 7   | A     | 1944 | U    |
| 7   | A     | 1946 | U    |
| 7   | A     | 1953 | A    |
| 7   | A     | 1955 | U    |
| 7   | A     | 1956 | U    |
| 7   | A     | 1960 | A    |
| 7   | A     | 1964 | G    |
| 7   | A     | 1966 | A    |
| 7   | A     | 1967 | C    |
| 7   | A     | 1970 | A    |
| 7   | A     | 1971 | U    |
| 7   | A     | 1972 | G    |
| 7   | A     | 1989 | G    |
| 7   | A     | 1990 | C    |
| 7   | A     | 1991 | U    |
| 7   | A     | 1993 | U    |
| 7   | A     | 1997 | C    |
| 7   | A     | 2001 | C    |
| 7   | A     | 2002 | G    |
| 7   | A     | 2013 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 2022 | U    |
| 7   | A     | 2023 | C    |
| 7   | A     | 2025 | C    |
| 7   | A     | 2026 | U    |
| 7   | A     | 2030 | A    |
| 7   | A     | 2031 | A    |
| 7   | A     | 2032 | G    |
| 7   | A     | 2033 | A    |
| 7   | A     | 2035 | G    |
| 7   | A     | 2043 | C    |
| 7   | A     | 2055 | C    |
| 7   | A     | 2056 | G    |
| 7   | A     | 2059 | A    |
| 7   | A     | 2060 | A    |
| 7   | A     | 2061 | G    |
| 7   | A     | 2062 | A    |
| 7   | A     | 2069 | G    |
| 7   | A     | 2075 | U    |
| 7   | A     | 2093 | G    |
| 7   | A     | 2095 | A    |
| 7   | A     | 2098 | U    |
| 7   | A     | 2100 | G    |
| 7   | A     | 2102 | G    |
| 7   | A     | 2107 | G    |
| 7   | A     | 2109 | U    |
| 7   | A     | 2110 | G    |
| 7   | A     | 2111 | U    |
| 7   | A     | 2112 | G    |
| 7   | A     | 2113 | U    |
| 7   | A     | 2115 | G    |
| 7   | A     | 2116 | G    |
| 7   | A     | 2118 | U    |
| 7   | A     | 2119 | A    |
| 7   | A     | 2120 | G    |
| 7   | A     | 2121 | G    |
| 7   | A     | 2123 | G    |
| 7   | A     | 2124 | G    |
| 7   | A     | 2125 | G    |
| 7   | A     | 2126 | A    |
| 7   | A     | 2127 | G    |
| 7   | A     | 2128 | G    |
| 7   | A     | 2130 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 2132 | U    |
| 7   | A     | 2135 | A    |
| 7   | A     | 2137 | U    |
| 7   | A     | 2140 | G    |
| 7   | A     | 2141 | G    |
| 7   | A     | 2145 | C    |
| 7   | A     | 2146 | C    |
| 7   | A     | 2147 | A    |
| 7   | A     | 2152 | G    |
| 7   | A     | 2157 | G    |
| 7   | A     | 2158 | A    |
| 7   | A     | 2162 | G    |
| 7   | A     | 2164 | C    |
| 7   | A     | 2165 | C    |
| 7   | A     | 2167 | U    |
| 7   | A     | 2169 | A    |
| 7   | A     | 2170 | A    |
| 7   | A     | 2171 | A    |
| 7   | A     | 2172 | U    |
| 7   | A     | 2173 | A    |
| 7   | A     | 2175 | C    |
| 7   | A     | 2178 | C    |
| 7   | A     | 2182 | U    |
| 7   | A     | 2183 | A    |
| 7   | A     | 2189 | U    |
| 7   | A     | 2198 | A    |
| 7   | A     | 2203 | U    |
| 7   | A     | 2204 | G    |
| 7   | A     | 2211 | A    |
| 7   | A     | 2212 | A    |
| 7   | A     | 2213 | U    |
| 7   | A     | 2214 | C    |
| 7   | A     | 2223 | G    |
| 7   | A     | 2225 | A    |
| 7   | A     | 2228 | G    |
| 7   | A     | 2238 | G    |
| 7   | A     | 2239 | G    |
| 7   | A     | 2242 | G    |
| 7   | A     | 2243 | U    |
| 7   | A     | 2250 | G    |
| 7   | A     | 2251 | G    |
| 7   | A     | 2252 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 2255 | G    |
| 7   | A     | 2257 | U    |
| 7   | A     | 2259 | U    |
| 7   | A     | 2266 | A    |
| 7   | A     | 2279 | G    |
| 7   | A     | 2283 | C    |
| 7   | A     | 2287 | A    |
| 7   | A     | 2288 | A    |
| 7   | A     | 2289 | G    |
| 7   | A     | 2297 | A    |
| 7   | A     | 2305 | U    |
| 7   | A     | 2309 | A    |
| 7   | A     | 2318 | G    |
| 7   | A     | 2319 | G    |
| 7   | A     | 2322 | A    |
| 7   | A     | 2325 | G    |
| 7   | A     | 2327 | A    |
| 7   | A     | 2330 | G    |
| 7   | A     | 2331 | G    |
| 7   | A     | 2333 | A    |
| 7   | A     | 2335 | A    |
| 7   | A     | 2338 | C    |
| 7   | A     | 2344 | U    |
| 7   | A     | 2345 | G    |
| 7   | A     | 2346 | A    |
| 7   | A     | 2347 | C    |
| 7   | A     | 2354 | C    |
| 7   | A     | 2357 | G    |
| 7   | A     | 2358 | A    |
| 7   | A     | 2361 | G    |
| 7   | A     | 2376 | A    |
| 7   | A     | 2383 | G    |
| 7   | A     | 2384 | U    |
| 7   | A     | 2385 | C    |
| 7   | A     | 2390 | U    |
| 7   | A     | 2402 | U    |
| 7   | A     | 2403 | C    |
| 7   | A     | 2404 | U    |
| 7   | A     | 2406 | A    |
| 7   | A     | 2407 | A    |
| 7   | A     | 2420 | C    |
| 7   | A     | 2423 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 2425 | A    |
| 7   | A     | 2427 | C    |
| 7   | A     | 2428 | G    |
| 7   | A     | 2429 | G    |
| 7   | A     | 2430 | A    |
| 7   | A     | 2432 | A    |
| 7   | A     | 2435 | A    |
| 7   | A     | 2441 | U    |
| 7   | A     | 2447 | G    |
| 7   | A     | 2448 | A    |
| 7   | A     | 2455 | G    |
| 7   | A     | 2463 | C    |
| 7   | A     | 2464 | G    |
| 7   | A     | 2469 | A    |
| 7   | A     | 2470 | G    |
| 7   | A     | 2474 | U    |
| 7   | A     | 2476 | A    |
| 7   | A     | 2478 | A    |
| 7   | A     | 2479 | U    |
| 7   | A     | 2480 | C    |
| 7   | A     | 2484 | G    |
| 7   | A     | 2490 | G    |
| 7   | A     | 2491 | U    |
| 7   | A     | 2498 | C    |
| 7   | A     | 2500 | U    |
| 7   | A     | 2502 | G    |
| 7   | A     | 2503 | A    |
| 7   | A     | 2504 | U    |
| 7   | A     | 2505 | G    |
| 7   | A     | 2507 | C    |
| 7   | A     | 2508 | G    |
| 7   | A     | 2518 | A    |
| 7   | A     | 2520 | C    |
| 7   | A     | 2527 | C    |
| 7   | A     | 2529 | G    |
| 7   | A     | 2547 | A    |
| 7   | A     | 2552 | U    |
| 7   | A     | 2554 | U    |
| 7   | A     | 2556 | C    |
| 7   | A     | 2558 | C    |
| 7   | A     | 2566 | A    |
| 7   | A     | 2567 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 2572 | A    |
| 7   | A     | 2576 | G    |
| 7   | A     | 2582 | G    |
| 7   | A     | 2585 | U    |
| 7   | A     | 2586 | U    |
| 7   | A     | 2588 | G    |
| 7   | A     | 2596 | U    |
| 7   | A     | 2597 | G    |
| 7   | A     | 2602 | A    |
| 7   | A     | 2609 | U    |
| 7   | A     | 2610 | C    |
| 7   | A     | 2613 | U    |
| 7   | A     | 2629 | U    |
| 7   | A     | 2630 | G    |
| 7   | A     | 2635 | A    |
| 7   | A     | 2636 | C    |
| 7   | A     | 2645 | G    |
| 7   | A     | 2646 | C    |
| 7   | A     | 2654 | A    |
| 7   | A     | 2661 | G    |
| 7   | A     | 2663 | G    |
| 7   | A     | 2669 | G    |
| 7   | A     | 2680 | U    |
| 7   | A     | 2682 | A    |
| 7   | A     | 2689 | U    |
| 7   | A     | 2690 | U    |
| 7   | A     | 2714 | G    |
| 7   | A     | 2722 | G    |
| 7   | A     | 2724 | U    |
| 7   | A     | 2726 | A    |
| 7   | A     | 2733 | A    |
| 7   | A     | 2744 | G    |
| 7   | A     | 2748 | A    |
| 7   | A     | 2757 | A    |
| 7   | A     | 2776 | A    |
| 7   | A     | 2778 | A    |
| 7   | A     | 2779 | U    |
| 7   | A     | 2793 | C    |
| 7   | A     | 2799 | A    |
| 7   | A     | 2807 | U    |
| 7   | A     | 2808 | G    |
| 7   | A     | 2818 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 2820 | A    |
| 7   | A     | 2826 | A    |
| 7   | A     | 2833 | U    |
| 7   | A     | 2835 | A    |
| 7   | A     | 2836 | U    |
| 7   | A     | 2843 | G    |
| 7   | A     | 2846 | G    |
| 7   | A     | 2848 | G    |
| 7   | A     | 2849 | U    |
| 7   | A     | 2867 | G    |
| 7   | A     | 2872 | A    |
| 7   | A     | 2873 | A    |
| 7   | A     | 2879 | A    |
| 7   | A     | 2880 | C    |
| 7   | A     | 2883 | A    |
| 7   | A     | 2887 | A    |
| 7   | A     | 2891 | U    |
| 7   | A     | 2893 | A    |
| 7   | A     | 2903 | U    |
| 8   | B     | 3    | A    |
| 8   | B     | 4    | U    |
| 8   | B     | 6    | G    |
| 8   | B     | 7    | A    |
| 8   | B     | 8    | A    |
| 8   | B     | 9    | G    |
| 8   | B     | 32   | A    |
| 8   | B     | 37   | U    |
| 8   | B     | 39   | G    |
| 8   | B     | 42   | G    |
| 8   | B     | 43   | C    |
| 8   | B     | 44   | A    |
| 8   | B     | 47   | C    |
| 8   | B     | 48   | C    |
| 8   | B     | 49   | U    |
| 8   | B     | 50   | A    |
| 8   | B     | 51   | A    |
| 8   | B     | 52   | C    |
| 8   | B     | 61   | G    |
| 8   | B     | 62   | U    |
| 8   | B     | 63   | C    |
| 8   | B     | 65   | A    |
| 8   | B     | 67   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 71  | A    |
| 8   | B     | 73  | C    |
| 8   | B     | 74  | A    |
| 8   | B     | 76  | G    |
| 8   | B     | 77  | A    |
| 8   | B     | 78  | A    |
| 8   | B     | 79  | G    |
| 8   | B     | 80  | A    |
| 8   | B     | 81  | A    |
| 8   | B     | 83  | C    |
| 8   | B     | 87  | C    |
| 8   | B     | 88  | U    |
| 8   | B     | 90  | C    |
| 8   | B     | 91  | U    |
| 8   | B     | 96  | U    |
| 8   | B     | 97  | G    |
| 8   | B     | 98  | A    |
| 8   | B     | 100 | G    |
| 8   | B     | 104 | G    |
| 8   | B     | 110 | C    |
| 8   | B     | 115 | G    |
| 8   | B     | 116 | A    |
| 8   | B     | 120 | A    |
| 8   | B     | 121 | U    |
| 8   | B     | 122 | G    |
| 8   | B     | 125 | U    |
| 8   | B     | 126 | G    |
| 8   | B     | 127 | G    |
| 8   | B     | 130 | A    |
| 8   | B     | 131 | A    |
| 8   | B     | 132 | C    |
| 8   | B     | 133 | U    |
| 8   | B     | 137 | U    |
| 8   | B     | 140 | U    |
| 8   | B     | 141 | G    |
| 8   | B     | 144 | G    |
| 8   | B     | 145 | G    |
| 8   | B     | 149 | A    |
| 8   | B     | 154 | U    |
| 8   | B     | 155 | A    |
| 8   | B     | 156 | C    |
| 8   | B     | 163 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 168 | G    |
| 8   | B     | 170 | U    |
| 8   | B     | 171 | A    |
| 8   | B     | 173 | U    |
| 8   | B     | 177 | G    |
| 8   | B     | 180 | U    |
| 8   | B     | 182 | A    |
| 8   | B     | 183 | C    |
| 8   | B     | 184 | G    |
| 8   | B     | 189 | A    |
| 8   | B     | 195 | A    |
| 8   | B     | 197 | A    |
| 8   | B     | 200 | G    |
| 8   | B     | 201 | G    |
| 8   | B     | 204 | G    |
| 8   | B     | 205 | A    |
| 8   | B     | 207 | C    |
| 8   | B     | 208 | U    |
| 8   | B     | 209 | U    |
| 8   | B     | 210 | C    |
| 8   | B     | 212 | G    |
| 8   | B     | 215 | C    |
| 8   | B     | 216 | U    |
| 8   | B     | 219 | U    |
| 8   | B     | 220 | G    |
| 8   | B     | 222 | C    |
| 8   | B     | 224 | U    |
| 8   | B     | 226 | G    |
| 8   | B     | 240 | G    |
| 8   | B     | 244 | U    |
| 8   | B     | 245 | U    |
| 8   | B     | 247 | G    |
| 8   | B     | 251 | G    |
| 8   | B     | 254 | G    |
| 8   | B     | 265 | G    |
| 8   | B     | 266 | G    |
| 8   | B     | 267 | C    |
| 8   | B     | 281 | G    |
| 8   | B     | 289 | G    |
| 8   | B     | 291 | U    |
| 8   | B     | 293 | G    |
| 8   | B     | 295 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 298 | A    |
| 8   | B     | 299 | G    |
| 8   | B     | 300 | A    |
| 8   | B     | 304 | U    |
| 8   | B     | 309 | A    |
| 8   | B     | 321 | A    |
| 8   | B     | 325 | A    |
| 8   | B     | 327 | A    |
| 8   | B     | 328 | C    |
| 8   | B     | 329 | A    |
| 8   | B     | 330 | C    |
| 8   | B     | 332 | G    |
| 8   | B     | 337 | G    |
| 8   | B     | 345 | C    |
| 8   | B     | 346 | G    |
| 8   | B     | 347 | G    |
| 8   | B     | 348 | G    |
| 8   | B     | 352 | C    |
| 8   | B     | 354 | G    |
| 8   | B     | 359 | G    |
| 8   | B     | 367 | U    |
| 8   | B     | 371 | A    |
| 8   | B     | 372 | C    |
| 8   | B     | 373 | A    |
| 8   | B     | 380 | G    |
| 8   | B     | 384 | G    |
| 8   | B     | 388 | G    |
| 8   | B     | 392 | C    |
| 8   | B     | 393 | A    |
| 8   | B     | 396 | C    |
| 8   | B     | 397 | A    |
| 8   | B     | 398 | U    |
| 8   | B     | 401 | C    |
| 8   | B     | 406 | G    |
| 8   | B     | 411 | A    |
| 8   | B     | 412 | A    |
| 8   | B     | 413 | G    |
| 8   | B     | 414 | A    |
| 8   | B     | 419 | C    |
| 8   | B     | 421 | U    |
| 8   | B     | 422 | C    |
| 8   | B     | 423 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 424 | G    |
| 8   | B     | 428 | G    |
| 8   | B     | 429 | U    |
| 8   | B     | 434 | U    |
| 8   | B     | 440 | C    |
| 8   | B     | 443 | C    |
| 8   | B     | 444 | G    |
| 8   | B     | 447 | G    |
| 8   | B     | 453 | G    |
| 8   | B     | 454 | G    |
| 8   | B     | 455 | G    |
| 8   | B     | 456 | A    |
| 8   | B     | 458 | U    |
| 8   | B     | 463 | U    |
| 8   | B     | 465 | A    |
| 8   | B     | 467 | U    |
| 8   | B     | 468 | A    |
| 8   | B     | 469 | C    |
| 8   | B     | 471 | U    |
| 8   | B     | 472 | U    |
| 8   | B     | 476 | U    |
| 8   | B     | 478 | A    |
| 8   | B     | 479 | U    |
| 8   | B     | 480 | U    |
| 8   | B     | 484 | G    |
| 8   | B     | 485 | U    |
| 8   | B     | 486 | U    |
| 8   | B     | 492 | C    |
| 8   | B     | 495 | A    |
| 8   | B     | 496 | A    |
| 8   | B     | 498 | A    |
| 8   | B     | 499 | A    |
| 8   | B     | 503 | C    |
| 8   | B     | 505 | G    |
| 8   | B     | 508 | U    |
| 8   | B     | 512 | U    |
| 8   | B     | 518 | C    |
| 8   | B     | 521 | G    |
| 8   | B     | 527 | G    |
| 8   | B     | 532 | A    |
| 8   | B     | 533 | A    |
| 8   | B     | 536 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 547 | A    |
| 8   | B     | 556 | C    |
| 8   | B     | 558 | G    |
| 8   | B     | 559 | A    |
| 8   | B     | 563 | A    |
| 8   | B     | 572 | A    |
| 8   | B     | 573 | A    |
| 8   | B     | 576 | C    |
| 8   | B     | 577 | G    |
| 8   | B     | 586 | C    |
| 8   | B     | 592 | G    |
| 8   | B     | 595 | A    |
| 8   | B     | 596 | A    |
| 8   | B     | 601 | G    |
| 8   | B     | 607 | A    |
| 8   | B     | 611 | C    |
| 8   | B     | 613 | C    |
| 8   | B     | 615 | G    |
| 8   | B     | 619 | U    |
| 8   | B     | 621 | A    |
| 8   | B     | 630 | A    |
| 8   | B     | 639 | G    |
| 8   | B     | 652 | U    |
| 8   | B     | 653 | U    |
| 8   | B     | 660 | C    |
| 8   | B     | 665 | A    |
| 8   | B     | 676 | A    |
| 8   | B     | 695 | A    |
| 8   | B     | 702 | A    |
| 8   | B     | 703 | G    |
| 8   | B     | 718 | A    |
| 8   | B     | 720 | C    |
| 8   | B     | 721 | G    |
| 8   | B     | 723 | U    |
| 8   | B     | 724 | G    |
| 8   | B     | 731 | G    |
| 8   | B     | 733 | G    |
| 8   | B     | 734 | G    |
| 8   | B     | 747 | A    |
| 8   | B     | 748 | G    |
| 8   | B     | 755 | G    |
| 8   | B     | 758 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 763 | G    |
| 8   | B     | 766 | A    |
| 8   | B     | 774 | G    |
| 8   | B     | 777 | A    |
| 8   | B     | 793 | U    |
| 8   | B     | 794 | A    |
| 8   | B     | 810 | C    |
| 8   | B     | 812 | G    |
| 8   | B     | 813 | U    |
| 8   | B     | 814 | A    |
| 8   | B     | 815 | A    |
| 8   | B     | 817 | C    |
| 8   | B     | 821 | G    |
| 8   | B     | 826 | C    |
| 8   | B     | 828 | U    |
| 8   | B     | 835 | U    |
| 8   | B     | 840 | C    |
| 8   | B     | 841 | C    |
| 8   | B     | 842 | U    |
| 8   | B     | 843 | U    |
| 8   | B     | 844 | G    |
| 8   | B     | 846 | G    |
| 8   | B     | 849 | G    |
| 8   | B     | 873 | A    |
| 8   | B     | 879 | C    |
| 8   | B     | 885 | G    |
| 8   | B     | 887 | G    |
| 8   | B     | 889 | A    |
| 8   | B     | 910 | C    |
| 8   | B     | 914 | A    |
| 8   | B     | 918 | A    |
| 8   | B     | 919 | A    |
| 8   | B     | 921 | U    |
| 8   | B     | 926 | G    |
| 8   | B     | 933 | G    |
| 8   | B     | 934 | C    |
| 8   | B     | 937 | A    |
| 8   | B     | 948 | C    |
| 8   | B     | 955 | U    |
| 8   | B     | 960 | U    |
| 8   | B     | 969 | A    |
| 8   | B     | 971 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | B     | 974  | A    |
| 8   | B     | 975  | A    |
| 8   | B     | 976  | G    |
| 8   | B     | 977  | A    |
| 8   | B     | 980  | C    |
| 8   | B     | 983  | A    |
| 8   | B     | 984  | C    |
| 8   | B     | 987  | G    |
| 8   | B     | 988  | G    |
| 8   | B     | 989  | U    |
| 8   | B     | 991  | U    |
| 8   | B     | 992  | U    |
| 8   | B     | 993  | G    |
| 8   | B     | 994  | A    |
| 8   | B     | 995  | C    |
| 8   | B     | 1001 | C    |
| 8   | B     | 1002 | G    |
| 8   | B     | 1004 | A    |
| 8   | B     | 1005 | A    |
| 8   | B     | 1008 | U    |
| 8   | B     | 1009 | U    |
| 8   | B     | 1012 | A    |
| 8   | B     | 1017 | U    |
| 8   | B     | 1022 | A    |
| 8   | B     | 1023 | U    |
| 8   | B     | 1026 | G    |
| 8   | B     | 1029 | U    |
| 8   | B     | 1031 | C    |
| 8   | B     | 1032 | G    |
| 8   | B     | 1033 | G    |
| 8   | B     | 1036 | A    |
| 8   | B     | 1039 | G    |
| 8   | B     | 1044 | A    |
| 8   | B     | 1054 | C    |
| 8   | B     | 1065 | U    |
| 8   | B     | 1073 | U    |
| 8   | B     | 1085 | U    |
| 8   | B     | 1094 | G    |
| 8   | B     | 1095 | U    |
| 8   | B     | 1101 | A    |
| 8   | B     | 1102 | A    |
| 8   | B     | 1108 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | B     | 1126 | U    |
| 8   | B     | 1127 | G    |
| 8   | B     | 1129 | C    |
| 8   | B     | 1130 | A    |
| 8   | B     | 1132 | C    |
| 8   | B     | 1133 | G    |
| 8   | B     | 1135 | U    |
| 8   | B     | 1136 | C    |
| 8   | B     | 1137 | C    |
| 8   | B     | 1138 | G    |
| 8   | B     | 1139 | G    |
| 8   | B     | 1140 | C    |
| 8   | B     | 1141 | C    |
| 8   | B     | 1142 | G    |
| 8   | B     | 1143 | G    |
| 8   | B     | 1145 | A    |
| 8   | B     | 1159 | U    |
| 8   | B     | 1160 | G    |
| 8   | B     | 1161 | C    |
| 8   | B     | 1162 | C    |
| 8   | B     | 1168 | U    |
| 8   | B     | 1171 | A    |
| 8   | B     | 1179 | A    |
| 8   | B     | 1182 | G    |
| 8   | B     | 1184 | G    |
| 8   | B     | 1193 | G    |
| 8   | B     | 1196 | A    |
| 8   | B     | 1197 | A    |
| 8   | B     | 1202 | U    |
| 8   | B     | 1212 | U    |
| 8   | B     | 1213 | A    |
| 8   | B     | 1224 | U    |
| 8   | B     | 1227 | A    |
| 8   | B     | 1233 | G    |
| 8   | B     | 1240 | U    |
| 8   | B     | 1241 | G    |
| 8   | B     | 1242 | G    |
| 8   | B     | 1249 | C    |
| 8   | B     | 1257 | A    |
| 8   | B     | 1258 | G    |
| 8   | B     | 1262 | C    |
| 8   | B     | 1271 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | B     | 1272 | G    |
| 8   | B     | 1275 | A    |
| 8   | B     | 1280 | A    |
| 8   | B     | 1285 | A    |
| 8   | B     | 1286 | U    |
| 8   | B     | 1287 | A    |
| 8   | B     | 1289 | A    |
| 8   | B     | 1290 | G    |
| 8   | B     | 1292 | G    |
| 8   | B     | 1293 | C    |
| 8   | B     | 1296 | C    |
| 8   | B     | 1298 | U    |
| 8   | B     | 1299 | A    |
| 8   | B     | 1300 | G    |
| 8   | B     | 1301 | U    |
| 8   | B     | 1302 | C    |
| 8   | B     | 1303 | C    |
| 8   | B     | 1304 | G    |
| 8   | B     | 1305 | G    |
| 8   | B     | 1310 | G    |
| 8   | B     | 1312 | G    |
| 8   | B     | 1317 | C    |
| 8   | B     | 1318 | A    |
| 8   | B     | 1320 | C    |
| 8   | B     | 1322 | C    |
| 8   | B     | 1331 | G    |
| 8   | B     | 1336 | C    |
| 8   | B     | 1340 | A    |
| 8   | B     | 1346 | A    |
| 8   | B     | 1348 | U    |
| 8   | B     | 1353 | G    |
| 8   | B     | 1363 | A    |
| 8   | B     | 1364 | U    |
| 8   | B     | 1368 | A    |
| 8   | B     | 1370 | G    |
| 8   | B     | 1378 | C    |
| 8   | B     | 1380 | U    |
| 8   | B     | 1385 | G    |
| 8   | B     | 1397 | C    |
| 8   | B     | 1398 | A    |
| 8   | B     | 1402 | C    |
| 8   | B     | 1405 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | B     | 1419 | G    |
| 8   | B     | 1429 | A    |
| 8   | B     | 1431 | A    |
| 8   | B     | 1432 | G    |
| 8   | B     | 1440 | U    |
| 8   | B     | 1446 | A    |
| 8   | B     | 1448 | C    |
| 8   | B     | 1452 | C    |
| 8   | B     | 1458 | G    |
| 8   | B     | 1464 | U    |
| 8   | B     | 1475 | G    |
| 8   | B     | 1487 | G    |
| 8   | B     | 1492 | A    |
| 8   | B     | 1494 | G    |
| 8   | B     | 1497 | G    |
| 8   | B     | 1503 | A    |
| 8   | B     | 1506 | U    |
| 8   | B     | 1517 | G    |
| 8   | B     | 1525 | G    |
| 8   | B     | 1528 | U    |
| 8   | B     | 1529 | G    |
| 8   | B     | 1530 | G    |
| 8   | B     | 1534 | A    |
| 8   | B     | 1535 | C    |
| 8   | B     | 1536 | C    |
| 8   | B     | 1540 | U    |
| 30  | X     | 3    | G    |
| 30  | X     | 4    | U    |
| 30  | X     | 5    | G    |
| 30  | X     | 6    | A    |
| 30  | X     | 13   | C    |
| 30  | X     | 14   | A    |
| 30  | X     | 15   | G    |
| 30  | X     | 19   | G    |
| 30  | X     | 20   | G    |
| 30  | X     | 21   | A    |
| 30  | X     | 22   | G    |
| 30  | X     | 29   | U    |
| 30  | X     | 33   | U    |
| 30  | X     | 39   | G    |
| 30  | X     | 41   | A    |
| 30  | X     | 44   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | X     | 45  | G    |
| 30  | X     | 48  | C    |
| 30  | X     | 49  | G    |
| 30  | X     | 53  | G    |
| 30  | X     | 57  | G    |
| 30  | X     | 58  | A    |
| 30  | X     | 59  | U    |
| 30  | X     | 60  | C    |
| 30  | X     | 63  | G    |
| 30  | X     | 65  | C    |
| 30  | X     | 68  | C    |
| 30  | X     | 70  | C    |
| 30  | X     | 71  | C    |
| 30  | X     | 73  | A    |
| 31  | Z     | 3   | G    |
| 31  | Z     | 6   | G    |
| 31  | Z     | 14  | A    |
| 31  | Z     | 19  | G    |
| 31  | Z     | 20  | U    |
| 31  | Z     | 24  | G    |
| 31  | Z     | 25  | C    |
| 31  | Z     | 26  | A    |
| 31  | Z     | 29  | U    |
| 31  | Z     | 32  | C    |
| 31  | Z     | 33  | U    |
| 31  | Z     | 36  | U    |
| 31  | Z     | 49  | G    |
| 31  | Z     | 50  | C    |
| 31  | Z     | 51  | A    |
| 31  | Z     | 57  | G    |
| 31  | Z     | 59  | A    |
| 31  | Z     | 63  | U    |
| 31  | Z     | 68  | G    |
| 31  | Z     | 71  | C    |
| 31  | Z     | 73  | A    |
| 31  | Z     | 74  | C    |
| 31  | Z     | 75  | C    |
| 31  | Z     | 76  | A    |
| 32  | a     | 3   | C    |
| 32  | a     | 15  | A    |
| 32  | a     | 17  | C    |
| 32  | a     | 24  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | a     | 25  | U    |
| 32  | a     | 31  | C    |
| 32  | a     | 32  | U    |
| 32  | a     | 35  | C    |
| 32  | a     | 44  | G    |
| 32  | a     | 51  | G    |
| 32  | a     | 53  | A    |
| 32  | a     | 56  | G    |
| 32  | a     | 66  | A    |
| 32  | a     | 83  | G    |
| 32  | a     | 88  | C    |
| 32  | a     | 89  | U    |
| 32  | a     | 90  | C    |
| 32  | a     | 91  | C    |
| 32  | a     | 99  | A    |
| 32  | a     | 109 | A    |
| 32  | a     | 119 | A    |
| 56  | y     | 3   | A    |
| 56  | y     | 7   | G    |
| 56  | y     | 13  | C    |
| 56  | y     | 16  | U    |
| 56  | y     | 17  | C    |
| 56  | y     | 18  | G    |
| 56  | y     | 19  | U    |
| 56  | y     | 20  | U    |
| 56  | y     | 21  | A    |
| 56  | y     | 22  | G    |
| 56  | y     | 33  | U    |
| 56  | y     | 36  | C    |
| 56  | y     | 48  | C    |
| 56  | y     | 49  | G    |
| 56  | y     | 51  | G    |
| 56  | y     | 69  | U    |
| 56  | y     | 71  | C    |
| 56  | y     | 75  | C    |
| 56  | y     | 76  | A    |

All (17) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 141 | G    |
| 7   | A     | 244 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 271  | G    |
| 7   | A     | 297  | G    |
| 7   | A     | 404  | A    |
| 7   | A     | 897  | C    |
| 7   | A     | 975  | A    |
| 7   | A     | 1730 | C    |
| 7   | A     | 1904 | G    |
| 7   | A     | 1913 | A    |
| 7   | A     | 2317 | A    |
| 7   | A     | 2346 | A    |
| 7   | A     | 2756 | U    |
| 8   | B     | 115  | G    |
| 8   | B     | 428  | G    |
| 8   | B     | 1201 | A    |
| 31  | Z     | 13   | C    |

#### 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](#)

There are no chain breaks in this entry.

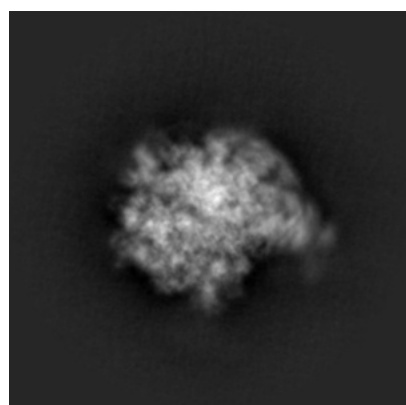
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30611. These allow visual inspection of the internal detail of the map and identification of artifacts.

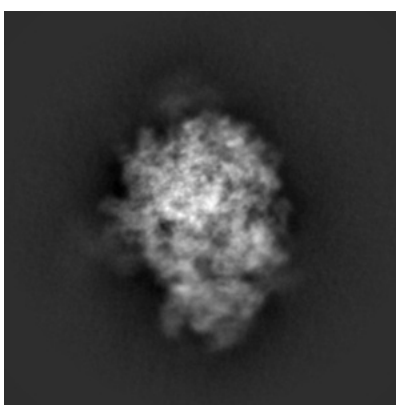
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

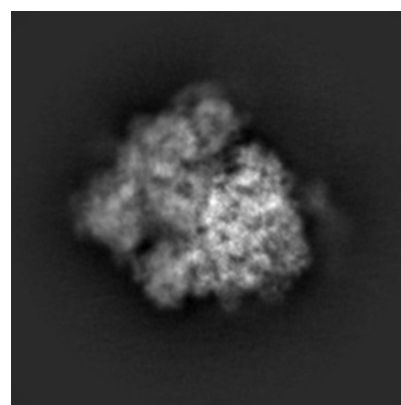
#### 6.1.1 Primary map



X



Y

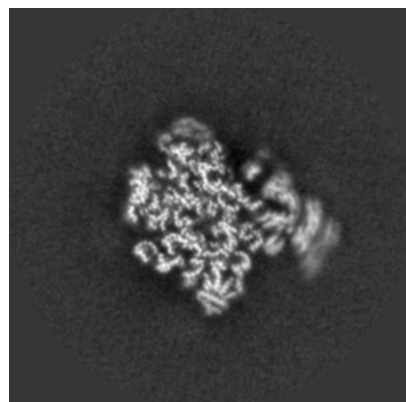


Z

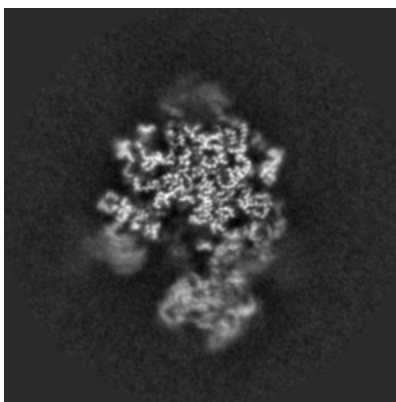
The images above show the map projected in three orthogonal directions.

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

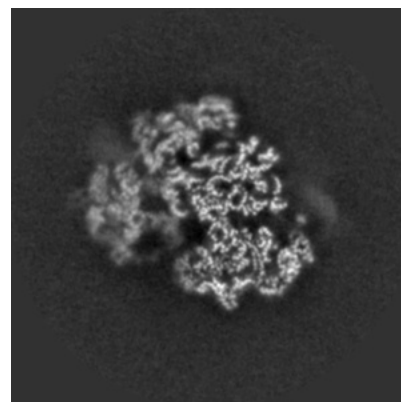
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

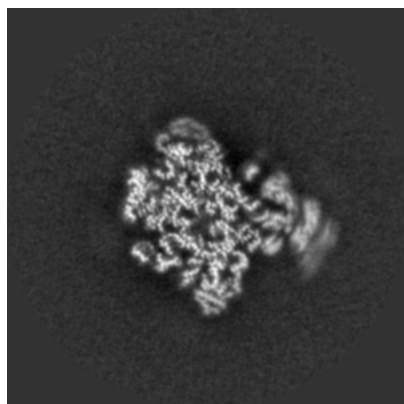


Z Index: 160

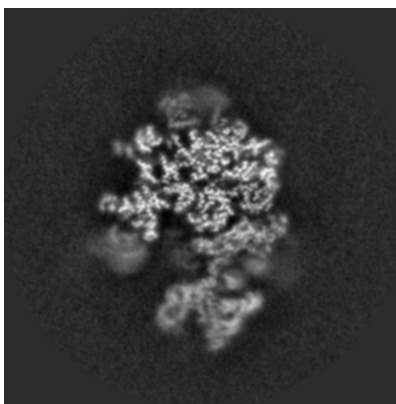
The images above show central slices of the map in three orthogonal directions.

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

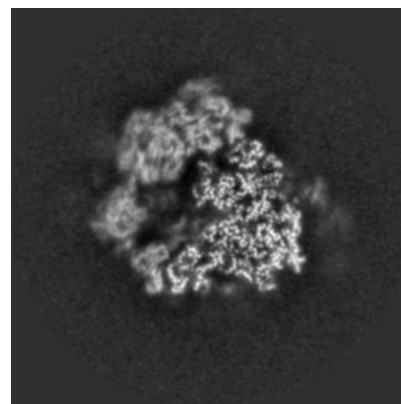
### 6.3.1 Primary map



X Index: 161



Y Index: 165

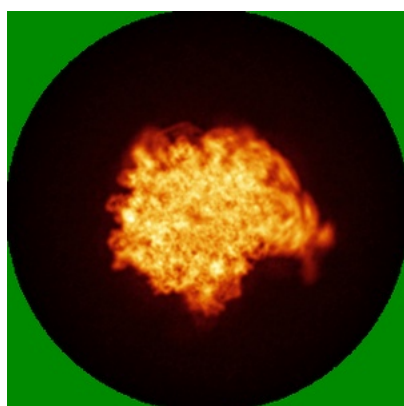


Z Index: 147

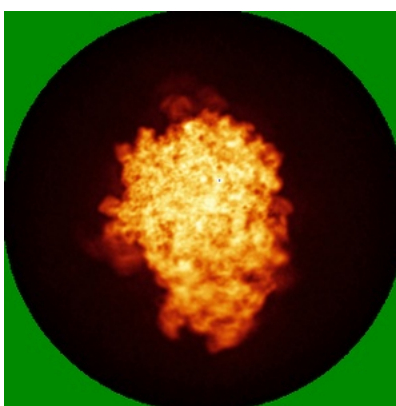
The images above show the largest variance slices of the map in three orthogonal directions.

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

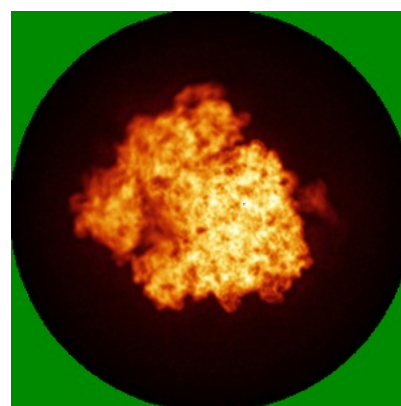
### 6.4.1 Primary map



X



Y



Z

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

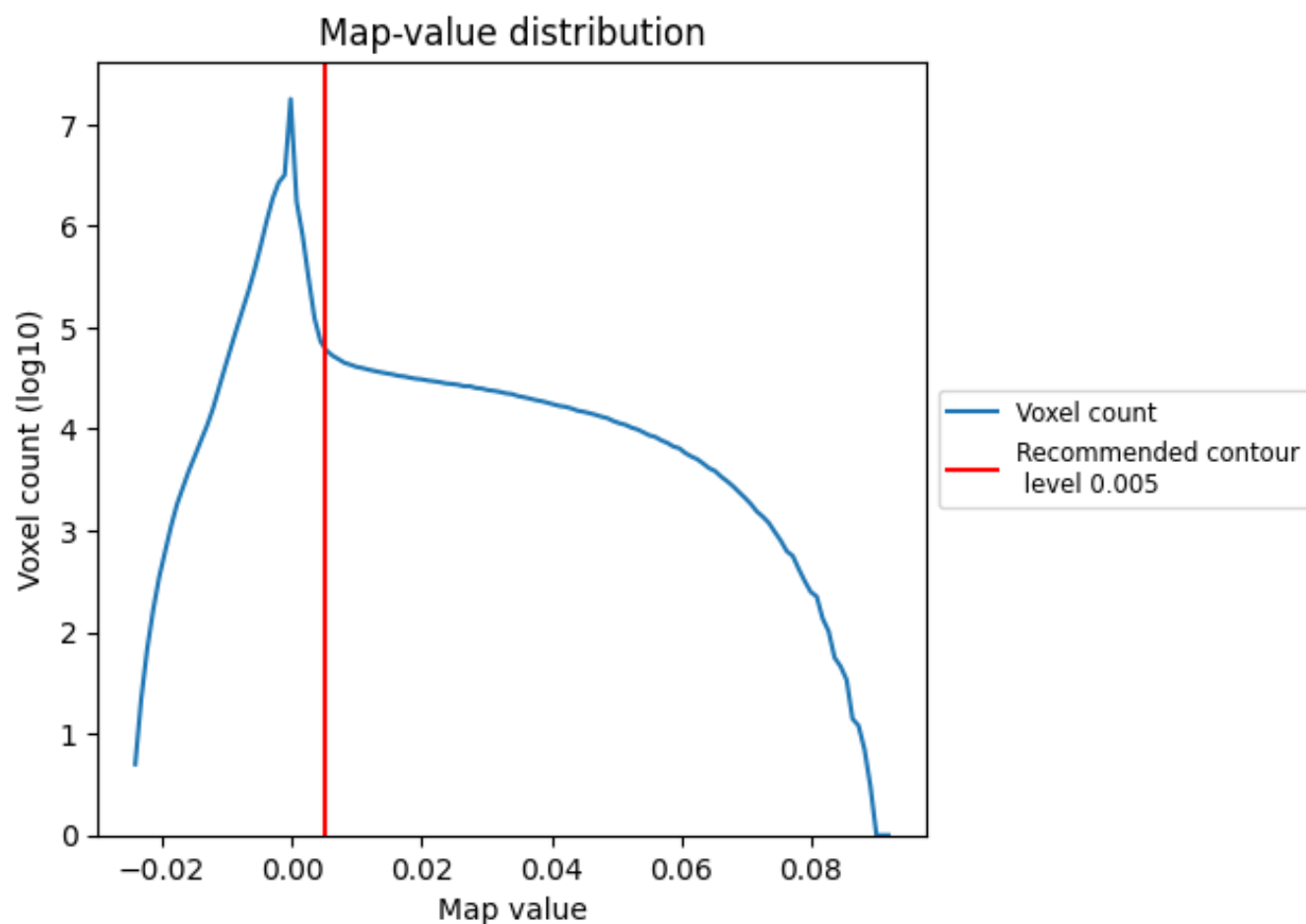
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

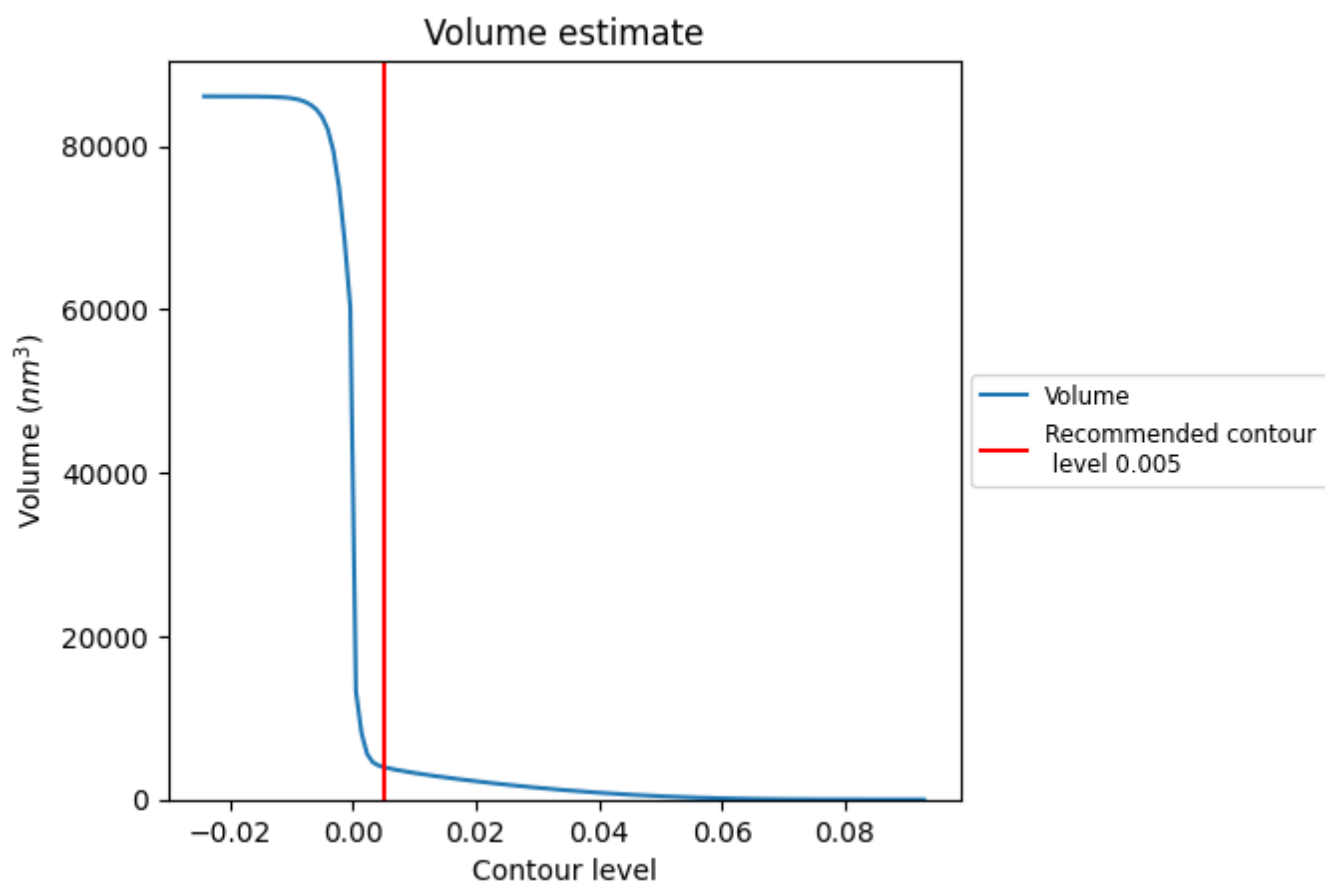
This section contains the results of statistical analysis of the map.

### 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.

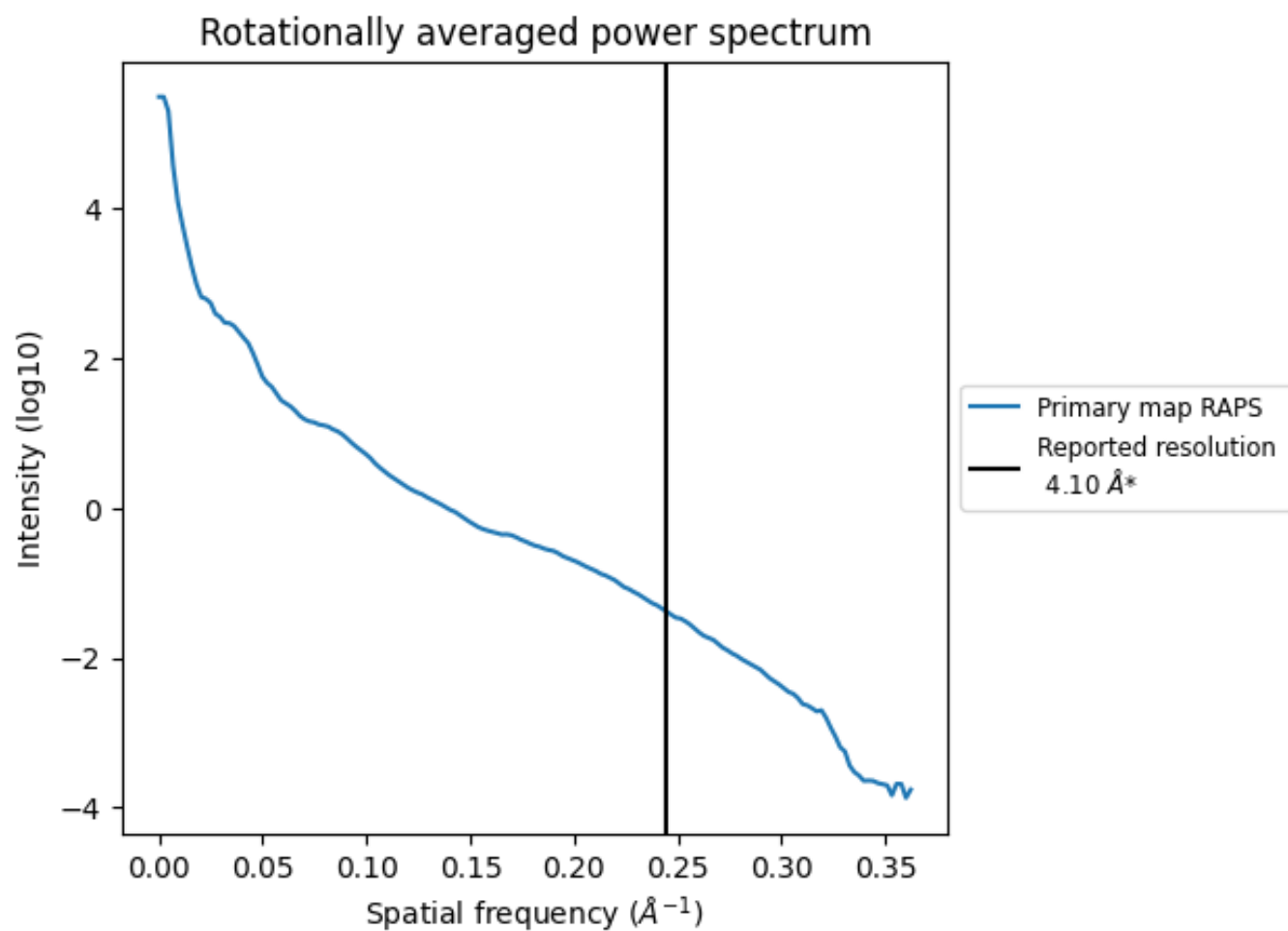
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3991  $\text{nm}^3$ ; this corresponds to an approximate mass of 3605 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 ⓘ

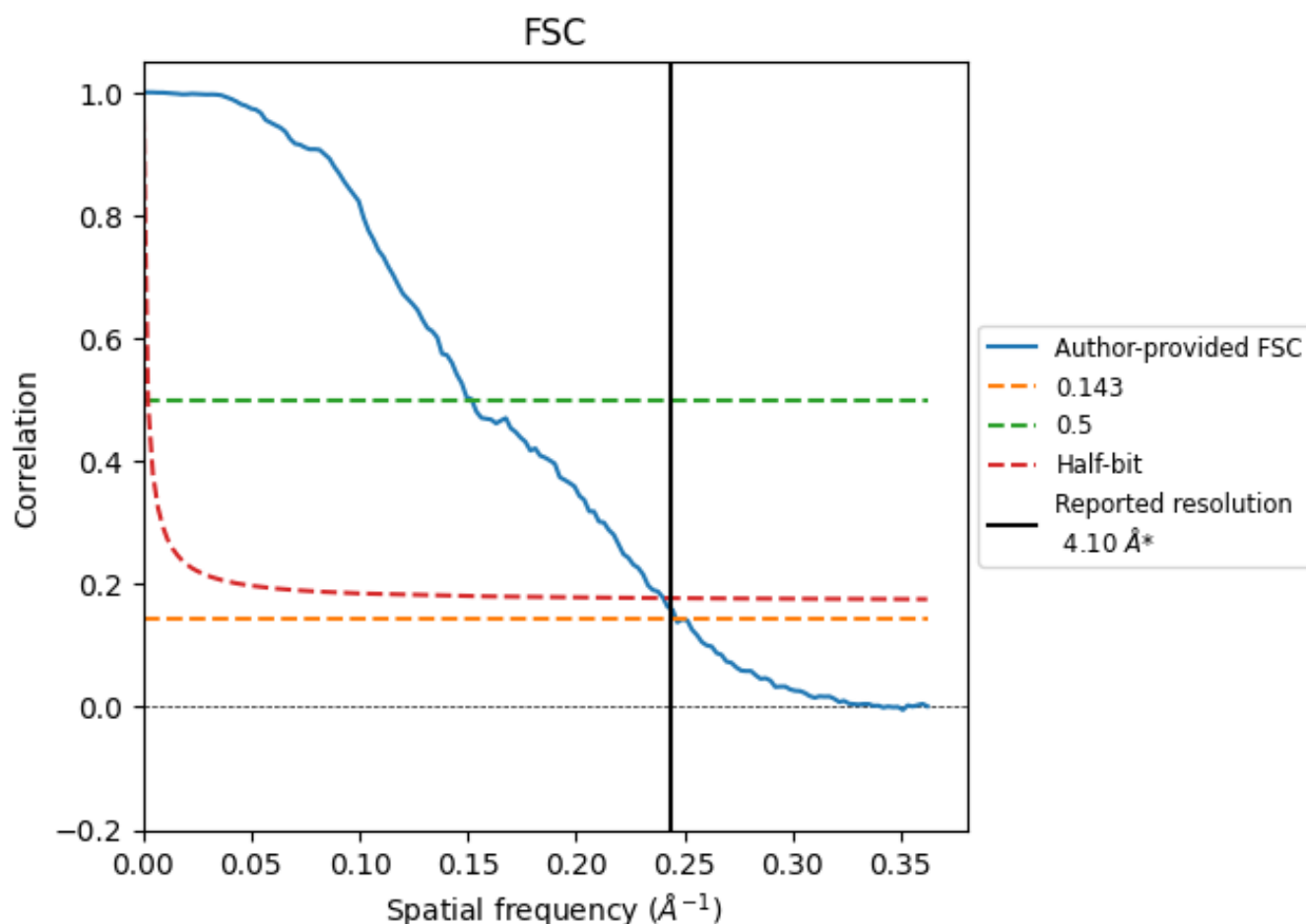


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

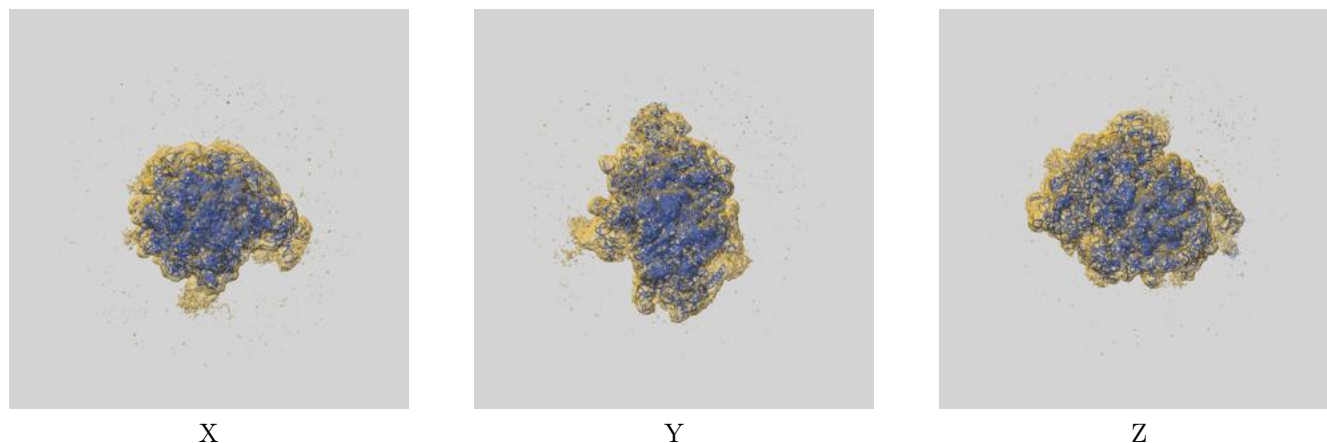
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.10                               | -    | -        |
| Author-provided FSC curve | 4.06                               | 6.59 | 4.16     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

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

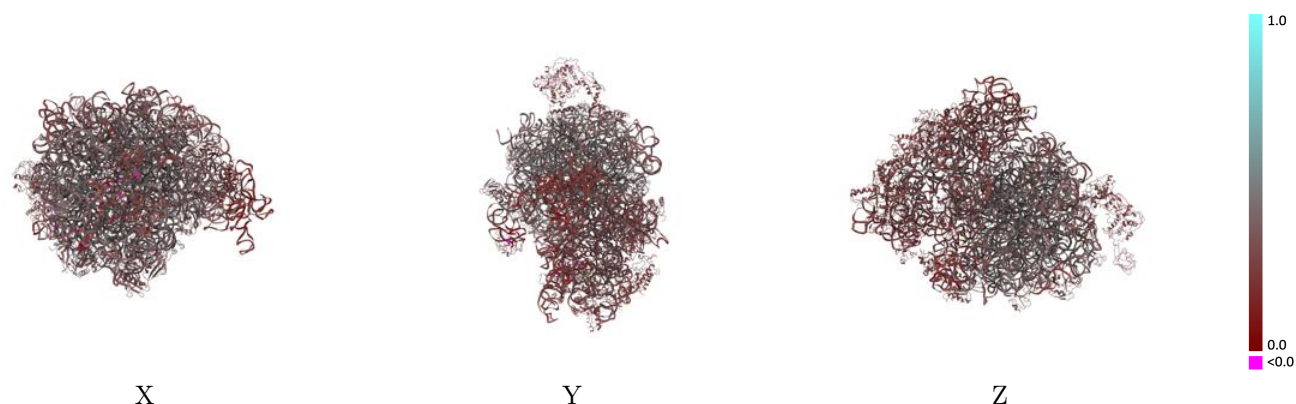
This section contains information regarding the fit between EMDB map EMD-30611 and PDB model 7D80. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

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



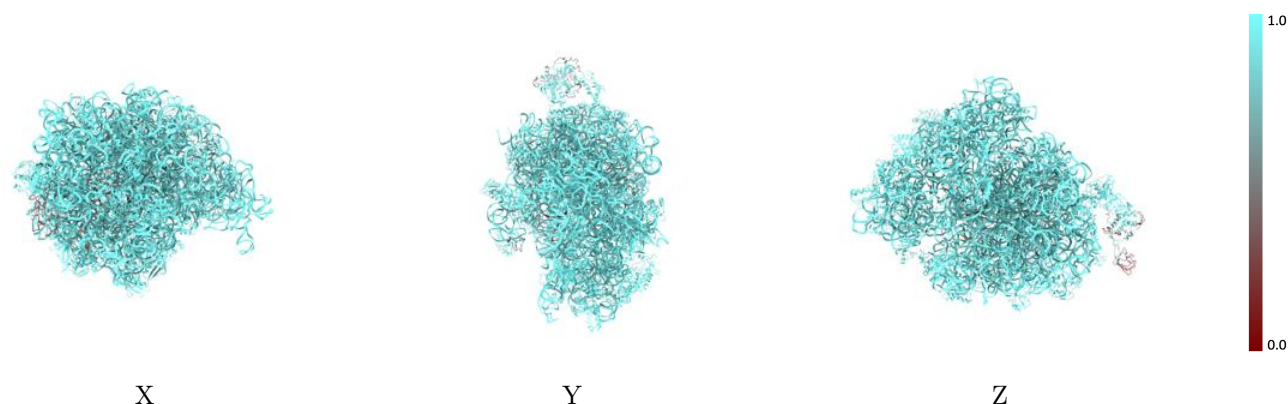
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



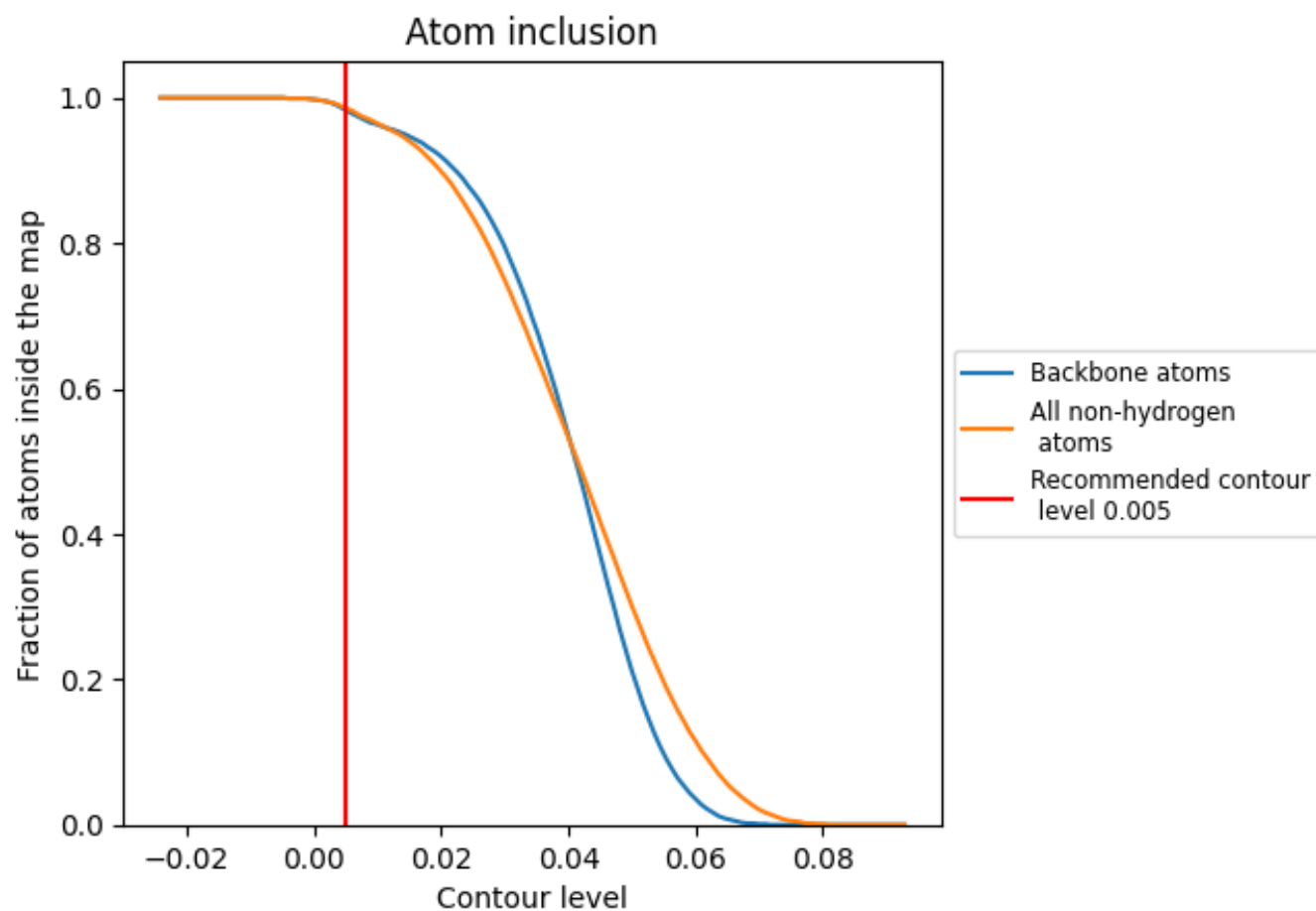
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 99% 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 (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9860   |  0.3390   |
| 0     |  0.9750   |  0.3790   |
| 1     |  0.9940   |  0.3960   |
| 2     |  1.0000   |  0.3610   |
| 3     |  0.9890   |  0.2710   |
| 5     |  0.6750   |  0.2400   |
| 6     |  1.0000   |  0.3920   |
| A     |  0.9990   |  0.3870   |
| B     |  1.0000   |  0.3000   |
| C     |  1.0000   |  0.2690   |
| D     |  0.9980   |  0.2850   |
| E     |  1.0000   |  0.2120   |
| F     |  0.9980   |  0.3040   |
| G     |  0.9940   |  0.2860   |
| H     |  0.9990  |  0.2410  |
| I     |  0.9990 |  0.2790 |
| J     |  1.0000 |  0.2260 |
| K     |  0.9970 |  0.2560 |
| L     |  0.9970 |  0.2910 |
| M     |  0.9940 |  0.2620 |
| N     |  0.9980 |  0.2210 |
| O     |  1.0000 |  0.2350 |
| P     |  0.9960 |  0.2560 |
| Q     |  0.9980 |  0.2510 |
| R     |  1.0000 |  0.2680 |
| S     |  1.0000 |  0.3140 |
| T     |  0.9980 |  0.2050 |
| U     |  0.9970 |  0.2250 |
| V     |  0.9930 |  0.2600 |
| W     |  0.9950 |  0.3610 |
| X     |  0.9980 |  0.2180 |
| Z     |  0.5280 |  0.2640 |
| a     |  1.0000 |  0.3520 |
| b     |  0.9910 |  0.4030 |
| c     |  0.9940 |  0.4000 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| d     |  0.9970   |  0.3740   |
| e     |  0.9990   |  0.2550   |
| f     |  1.0000   |  0.3330   |
| g     |  1.0000   |  0.3360   |
| h     |  0.8800   |  0.1720   |
| i     |  0.9960   |  0.3910   |
| j     |  0.9910   |  0.4010   |
| k     |  0.9950   |  0.3920   |
| l     |  0.9970   |  0.3940   |
| m     |  0.9980   |  0.3800   |
| n     |  1.0000   |  0.3220   |
| o     |  0.9930   |  0.3830   |
| p     |  0.9990   |  0.3670   |
| q     |  0.9960   |  0.4020   |
| r     |  0.9920   |  0.3850   |
| s     |  0.9960   |  0.3580   |
| t     |  1.0000   |  0.3620   |
| u     |  0.9980  |  0.4010  |
| v     |  0.9970 |  0.3730 |
| w     |  1.0000 |  0.2840 |
| x     |  0.9950 |  0.3850 |
| y     |  0.9700 |  0.2890 |
| z     |  0.9880 |  0.3580 |