



## Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 10:30 am BST

PDB ID : 8P18 / pdb\_00008p18  
EMDB ID : EMD-17348  
Title : E167K RF2 on E. coli 70S release complex with UGG (Structure III)  
Authors : Pundir, S.; Larsson, D.S.D.; Selmer, M.; Sanyal, S.  
Deposited on : 2023-05-11  
Resolution : 2.77 Å(reported)  
Based on initial models : 1GQE, 8B0X, 7K00, 5MDV

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

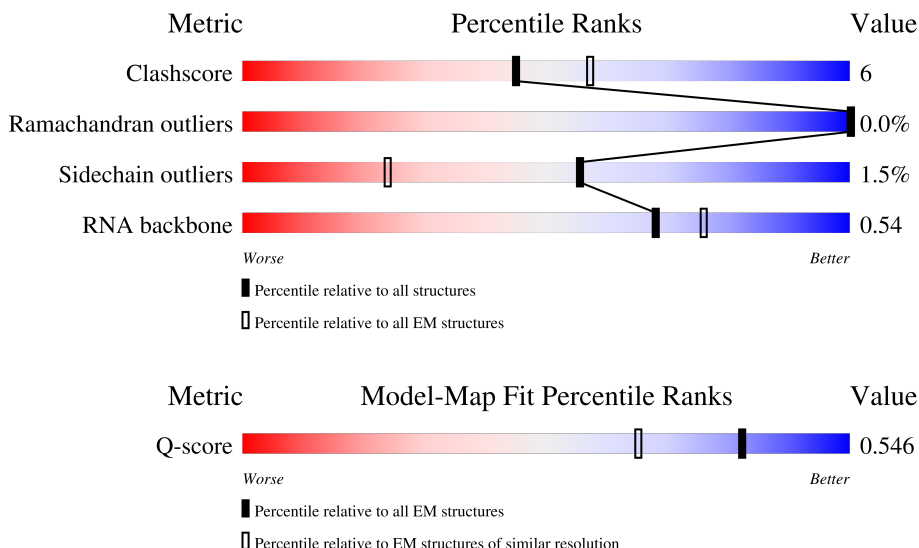
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.77 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                       | 10695 ( 2.27 - 3.27 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 2     | 1542   |                  |
| 2   | g     | 241    |                  |
| 3   | h     | 233    |                  |

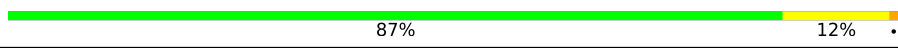
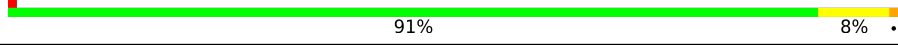
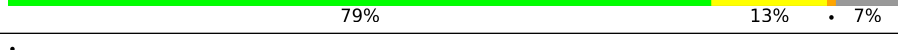
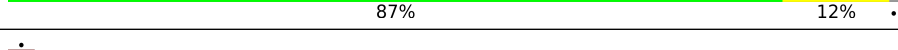
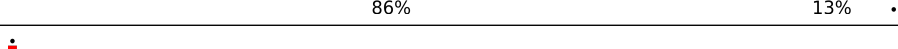
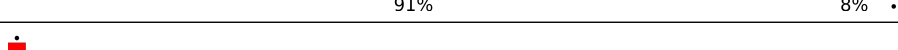
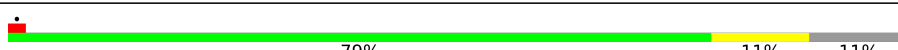
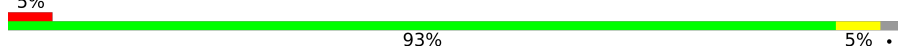
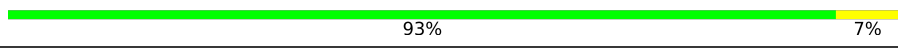
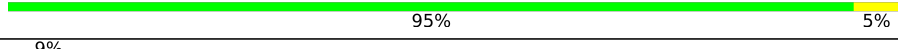
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | i     | 206    |                  |
| 5   | j     | 167    |                  |
| 6   | k     | 135    |                  |
| 7   | l     | 179    |                  |
| 8   | m     | 130    |                  |
| 9   | n     | 130    |                  |
| 10  | o     | 103    |                  |
| 11  | p     | 129    |                  |
| 12  | q     | 124    |                  |
| 13  | r     | 118    |                  |
| 14  | s     | 101    |                  |
| 15  | t     | 89     |                  |
| 16  | u     | 82     |                  |
| 17  | v     | 84     |                  |
| 18  | w     | 75     |                  |
| 19  | x     | 92     |                  |
| 20  | y     | 87     |                  |
| 21  | z     | 71     |                  |
| 22  | 4     | 49     |                  |
| 23  | 5     | 76     |                  |
| 24  | 1     | 2904   |                  |
| 25  | 3     | 120    |                  |
| 26  | B     | 273    |                  |
| 27  | C     | 209    |                  |
| 28  | D     | 201    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | E     | 179    |    |
| 30  | F     | 177    |    |
| 31  | J     | 142    |    |
| 32  | K     | 123    |    |
| 33  | L     | 144    |    |
| 34  | M     | 136    |    |
| 35  | N     | 127    |    |
| 36  | O     | 117    |    |
| 37  | P     | 115    |    |
| 38  | Q     | 118    |    |
| 39  | R     | 103    |    |
| 40  | S     | 110    |  |
| 41  | T     | 100    |  |
| 42  | U     | 104    |  |
| 43  | V     | 94     |  |
| 44  | W     | 85     |  |
| 45  | X     | 78     |  |
| 46  | Y     | 63     |  |
| 47  | Z     | 59     |  |
| 48  | b     | 57     |  |
| 49  | c     | 55     |  |
| 50  | d     | 46     |  |
| 51  | e     | 65     |  |
| 52  | f     | 38     |  |
| 53  | a     | 70     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | I     | 142    |                  |
| 55  | 6     | 365    |                  |
| 56  | G     | 149    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58  | SPD  | 2     | 1687 | -         | -        | X       | -                |

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 148603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | 2     | 1536     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32966 | 14711 | 6044 | 10675 | 1536 |         |       |

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | g     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1753  | 1109 | 315 | 321 | 8 |         |       |

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | h     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1648  | 1043 | 309 | 292 | 4 |         |       |

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | j     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 717 | 217 | 212 | 6 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | k     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 530 | 151 | 151 | 7 |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | l     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1214  | 756 | 235 | 219 | 4 |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | m     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | n     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | o     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | p     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 173 | 161 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| p     | 119     | IAS      | ASN    | variant | UNP P0A7R9 |

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | q     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |       |

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | r     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 552 | 179 | 157 | 3 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | s     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | t     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | u     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 403 | 127 | 112 | 1 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | v     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 641   | 406 | 120 | 112 | 3 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 18  | w     | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 345 | 102 | 96 | 1 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | x     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 427 | 127 | 112 | 2 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | y     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 21  | z     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 589   | 366 | 125 | 97 | 1 |         |       |

- Molecule 22 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | 4     | 26       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 562   | 251 | 104 | 181 | 26 |         |       |

- Molecule 23 is a RNA chain called tRNA(fMet).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | 5     | 76       | Total | C   | N   | O   | P  | 2       | 0     |
|     |       |          | 1665  | 742 | 302 | 543 | 78 |         |       |

- Molecule 24 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 24  | 1     | 2899     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62252 | 27778 | 11456 | 20119 | 2899 |         |       |

- Molecule 25 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 25  | 3     | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2549  | 1135 | 466 | 829 | 119 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | B     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | C     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 980 | 288 | 294 | 4 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | D     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | E     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | F     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1313  | 826 | 241 | 244 | 2 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | J     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | K     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | L     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | M     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 686 | 205 | 177 | 7 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| M     | 82      | MS6      | MET    | variant | UNP P0ADY7 |

- Molecule 35 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | N     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 585 | 194 | 161 | 5 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 36  | O     | 116      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | P     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 38  | Q     | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | R     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | S     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | T     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | U     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | V     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | W     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 582   | 360 | 117 | 104 | 1 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | X     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46  | Y     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47  | Z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48  | b     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | c     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 417   | 269 | 76 | 72 |   |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | d     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 51  | e     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52  | f     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 53 is a protein called Large ribosomal subunit protein bL31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53  | a     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 480   | 299 | 90 | 85 | 6 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | I     | 68       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 484   | 298 | 89 | 94 | 3 |         |       |

- Molecule 55 is a protein called Peptide chain release factor RF2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | 6     | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2855  | 1757 | 501 | 587 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| 6     | 167     | LYS      | GLU    | engineered mutation | UNP P07012 |

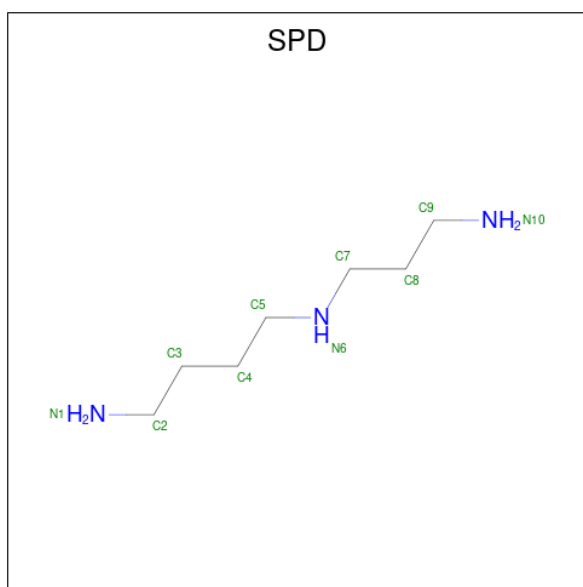
- Molecule 56 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | G     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 57  | 2     | 91       | Total | Mg  | 0       |
|     |       |          | 91    | 91  |         |
| 57  | s     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | 5     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 57  | 1     | 219      | Total | Mg  | 0       |
|     |       |          | 219   | 219 |         |
| 57  | 3     | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 57  | B     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | C     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | b     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 58 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).

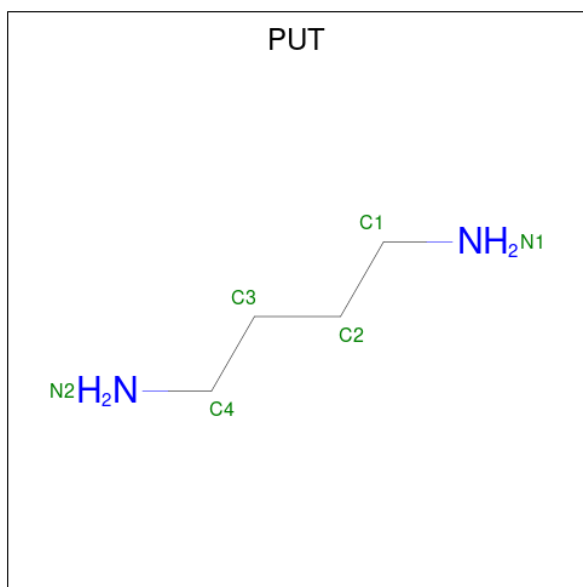


| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 58  | 2     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 2     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 58  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 59  | 2     | 35       | Total | K  | 0       |
|     |       |          | 35    | 35 |         |
| 59  | 1     | 92       | Total | K  | 0       |
|     |       |          | 92    | 92 |         |

- Molecule 60 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).



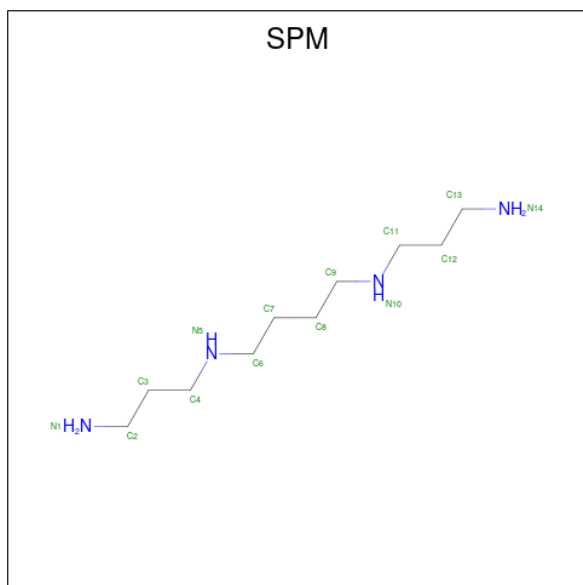
| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 60  | 2     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | 2     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

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| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 60  | 1     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | C     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 60  | Z     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

- Molecule 61 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 61  | 1     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 62  | f     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 62  | a     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

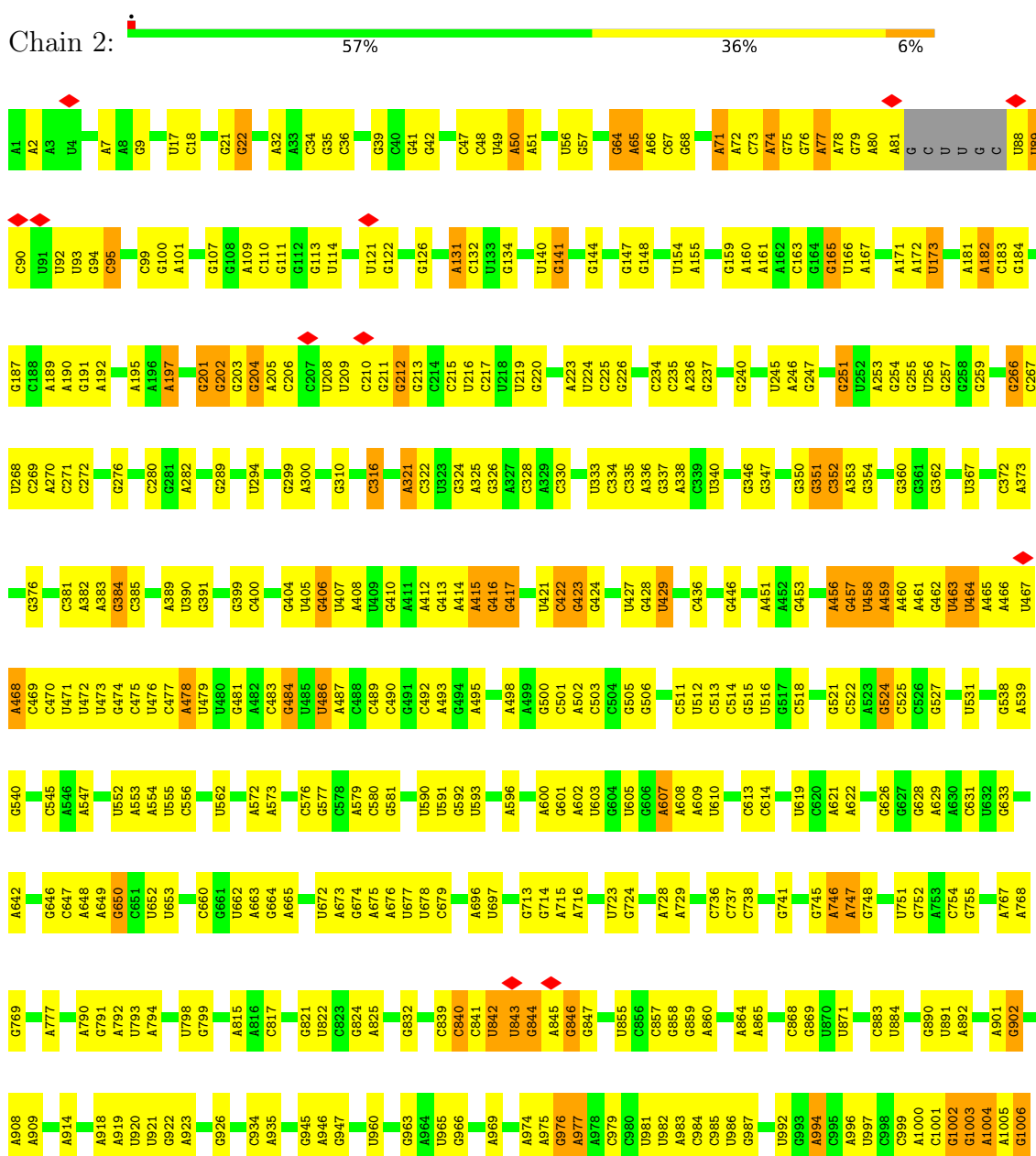
- Molecule 63 is water.

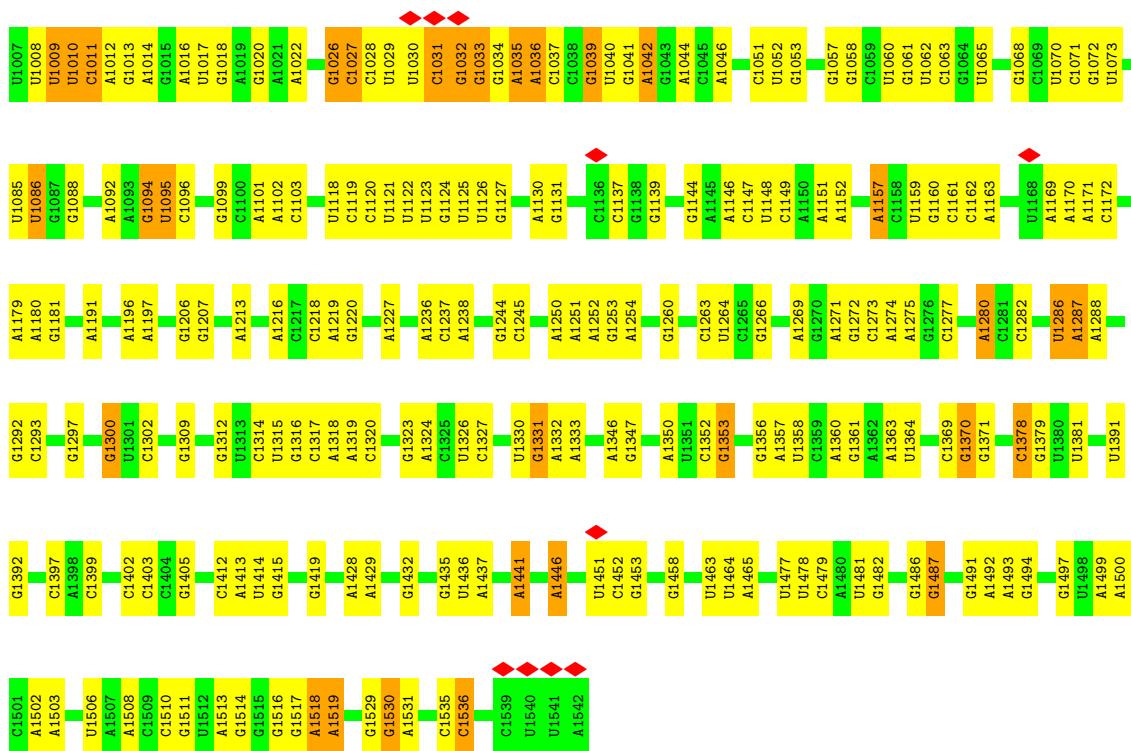
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 63  | 1     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

### 3 Residue-property plots

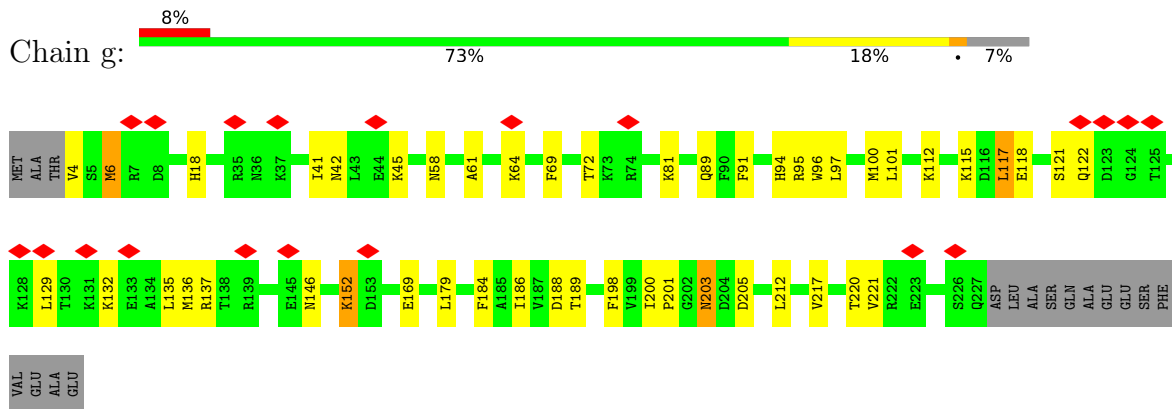
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S rRNA

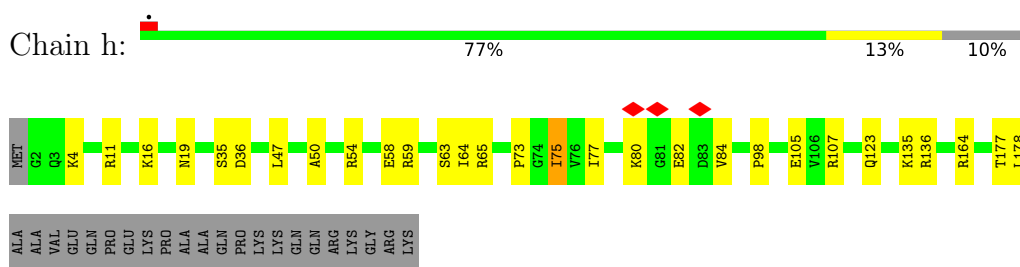




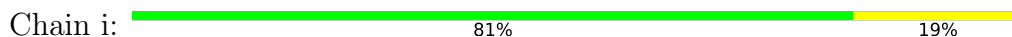
• Molecule 2: Small ribosomal subunit protein uS2

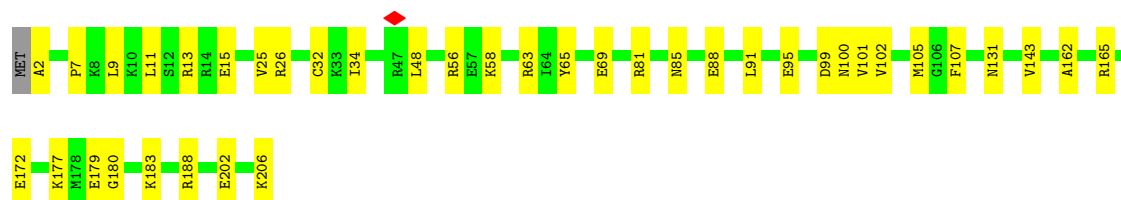


• Molecule 3: Small ribosomal subunit protein uS3

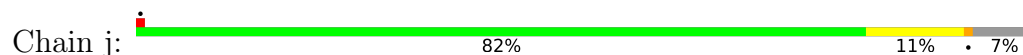


• Molecule 4: Small ribosomal subunit protein uS4

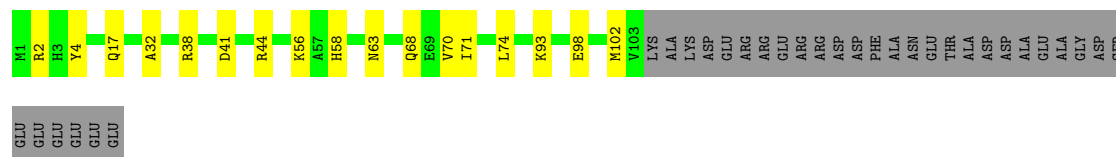




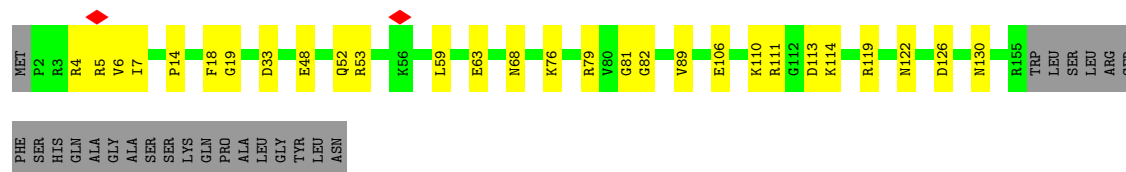
- Molecule 5: Small ribosomal subunit protein uS5



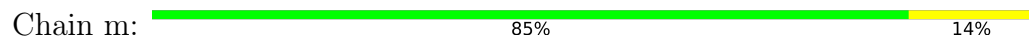
- Molecule 6: 30S ribosomal protein S6



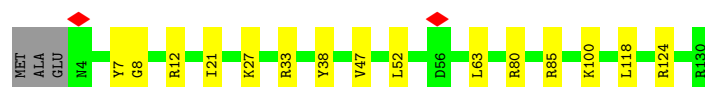
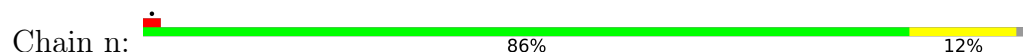
- Molecule 7: 30S ribosomal protein S7



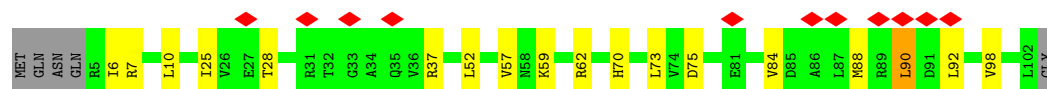
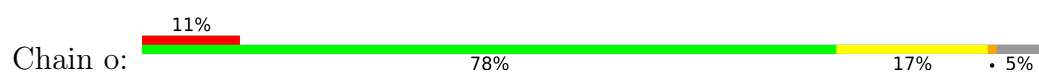
- Molecule 8: Small ribosomal subunit protein uS8



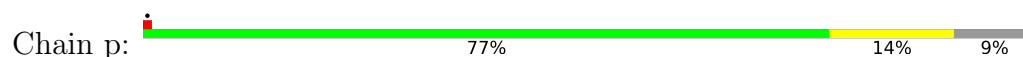
- Molecule 9: Small ribosomal subunit protein uS9



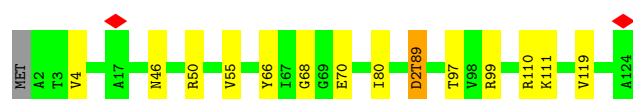
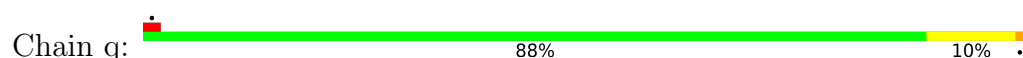
- Molecule 10: Small ribosomal subunit protein uS10



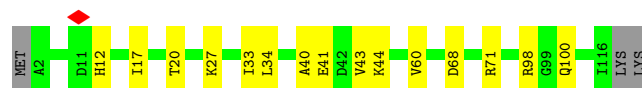
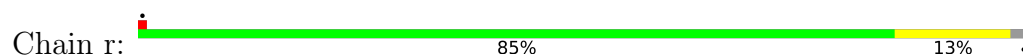
- Molecule 11: Small ribosomal subunit protein uS11



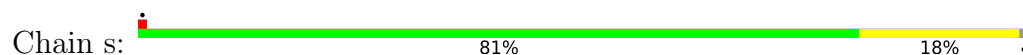
- Molecule 12: Small ribosomal subunit protein uS12



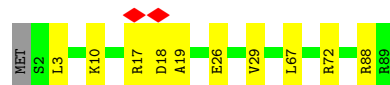
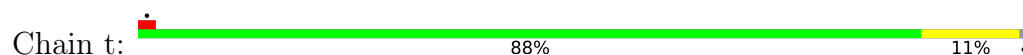
- Molecule 13: Small ribosomal subunit protein uS13



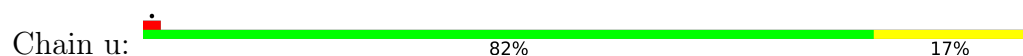
- Molecule 14: Small ribosomal subunit protein uS14



- Molecule 15: Small ribosomal subunit protein uS15



- Molecule 16: Small ribosomal subunit protein bS16

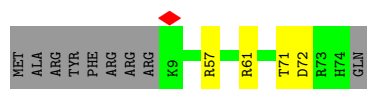
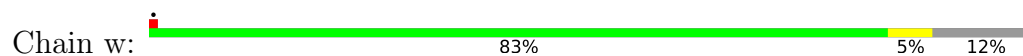




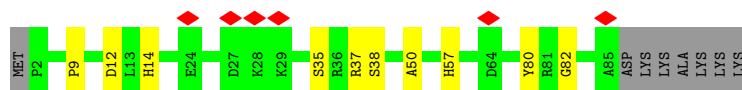
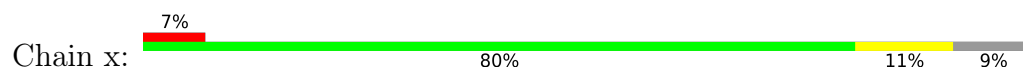
- Molecule 17: Small ribosomal subunit protein uS17



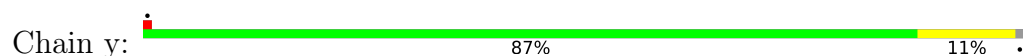
- Molecule 18: Small ribosomal subunit protein bS18



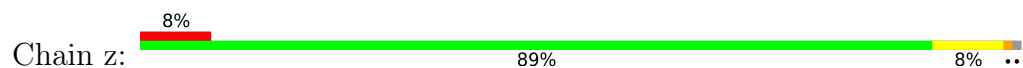
- Molecule 19: Small ribosomal subunit protein uS19



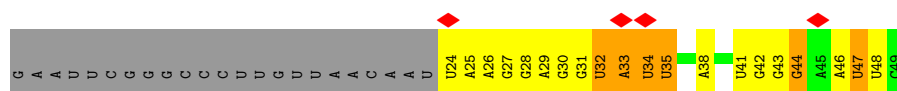
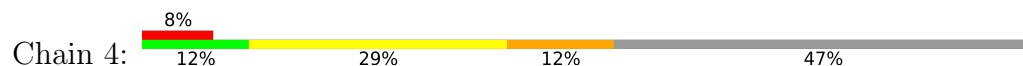
- Molecule 20: Small ribosomal subunit protein bS20



- Molecule 21: Small ribosomal subunit protein bS21



- Molecule 22: mRNA



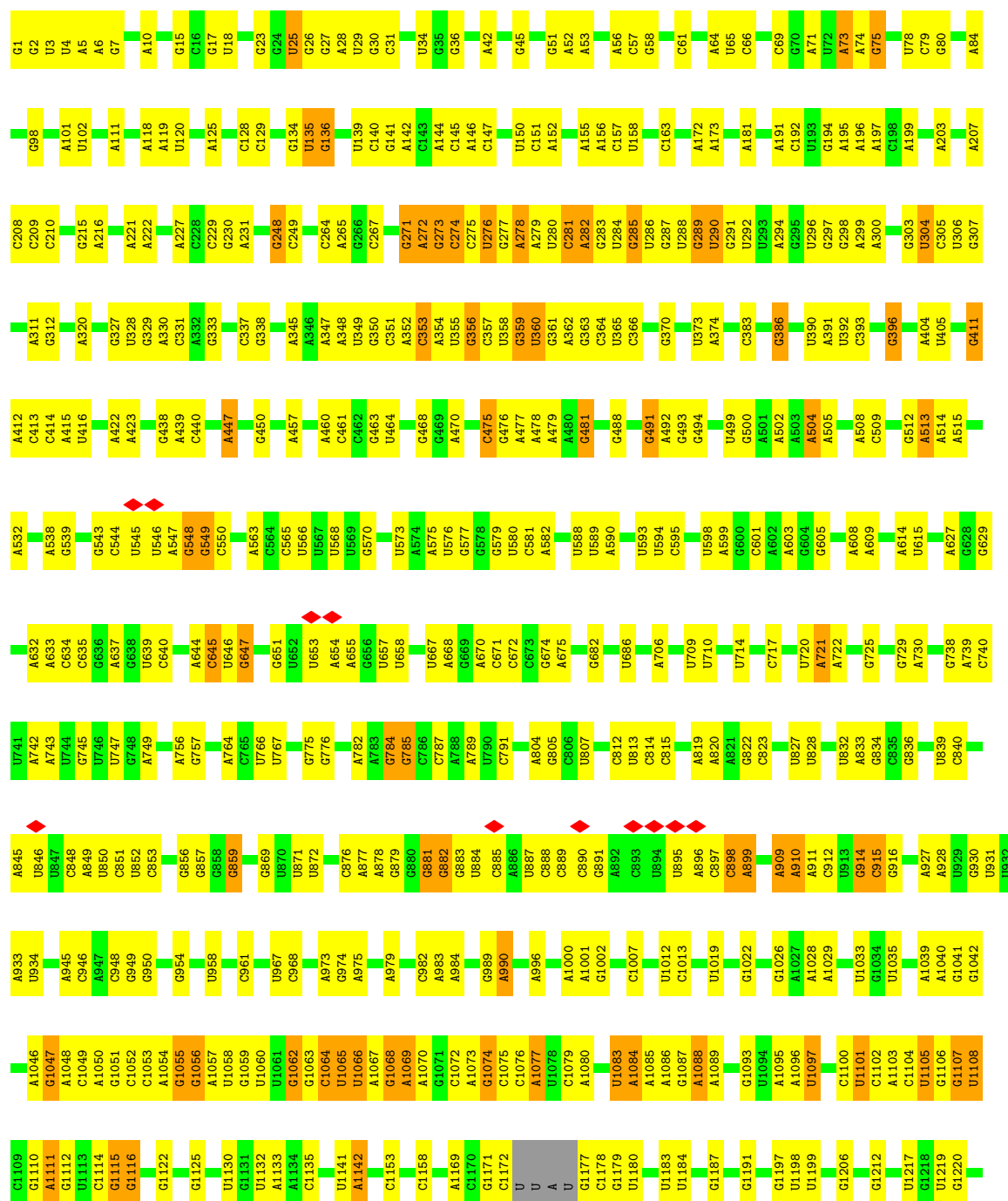
- Molecule 23: tRNA(fMet)

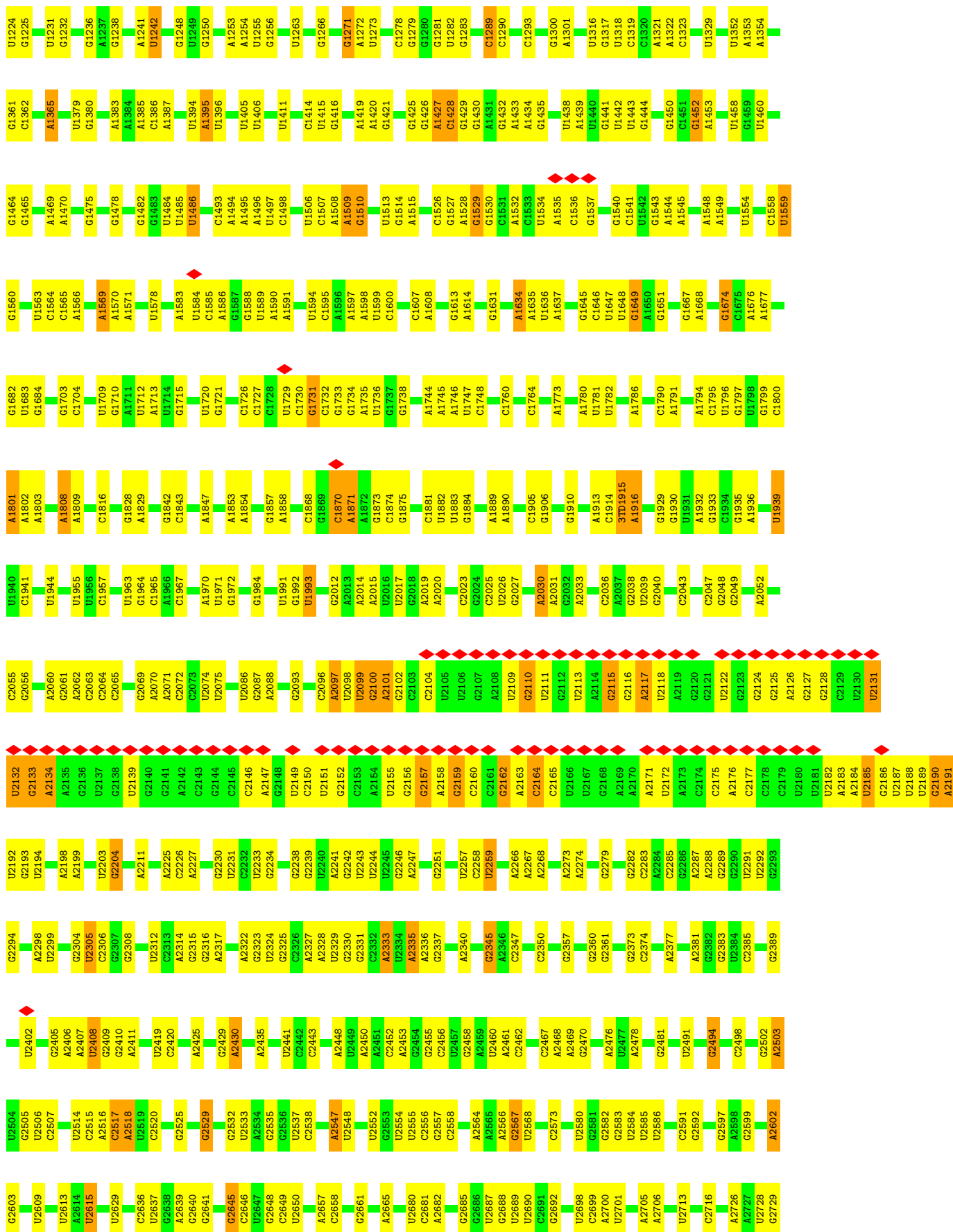
Chain 5:  51% 39% 9%

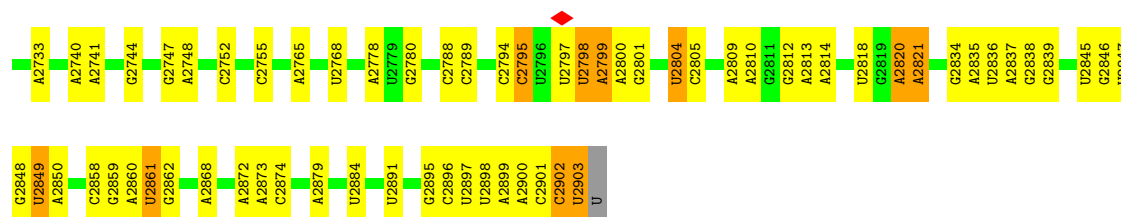


• Molecule 24: 23S rRNA

Chain 1:  61% 34% 5%

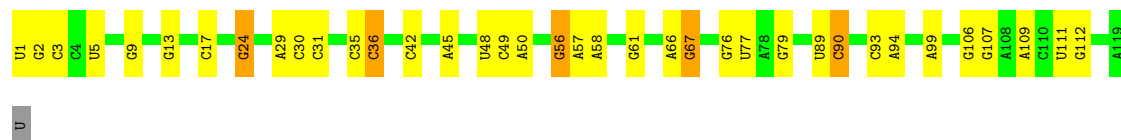






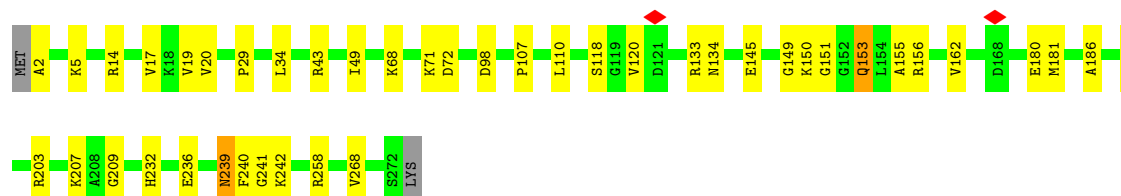
• Molecule 25: 5S rRNA

Chain 3: 68% 27%



• Molecule 26: 50S ribosomal protein L2

Chain B: 84% 15%



• Molecule 27: 50S ribosomal protein L3

Chain C: 89% 11%



• Molecule 28: 50S ribosomal protein L4

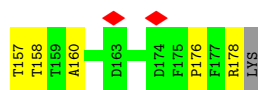
Chain D: 89% 11%



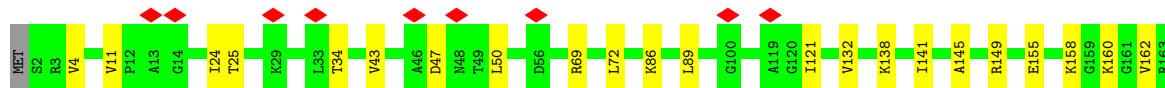
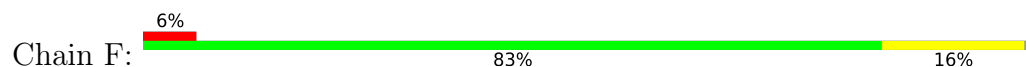
• Molecule 29: 50S ribosomal protein L5

Chain E: 79% 20%

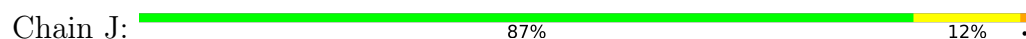




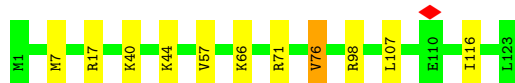
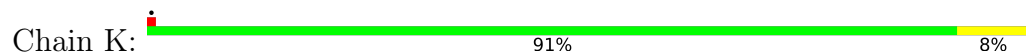
- Molecule 30: 50S ribosomal protein L6



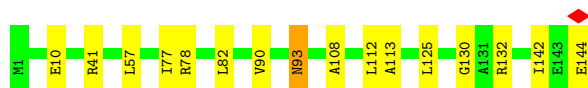
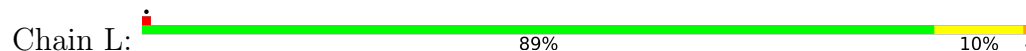
- Molecule 31: 50S ribosomal protein L13



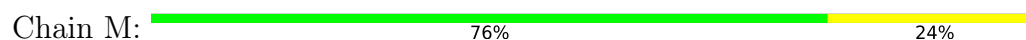
- Molecule 32: 50S ribosomal protein L14



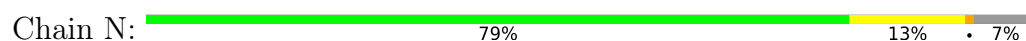
- Molecule 33: 50S ribosomal protein L15

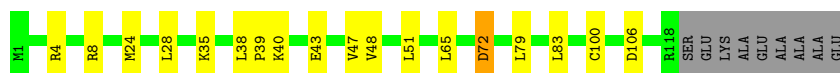


- Molecule 34: Large ribosomal subunit protein uL16

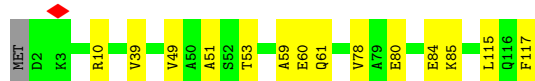
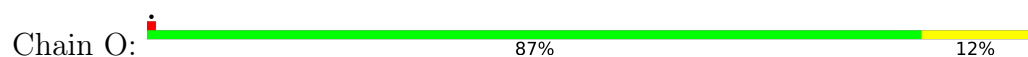


- Molecule 35: 50S ribosomal protein L17

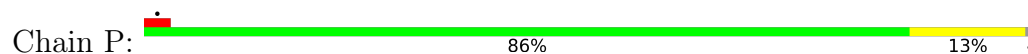




- Molecule 36: 50S ribosomal protein L18



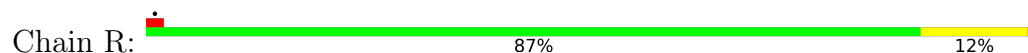
- Molecule 37: 50S ribosomal protein L19



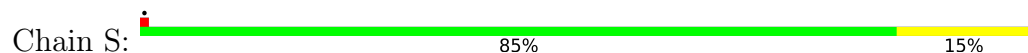
- Molecule 38: 50S ribosomal protein L20



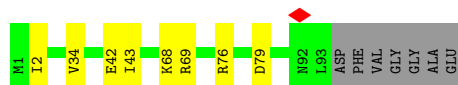
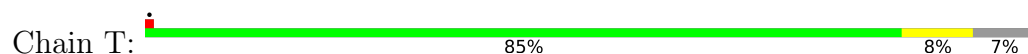
- Molecule 39: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L22

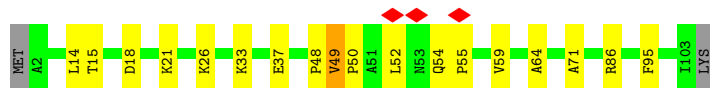


- Molecule 41: 50S ribosomal protein L23



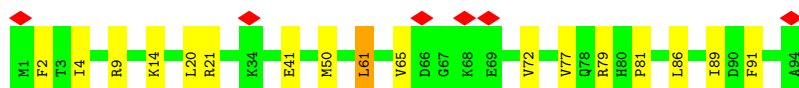
- Molecule 42: 50S ribosomal protein L24

Chain U:  81% 16% ..



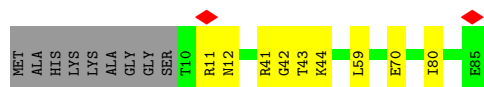
- Molecule 43: 50S ribosomal protein L25

Chain V:  6% 82% 17% .



- Molecule 44: 50S ribosomal protein L27

Chain W:  79% 11% 11%



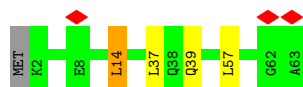
- Molecule 45: 50S ribosomal protein L28

Chain X:  85% 14% .



- Molecule 46: 50S ribosomal protein L29

Chain Y:  5% 92% 5% ..



- Molecule 47: 50S ribosomal protein L30

Chain Z:  5% 93% 5% .



- Molecule 48: 50S ribosomal protein L32

Chain b:  88% 11% .



## • Molecule 49: 50S ribosomal protein L33

Chain c:  78% 15% 7%

## • Molecule 50: 50S ribosomal protein L34

Chain d:  93% 7%

## • Molecule 51: 50S ribosomal protein L35

Chain e:  78% 20% 2%

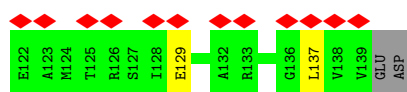
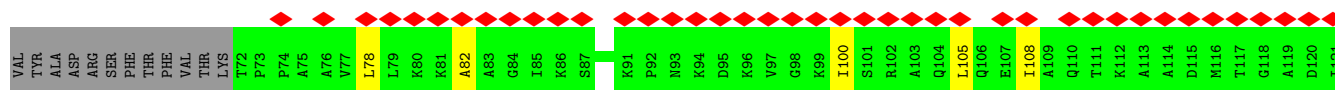
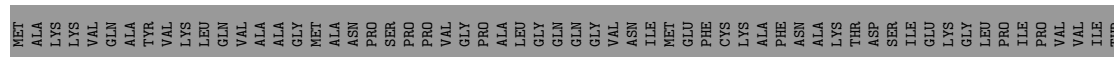
## • Molecule 52: 50S ribosomal protein L36

Chain f:  95% 5%

## • Molecule 53: Large ribosomal subunit protein bL31

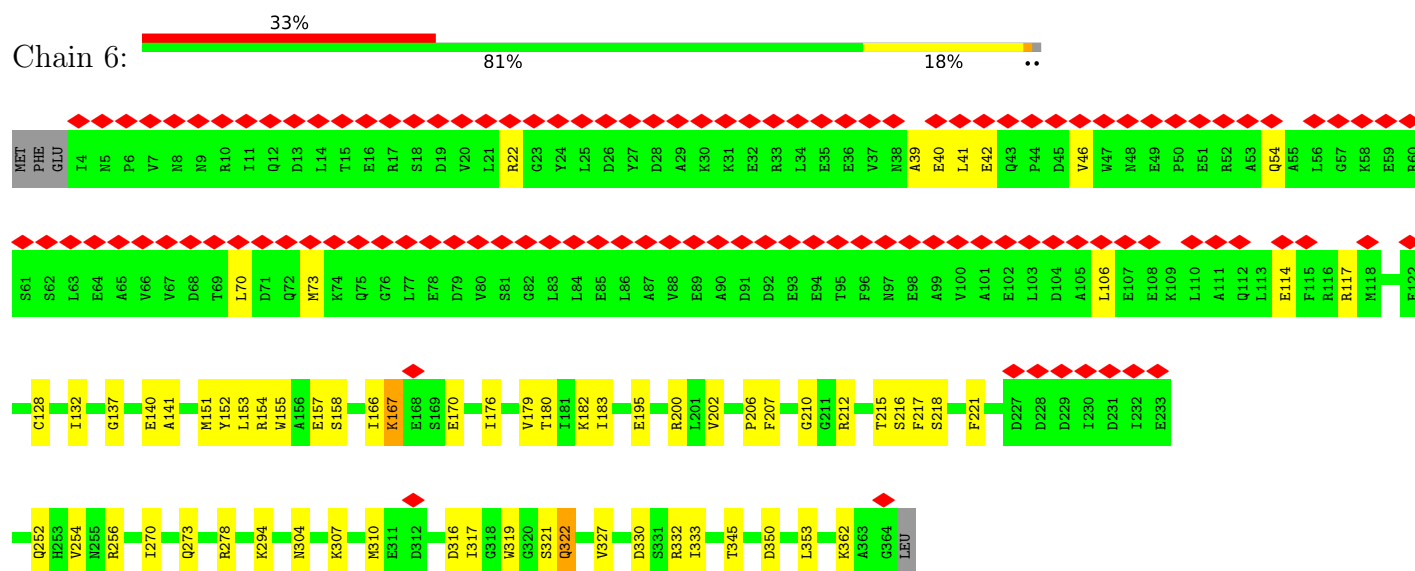
Chain a:  9% 67% 17% 5%

## • Molecule 54: 50S ribosomal protein L11

Chain I:  37% 43% 5% 52%

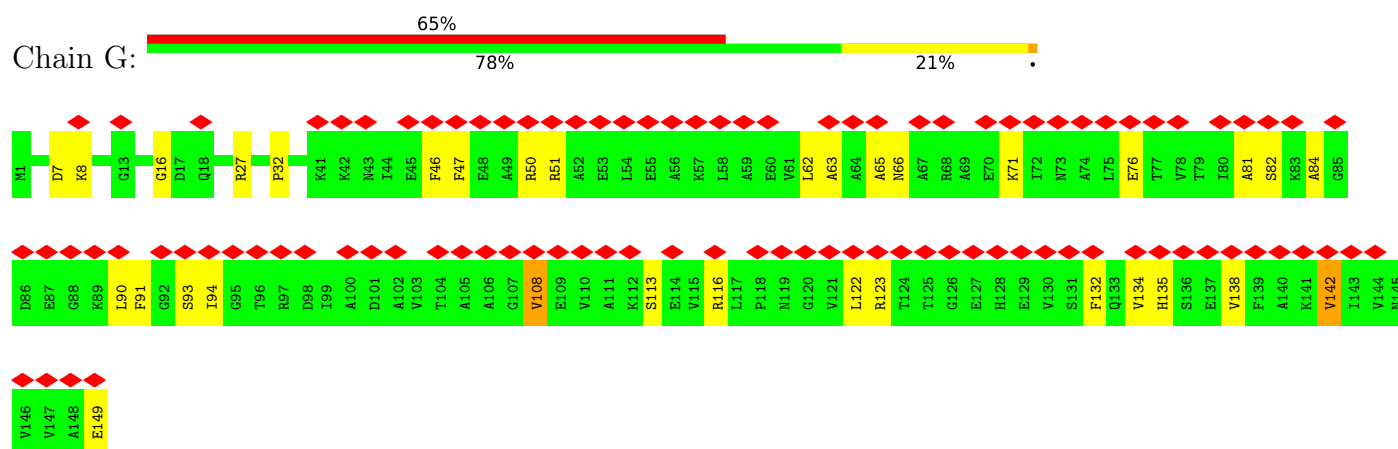
- Molecule 55: Peptide chain release factor RF2

Chain 6:



- Molecule 56: 50S ribosomal protein L9

Chain G:



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 21004                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 38.14                                   | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1300                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 1.261                                   | Depositor |
| Minimum map value                    | -0.428                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.056                                   | Depositor |
| Recommended contour level            | 0.19                                    | Depositor |
| Map size (Å)                         | 433.44598, 433.44598, 433.44598         | wwPDB     |
| Map dimensions                       | 520, 520, 520                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.83355, 0.83355, 0.83355               | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 3TD, D2T, OMU, H2U, G7M, MG, OMC, 4OC, 5MC, SPD, MA6, PUT, 1MG, 5MU, K, OMG, ZN, UR3, 2MA, 6MZ, 4D4, MEQ, 2MG, SPM, IAS, MS6

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$   |
| 1   | 2     | 0.31         | 0/36631     | 0.31        | 0/57136       |
| 2   | g     | 0.21         | 0/1784      | 0.32        | 0/2403        |
| 3   | h     | 0.25         | 0/1675      | 0.32        | 0/2256        |
| 4   | i     | 0.24         | 0/1665      | 0.28        | 0/2227        |
| 5   | j     | 0.28         | 0/1165      | 0.35        | 0/1568        |
| 6   | k     | 0.23         | 0/858       | 0.31        | 0/1160        |
| 7   | l     | 0.20         | 0/1230      | 0.30        | 0/1649        |
| 8   | m     | 0.27         | 0/989       | 0.31        | 0/1326        |
| 9   | n     | 0.22         | 0/1034      | 0.29        | 0/1375        |
| 10  | o     | 0.23         | 0/796       | 0.34        | 0/1077        |
| 11  | p     | 0.25         | 0/884       | 0.34        | 0/1191        |
| 12  | q     | 0.28         | 0/960       | 0.33        | 0/1286        |
| 13  | r     | 0.21         | 0/900       | 0.29        | 0/1204        |
| 14  | s     | 0.24         | 0/817       | 0.27        | 0/1088        |
| 15  | t     | 0.24         | 0/722       | 0.29        | 0/964         |
| 16  | u     | 0.26         | 0/653       | 0.32        | 0/877         |
| 17  | v     | 0.24         | 0/650       | 0.31        | 0/871         |
| 18  | w     | 0.26         | 0/553       | 0.31        | 0/742         |
| 19  | x     | 0.21         | 0/685       | 0.27        | 0/922         |
| 20  | y     | 0.24         | 0/676       | 0.28        | 0/895         |
| 21  | z     | 0.22         | 0/597       | 0.27        | 0/792         |
| 22  | 4     | 0.25         | 0/630       | 0.37        | 0/981         |
| 23  | 5     | 0.28         | 0/1859      | 0.30        | 0/2894        |
| 24  | 1     | 0.35         | 0/69147     | 0.32        | 0/107869      |
| 25  | 3     | 0.27         | 0/2850      | 0.27        | 0/4444        |
| 26  | B     | 0.33         | 0/2121      | 0.35        | 0/2852        |
| 27  | C     | 0.31         | 0/1576      | 0.32        | 0/2119        |
| 28  | D     | 0.28         | 0/1571      | 0.31        | 0/2113        |
| 29  | E     | 0.22         | 0/1434      | 0.32        | 0/1926        |
| 30  | F     | 0.22         | 0/1333      | 0.35        | 1/1805 (0.1%) |
| 31  | J     | 0.29         | 0/1152      | 0.28        | 0/1551        |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 32  | K     | 0.30         | 0/955    | 0.33        | 0/1279          |
| 33  | L     | 0.29         | 0/1062   | 0.31        | 0/1413          |
| 34  | M     | 0.30         | 0/1073   | 0.32        | 0/1433          |
| 35  | N     | 0.31         | 0/958    | 0.35        | 0/1281          |
| 36  | O     | 0.23         | 0/902    | 0.33        | 0/1209          |
| 37  | P     | 0.29         | 0/929    | 0.32        | 0/1242          |
| 38  | Q     | 0.33         | 0/960    | 0.32        | 0/1278          |
| 39  | R     | 0.29         | 0/829    | 0.37        | 0/1107          |
| 40  | S     | 0.30         | 0/864    | 0.31        | 0/1156          |
| 41  | T     | 0.26         | 0/744    | 0.33        | 0/994           |
| 42  | U     | 0.25         | 0/787    | 0.31        | 0/1051          |
| 43  | V     | 0.25         | 0/766    | 0.34        | 0/1025          |
| 44  | W     | 0.30         | 0/589    | 0.37        | 0/779           |
| 45  | X     | 0.31         | 0/635    | 0.31        | 0/848           |
| 46  | Y     | 0.22         | 0/502    | 0.24        | 0/667           |
| 47  | Z     | 0.28         | 0/453    | 0.35        | 0/605           |
| 48  | b     | 0.29         | 0/450    | 0.31        | 0/599           |
| 49  | c     | 0.26         | 0/424    | 0.33        | 0/565           |
| 50  | d     | 0.32         | 0/380    | 0.29        | 0/498           |
| 51  | e     | 0.29         | 0/513    | 0.32        | 0/676           |
| 52  | f     | 0.32         | 0/303    | 0.35        | 0/397           |
| 53  | a     | 0.17         | 0/488    | 0.30        | 0/649           |
| 54  | I     | 0.15         | 0/486    | 0.38        | 0/650           |
| 55  | 6     | 0.24         | 0/2884   | 0.33        | 0/3885          |
| 56  | G     | 0.18         | 0/1122   | 0.34        | 0/1515          |
| All | All   | 0.32         | 0/159655 | 0.32        | 1/238364 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | F     | 47  | ASP  | CB-CA-C | -5.30 | 110.02      | 117.23   |

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 32966 | 0        | 16605    | 440     | 0            |
| 2   | g     | 1753  | 0        | 1780     | 27      | 0            |
| 3   | h     | 1648  | 0        | 1722     | 17      | 0            |
| 4   | i     | 1643  | 0        | 1707     | 27      | 0            |
| 5   | j     | 1152  | 0        | 1196     | 14      | 0            |
| 6   | k     | 839   | 0        | 833      | 9       | 0            |
| 7   | l     | 1214  | 0        | 1267     | 19      | 0            |
| 8   | m     | 979   | 0        | 1031     | 14      | 0            |
| 9   | n     | 1022  | 0        | 1070     | 11      | 0            |
| 10  | o     | 786   | 0        | 828      | 10      | 0            |
| 11  | p     | 877   | 0        | 884      | 11      | 0            |
| 12  | q     | 957   | 0        | 1017     | 9       | 0            |
| 13  | r     | 891   | 0        | 952      | 11      | 0            |
| 14  | s     | 805   | 0        | 844      | 12      | 0            |
| 15  | t     | 714   | 0        | 734      | 7       | 0            |
| 16  | u     | 643   | 0        | 661      | 9       | 0            |
| 17  | v     | 641   | 0        | 682      | 16      | 0            |
| 18  | w     | 544   | 0        | 565      | 3       | 0            |
| 19  | x     | 668   | 0        | 693      | 6       | 0            |
| 20  | y     | 670   | 0        | 719      | 6       | 0            |
| 21  | z     | 589   | 0        | 629      | 5       | 0            |
| 22  | 4     | 562   | 0        | 279      | 24      | 0            |
| 23  | 5     | 1665  | 0        | 848      | 12      | 0            |
| 24  | 1     | 62252 | 0        | 31312    | 605     | 0            |
| 25  | 3     | 2549  | 0        | 1291     | 24      | 0            |
| 26  | B     | 2082  | 0        | 2154     | 31      | 0            |
| 27  | C     | 1566  | 0        | 1618     | 13      | 0            |
| 28  | D     | 1552  | 0        | 1619     | 13      | 0            |
| 29  | E     | 1410  | 0        | 1444     | 23      | 0            |
| 30  | F     | 1313  | 0        | 1358     | 15      | 0            |
| 31  | J     | 1129  | 0        | 1162     | 14      | 0            |
| 32  | K     | 946   | 0        | 1023     | 8       | 0            |
| 33  | L     | 1053  | 0        | 1129     | 11      | 0            |
| 34  | M     | 1075  | 0        | 1145     | 22      | 0            |
| 35  | N     | 945   | 0        | 989      | 11      | 0            |
| 36  | O     | 892   | 0        | 923      | 8       | 0            |
| 37  | P     | 917   | 0        | 962      | 11      | 0            |
| 38  | Q     | 947   | 0        | 1019     | 8       | 0            |
| 39  | R     | 816   | 0        | 839      | 7       | 0            |
| 40  | S     | 857   | 0        | 922      | 11      | 0            |
| 41  | T     | 738   | 0        | 807      | 3       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 42  | U     | 779    | 0        | 830      | 10      | 0            |
| 43  | V     | 753    | 0        | 780      | 11      | 0            |
| 44  | W     | 582    | 0        | 599      | 6       | 0            |
| 45  | X     | 625    | 0        | 652      | 8       | 0            |
| 46  | Y     | 501    | 0        | 531      | 2       | 0            |
| 47  | Z     | 449    | 0        | 488      | 2       | 0            |
| 48  | b     | 444    | 0        | 458      | 5       | 0            |
| 49  | c     | 417    | 0        | 451      | 5       | 0            |
| 50  | d     | 377    | 0        | 418      | 3       | 0            |
| 51  | e     | 504    | 0        | 572      | 8       | 0            |
| 52  | f     | 302    | 0        | 340      | 1       | 0            |
| 53  | a     | 480    | 0        | 478      | 9       | 0            |
| 54  | I     | 484    | 0        | 521      | 3       | 0            |
| 55  | 6     | 2855   | 0        | 2756     | 38      | 0            |
| 56  | G     | 1111   | 0        | 1148     | 20      | 0            |
| 57  | 1     | 219    | 0        | 0        | 0       | 0            |
| 57  | 2     | 91     | 0        | 0        | 0       | 0            |
| 57  | 3     | 5      | 0        | 0        | 0       | 0            |
| 57  | 5     | 2      | 0        | 0        | 0       | 0            |
| 57  | B     | 1      | 0        | 0        | 0       | 0            |
| 57  | C     | 1      | 0        | 0        | 0       | 0            |
| 57  | b     | 1      | 0        | 0        | 0       | 0            |
| 57  | s     | 1      | 0        | 0        | 0       | 0            |
| 58  | 1     | 110    | 0        | 209      | 3       | 0            |
| 58  | 2     | 20     | 0        | 38       | 7       | 0            |
| 59  | 1     | 92     | 0        | 0        | 0       | 0            |
| 59  | 2     | 35     | 0        | 0        | 0       | 0            |
| 60  | 1     | 54     | 0        | 108      | 4       | 0            |
| 60  | 2     | 12     | 0        | 24       | 4       | 0            |
| 60  | C     | 6      | 0        | 12       | 1       | 0            |
| 60  | Z     | 6      | 0        | 12       | 0       | 0            |
| 61  | 1     | 14     | 0        | 26       | 0       | 0            |
| 62  | a     | 1      | 0        | 0        | 0       | 0            |
| 62  | f     | 1      | 0        | 0        | 0       | 0            |
| 63  | 1     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 148603 | 0        | 100713   | 1548    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1548) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2:1028:C:N4     | 1:2:1033:G:O6      | 2.09                     | 0.84              |
| 24:1:1056:G:H4'   | 24:1:1086:A:H8     | 1.41                     | 0.83              |
| 1:2:946:A:H2'     | 1:2:947:G:C8       | 2.15                     | 0.81              |
| 24:1:568:U:H1'    | 24:1:2030:6MZ:H9C1 | 1.63                     | 0.80              |
| 24:1:2100:G:H1    | 24:1:2189:U:H3     | 1.32                     | 0.78              |
| 29:E:158:THR:HG22 | 29:E:160:ALA:H     | 1.47                     | 0.78              |
| 24:1:1178:C:H2'   | 24:1:1179:G:H8     | 1.50                     | 0.77              |
| 56:G:84:ALA:HB2   | 56:G:90:LEU:HD23   | 1.67                     | 0.76              |
| 1:2:1312:G:OP2    | 53:a:63:ARG:NH2    | 2.19                     | 0.75              |
| 1:2:81:A:N6       | 1:2:88:U:O4        | 2.17                     | 0.75              |
| 24:1:1063:G:O2'   | 24:1:1064:C:O5'    | 2.05                     | 0.74              |
| 1:2:673:A:H2'     | 1:2:674:G:C8       | 2.21                     | 0.74              |
| 24:1:1105:U:H2'   | 24:1:1106:G:H8     | 1.52                     | 0.74              |
| 4:i:172:GLU:HG3   | 4:i:183:LYS:HD2    | 1.68                     | 0.74              |
| 24:1:1105:U:H2'   | 24:1:1106:G:C8     | 2.22                     | 0.73              |
| 26:B:107:PRO:HD2  | 26:B:110:LEU:HD22  | 1.70                     | 0.73              |
| 45:X:74:ARG:NH1   | 45:X:76:GLU:OE2    | 2.21                     | 0.72              |
| 1:2:754:C:OP1     | 15:t:72:ARG:NH2    | 2.23                     | 0.72              |
| 1:2:1009:U:H3     | 1:2:1020:G:H1      | 1.37                     | 0.72              |
| 1:2:946:A:H2'     | 1:2:947:G:H8       | 1.52                     | 0.72              |
| 55:6:117:ARG:NH2  | 55:6:362:LYS:O     | 2.23                     | 0.71              |
| 3:h:73:PRO:HG3    | 3:h:105:GLU:HG2    | 1.72                     | 0.71              |
| 34:M:77:PRO:HG2   | 34:M:80:VAL:HG21   | 1.70                     | 0.71              |
| 56:G:81:ALA:HB1   | 56:G:149:GLU:HB2   | 1.71                     | 0.71              |
| 24:1:954:G:OP2    | 34:M:16:ARG:NH1    | 2.22                     | 0.71              |
| 24:1:1478:G:H1    | 24:1:1513:U:H3     | 1.38                     | 0.71              |
| 25:3:17:C:O2      | 25:3:67:G:N2       | 2.16                     | 0.71              |
| 25:3:36:C:N4      | 25:3:49:C:O2       | 2.24                     | 0.71              |
| 1:2:415:A:H3'     | 1:2:416:G:H8       | 1.55                     | 0.71              |
| 4:i:48:LEU:HD21   | 4:i:56:ARG:HG3     | 1.71                     | 0.71              |
| 25:3:1:U:H2'      | 25:3:2:G:H8        | 1.56                     | 0.70              |
| 42:U:26:LYS:HD3   | 42:U:37:GLU:HB3    | 1.73                     | 0.70              |
| 1:2:664:G:H22     | 1:2:741:G:H1       | 1.39                     | 0.70              |
| 3:h:35:SER:OG     | 3:h:59:ARG:NH2     | 2.25                     | 0.70              |
| 22:4:47:U:H5'     | 22:4:48:U:H5''     | 1.74                     | 0.70              |
| 24:1:1102:C:H2'   | 24:1:1103:A:H8     | 1.55                     | 0.69              |
| 1:2:842:U:H4'     | 1:2:846:G:N1       | 2.06                     | 0.69              |
| 1:2:1323:G:H2'    | 1:2:1324:A:C8      | 2.28                     | 0.69              |
| 7:l:113:ASP:OD2   | 7:l:122:ASN:ND2    | 2.25                     | 0.69              |
| 9:n:52:LEU:HD11   | 9:n:63:LEU:HD11    | 1.73                     | 0.69              |
| 5:j:164:ILE:O     | 8:m:114:ARG:NH2    | 2.26                     | 0.68              |
| 1:2:1086:U:H3     | 1:2:1099:G:H22     | 1.41                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:324:G:O2'    | 58:2:1687:SPD:N10 | 2.27                     | 0.68              |
| 24:1:1068:G:N2   | 24:1:1095:A:O2'   | 2.27                     | 0.68              |
| 55:6:330:ASP:OD2 | 55:6:332:ARG:NH1  | 2.27                     | 0.67              |
| 31:J:125:TYR:OH  | 31:J:132:HIS:NE2  | 2.27                     | 0.67              |
| 1:2:1218:C:H2'   | 1:2:1219:A:C8     | 2.30                     | 0.67              |
| 3:h:77:ILE:HA    | 3:h:84:VAL:HG23   | 1.77                     | 0.67              |
| 24:1:1944:U:H5'' | 60:1:3330:PUT:H22 | 1.76                     | 0.67              |
| 15:t:18:ASP:OD1  | 15:t:19:ALA:N     | 2.28                     | 0.67              |
| 30:F:24:ILE:HD11 | 30:F:43:VAL:HG11  | 1.75                     | 0.66              |
| 24:1:1058:U:H2'  | 24:1:1059:G:C8    | 2.30                     | 0.66              |
| 3:h:58:GLU:OE1   | 3:h:65:ARG:NH1    | 2.29                     | 0.66              |
| 24:1:1069:A:O2'  | 24:1:1073:A:N6    | 2.28                     | 0.66              |
| 24:1:1747:U:H2'  | 24:1:1748:C:C6    | 2.31                     | 0.66              |
| 1:2:1297:G:O2'   | 7:l:114:LYS:NZ    | 2.26                     | 0.66              |
| 24:1:1434:A:H2'  | 24:1:1435:G:C8    | 2.31                     | 0.66              |
| 24:1:1590:A:H2'  | 24:1:1591:A:C8    | 2.31                     | 0.66              |
| 1:2:93:U:H2'     | 1:2:95:C:H5       | 1.62                     | 0.65              |
| 24:1:1076:C:H2'  | 24:1:1077:A:C8    | 2.31                     | 0.65              |
| 56:G:113:SER:O   | 56:G:116:ARG:NH1  | 2.29                     | 0.65              |
| 17:v:18:GLU:O    | 17:v:51:ASN:ND2   | 2.29                     | 0.65              |
| 24:1:1434:A:H2'  | 24:1:1435:G:H8    | 1.61                     | 0.65              |
| 33:L:93:ASN:OD1  | 33:L:93:ASN:N     | 2.24                     | 0.65              |
| 42:U:14:LEU:HD11 | 42:U:71:ALA:HB2   | 1.77                     | 0.65              |
| 1:2:999:C:N3     | 1:2:1042:A:N6     | 2.44                     | 0.65              |
| 24:1:284:U:H2'   | 24:1:285:G:C8     | 2.31                     | 0.65              |
| 7:l:113:ASP:HB2  | 7:l:119:ARG:HG3   | 1.78                     | 0.65              |
| 24:1:2328:A:H2'  | 24:1:2329:U:C6    | 2.31                     | 0.65              |
| 24:1:2134:A:N6   | 24:1:2157:G:O2'   | 2.30                     | 0.65              |
| 24:1:1802:A:H2'  | 24:1:1803:A:C8    | 2.33                     | 0.65              |
| 24:1:2133:G:O2'  | 24:1:2157:G:N2    | 2.30                     | 0.65              |
| 1:2:269:C:H2'    | 1:2:270:A:C8      | 2.32                     | 0.64              |
| 1:2:316:C:H5'    | 60:2:1728:PUT:H31 | 1.77                     | 0.64              |
| 2:g:18:HIS:NE2   | 2:g:205:ASP:OD2   | 2.30                     | 0.64              |
| 1:2:92:U:H2'     | 1:2:93:U:C6       | 2.32                     | 0.64              |
| 13:r:12:HIS:O    | 13:r:44:LYS:NZ    | 2.25                     | 0.64              |
| 26:B:239:ASN:OD1 | 26:B:239:ASN:N    | 2.30                     | 0.64              |
| 25:3:1:U:H2'     | 25:3:2:G:C8       | 2.33                     | 0.64              |
| 34:M:66:ARG:NH1  | 34:M:104:GLU:OE2  | 2.31                     | 0.64              |
| 53:a:41:HIS:HB3  | 53:a:44:PHE:HD2   | 1.63                     | 0.64              |
| 1:2:1152:A:OP1   | 10:o:70:HIS:ND1   | 2.28                     | 0.64              |
| 24:1:1469:A:H2'  | 24:1:1470:A:C8    | 2.33                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:B:29:PRO:HG2  | 26:B:34:LEU:HD11  | 1.79                     | 0.63              |
| 36:O:39:VAL:HB   | 36:O:49:VAL:HG22  | 1.79                     | 0.63              |
| 1:2:310:G:H5''   | 16:u:31:ARG:HB2   | 1.80                     | 0.63              |
| 1:2:677:U:H3     | 1:2:713:G:H22     | 1.47                     | 0.63              |
| 1:2:1356:G:H2'   | 1:2:1357:A:C8     | 2.34                     | 0.63              |
| 1:2:352:C:H5'    | 60:2:1728:PUT:H42 | 1.80                     | 0.63              |
| 1:2:1032:G:H2'   | 1:2:1033:G:H4'    | 1.81                     | 0.63              |
| 1:2:416:G:H2'    | 1:2:417:G:H8      | 1.62                     | 0.63              |
| 24:1:75:G:H22    | 24:1:111:A:H2     | 1.47                     | 0.63              |
| 27:C:1:MET:HB3   | 27:C:205:PRO:HG2  | 1.79                     | 0.63              |
| 24:1:848:C:H2'   | 24:1:849:A:H8     | 1.63                     | 0.63              |
| 24:1:1102:C:H2'  | 24:1:1103:A:C8    | 2.33                     | 0.63              |
| 24:1:249:C:O2    | 51:e:12:LYS:NZ    | 2.32                     | 0.63              |
| 24:1:1796:U:H2'  | 24:1:1797:G:H8    | 1.64                     | 0.63              |
| 24:1:2193:G:H2'  | 24:1:2194:U:C6    | 2.34                     | 0.63              |
| 34:M:53:MET:HG3  | 34:M:120:ALA:HB2  | 1.81                     | 0.63              |
| 55:6:200:ARG:HD3 | 55:6:202:VAL:HG23 | 1.81                     | 0.63              |
| 13:r:17:ILE:O    | 13:r:20:THR:HG22  | 1.99                     | 0.63              |
| 1:2:714:G:H2'    | 1:2:715:A:C8      | 2.34                     | 0.62              |
| 22:4:29:A:H2'    | 22:4:30:G:H8      | 1.63                     | 0.62              |
| 24:1:447:A:O2'   | 58:1:3209:SPD:H82 | 1.98                     | 0.62              |
| 3:h:19:ASN:OD1   | 3:h:54:ARG:NH2    | 2.32                     | 0.62              |
| 1:2:1027:C:H2'   | 1:2:1028:C:C6     | 2.35                     | 0.62              |
| 11:p:67:ALA:HB2  | 11:p:96:THR:HG23  | 1.81                     | 0.62              |
| 24:1:1084:A:H2'  | 24:1:1085:A:C8    | 2.35                     | 0.62              |
| 24:1:1177:G:H2'  | 24:1:1178:C:C6    | 2.34                     | 0.62              |
| 43:V:4:ILE:HG12  | 43:V:50:MET:HE1   | 1.80                     | 0.62              |
| 1:2:492:C:H2'    | 1:2:493:A:C8      | 2.35                     | 0.62              |
| 1:2:842:U:H3'    | 1:2:843:U:H5''    | 1.83                     | 0.61              |
| 1:2:843:U:H3'    | 1:2:844:G:H5''    | 1.81                     | 0.61              |
| 16:u:4:ILE:HG12  | 16:u:21:VAL:HG22  | 1.81                     | 0.61              |
| 24:1:848:C:H2'   | 24:1:849:A:C8     | 2.35                     | 0.61              |
| 26:B:200:HIS:HE1 | 26:B:203:ARG:HH21 | 1.47                     | 0.61              |
| 1:2:255:G:O3'    | 17:v:19:LYS:NZ    | 2.34                     | 0.61              |
| 24:1:1386:C:H2'  | 24:1:1387:A:C8    | 2.35                     | 0.61              |
| 1:2:93:U:H2'     | 1:2:95:C:C5       | 2.36                     | 0.61              |
| 19:x:50:ALA:HB1  | 19:x:57:HIS:HB3   | 1.82                     | 0.61              |
| 24:1:1178:C:H2'  | 24:1:1179:G:C8    | 2.33                     | 0.61              |
| 23:5:18:G:H21    | 23:5:58:A:H5'     | 1.65                     | 0.61              |
| 28:D:111:GLU:OE1 | 28:D:115:GLN:NE2  | 2.32                     | 0.61              |
| 29:E:116:GLY:HA3 | 29:E:178:ARG:HB3  | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:L:112:LEU:HD12 | 33:L:130:GLY:HA3  | 1.82                     | 0.61              |
| 47:Z:41:THR:HG22  | 47:Z:43:ALA:H     | 1.65                     | 0.61              |
| 3:h:16:LYS:NZ     | 3:h:181:ASP:OD1   | 2.34                     | 0.60              |
| 34:M:42:THR:HG22  | 34:M:93:VAL:HG12  | 1.82                     | 0.60              |
| 1:2:197:A:N1      | 1:2:220:G:O2'     | 2.31                     | 0.60              |
| 24:1:5:A:H2'      | 24:1:6:A:C8       | 2.36                     | 0.60              |
| 24:1:2336:A:H61   | 44:W:43:THR:HG21  | 1.66                     | 0.60              |
| 24:1:210:C:OP1    | 50:d:29:GLN:NE2   | 2.33                     | 0.60              |
| 12:q:110:ARG:HB3  | 12:q:119:VAL:HG21 | 1.82                     | 0.60              |
| 24:1:833:A:H2'    | 24:1:834:G:C8     | 2.37                     | 0.60              |
| 1:2:662:U:H2'     | 1:2:663:A:C8      | 2.37                     | 0.60              |
| 1:2:475:C:H2'     | 1:2:476:U:C6      | 2.36                     | 0.60              |
| 1:2:1071:C:H2'    | 1:2:1072:G:H8     | 1.66                     | 0.60              |
| 1:2:674:G:H2'     | 1:2:675:A:H8      | 1.66                     | 0.60              |
| 24:1:1083:U:O2'   | 24:1:1085:A:OP2   | 2.15                     | 0.60              |
| 24:1:1084:A:N3    | 24:1:1105:U:O2'   | 2.30                     | 0.59              |
| 24:1:2529:G:H4'   | 30:F:175:LYS:HG2  | 1.84                     | 0.59              |
| 1:2:501:C:H2'     | 1:2:502:A:H8      | 1.67                     | 0.59              |
| 24:1:272:A:H2'    | 24:1:273:G:C8     | 2.37                     | 0.59              |
| 56:G:71:LYS:HE3   | 56:G:108:VAL:HG13 | 1.82                     | 0.59              |
| 1:2:147:G:H2'     | 1:2:148:G:C8      | 2.38                     | 0.59              |
| 9:n:118:LEU:HD22  | 9:n:124:ARG:HG2   | 1.83                     | 0.59              |
| 24:1:494:G:H4'    | 40:S:6:LYS:HB2    | 1.84                     | 0.59              |
| 24:1:2874:C:H5''  | 35:N:4:ARG:HH21   | 1.68                     | 0.59              |
| 24:1:538:A:O2'    | 31:J:9:GLU:OE2    | 2.20                     | 0.59              |
| 1:2:337:G:H2'     | 1:2:338:A:C8      | 2.38                     | 0.59              |
| 24:1:593:U:H2'    | 24:1:594:U:C6     | 2.38                     | 0.59              |
| 1:2:405:U:O4      | 4:i:2:ALA:N       | 2.35                     | 0.59              |
| 24:1:549:G:H2'    | 24:1:550:C:C6     | 2.38                     | 0.59              |
| 24:1:1509:A:HO2'  | 24:1:1510:G:H8    | 1.51                     | 0.59              |
| 25:3:66:A:H61     | 25:3:107:G:H2'    | 1.68                     | 0.59              |
| 25:3:76:G:OP1     | 43:V:9:ARG:NH1    | 2.30                     | 0.59              |
| 1:2:842:U:H2'     | 1:2:844:G:H5'     | 1.85                     | 0.59              |
| 1:2:1402:4OC:HM22 | 1:2:1403:C:H5'    | 1.84                     | 0.59              |
| 1:2:1391:U:H2'    | 1:2:1392:G:C8     | 2.38                     | 0.58              |
| 24:1:639:U:H2'    | 24:1:640:C:C6     | 2.37                     | 0.58              |
| 24:1:1450:G:N2    | 24:1:1452:G:O6    | 2.36                     | 0.58              |
| 1:2:840:C:N3      | 1:2:842:U:H5'     | 2.18                     | 0.58              |
| 14:s:34:VAL:O     | 14:s:41:ARG:NH2   | 2.36                     | 0.58              |
| 24:1:1266:G:O2'   | 24:1:2012:G:O6    | 2.21                     | 0.58              |
| 1:2:458:U:H2'     | 1:2:459:A:C8      | 2.39                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:1:2547:A:H2'   | 24:1:2548:U:C6    | 2.38                     | 0.58              |
| 29:E:62:GLY:O     | 29:E:95:ARG:NH2   | 2.36                     | 0.58              |
| 22:4:42:G:H22     | 55:6:140:GLU:HG2  | 1.69                     | 0.58              |
| 24:1:1720:U:H2'   | 24:1:1721:G:O4'   | 2.03                     | 0.58              |
| 24:1:2193:G:H2'   | 24:1:2194:U:H6    | 1.67                     | 0.58              |
| 55:6:41:LEU:HA    | 55:6:46:VAL:HG11  | 1.84                     | 0.58              |
| 1:2:501:C:H2'     | 1:2:502:A:C8      | 2.39                     | 0.58              |
| 24:1:84:A:N1      | 24:1:98:G:O2'     | 2.35                     | 0.58              |
| 26:B:120:VAL:HG22 | 56:G:91:PHE:HB3   | 1.84                     | 0.58              |
| 1:2:475:C:H2'     | 1:2:476:U:H6      | 1.69                     | 0.58              |
| 1:2:1347:G:O6     | 9:n:12:ARG:NH2    | 2.35                     | 0.58              |
| 19:x:35:SER:OG    | 19:x:38:SER:OG    | 2.20                     | 0.58              |
| 24:1:1198:U:H2'   | 24:1:1199:U:C6    | 2.39                     | 0.58              |
| 33:L:57:LEU:HD22  | 51:e:54:ASP:HB3   | 1.85                     | 0.58              |
| 24:1:155:A:H2'    | 24:1:156:A:C8     | 2.38                     | 0.58              |
| 24:1:1199:U:H1'   | 38:Q:4:VAL:HG22   | 1.85                     | 0.57              |
| 24:1:2291:U:H2'   | 24:1:2292:U:C6    | 2.39                     | 0.57              |
| 54:I:100:ILE:HD11 | 54:I:137:LEU:HD23 | 1.85                     | 0.57              |
| 2:g:72:THR:OG1    | 2:g:169:GLU:OE2   | 2.21                     | 0.57              |
| 24:1:1794:A:H2'   | 24:1:1795:C:C6    | 2.39                     | 0.57              |
| 1:2:746:A:H2'     | 1:2:747:A:C8      | 2.39                     | 0.57              |
| 1:2:1062:U:H2'    | 1:2:1063:C:C6     | 2.38                     | 0.57              |
| 8:m:77:ARG:NH1    | 8:m:79:SER:O      | 2.37                     | 0.57              |
| 9:n:33:ARG:HH21   | 9:n:38:TYR:HA     | 1.70                     | 0.57              |
| 24:1:856:G:H2'    | 24:1:857:G:C8     | 2.39                     | 0.57              |
| 55:6:39:ALA:O     | 55:6:42:GLU:HG3   | 2.03                     | 0.57              |
| 24:1:1796:U:H2'   | 24:1:1797:G:C8    | 2.39                     | 0.57              |
| 1:2:219:U:H2'     | 1:2:220:G:H8      | 1.70                     | 0.57              |
| 1:2:1266:G:N2     | 1:2:1269:A:OP2    | 2.34                     | 0.57              |
| 3:h:36:ASP:OD1    | 3:h:59:ARG:NH2    | 2.34                     | 0.57              |
| 6:k:38:ARG:NH1    | 6:k:98:GLU:O      | 2.37                     | 0.57              |
| 24:1:1086:A:H4'   | 24:1:1103:A:C2    | 2.40                     | 0.57              |
| 1:2:17:U:H2'      | 1:2:18:C:C6       | 2.39                     | 0.57              |
| 4:i:202:GLU:OE1   | 5:j:112:ARG:NH1   | 2.37                     | 0.57              |
| 24:1:281:C:H2'    | 24:1:282:A:C8     | 2.40                     | 0.57              |
| 30:F:50:LEU:HD13  | 30:F:72:LEU:HD23  | 1.87                     | 0.57              |
| 1:2:416:G:H2'     | 1:2:417:G:C8      | 2.40                     | 0.57              |
| 1:2:843:U:H5      | 1:2:844:G:C4      | 2.23                     | 0.57              |
| 1:2:1031:C:O2'    | 1:2:1032:G:N2     | 2.37                     | 0.57              |
| 24:1:356:G:H2'    | 24:1:357:C:C6     | 2.39                     | 0.57              |
| 29:E:98:GLU:OE2   | 53:a:25:ARG:NH1   | 2.37                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 52:f:16:ILE:HD13 | 52:f:25:VAL:HG22  | 1.87                     | 0.57              |
| 1:2:326:G:O6     | 58:2:1687:SPD:N10 | 2.37                     | 0.57              |
| 1:2:1397:C:OP2   | 5:j:29:ARG:NH2    | 2.37                     | 0.57              |
| 1:2:476:U:H2'    | 1:2:477:C:C6      | 2.39                     | 0.56              |
| 1:2:1535:C:H2'   | 1:2:1536:C:C6     | 2.39                     | 0.56              |
| 10:o:7:ARG:HD3   | 10:o:73:LEU:HD11  | 1.87                     | 0.56              |
| 24:1:2285:C:OP2  | 49:c:6:ARG:NH1    | 2.38                     | 0.56              |
| 24:1:2305:U:H5'' | 29:E:131:GLY:HA3  | 1.86                     | 0.56              |
| 17:v:25:ILE:HB   | 17:v:42:THR:HG23  | 1.87                     | 0.56              |
| 24:1:2191:A:H2'  | 24:1:2192:U:C6    | 2.40                     | 0.56              |
| 24:1:2233:U:H2'  | 24:1:2234:G:C8    | 2.40                     | 0.56              |
| 26:B:71:LYS:O    | 26:B:118:SER:OG   | 2.23                     | 0.56              |
| 1:2:1011:C:H2'   | 1:2:1012:A:C8     | 2.41                     | 0.56              |
| 1:2:1119:C:OP1   | 9:n:85:ARG:NH2    | 2.38                     | 0.56              |
| 5:j:13:GLU:HG2   | 5:j:39:VAL:HG12   | 1.87                     | 0.56              |
| 22:4:29:A:H2'    | 22:4:30:G:C8      | 2.39                     | 0.56              |
| 26:B:200:HIS:CE1 | 26:B:203:ARG:HH21 | 2.22                     | 0.56              |
| 38:Q:86:ALA:HB2  | 38:Q:116:ALA:HB2  | 1.88                     | 0.56              |
| 1:2:1004:A:H2'   | 1:2:1005:A:O4'    | 2.05                     | 0.56              |
| 24:1:2567:G:H2'  | 24:1:2568:U:C6    | 2.41                     | 0.56              |
| 28:D:6:LYS:HA    | 28:D:9:GLN:HE21   | 1.71                     | 0.56              |
| 24:1:2514:U:H2'  | 24:1:2515:C:C6    | 2.40                     | 0.56              |
| 1:2:390:U:H2'    | 1:2:391:G:C8      | 2.40                     | 0.56              |
| 1:2:466:A:H2'    | 1:2:468:A:C8      | 2.40                     | 0.56              |
| 2:g:115:LYS:NZ   | 2:g:152:LYS:O     | 2.31                     | 0.56              |
| 24:1:588:U:H2'   | 24:1:589:U:C6     | 2.41                     | 0.56              |
| 24:1:1746:A:H2'  | 24:1:1747:U:C6    | 2.40                     | 0.56              |
| 1:2:891:U:H2'    | 1:2:892:A:H8      | 1.71                     | 0.56              |
| 12:q:55:VAL:HG21 | 12:q:80:ILE:HD11  | 1.88                     | 0.56              |
| 23:5:21:A:H61    | 23:5:46:G:H2'     | 1.70                     | 0.56              |
| 55:6:140:GLU:OE1 | 55:6:206:PRO:HD2  | 2.05                     | 0.56              |
| 55:6:170:GLU:HA  | 55:6:176:ILE:HA   | 1.87                     | 0.56              |
| 24:1:2304:G:H22  | 24:1:2312:U:H3    | 1.52                     | 0.56              |
| 25:3:17:C:N3     | 25:3:67:G:N1      | 2.35                     | 0.56              |
| 1:2:842:U:H4'    | 1:2:846:G:C2      | 2.40                     | 0.56              |
| 1:2:1463:U:H2'   | 1:2:1464:U:C6     | 2.41                     | 0.56              |
| 24:1:1432:G:H2'  | 24:1:1433:A:C8    | 2.41                     | 0.56              |
| 24:1:2176:A:H2'  | 24:1:2177:C:C6    | 2.41                     | 0.56              |
| 1:2:189:A:H2'    | 1:2:190:A:C8      | 2.42                     | 0.55              |
| 1:2:201:G:H1     | 1:2:216:U:H3      | 1.52                     | 0.55              |
| 1:2:524:G:H2'    | 1:2:525:C:C6      | 2.41                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:m:11:LEU:HD22  | 8:m:75:ILE:HD11  | 1.89                     | 0.55              |
| 1:2:269:C:H2'    | 1:2:270:A:H8     | 1.69                     | 0.55              |
| 24:1:581:C:H2'   | 24:1:582:A:C8    | 2.41                     | 0.55              |
| 24:1:2086:U:H2'  | 24:1:2087:G:C8   | 2.41                     | 0.55              |
| 24:1:2452:C:H2'  | 24:1:2453:A:C8   | 2.41                     | 0.55              |
| 56:G:63:ALA:HA   | 56:G:66:ASN:HD22 | 1.71                     | 0.55              |
| 24:1:1083:U:O2'  | 24:1:1084:A:O5'  | 2.24                     | 0.55              |
| 24:1:1590:A:H2'  | 24:1:1591:A:H8   | 1.71                     | 0.55              |
| 1:2:235:C:H2'    | 1:2:236:A:C8     | 2.42                     | 0.55              |
| 24:1:191:A:H2'   | 24:1:192:C:C6    | 2.42                     | 0.55              |
| 24:1:849:A:H2'   | 24:1:850:U:C6    | 2.42                     | 0.55              |
| 1:2:945:G:C2     | 1:2:946:A:C8     | 2.94                     | 0.55              |
| 1:2:1124:G:N2    | 1:2:1125:U:O4    | 2.34                     | 0.55              |
| 24:1:742:A:H2'   | 24:1:743:A:C8    | 2.42                     | 0.55              |
| 24:1:1361:G:H2'  | 24:1:1362:C:C6   | 2.41                     | 0.55              |
| 24:1:2162:G:OP2  | 24:1:2164:C:N4   | 2.38                     | 0.55              |
| 29:E:140:GLU:HG3 | 53:a:28:VAL:HG12 | 1.87                     | 0.55              |
| 31:J:128:ASN:ND2 | 31:J:128:ASN:O   | 2.40                     | 0.55              |
| 55:6:217:PHE:CZ  | 55:6:319:TRP:HA  | 2.42                     | 0.55              |
| 1:2:204:G:H3'    | 1:2:205:A:H8     | 1.70                     | 0.55              |
| 7:l:79:ARG:HH11  | 7:l:82:GLY:HA2   | 1.72                     | 0.55              |
| 17:v:47:HIS:HB3  | 17:v:74:THR:HG22 | 1.89                     | 0.55              |
| 16:u:40:ASN:HB3  | 16:u:43:ALA:HB2  | 1.88                     | 0.55              |
| 24:1:155:A:H2'   | 24:1:156:A:H8    | 1.70                     | 0.55              |
| 24:1:1799:G:OP1  | 26:B:258:ARG:NH1 | 2.33                     | 0.55              |
| 24:1:2804:U:H2'  | 24:1:2805:C:C6   | 2.42                     | 0.55              |
| 56:G:82:SER:O    | 56:G:149:GLU:N   | 2.32                     | 0.55              |
| 1:2:1350:A:O2'   | 7:l:33:ASP:OD1   | 2.24                     | 0.55              |
| 5:j:159:LYS:HB2  | 5:j:164:ILE:HD13 | 1.87                     | 0.55              |
| 24:1:373:U:H2'   | 24:1:374:A:H8    | 1.71                     | 0.55              |
| 24:1:414:C:H2'   | 24:1:415:A:C8    | 2.42                     | 0.55              |
| 1:2:660:C:O2     | 1:2:745:G:N2     | 2.19                     | 0.55              |
| 24:1:668:A:H2'   | 24:1:670:A:H62   | 1.72                     | 0.55              |
| 24:1:357:C:H2'   | 24:1:358:U:C6    | 2.42                     | 0.54              |
| 24:1:1842:G:H2'  | 24:1:1843:C:H6   | 1.72                     | 0.54              |
| 1:2:216:U:H2'    | 1:2:217:C:C6     | 2.42                     | 0.54              |
| 22:4:27:G:H2'    | 22:4:28:G:H8     | 1.72                     | 0.54              |
| 24:1:1028:A:H2'  | 24:1:1029:A:C8   | 2.41                     | 0.54              |
| 24:1:2149:U:H2'  | 24:1:2150:C:C6   | 2.42                     | 0.54              |
| 24:1:2327:A:H2'  | 24:1:2328:A:C8   | 2.42                     | 0.54              |
| 24:1:2599:G:C8   | 26:B:236:GLU:HG2 | 2.42                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:g:4:VAL:HG21   | 2:g:212:LEU:HD21  | 1.90                     | 0.54              |
| 24:1:1405:U:H2'  | 24:1:1406:U:C6    | 2.41                     | 0.54              |
| 24:1:2329:U:H2'  | 24:1:2330:G:C8    | 2.42                     | 0.54              |
| 1:2:382:A:H2'    | 1:2:383:A:C8      | 2.42                     | 0.54              |
| 6:k:41:ASP:OD1   | 6:k:58:HIS:NE2    | 2.37                     | 0.54              |
| 12:q:70:GLU:N    | 12:q:70:GLU:OE1   | 2.40                     | 0.54              |
| 24:1:2537:U:H2'  | 24:1:2538:C:C6    | 2.42                     | 0.54              |
| 1:2:340:U:OP2    | 32:K:98:ARG:NH2   | 2.40                     | 0.54              |
| 28:D:21:ARG:HD3  | 28:D:106:LYS:HB3  | 1.88                     | 0.54              |
| 1:2:76:G:H1      | 1:2:93:U:H3       | 1.55                     | 0.54              |
| 1:2:539:A:H2'    | 1:2:540:G:C8      | 2.42                     | 0.54              |
| 1:2:859:G:H2'    | 1:2:860:A:C8      | 2.43                     | 0.54              |
| 11:p:17:SER:HA   | 11:p:79:ILE:HA    | 1.90                     | 0.54              |
| 14:s:47:LYS:O    | 14:s:50:THR:OG1   | 2.26                     | 0.54              |
| 30:F:86:LYS:HG2  | 30:F:132:VAL:HG22 | 1.90                     | 0.54              |
| 34:M:136:MET:HG2 | 43:V:77:VAL:HG12  | 1.88                     | 0.54              |
| 24:1:1052:C:H2'  | 24:1:1053:C:C6    | 2.43                     | 0.54              |
| 1:2:1151:A:HO2'  | 1:2:1152:A:H8     | 1.53                     | 0.54              |
| 24:1:1589:U:H2'  | 24:1:1590:A:H8    | 1.73                     | 0.54              |
| 24:1:2064:C:H2'  | 24:1:2065:C:C6    | 2.43                     | 0.54              |
| 24:1:2728:U:HO2' | 24:1:2729:G:H8    | 1.56                     | 0.54              |
| 1:2:1026:G:O2'   | 1:2:1027:C:OP1    | 2.24                     | 0.54              |
| 24:1:306:U:H2'   | 24:1:307:G:O4'    | 2.08                     | 0.54              |
| 24:1:1019:U:OP1  | 24:1:1035:U:O2'   | 2.22                     | 0.54              |
| 24:1:1808:A:H3'  | 24:1:1809:A:C8    | 2.43                     | 0.54              |
| 1:2:1530:G:H2'   | 1:2:1531:A:C8     | 2.43                     | 0.54              |
| 33:L:108:ALA:HB3 | 33:L:125:LEU:HD22 | 1.89                     | 0.54              |
| 1:2:324:G:H4'    | 58:2:1687:SPD:H91 | 1.90                     | 0.53              |
| 26:B:120:VAL:CG2 | 56:G:91:PHE:HB3   | 2.38                     | 0.53              |
| 53:a:11:GLU:HA   | 53:a:25:ARG:HA    | 1.90                     | 0.53              |
| 24:1:172:A:H2'   | 24:1:173:A:C8     | 2.43                     | 0.53              |
| 24:1:1494:A:H2'  | 24:1:1495:A:C8    | 2.43                     | 0.53              |
| 24:1:1941:C:OP2  | 60:1:3330:PUT:N1  | 2.41                     | 0.53              |
| 24:1:2096:C:H2'  | 24:1:2097:A:C8    | 2.43                     | 0.53              |
| 56:G:7:ASP:OD1   | 56:G:8:LYS:N      | 2.38                     | 0.53              |
| 1:2:600:A:H2'    | 1:2:601:G:H8      | 1.73                     | 0.53              |
| 1:2:977:A:O2'    | 1:2:979:C:OP2     | 2.23                     | 0.53              |
| 24:1:594:U:H2'   | 24:1:595:C:C6     | 2.43                     | 0.53              |
| 40:S:4:ILE:HG12  | 40:S:106:VAL:HG22 | 1.89                     | 0.53              |
| 4:i:172:GLU:OE2  | 4:i:183:LYS:NZ    | 2.39                     | 0.53              |
| 12:q:50:ARG:HB3  | 12:q:66:TYR:HE1   | 1.73                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 24:1:581:C:H2'   | 24:1:582:A:H8    | 1.72                     | 0.53              |
| 3:h:63:SER:OG    | 3:h:64:ILE:N     | 2.39                     | 0.53              |
| 22:4:47:U:H5'    | 22:4:48:U:C5'    | 2.39                     | 0.53              |
| 24:1:807:U:OP2   | 33:L:41:ARG:NH2  | 2.41                     | 0.53              |
| 24:1:1842:G:H2'  | 24:1:1843:C:C6   | 2.43                     | 0.53              |
| 1:2:713:G:H2'    | 1:2:714:G:C8     | 2.44                     | 0.53              |
| 24:1:197:A:N6    | 24:1:2430:A:O2'  | 2.40                     | 0.53              |
| 24:1:2408:U:H2'  | 24:1:2409:G:C8   | 2.44                     | 0.53              |
| 1:2:235:C:H2'    | 1:2:236:A:H8     | 1.73                     | 0.53              |
| 1:2:673:A:H2'    | 1:2:674:G:H8     | 1.70                     | 0.53              |
| 5:j:115:LEU:HD13 | 5:j:123:VAL:HG11 | 1.91                     | 0.53              |
| 1:2:56:U:H2'     | 1:2:57:G:C8      | 2.43                     | 0.53              |
| 24:1:64:A:H2'    | 24:1:65:U:C6     | 2.44                     | 0.53              |
| 24:1:2698:U:H2'  | 24:1:2699:C:C6   | 2.43                     | 0.53              |
| 37:P:6:LYS:O     | 37:P:10:GLN:HG2  | 2.09                     | 0.53              |
| 45:X:41:GLU:OE1  | 45:X:44:LYS:NZ   | 2.40                     | 0.53              |
| 1:2:131:A:H2'    | 1:2:132:C:C6     | 2.44                     | 0.53              |
| 1:2:1051:C:H2'   | 1:2:1052:U:C6    | 2.44                     | 0.53              |
| 24:1:709:U:H2'   | 24:1:710:U:C6    | 2.43                     | 0.53              |
| 24:1:887:U:O2'   | 24:1:889:C:OP2   | 2.22                     | 0.53              |
| 1:2:333:U:OP1    | 20:y:2:ALA:N     | 2.42                     | 0.53              |
| 8:m:50:LYS:HE2   | 8:m:52:GLU:HG2   | 1.91                     | 0.53              |
| 24:1:1028:A:N6   | 24:1:1125:G:H2'  | 2.24                     | 0.53              |
| 24:1:1438:U:H2'  | 24:1:1439:A:H8   | 1.74                     | 0.53              |
| 42:U:18:ASP:HB3  | 42:U:21:LYS:HD2  | 1.90                     | 0.53              |
| 24:1:2052:A:H4'  | 27:C:148:GLN:O   | 2.08                     | 0.52              |
| 26:B:5:LYS:NZ    | 26:B:14:ARG:O    | 2.43                     | 0.52              |
| 55:6:304:ASN:HA  | 55:6:307:LYS:HE2 | 1.91                     | 0.52              |
| 1:2:384:G:H2'    | 1:2:385:C:C6     | 2.44                     | 0.52              |
| 24:1:1386:C:H2'  | 24:1:1387:A:H8   | 1.74                     | 0.52              |
| 24:1:1469:A:H2'  | 24:1:1470:A:H8   | 1.74                     | 0.52              |
| 1:2:41:G:H2'     | 1:2:42:G:H8      | 1.73                     | 0.52              |
| 1:2:728:A:H2'    | 1:2:729:A:C8     | 2.43                     | 0.52              |
| 21:z:31:GLU:OE2  | 21:z:34:ARG:NH2  | 2.42                     | 0.52              |
| 24:1:1084:A:H8   | 24:1:1084:A:OP1  | 1.92                     | 0.52              |
| 24:1:1682:G:H2'  | 24:1:1683:U:C6   | 2.44                     | 0.52              |
| 25:3:66:A:N6     | 25:3:107:G:H2'   | 2.24                     | 0.52              |
| 26:B:5:LYS:HD2   | 26:B:17:VAL:HG22 | 1.92                     | 0.52              |
| 1:2:216:U:H4'    | 1:2:464:U:H4'    | 1.91                     | 0.52              |
| 1:2:472:U:H2'    | 1:2:473:U:C6     | 2.44                     | 0.52              |
| 1:2:1332:A:H2'   | 1:2:1333:A:C8    | 2.45                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:n:21:ILE:HG12  | 9:n:63:LEU:HD22   | 1.90                     | 0.52              |
| 24:1:1039:A:H2'  | 24:1:1040:A:O4'   | 2.09                     | 0.52              |
| 1:2:1287:A:H2'   | 1:2:1288:A:C8     | 2.45                     | 0.52              |
| 35:N:8:ARG:HD2   | 35:N:43:GLU:HG2   | 1.90                     | 0.52              |
| 1:2:674:G:H2'    | 1:2:675:A:C8      | 2.45                     | 0.52              |
| 24:1:629:G:N3    | 24:1:639:U:O2'    | 2.43                     | 0.52              |
| 24:1:832:U:H2'   | 24:1:833:A:C8     | 2.45                     | 0.52              |
| 24:1:2602:A:C6   | 55:6:254:VAL:HG13 | 2.45                     | 0.52              |
| 1:2:842:U:H3'    | 1:2:843:U:C5'     | 2.40                     | 0.52              |
| 1:2:1356:G:H2'   | 1:2:1357:A:H8     | 1.72                     | 0.52              |
| 11:p:87:LYS:HB2  | 11:p:113:VAL:HG23 | 1.91                     | 0.52              |
| 34:M:20:LEU:HD13 | 43:V:81:PRO:HG2   | 1.92                     | 0.52              |
| 43:V:2:PHE:HB2   | 43:V:61:LEU:HD12  | 1.90                     | 0.52              |
| 24:1:859:G:O2'   | 24:1:916:G:O6     | 2.27                     | 0.52              |
| 24:1:1064:C:O2'  | 24:1:1065:U:H5'   | 2.09                     | 0.52              |
| 31:J:34:ARG:HG3  | 31:J:39:LYS:HB2   | 1.92                     | 0.52              |
| 41:T:2:ILE:HD13  | 41:T:42:GLU:HG2   | 1.92                     | 0.52              |
| 42:U:49:VAL:HG23 | 42:U:52:LEU:O     | 2.09                     | 0.52              |
| 1:2:206:C:H42    | 1:2:213:G:H22     | 1.57                     | 0.52              |
| 4:i:25:VAL:HG23  | 4:i:26:ARG:HG2    | 1.91                     | 0.52              |
| 55:6:218:SER:HA  | 55:6:317:ILE:HD11 | 1.90                     | 0.52              |
| 1:2:76:G:H2'     | 1:2:77:A:C8       | 2.44                     | 0.52              |
| 11:p:81:ASN:OD1  | 11:p:106:ARG:HB3  | 2.10                     | 0.52              |
| 12:q:4:VAL:HG23  | 17:v:34:TYR:HB3   | 1.91                     | 0.52              |
| 15:t:17:ARG:NH1  | 15:t:26:GLU:OE1   | 2.43                     | 0.52              |
| 24:1:3:U:H2'     | 24:1:4:U:C6       | 2.45                     | 0.52              |
| 1:2:1360:A:OP2   | 14:s:75:ARG:NH2   | 2.43                     | 0.51              |
| 7:l:59:LEU:O     | 7:l:63:GLU:HG2    | 2.10                     | 0.51              |
| 24:1:1000:A:H2'  | 24:1:1001:A:C8    | 2.45                     | 0.51              |
| 22:4:33:A:H4'    | 22:4:34:U:N3      | 2.24                     | 0.51              |
| 24:1:729:G:C6    | 26:B:207:LYS:HB2  | 2.45                     | 0.51              |
| 25:3:5:U:OP1     | 25:3:61:G:O2'     | 2.20                     | 0.51              |
| 28:D:7:ASP:N     | 28:D:7:ASP:OD1    | 2.37                     | 0.51              |
| 30:F:25:THR:HG22 | 30:F:34:THR:HG23  | 1.91                     | 0.51              |
| 17:v:53:CYS:SG   | 17:v:75:LEU:HD11  | 2.51                     | 0.51              |
| 24:1:849:A:H2'   | 24:1:850:U:H6     | 1.75                     | 0.51              |
| 24:1:1086:A:H4'  | 24:1:1103:A:H2    | 1.73                     | 0.51              |
| 24:1:2798:U:H4'  | 24:1:2799:A:H5'   | 1.90                     | 0.51              |
| 53:a:45:THR:O    | 53:a:47:LYS:NZ    | 2.43                     | 0.51              |
| 1:2:126:G:OP1    | 1:2:605:U:O2'     | 2.18                     | 0.51              |
| 7:l:18:PHE:HB3   | 7:l:59:LEU:HD11   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 24:1:390:U:H4'   | 24:1:391:A:H5'   | 1.92                     | 0.51              |
| 24:1:5:A:H2'     | 24:1:6:A:H8      | 1.72                     | 0.51              |
| 24:1:347:A:H2'   | 24:1:348:A:C8    | 2.46                     | 0.51              |
| 24:1:1059:G:H2'  | 24:1:1060:U:C5   | 2.45                     | 0.51              |
| 24:1:1528:A:OP2  | 24:1:1543:G:N2   | 2.40                     | 0.51              |
| 24:1:1801:A:C8   | 24:1:2203:U:H2'  | 2.46                     | 0.51              |
| 24:1:2597:G:H5'  | 26:B:241:GLY:HA3 | 1.92                     | 0.51              |
| 24:1:2747:G:O6   | 24:1:2755:C:H5'' | 2.11                     | 0.51              |
| 24:1:2898:U:H2'  | 24:1:2899:A:H8   | 1.76                     | 0.51              |
| 32:K:40:LYS:HE3  | 32:K:57:VAL:HG12 | 1.93                     | 0.51              |
| 1:2:1273:C:H2'   | 1:2:1274:A:O4'   | 2.10                     | 0.51              |
| 24:1:1062:G:C6   | 24:1:1077:A:C6   | 2.99                     | 0.51              |
| 1:2:476:U:H2'    | 1:2:477:C:H6     | 1.74                     | 0.51              |
| 1:2:555:U:H2'    | 1:2:556:C:C6     | 2.45                     | 0.51              |
| 1:2:1014:A:C2    | 1:2:1219:A:H1'   | 2.46                     | 0.51              |
| 24:1:457:A:N1    | 24:1:470:A:H5''  | 2.24                     | 0.51              |
| 24:1:475:C:O2    | 24:1:479:A:N6    | 2.35                     | 0.51              |
| 24:1:644:A:H2'   | 24:1:645:C:O4'   | 2.10                     | 0.51              |
| 24:1:851:C:H2'   | 24:1:852:U:C6    | 2.46                     | 0.51              |
| 24:1:1548:A:H2'  | 24:1:1549:A:C8   | 2.45                     | 0.51              |
| 24:1:2175:C:H2'  | 24:1:2176:A:C8   | 2.46                     | 0.51              |
| 27:C:152:PRO:HG3 | 27:C:156:PHE:CZ  | 2.46                     | 0.51              |
| 1:2:1162:C:H2'   | 1:2:1163:A:H8    | 1.75                     | 0.51              |
| 22:4:44:G:C5     | 55:6:212:ARG:HD3 | 2.46                     | 0.51              |
| 24:1:151:C:H2'   | 24:1:152:A:H8    | 1.76                     | 0.51              |
| 24:1:645:C:H2'   | 24:1:647:G:C8    | 2.46                     | 0.51              |
| 24:1:1062:G:H2'  | 24:1:1063:G:C8   | 2.45                     | 0.51              |
| 24:1:2246:G:H2'  | 24:1:2247:A:C8   | 2.46                     | 0.51              |
| 27:C:55:LYS:HD3  | 27:C:60:VAL:HG22 | 1.93                     | 0.51              |
| 1:2:376:G:H5''   | 16:u:5:ARG:HB2   | 1.93                     | 0.51              |
| 22:4:24:U:H2'    | 22:4:25:A:H8     | 1.75                     | 0.51              |
| 24:1:275:C:H2'   | 24:1:276:U:O4'   | 2.11                     | 0.51              |
| 24:1:634:C:H2'   | 24:1:635:C:C6    | 2.46                     | 0.51              |
| 24:1:2328:A:H2'  | 24:1:2329:U:H6   | 1.75                     | 0.51              |
| 55:6:41:LEU:HD23 | 55:6:46:VAL:HG21 | 1.92                     | 0.51              |
| 1:2:1130:A:H2'   | 1:2:1131:G:H8    | 1.76                     | 0.51              |
| 4:i:15:GLU:OE2   | 4:i:63:ARG:NH1   | 2.44                     | 0.51              |
| 24:1:1115:G:O2'  | 24:1:1116:G:O5'  | 2.29                     | 0.51              |
| 24:1:1794:A:H2'  | 24:1:1795:C:H6   | 1.74                     | 0.51              |
| 24:1:2025:C:H2'  | 24:1:2026:U:C6   | 2.45                     | 0.51              |
| 1:2:1095:U:H2'   | 1:2:1096:C:C6    | 2.46                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1314:C:H2'   | 1:2:1315:U:C6     | 2.46                     | 0.50              |
| 3:h:47:LEU:HB3   | 3:h:50:ALA:HB3    | 1.93                     | 0.50              |
| 24:1:2408:U:H2'  | 24:1:2409:G:H8    | 1.75                     | 0.50              |
| 27:C:56:LYS:HB2  | 27:C:59:ARG:HB2   | 1.93                     | 0.50              |
| 31:J:114:LEU:HG  | 31:J:118:MET:HE3  | 1.92                     | 0.50              |
| 32:K:7:MET:HE1   | 32:K:44:LYS:HG3   | 1.92                     | 0.50              |
| 1:2:660:C:N3     | 1:2:745:G:N1      | 2.38                     | 0.50              |
| 1:2:1513:A:H2'   | 1:2:1514:G:C8     | 2.46                     | 0.50              |
| 24:1:320:A:N3    | 28:D:163:ASN:ND2  | 2.56                     | 0.50              |
| 24:1:414:C:H2'   | 24:1:415:A:H8     | 1.75                     | 0.50              |
| 24:1:2901:C:H2'  | 24:1:2902:C:C6    | 2.46                     | 0.50              |
| 1:2:459:A:H2'    | 1:2:460:A:C8      | 2.47                     | 0.50              |
| 1:2:600:A:H2'    | 1:2:601:G:C8      | 2.46                     | 0.50              |
| 1:2:613:C:H2'    | 1:2:614:C:C6      | 2.46                     | 0.50              |
| 1:2:868:C:H2'    | 1:2:869:G:O4'     | 2.11                     | 0.50              |
| 24:1:549:G:H2'   | 24:1:550:C:H6     | 1.76                     | 0.50              |
| 24:1:1484:U:H2'  | 24:1:1485:U:C6    | 2.46                     | 0.50              |
| 25:3:77:U:OP1    | 43:V:21:ARG:NH1   | 2.37                     | 0.50              |
| 25:3:90:C:H5'    | 34:M:18:ARG:HG2   | 1.93                     | 0.50              |
| 1:2:41:G:H2'     | 1:2:42:G:C8       | 2.47                     | 0.50              |
| 1:2:335:C:H2'    | 1:2:336:A:H8      | 1.76                     | 0.50              |
| 1:2:1120:C:H2'   | 1:2:1121:U:H6     | 1.75                     | 0.50              |
| 13:r:33:ILE:HD13 | 13:r:60:VAL:HG22  | 1.93                     | 0.50              |
| 24:1:504:A:N3    | 24:1:504:A:H2'    | 2.27                     | 0.50              |
| 24:1:813:U:H2'   | 24:1:814:C:C6     | 2.47                     | 0.50              |
| 24:1:1248:G:OP1  | 28:D:44:ARG:NH1   | 2.39                     | 0.50              |
| 24:1:1438:U:H2'  | 24:1:1439:A:C8    | 2.45                     | 0.50              |
| 24:1:2331:G:O2'  | 44:W:43:THR:HG22  | 2.11                     | 0.50              |
| 24:1:2641:G:H5'' | 31:J:78:THR:HB    | 1.92                     | 0.50              |
| 1:2:1147:C:O2'   | 9:n:7:TYR:OH      | 2.25                     | 0.50              |
| 1:2:1171:A:H2'   | 1:2:1172:C:C6     | 2.47                     | 0.50              |
| 12:q:68:GLY:O    | 12:q:99:ARG:NH1   | 2.42                     | 0.50              |
| 24:1:548:G:H2'   | 24:1:549:G:H1'    | 1.92                     | 0.50              |
| 24:1:2591:C:H2'  | 24:1:2592:G:C8    | 2.46                     | 0.50              |
| 29:E:52:ASN:HB2  | 29:E:150:ARG:HH22 | 1.76                     | 0.50              |
| 24:1:2:G:H2'     | 24:1:3:U:C6       | 2.47                     | 0.50              |
| 42:U:50:PRO:O    | 42:U:54:GLN:NE2   | 2.44                     | 0.50              |
| 1:2:353:A:C5     | 60:2:1728:PUT:H32 | 2.46                     | 0.50              |
| 1:2:1060:U:H2'   | 1:2:1061:G:H8     | 1.76                     | 0.50              |
| 24:1:351:C:H2'   | 24:1:352:A:C8     | 2.46                     | 0.50              |
| 24:1:839:U:H2'   | 24:1:840:C:C6     | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 39:R:36:ALA:HA   | 39:R:58:VAL:HG23 | 1.94                     | 0.50              |
| 8:m:39:VAL:HG21  | 8:m:110:VAL:HG12 | 1.93                     | 0.50              |
| 24:1:543:G:H2'   | 24:1:544:C:O4'   | 2.12                     | 0.50              |
| 24:1:1046:A:H3'  | 24:1:1047:G:H5'  | 1.93                     | 0.50              |
| 35:N:28:LEU:HD23 | 35:N:48:VAL:HG21 | 1.94                     | 0.50              |
| 1:2:463:U:H2'    | 1:2:464:U:C6     | 2.47                     | 0.50              |
| 1:2:470:C:H2'    | 1:2:471:U:C6     | 2.47                     | 0.50              |
| 1:2:554:A:H2'    | 1:2:555:U:C6     | 2.47                     | 0.50              |
| 24:1:1361:G:H2'  | 24:1:1362:C:H6   | 1.77                     | 0.50              |
| 24:1:2532:G:O2'  | 24:1:2657:A:N1   | 2.44                     | 0.50              |
| 24:1:2591:C:H2'  | 24:1:2592:G:H8   | 1.75                     | 0.50              |
| 28:D:5:LEU:O     | 28:D:9:GLN:NE2   | 2.45                     | 0.50              |
| 1:2:294:U:OP1    | 1:2:610:U:O2'    | 2.28                     | 0.49              |
| 4:i:9:LEU:HD13   | 4:i:32:CYS:HB3   | 1.93                     | 0.49              |
| 24:1:288:U:H2'   | 24:1:289:G:C8    | 2.47                     | 0.49              |
| 24:1:2131:U:H5'  | 24:1:2132:U:H5'' | 1.93                     | 0.49              |
| 24:1:2849:U:H4'  | 24:1:2868:A:C2   | 2.46                     | 0.49              |
| 40:S:86:MET:HB2  | 40:S:96:ILE:HG12 | 1.93                     | 0.49              |
| 1:2:745:G:H2'    | 1:2:746:A:C8     | 2.47                     | 0.49              |
| 24:1:871:U:H2'   | 24:1:872:U:C6    | 2.48                     | 0.49              |
| 24:1:1059:G:H3'  | 24:1:1060:U:H2'  | 1.93                     | 0.49              |
| 24:1:1443:U:H2'  | 24:1:1444:G:H8   | 1.77                     | 0.49              |
| 24:1:1799:G:O2'  | 26:B:180:GLU:OE2 | 2.20                     | 0.49              |
| 24:1:2788:C:H2'  | 24:1:2789:C:C6   | 2.46                     | 0.49              |
| 44:W:11:ARG:O    | 44:W:12:ASN:ND2  | 2.45                     | 0.49              |
| 1:2:1162:C:H2'   | 1:2:1163:A:C8    | 2.47                     | 0.49              |
| 10:o:25:ILE:HG13 | 10:o:92:LEU:HD11 | 1.95                     | 0.49              |
| 24:1:1141:U:H4'  | 24:1:1142:A:O4'  | 2.12                     | 0.49              |
| 24:1:2115:G:O2'  | 24:1:2117:A:N6   | 2.45                     | 0.49              |
| 24:1:2469:A:H2'  | 24:1:2470:G:O4'  | 2.12                     | 0.49              |
| 55:6:22:ARG:HG2  | 55:6:70:LEU:HD13 | 1.95                     | 0.49              |
| 1:2:77:A:H2'     | 1:2:78:A:C8      | 2.46                     | 0.49              |
| 1:2:236:A:H2'    | 1:2:237:G:C8     | 2.47                     | 0.49              |
| 1:2:459:A:H2'    | 1:2:460:A:H8     | 1.76                     | 0.49              |
| 1:2:1119:C:H2'   | 1:2:1120:C:H6    | 1.77                     | 0.49              |
| 1:2:1314:C:H2'   | 1:2:1315:U:H6    | 1.78                     | 0.49              |
| 2:g:97:LEU:H     | 2:g:100:MET:HE3  | 1.76                     | 0.49              |
| 24:1:355:U:H2'   | 24:1:356:G:C8    | 2.47                     | 0.49              |
| 24:1:739:A:H1'   | 24:1:740:C:H5    | 1.78                     | 0.49              |
| 24:1:1509:A:O2'  | 24:1:1510:G:H8   | 1.94                     | 0.49              |
| 36:O:51:ALA:HB3  | 36:O:78:VAL:HB   | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:21:G:H2'      | 1:2:22:G:C8       | 2.48                     | 0.49              |
| 1:2:337:G:H2'     | 1:2:338:A:H8      | 1.77                     | 0.49              |
| 1:2:1286:U:H2'    | 1:2:1287:A:H5'    | 1.93                     | 0.49              |
| 11:p:85:MET:HE3   | 11:p:113:VAL:HG11 | 1.94                     | 0.49              |
| 20:y:67:ILE:HB    | 20:y:71:LYS:HD3   | 1.95                     | 0.49              |
| 24:1:30:G:H2'     | 24:1:31:C:C6      | 2.47                     | 0.49              |
| 24:1:150:U:H2'    | 24:1:151:C:C6     | 2.48                     | 0.49              |
| 24:1:576:U:H2'    | 24:1:577:G:C8     | 2.47                     | 0.49              |
| 24:1:1197:G:H2'   | 24:1:1198:U:H6    | 1.78                     | 0.49              |
| 24:1:2014:A:H2'   | 24:1:2015:A:C8    | 2.48                     | 0.49              |
| 26:B:72:ASP:OD1   | 26:B:72:ASP:N     | 2.42                     | 0.49              |
| 1:2:1005:A:C5     | 1:2:1006:G:H1'    | 2.48                     | 0.49              |
| 1:2:1237:C:H4'    | 1:2:1300:G:H22    | 1.78                     | 0.49              |
| 10:o:59:LYS:HE2   | 10:o:62:ARG:NH2   | 2.27                     | 0.49              |
| 24:1:2109:U:H2'   | 24:1:2110:G:C8    | 2.48                     | 0.49              |
| 24:1:2820:A:O2'   | 24:1:2821:A:OP1   | 2.30                     | 0.49              |
| 32:K:76:VAL:HG13  | 37:P:73:VAL:HB    | 1.94                     | 0.49              |
| 44:W:59:LEU:HD12  | 44:W:80:ILE:HD12  | 1.93                     | 0.49              |
| 1:2:514:C:H2'     | 1:2:515:G:H8      | 1.76                     | 0.49              |
| 1:2:769:G:H4'     | 1:2:1513:A:H4'    | 1.94                     | 0.49              |
| 3:h:63:SER:OG     | 3:h:98:PRO:O      | 2.19                     | 0.49              |
| 24:1:281:C:H2'    | 24:1:282:A:H8     | 1.77                     | 0.49              |
| 24:1:1353:A:H2'   | 24:1:1354:A:C8    | 2.48                     | 0.49              |
| 1:2:1244:G:H2'    | 1:2:1245:C:C6     | 2.48                     | 0.49              |
| 24:1:675:A:N3     | 24:1:2443:C:O2'   | 2.44                     | 0.49              |
| 7:l:68:ASN:ND2    | 7:l:130:ASN:OD1   | 2.46                     | 0.49              |
| 14:s:3:LYS:HB2    | 14:s:6:MET:HG2    | 1.94                     | 0.49              |
| 24:1:274:C:H2'    | 24:1:275:C:O4'    | 2.12                     | 0.49              |
| 24:1:2430:A:N3    | 24:1:2430:A:H2'   | 2.28                     | 0.49              |
| 24:1:2780:G:OP2   | 31:J:120:ARG:HD3  | 2.13                     | 0.49              |
| 42:U:86:ARG:HG3   | 42:U:95:PHE:CE1   | 2.48                     | 0.49              |
| 55:6:316:ASP:O    | 55:6:321:SER:OG   | 2.28                     | 0.49              |
| 1:2:1017:U:H2'    | 1:2:1018:G:C8     | 2.48                     | 0.49              |
| 4:i:91:LEU:HD12   | 4:i:188:ARG:HD3   | 1.94                     | 0.49              |
| 54:I:105:LEU:HD13 | 54:I:129:GLU:HG2  | 1.94                     | 0.49              |
| 1:2:460:A:H2'     | 1:2:461:A:H8      | 1.77                     | 0.48              |
| 1:2:652:U:O4      | 1:2:752:G:O2'     | 2.22                     | 0.48              |
| 24:1:1278:C:H2'   | 24:1:1279:G:H8    | 1.78                     | 0.48              |
| 24:1:1744:A:H3'   | 24:1:1745:A:H8    | 1.77                     | 0.48              |
| 24:1:2419:U:H4'   | 49:c:22:THR:HG21  | 1.95                     | 0.48              |
| 13:r:40:ALA:HB3   | 13:r:43:VAL:HG23  | 1.93                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:1:979:A:H2'   | 24:1:982:C:H42    | 1.78                     | 0.48              |
| 24:1:2649:C:H2'  | 24:1:2650:U:H6    | 1.77                     | 0.48              |
| 1:2:1123:U:O2'   | 1:2:1124:G:H5'    | 2.14                     | 0.48              |
| 2:g:69:PHE:HE1   | 2:g:89:GLN:HB2    | 1.79                     | 0.48              |
| 24:1:1441:G:H2'  | 24:1:1442:U:C6    | 2.48                     | 0.48              |
| 24:1:2554:U:H2'  | 24:1:2555:U:C6    | 2.48                     | 0.48              |
| 37:P:33:VAL:HG22 | 37:P:38:LYS:HG3   | 1.95                     | 0.48              |
| 40:S:24:ILE:HD13 | 40:S:36:LEU:HD11  | 1.95                     | 0.48              |
| 1:2:206:C:N4     | 1:2:213:G:H22     | 2.11                     | 0.48              |
| 1:2:212:G:C4     | 1:2:213:G:C8      | 3.01                     | 0.48              |
| 1:2:1218:C:H2'   | 1:2:1219:A:H8     | 1.77                     | 0.48              |
| 22:4:44:G:H1     | 55:6:210:GLY:HA3  | 1.79                     | 0.48              |
| 24:1:608:A:H2'   | 24:1:609:A:C8     | 2.48                     | 0.48              |
| 24:1:910:A:H2'   | 24:1:911:A:C8     | 2.48                     | 0.48              |
| 24:1:1484:U:H2'  | 24:1:1485:U:H6    | 1.76                     | 0.48              |
| 24:1:1889:A:H2'  | 24:1:1890:A:C8    | 2.49                     | 0.48              |
| 24:1:2192:U:H2'  | 24:1:2193:G:C8    | 2.48                     | 0.48              |
| 30:F:138:LYS:O   | 30:F:141:ILE:HG13 | 2.13                     | 0.48              |
| 1:2:190:A:O5'    | 1:2:190:A:H8      | 1.97                     | 0.48              |
| 20:y:57:ILE:O    | 20:y:61:GLN:HG2   | 2.13                     | 0.48              |
| 24:1:6:A:H2'     | 24:1:7:G:C8       | 2.49                     | 0.48              |
| 29:E:37:ASN:HB3  | 29:E:153:ASP:OD1  | 2.14                     | 0.48              |
| 56:G:62:LEU:O    | 56:G:66:ASN:ND2   | 2.46                     | 0.48              |
| 1:2:538:G:H5''   | 12:q:111:LYS:HB2  | 1.96                     | 0.48              |
| 4:i:85:ASN:HB3   | 4:i:88:GLU:HG3    | 1.96                     | 0.48              |
| 6:k:17:GLN:N     | 6:k:17:GLN:OE1    | 2.46                     | 0.48              |
| 24:1:1316:U:H2'  | 24:1:1317:G:H8    | 1.77                     | 0.48              |
| 24:1:1485:U:H2'  | 24:1:1486:U:C6    | 2.49                     | 0.48              |
| 26:B:153:GLN:HA  | 26:B:156:ARG:HD3  | 1.95                     | 0.48              |
| 45:X:60:ASP:OD2  | 56:G:27:ARG:NH2   | 2.44                     | 0.48              |
| 1:2:415:A:H3'    | 1:2:416:G:C8      | 2.43                     | 0.48              |
| 1:2:470:C:H2'    | 1:2:471:U:H6      | 1.78                     | 0.48              |
| 1:2:477:C:H2'    | 1:2:478:A:C8      | 2.49                     | 0.48              |
| 1:2:981:U:OP1    | 14:s:9:ARG:NH1    | 2.45                     | 0.48              |
| 24:1:203:A:H61   | 60:1:3331:PUT:H31 | 1.79                     | 0.48              |
| 24:1:1589:U:H2'  | 24:1:1590:A:C8    | 2.49                     | 0.48              |
| 24:1:2159:G:H2'  | 24:1:2160:C:C6    | 2.48                     | 0.48              |
| 29:E:36:LEU:HD22 | 29:E:154:ILE:HG12 | 1.95                     | 0.48              |
| 56:G:46:PHE:CZ   | 56:G:50:ARG:HD3   | 2.49                     | 0.48              |
| 1:2:204:G:C4     | 1:2:205:A:C8      | 3.02                     | 0.48              |
| 1:2:390:U:H2'    | 1:2:391:G:H8      | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:514:C:C2      | 1:2:515:G:C8      | 3.02                     | 0.48              |
| 1:2:844:G:H3'     | 1:2:844:G:N3      | 2.28                     | 0.48              |
| 1:2:1013:G:N2     | 1:2:1016:A:OP2    | 2.40                     | 0.48              |
| 24:1:756:A:H2'    | 24:1:757:G:O4'    | 2.13                     | 0.48              |
| 24:1:1564:C:H2'   | 24:1:1565:C:C6    | 2.48                     | 0.48              |
| 24:1:2557:G:H2'   | 24:1:2558:C:C6    | 2.49                     | 0.48              |
| 30:F:121:ILE:HD12 | 30:F:141:ILE:HG22 | 1.95                     | 0.48              |
| 1:2:56:U:H2'      | 1:2:57:G:H8       | 1.78                     | 0.48              |
| 1:2:737:C:H2'     | 1:2:738:C:H6      | 1.79                     | 0.48              |
| 1:2:1008:U:C2     | 1:2:1022:A:C2     | 3.02                     | 0.48              |
| 24:1:172:A:H2'    | 24:1:173:A:H8     | 1.79                     | 0.48              |
| 24:1:839:U:H1'    | 24:1:1191:G:H1'   | 1.95                     | 0.48              |
| 24:1:2273:A:H2'   | 24:1:2274:A:C8    | 2.48                     | 0.48              |
| 24:1:2645:G:OP2   | 24:1:2645:G:N2    | 2.36                     | 0.48              |
| 30:F:164:TYR:HB2  | 30:F:167:GLU:HB3  | 1.95                     | 0.48              |
| 1:2:171:A:H2'     | 1:2:172:A:C8      | 2.49                     | 0.48              |
| 1:2:642:A:N7      | 8:m:107:SER:HA    | 2.29                     | 0.48              |
| 1:2:1011:C:H2'    | 1:2:1012:A:H8     | 1.78                     | 0.48              |
| 2:g:58:ASN:ND2    | 2:g:220:THR:O     | 2.47                     | 0.48              |
| 11:p:35:THR:HG22  | 11:p:41:ALA:HA    | 1.96                     | 0.48              |
| 14:s:79:LEU:HB2   | 14:s:84:VAL:HG23  | 1.96                     | 0.48              |
| 24:1:279:A:H61    | 24:1:360:U:C2'    | 2.27                     | 0.48              |
| 24:1:1096:A:H2'   | 24:1:1097:U:O4'   | 2.14                     | 0.48              |
| 24:1:2185:U:H2'   | 24:1:2186:G:C8    | 2.49                     | 0.48              |
| 30:F:89:LEU:HG    | 30:F:162:VAL:HG22 | 1.96                     | 0.48              |
| 38:Q:50:ARG:O     | 38:Q:54:LYS:NZ    | 2.46                     | 0.48              |
| 1:2:259:G:O6      | 60:2:1727:PUT:N2  | 2.35                     | 0.47              |
| 1:2:270:A:H2'     | 1:2:271:C:C6      | 2.50                     | 0.47              |
| 1:2:842:U:H4'     | 1:2:846:G:C6      | 2.49                     | 0.47              |
| 1:2:1068:G:N7     | 1:2:1094:G:H2'    | 2.28                     | 0.47              |
| 1:2:1463:U:H2'    | 1:2:1464:U:H6     | 1.78                     | 0.47              |
| 1:2:1477:U:H2'    | 1:2:1478:U:C6     | 2.49                     | 0.47              |
| 4:i:172:GLU:O     | 4:i:180:GLY:HA2   | 2.14                     | 0.47              |
| 24:1:78:U:H2'     | 24:1:79:C:C6      | 2.49                     | 0.47              |
| 24:1:632:A:H2'    | 24:1:633:A:C8     | 2.49                     | 0.47              |
| 24:1:1631:G:H1'   | 24:1:1635:A:H61   | 1.78                     | 0.47              |
| 24:1:2455:G:H2'   | 24:1:2456:C:C6    | 2.49                     | 0.47              |
| 28:D:91:ASP:OD1   | 28:D:93:SER:OG    | 2.21                     | 0.47              |
| 1:2:223:A:H2'     | 1:2:224:U:C6      | 2.49                     | 0.47              |
| 1:2:1530:G:H2'    | 1:2:1531:A:H8     | 1.79                     | 0.47              |
| 2:g:132:LYS:O     | 2:g:136:MET:HG3   | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:k:4:TYR:CE1     | 6:k:71:ILE:HG13   | 2.50                     | 0.47              |
| 24:1:1114:C:O2'   | 24:1:1115:G:H5'   | 2.13                     | 0.47              |
| 24:1:2204:G:H4'   | 26:B:150:LYS:HD3  | 1.96                     | 0.47              |
| 24:1:2312:U:H5'   | 29:E:85:ILE:HD11  | 1.95                     | 0.47              |
| 26:B:2:ALA:N      | 26:B:20:VAL:O     | 2.47                     | 0.47              |
| 37:P:100:LEU:HD11 | 37:P:110:ILE:HD11 | 1.96                     | 0.47              |
| 51:e:62:LEU:HB3   | 51:e:65:ALA:HB2   | 1.96                     | 0.47              |
| 1:2:500:G:H2'     | 1:2:501:C:C6      | 2.49                     | 0.47              |
| 1:2:545:C:H5'     | 4:i:69:GLU:HB2    | 1.96                     | 0.47              |
| 1:2:649:A:H2'     | 1:2:650:G:O4'     | 2.14                     | 0.47              |
| 7:l:14:PRO:HB2    | 7:l:19:GLY:HA2    | 1.96                     | 0.47              |
| 24:1:296:U:H2'    | 24:1:297:G:C8     | 2.48                     | 0.47              |
| 24:1:1649:G:O2'   | 35:N:106:ASP:OD2  | 2.20                     | 0.47              |
| 53:a:16:CYS:SG    | 53:a:17:SER:N     | 2.88                     | 0.47              |
| 1:2:109:A:H2'     | 1:2:326:G:N2      | 2.29                     | 0.47              |
| 1:2:321:A:H2'     | 1:2:322:C:C6      | 2.48                     | 0.47              |
| 1:2:473:U:H2'     | 1:2:474:G:H8      | 1.78                     | 0.47              |
| 1:2:613:C:OP1     | 4:i:81:ARG:NH1    | 2.43                     | 0.47              |
| 1:2:621:A:H2'     | 1:2:622:A:C8      | 2.50                     | 0.47              |
| 1:2:1441:A:N1     | 37:P:114:LEU:HD12 | 2.30                     | 0.47              |
| 24:1:927:A:H2'    | 24:1:928:A:C8     | 2.49                     | 0.47              |
| 24:1:1385:A:O2'   | 24:1:1396:U:O2    | 2.31                     | 0.47              |
| 24:1:1631:G:H1'   | 24:1:1635:A:N6    | 2.30                     | 0.47              |
| 24:1:2074:U:H2'   | 24:1:2075:U:C6    | 2.49                     | 0.47              |
| 24:1:2740:A:H2'   | 24:1:2741:A:C8    | 2.50                     | 0.47              |
| 49:c:25:LYS:NZ    | 49:c:51:GLU:OE1   | 2.31                     | 0.47              |
| 1:2:246:A:C2      | 1:2:282:A:C5      | 3.02                     | 0.47              |
| 1:2:745:G:O2'     | 1:2:746:A:H5'     | 2.14                     | 0.47              |
| 1:2:983:A:H5'     | 1:2:984:C:OP2     | 2.15                     | 0.47              |
| 1:2:1032:G:C6     | 1:2:1033:G:H1'    | 2.49                     | 0.47              |
| 1:2:1435:G:H2'    | 1:2:1436:U:C6     | 2.49                     | 0.47              |
| 1:2:1458:G:OP1    | 20:y:30:THR:OG1   | 2.29                     | 0.47              |
| 24:1:589:U:H2'    | 24:1:590:A:C8     | 2.50                     | 0.47              |
| 24:1:1321:A:C4    | 24:1:1322:A:C8    | 3.03                     | 0.47              |
| 24:1:2199:A:N1    | 24:1:2226:C:N4    | 2.63                     | 0.47              |
| 24:1:2850:A:N7    | 24:1:2868:A:O2'   | 2.46                     | 0.47              |
| 34:M:53:MET:HE1   | 34:M:103:TYR:CD1  | 2.49                     | 0.47              |
| 1:2:325:A:N7      | 58:2:1687:SPD:H71 | 2.29                     | 0.47              |
| 1:2:985:C:H2'     | 1:2:986:U:C6      | 2.50                     | 0.47              |
| 1:2:1516:2MG:N2   | 1:2:1519:MA6:OP2  | 2.46                     | 0.47              |
| 19:x:9:PRO:HD3    | 53:a:64:PHE:CG    | 2.49                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:5:21:A:N6     | 23:5:46:G:H2'     | 2.29                     | 0.47              |
| 24:1:1101:U:H2'  | 24:1:1102:C:O4'   | 2.14                     | 0.47              |
| 24:1:2039:U:H2'  | 24:1:2040:G:C8    | 2.50                     | 0.47              |
| 24:1:2809:A:H2'  | 24:1:2810:A:C8    | 2.49                     | 0.47              |
| 31:J:125:TYR:HH  | 31:J:132:HIS:CD2  | 2.32                     | 0.47              |
| 1:2:71:A:N1      | 1:2:99:C:O2'      | 2.43                     | 0.47              |
| 1:2:422:C:O2     | 1:2:423:G:N1      | 2.48                     | 0.47              |
| 1:2:974:A:OP1    | 14:s:69:ARG:NH2   | 2.48                     | 0.47              |
| 1:2:1118:U:H2'   | 1:2:1119:C:H6     | 1.80                     | 0.47              |
| 1:2:1253:G:H2'   | 1:2:1254:A:H8     | 1.80                     | 0.47              |
| 1:2:1309:G:N7    | 13:r:98:ARG:NH2   | 2.63                     | 0.47              |
| 1:2:1428:A:H2'   | 1:2:1429:A:O4'    | 2.15                     | 0.47              |
| 10:o:37:ARG:HB2  | 10:o:75:ASP:HB2   | 1.95                     | 0.47              |
| 24:1:784:G:H5'   | 24:1:785:G:OP1    | 2.14                     | 0.47              |
| 24:1:1056:G:H4'  | 24:1:1086:A:C8    | 2.33                     | 0.47              |
| 24:1:1710:G:H4'  | 24:1:2858:C:O2    | 2.15                     | 0.47              |
| 24:1:1791:A:N6   | 24:1:1828:G:O2'   | 2.44                     | 0.47              |
| 24:1:2233:U:H2'  | 24:1:2234:G:H8    | 1.78                     | 0.47              |
| 24:1:2564:A:OP1  | 24:1:2648:G:O2'   | 2.28                     | 0.47              |
| 24:1:2845:U:H2'  | 24:1:2846:G:C8    | 2.49                     | 0.47              |
| 25:3:29:A:H2'    | 25:3:30:C:C6      | 2.50                     | 0.47              |
| 29:E:50:LEU:HD11 | 29:E:67:ILE:HD12  | 1.97                     | 0.47              |
| 51:e:16:LYS:HE2  | 51:e:20:GLY:HA2   | 1.96                     | 0.47              |
| 1:2:107:G:OP2    | 58:2:1687:SPD:H82 | 2.14                     | 0.47              |
| 1:2:715:A:H2'    | 1:2:716:A:C8      | 2.49                     | 0.47              |
| 1:2:842:U:H2'    | 1:2:844:G:C5'     | 2.44                     | 0.47              |
| 7:l:5:ARG:NH2    | 7:l:7:ILE:O       | 2.46                     | 0.47              |
| 21:z:33:ARG:NH2  | 22:4:31:G:OP2     | 2.38                     | 0.47              |
| 24:1:52:A:H2'    | 24:1:53:A:C8      | 2.49                     | 0.47              |
| 1:2:64:G:H4'     | 1:2:65:A:H3'      | 1.95                     | 0.47              |
| 1:2:166:U:H2'    | 1:2:167:A:C8      | 2.50                     | 0.47              |
| 1:2:1008:U:H2'   | 1:2:1009:U:O4'    | 2.15                     | 0.47              |
| 1:2:1251:A:H2'   | 1:2:1252:A:C8     | 2.49                     | 0.47              |
| 5:j:164:ILE:HG22 | 5:j:165:LEU:HG    | 1.97                     | 0.47              |
| 9:n:100:LYS:HE3  | 9:n:100:LYS:HB3   | 1.60                     | 0.47              |
| 24:1:2:G:N1      | 24:1:2902:C:N3    | 2.63                     | 0.47              |
| 34:M:136:MET:O   | 43:V:79:ARG:NH2   | 2.24                     | 0.47              |
| 1:2:206:C:H42    | 1:2:213:G:H1      | 1.62                     | 0.47              |
| 1:2:216:U:H1'    | 1:2:466:A:H61     | 1.79                     | 0.47              |
| 1:2:299:G:H2'    | 1:2:300:A:C8      | 2.50                     | 0.47              |
| 1:2:428:G:OP2    | 4:i:7:PRO:HG2     | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:g:64:LYS:HA    | 2:g:64:LYS:HD3    | 1.66                     | 0.47              |
| 7:l:81:GLY:C     | 22:4:34:U:H5'     | 2.40                     | 0.47              |
| 17:v:19:LYS:HG3  | 17:v:48:ASP:O     | 2.15                     | 0.47              |
| 24:1:290:U:H3    | 24:1:350:G:H1     | 1.63                     | 0.47              |
| 24:1:1049:C:C2   | 24:1:1050:A:C8    | 3.03                     | 0.47              |
| 24:1:1594:U:H2'  | 24:1:1595:C:C6    | 2.50                     | 0.47              |
| 24:1:1703:G:H2'  | 24:1:1704:C:C6    | 2.50                     | 0.47              |
| 24:1:1735:A:H2'  | 24:1:1736:U:C6    | 2.50                     | 0.47              |
| 24:1:2184:A:H2'  | 24:1:2185:U:O4'   | 2.15                     | 0.47              |
| 28:D:97:ASN:HB2  | 28:D:100:MET:HG3  | 1.97                     | 0.47              |
| 1:2:268:U:H2'    | 1:2:269:C:C6      | 2.51                     | 0.46              |
| 1:2:696:A:H2'    | 1:2:697:U:H6      | 1.79                     | 0.46              |
| 1:2:839:C:H2'    | 1:2:840:C:C6      | 2.50                     | 0.46              |
| 1:2:1120:C:H2'   | 1:2:1121:U:C6     | 2.49                     | 0.46              |
| 1:2:1169:A:H2'   | 1:2:1170:A:C8     | 2.49                     | 0.46              |
| 1:2:1236:A:H2'   | 1:2:1237:C:C6     | 2.50                     | 0.46              |
| 2:g:94:HIS:ND1   | 2:g:146:ASN:O     | 2.48                     | 0.46              |
| 3:h:11:ARG:NH2   | 3:h:177:THR:O     | 2.48                     | 0.46              |
| 24:1:1429:G:H2'  | 24:1:1430:G:H8    | 1.80                     | 0.46              |
| 24:1:2333:A:H5'  | 24:1:2335:A:H1'   | 1.97                     | 0.46              |
| 1:2:335:C:H2'    | 1:2:336:A:C8      | 2.50                     | 0.46              |
| 1:2:738:C:OP1    | 6:k:2:ARG:NH1     | 2.42                     | 0.46              |
| 1:2:1009:U:O2    | 1:2:1020:G:N2     | 2.38                     | 0.46              |
| 1:2:1481:U:H2'   | 1:2:1482:G:C8     | 2.50                     | 0.46              |
| 22:4:24:U:H2'    | 22:4:25:A:C8      | 2.50                     | 0.46              |
| 24:1:305:C:H2'   | 24:1:306:U:C6     | 2.50                     | 0.46              |
| 24:1:851:C:H2'   | 24:1:852:U:H6     | 1.81                     | 0.46              |
| 24:1:1187:G:H5'' | 39:R:83:TYR:CE1   | 2.50                     | 0.46              |
| 24:1:2859:G:H2'  | 24:1:2860:A:C8    | 2.50                     | 0.46              |
| 31:J:92:MET:HE3  | 31:J:92:MET:HB3   | 1.87                     | 0.46              |
| 42:U:54:GLN:HG2  | 42:U:55:PRO:HD3   | 1.97                     | 0.46              |
| 45:X:39:TRP:HE1  | 45:X:41:GLU:HG2   | 1.80                     | 0.46              |
| 1:2:404:G:O2'    | 1:2:498:A:N1      | 2.43                     | 0.46              |
| 1:2:999:C:H2'    | 1:2:1000:A:H8     | 1.81                     | 0.46              |
| 8:m:29:SER:HB3   | 8:m:57:PRO:HB2    | 1.98                     | 0.46              |
| 24:1:580:U:H2'   | 24:1:581:C:C6     | 2.51                     | 0.46              |
| 24:1:1072:C:H2'  | 24:1:1093:G:O6    | 2.15                     | 0.46              |
| 24:1:2149:U:H2'  | 24:1:2150:C:H6    | 1.80                     | 0.46              |
| 25:3:93:C:H2'    | 25:3:94:A:H8      | 1.80                     | 0.46              |
| 27:C:25:THR:HG21 | 27:C:193:VAL:HG22 | 1.97                     | 0.46              |
| 27:C:56:LYS:O    | 27:C:60:VAL:HG23  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:522:C:H41     | 12:q:50:ARG:NH2  | 2.13                     | 0.46              |
| 2:g:6:MET:HE2     | 2:g:6:MET:HB2    | 1.82                     | 0.46              |
| 24:1:2518:A:H2'   | 24:1:2518:A:N3   | 2.30                     | 0.46              |
| 1:2:1071:C:H2'    | 1:2:1072:G:C8    | 2.48                     | 0.46              |
| 24:1:878:A:N7     | 24:1:899:A:H2    | 2.14                     | 0.46              |
| 24:1:1709:U:H2'   | 24:1:1710:G:C8   | 2.51                     | 0.46              |
| 24:1:2099:U:H3    | 24:1:2190:G:H1   | 1.63                     | 0.46              |
| 29:E:108:VAL:HG11 | 29:E:176:PRO:HG2 | 1.98                     | 0.46              |
| 4:i:177:LYS:HB2   | 4:i:179:GLU:HG2  | 1.98                     | 0.46              |
| 24:1:356:G:H2'    | 24:1:357:C:H6    | 1.79                     | 0.46              |
| 1:2:134:G:H1'     | 1:2:325:A:C5     | 2.50                     | 0.46              |
| 4:i:162:ALA:HA    | 4:i:165:ARG:HD3  | 1.98                     | 0.46              |
| 4:i:188:ARG:HD2   | 4:i:188:ARG:HA   | 1.76                     | 0.46              |
| 24:1:1442:U:H2'   | 24:1:1443:U:C6   | 2.51                     | 0.46              |
| 24:1:1645:G:H5''  | 24:1:1646:C:H5'  | 1.98                     | 0.46              |
| 24:1:1712:U:OP2   | 24:1:1713:A:O2'  | 2.33                     | 0.46              |
| 24:1:1747:U:H2'   | 24:1:1748:C:H6   | 1.78                     | 0.46              |
| 1:2:166:U:H2'     | 1:2:167:A:H8     | 1.80                     | 0.46              |
| 7:l:53:ARG:NH2    | 7:l:122:ASN:OD1  | 2.49                     | 0.46              |
| 10:o:28:THR:HG21  | 10:o:90:LEU:HG   | 1.96                     | 0.46              |
| 11:p:87:LYS:HD3   | 11:p:115:PRO:HD3 | 1.98                     | 0.46              |
| 24:1:364:C:H2'    | 24:1:365:U:C6    | 2.50                     | 0.46              |
| 24:1:1064:C:O2'   | 24:1:1065:U:C6   | 2.68                     | 0.46              |
| 24:1:1475:G:O2'   | 24:1:1514:G:O6   | 2.30                     | 0.46              |
| 24:1:1570:A:H2'   | 24:1:1571:A:C8   | 2.51                     | 0.46              |
| 24:1:1597:A:H5''  | 24:1:1598:A:H5'  | 1.98                     | 0.46              |
| 24:1:2291:U:H2'   | 24:1:2292:U:H6   | 1.77                     | 0.46              |
| 24:1:2902:C:H3'   | 24:1:2903:U:C6   | 2.51                     | 0.46              |
| 1:2:678:U:H2'     | 1:2:679:C:H6     | 1.81                     | 0.46              |
| 11:p:97:ILE:HG22  | 21:z:12:PHE:HZ   | 1.80                     | 0.46              |
| 24:1:881:G:H2'    | 24:1:882:G:C8    | 2.51                     | 0.46              |
| 24:1:2692:G:H1'   | 24:1:2847:U:H1'  | 1.98                     | 0.46              |
| 1:2:110:C:H2'     | 1:2:111:G:O4'    | 2.16                     | 0.46              |
| 1:2:1088:G:H4'    | 21:z:70:LEU:HD13 | 1.97                     | 0.46              |
| 4:i:105:MET:HE1   | 4:i:143:VAL:HB   | 1.98                     | 0.46              |
| 8:m:96:MET:HE2    | 8:m:99:LEU:HB2   | 1.98                     | 0.46              |
| 22:4:32:U:H4'     | 22:4:33:A:OP1    | 2.14                     | 0.46              |
| 24:1:570:G:H2'    | 24:1:2030:6MZ:N7 | 2.30                     | 0.46              |
| 24:1:1075:C:H2'   | 24:1:1076:C:O4'  | 2.16                     | 0.46              |
| 24:1:2836:U:H2'   | 24:1:2837:A:C8   | 2.51                     | 0.46              |
| 26:B:133:ARG:HB3  | 26:B:186:ALA:HB1 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:M:50:ARG:HD3  | 34:M:65:ILE:HD11  | 1.97                     | 0.46              |
| 11:p:86:VAL:HG21 | 11:p:97:ILE:HD11  | 1.99                     | 0.45              |
| 24:1:391:A:H1'   | 24:1:411:G:O4'    | 2.16                     | 0.45              |
| 24:1:651:G:H5'   | 51:e:19:LYS:HG3   | 1.98                     | 0.45              |
| 24:1:1485:U:H2'  | 24:1:1486:U:H6    | 1.81                     | 0.45              |
| 24:1:1780:A:H3'  | 24:1:1781:U:H2'   | 1.97                     | 0.45              |
| 33:L:10:GLU:H    | 33:L:10:GLU:CD    | 2.24                     | 0.45              |
| 40:S:20:VAL:HG11 | 40:S:44:ALA:HA    | 1.97                     | 0.45              |
| 56:G:16:GLY:HA2  | 56:G:47:PHE:CE2   | 2.51                     | 0.45              |
| 56:G:94:ILE:HB   | 56:G:122:LEU:HB2  | 1.97                     | 0.45              |
| 1:2:67:C:H2'     | 1:2:68:G:C8       | 2.51                     | 0.45              |
| 1:2:736:C:H2'    | 1:2:737:C:C6      | 2.51                     | 0.45              |
| 1:2:1005:A:H4'   | 1:2:1037:C:H1'    | 1.98                     | 0.45              |
| 24:1:17:G:H2'    | 24:1:18:U:C6      | 2.51                     | 0.45              |
| 24:1:909:A:H2'   | 24:1:912:C:H5     | 1.81                     | 0.45              |
| 24:1:2898:U:H2'  | 24:1:2899:A:C8    | 2.52                     | 0.45              |
| 1:2:35:G:H2'     | 1:2:36:C:C6       | 2.51                     | 0.45              |
| 1:2:234:C:H4'    | 17:v:66:PRO:HG3   | 1.97                     | 0.45              |
| 1:2:505:G:H2'    | 1:2:506:G:C8      | 2.51                     | 0.45              |
| 1:2:608:A:H2'    | 1:2:609:A:O4'     | 2.16                     | 0.45              |
| 24:1:1047:G:HO2' | 24:1:1110:G:H1    | 1.63                     | 0.45              |
| 24:1:1076:C:H2'  | 24:1:1077:A:H8    | 1.80                     | 0.45              |
| 24:1:2243:U:H2'  | 24:1:2244:U:C6    | 2.51                     | 0.45              |
| 25:3:2:G:H2'     | 25:3:3:C:H6       | 1.81                     | 0.45              |
| 29:E:14:LYS:H    | 29:E:14:LYS:HD2   | 1.82                     | 0.45              |
| 1:2:154:U:H2'    | 1:2:155:A:C8      | 2.51                     | 0.45              |
| 1:2:219:U:H2'    | 1:2:220:G:C8      | 2.51                     | 0.45              |
| 1:2:251:G:C6     | 1:2:266:G:C6      | 3.05                     | 0.45              |
| 15:t:10:LYS:HE2  | 15:t:10:LYS:HB3   | 1.80                     | 0.45              |
| 16:u:3:THR:HG22  | 16:u:66:THR:OG1   | 2.16                     | 0.45              |
| 24:1:1532:A:C6   | 24:1:1540:G:C6    | 3.04                     | 0.45              |
| 24:1:2246:G:H2'  | 24:1:2247:A:H8    | 1.81                     | 0.45              |
| 26:B:181:MET:HB3 | 26:B:268:VAL:HB   | 1.98                     | 0.45              |
| 27:C:35:THR:HG22 | 27:C:73:VAL:HG21  | 1.99                     | 0.45              |
| 30:F:149:ARG:HG3 | 30:F:162:VAL:O    | 2.16                     | 0.45              |
| 33:L:82:LEU:HD22 | 33:L:90:VAL:HG21  | 1.97                     | 0.45              |
| 33:L:132:ARG:HG3 | 33:L:142:ILE:HD12 | 1.99                     | 0.45              |
| 1:2:626:G:OP1    | 16:u:35:ARG:NH2   | 2.50                     | 0.45              |
| 1:2:891:U:H2'    | 1:2:892:A:C8      | 2.51                     | 0.45              |
| 1:2:1271:A:H2'   | 1:2:1272:G:C8     | 2.52                     | 0.45              |
| 4:i:11:LEU:O     | 4:i:15:GLU:HG2    | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:s:10:GLU:HG3  | 14:s:63:ARG:HD2  | 1.97                     | 0.45              |
| 24:1:69:C:O2     | 24:1:73:A:O2'    | 2.32                     | 0.45              |
| 24:1:468:G:N7    | 50:d:39:ARG:NH2  | 2.58                     | 0.45              |
| 24:1:488:G:H1'   | 24:1:492:A:N6    | 2.31                     | 0.45              |
| 24:1:667:U:H2'   | 24:1:668:A:O4'   | 2.15                     | 0.45              |
| 24:1:729:G:C5    | 26:B:207:LYS:HB2 | 2.52                     | 0.45              |
| 24:1:914:G:H5'   | 24:1:915:C:OP2   | 2.17                     | 0.45              |
| 24:1:1179:G:H2'  | 24:1:1180:U:C6   | 2.52                     | 0.45              |
| 24:1:2294:G:H5'' | 36:O:10:ARG:HD2  | 1.99                     | 0.45              |
| 24:1:2649:C:H2'  | 24:1:2650:U:C6   | 2.51                     | 0.45              |
| 46:Y:37:LEU:HG   | 46:Y:39:GLN:O    | 2.17                     | 0.45              |
| 1:2:842:U:C6     | 1:2:843:U:H5''   | 2.52                     | 0.45              |
| 2:g:118:GLU:O    | 2:g:122:GLN:HG2  | 2.17                     | 0.45              |
| 22:4:43:G:N7     | 55:6:215:THR:OG1 | 2.42                     | 0.45              |
| 24:1:276:U:HO2'  | 24:1:278:A:H8    | 1.63                     | 0.45              |
| 24:1:279:A:H2'   | 24:1:280:U:O4'   | 2.17                     | 0.45              |
| 24:1:2316:G:H2'  | 24:1:2317:A:H8   | 1.82                     | 0.45              |
| 27:C:32:ASN:N    | 27:C:32:ASN:HD22 | 2.12                     | 0.45              |
| 30:F:155:GLU:OE2 | 30:F:160:LYS:HB2 | 2.17                     | 0.45              |
| 36:O:53:THR:O    | 36:O:59:ALA:HB2  | 2.17                     | 0.45              |
| 45:X:3:ARG:O     | 45:X:12:PRO:HD3  | 2.16                     | 0.45              |
| 1:2:34:C:H2'     | 1:2:35:G:H8      | 1.81                     | 0.45              |
| 1:2:922:G:H2'    | 1:2:923:A:C8     | 2.52                     | 0.45              |
| 1:2:1035:A:C4    | 1:2:1036:A:C2    | 3.04                     | 0.45              |
| 1:2:1332:A:H2'   | 1:2:1333:A:H8    | 1.81                     | 0.45              |
| 24:1:2615:U:C2   | 48:b:4:GLN:HA    | 2.52                     | 0.45              |
| 25:3:48:U:H2'    | 25:3:49:C:C6     | 2.52                     | 0.45              |
| 1:2:456:A:H3'    | 1:2:457:G:H8     | 1.82                     | 0.45              |
| 1:2:855:U:OP2    | 1:2:871:U:N3     | 2.39                     | 0.45              |
| 2:g:217:VAL:HA   | 2:g:220:THR:HG22 | 1.99                     | 0.45              |
| 18:w:71:THR:OG1  | 18:w:72:ASP:N    | 2.50                     | 0.45              |
| 19:x:12:ASP:HB3  | 19:x:14:HIS:CE1  | 2.52                     | 0.45              |
| 22:4:34:U:H4'    | 22:4:35:U:C6     | 2.52                     | 0.45              |
| 24:1:145:C:H2'   | 24:1:146:A:C8    | 2.52                     | 0.45              |
| 24:1:577:G:O2'   | 24:1:1254:A:OP1  | 2.35                     | 0.45              |
| 24:1:1007:C:OP1  | 31:J:37:ARG:NH1  | 2.49                     | 0.45              |
| 24:1:1198:U:H2'  | 24:1:1199:U:H6   | 1.80                     | 0.45              |
| 24:1:2020:A:H5'  | 48:b:9:THR:CG2   | 2.46                     | 0.45              |
| 24:1:2420:C:OP1  | 51:e:34:THR:OG1  | 2.35                     | 0.45              |
| 24:1:2687:U:H2'  | 24:1:2688:G:O4'  | 2.17                     | 0.45              |
| 30:F:145:ALA:HB1 | 30:F:164:TYR:HE1 | 1.81                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 35:N:79:LEU:HD23  | 35:N:83:LEU:HD12 | 1.99                     | 0.45              |
| 41:T:76:ARG:NH2   | 41:T:79:ASP:OD1  | 2.50                     | 0.45              |
| 46:Y:14:LEU:HB3   | 46:Y:57:LEU:HD21 | 1.98                     | 0.45              |
| 1:2:253:A:H2'     | 1:2:254:G:C8     | 2.52                     | 0.45              |
| 1:2:465:A:H2'     | 1:2:466:A:C8     | 2.52                     | 0.45              |
| 1:2:908:A:H2'     | 1:2:909:A:C8     | 2.51                     | 0.45              |
| 24:1:1544:A:H2'   | 24:1:1545:A:C8   | 2.51                     | 0.45              |
| 31:J:76:HIS:CE1   | 31:J:85:LYS:HB2  | 2.51                     | 0.45              |
| 1:2:92:U:H2'      | 1:2:93:U:H6      | 1.81                     | 0.45              |
| 1:2:1148:U:H2'    | 1:2:1149:C:O4'   | 2.16                     | 0.45              |
| 1:2:1171:A:H2'    | 1:2:1172:C:H6    | 1.82                     | 0.45              |
| 1:2:1191:A:H5''   | 3:h:4:LYS:HE3    | 1.98                     | 0.45              |
| 1:2:1369:C:H2'    | 1:2:1370:G:C8    | 2.52                     | 0.45              |
| 22:4:31:G:H2'     | 22:4:32:U:C6     | 2.51                     | 0.45              |
| 24:1:413:C:H2'    | 24:1:414:C:H6    | 1.82                     | 0.45              |
| 24:1:1443:U:H2'   | 24:1:1444:G:C8   | 2.51                     | 0.45              |
| 24:1:1563:U:H2'   | 24:1:1564:C:C6   | 2.52                     | 0.45              |
| 36:O:115:LEU:HD23 | 36:O:115:LEU:HA  | 1.83                     | 0.45              |
| 1:2:113:G:H2'     | 1:2:114:U:C6     | 2.52                     | 0.44              |
| 1:2:999:C:H2'     | 1:2:1000:A:C8    | 2.52                     | 0.44              |
| 22:4:27:G:H2'     | 22:4:28:G:C8     | 2.52                     | 0.44              |
| 24:1:280:U:H2'    | 24:1:281:C:C6    | 2.53                     | 0.44              |
| 24:1:1394:U:H2'   | 24:1:1395:A:O4'  | 2.17                     | 0.44              |
| 24:1:1676:A:H2'   | 24:1:1677:A:O4'  | 2.16                     | 0.44              |
| 29:E:121:SER:HB2  | 29:E:128:TYR:CE1 | 2.52                     | 0.44              |
| 34:M:53:MET:HE3   | 34:M:53:MET:HB2  | 1.85                     | 0.44              |
| 35:N:72:ASP:OD1   | 35:N:72:ASP:N    | 2.50                     | 0.44              |
| 1:2:187:G:N2      | 1:2:190:A:OP2    | 2.44                     | 0.44              |
| 1:2:883:C:O2'     | 1:2:884:U:H5'    | 2.18                     | 0.44              |
| 1:2:1092:A:H5''   | 7:l:4:ARG:NH2    | 2.32                     | 0.44              |
| 1:2:1244:G:H2'    | 1:2:1245:C:H6    | 1.82                     | 0.44              |
| 1:2:1263:C:H2'    | 1:2:1264:U:C6    | 2.52                     | 0.44              |
| 1:2:1464:U:H2'    | 1:2:1465:A:H8    | 1.82                     | 0.44              |
| 24:1:151:C:H2'    | 24:1:152:A:C8    | 2.52                     | 0.44              |
| 24:1:499:U:H2'    | 24:1:500:G:O4'   | 2.17                     | 0.44              |
| 24:1:1506:U:H2'   | 24:1:1507:C:C6   | 2.52                     | 0.44              |
| 24:1:2469:A:H4'   | 34:M:55:ARG:CD   | 2.48                     | 0.44              |
| 24:1:2556:C:H2'   | 24:1:2557:G:O4'  | 2.16                     | 0.44              |
| 29:E:38:MET:HE3   | 29:E:57:LEU:HD13 | 2.00                     | 0.44              |
| 1:2:50:A:O2'      | 1:2:360:G:N2     | 2.50                     | 0.44              |
| 1:2:202:G:O2'     | 1:2:468:A:N3     | 2.46                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1040:U:H2'    | 1:2:1041:G:C8     | 2.51                     | 0.44              |
| 1:2:1319:A:O2'    | 1:2:1323:G:N7     | 2.41                     | 0.44              |
| 24:1:296:U:H2'    | 24:1:297:G:H8     | 1.82                     | 0.44              |
| 24:1:548:G:H2'    | 24:1:549:G:C1'    | 2.47                     | 0.44              |
| 24:1:1107:G:H2'   | 24:1:1108:U:C6    | 2.53                     | 0.44              |
| 24:1:1425:G:H2'   | 24:1:1426:G:C8    | 2.52                     | 0.44              |
| 24:1:1527:G:N1    | 24:1:1544:A:OP2   | 2.43                     | 0.44              |
| 24:1:2186:G:H2'   | 24:1:2187:U:O4'   | 2.17                     | 0.44              |
| 24:1:2460:U:C2    | 24:1:2461:A:C8    | 3.06                     | 0.44              |
| 55:6:270:ILE:HD11 | 55:6:294:LYS:HD3  | 1.99                     | 0.44              |
| 1:2:461:A:H2'     | 1:2:462:G:H8      | 1.82                     | 0.44              |
| 1:2:844:G:C2      | 1:2:846:G:H1'     | 2.51                     | 0.44              |
| 1:2:979:C:O2      | 14:s:59:ARG:HD2   | 2.16                     | 0.44              |
| 2:g:118:GLU:O     | 2:g:121:SER:OG    | 2.28                     | 0.44              |
| 13:r:100:GLN:N    | 13:r:100:GLN:OE1  | 2.51                     | 0.44              |
| 24:1:945:A:H1'    | 58:1:3203:SPD:H82 | 1.99                     | 0.44              |
| 24:1:1079:C:H2'   | 24:1:1080:A:C8    | 2.51                     | 0.44              |
| 24:1:1631:G:N1    | 24:1:1634:A:OP2   | 2.41                     | 0.44              |
| 24:1:2038:G:H2'   | 24:1:2039:U:O4'   | 2.17                     | 0.44              |
| 24:1:2373:G:H2'   | 24:1:2374:C:C6    | 2.52                     | 0.44              |
| 26:B:120:VAL:HG23 | 26:B:134:ASN:OD1  | 2.17                     | 0.44              |
| 1:2:160:A:H2'     | 1:2:161:A:O4'     | 2.17                     | 0.44              |
| 1:2:672:U:H2'     | 1:2:673:A:C8      | 2.53                     | 0.44              |
| 1:2:1319:A:C8     | 1:2:1323:G:C6     | 3.05                     | 0.44              |
| 2:g:203:ASN:ND2   | 2:g:205:ASP:H     | 2.16                     | 0.44              |
| 24:1:1:G:H2'      | 24:1:2:G:C8       | 2.53                     | 0.44              |
| 24:1:144:A:H2'    | 24:1:145:C:C6     | 2.52                     | 0.44              |
| 24:1:898:C:H2'    | 24:1:899:A:O4'    | 2.17                     | 0.44              |
| 24:1:950:G:H1     | 24:1:967:U:H3     | 1.65                     | 0.44              |
| 24:1:1289:C:H2'   | 24:1:1290:C:C6    | 2.53                     | 0.44              |
| 24:1:1496:A:H2'   | 24:1:1498:C:C5    | 2.52                     | 0.44              |
| 24:1:1874:C:H2'   | 24:1:1875:G:O4'   | 2.16                     | 0.44              |
| 33:L:77:ILE:HD13  | 33:L:108:ALA:HB1  | 1.99                     | 0.44              |
| 34:M:17:ASN:OD1   | 34:M:97:GLN:NE2   | 2.41                     | 0.44              |
| 1:2:628:G:H2'     | 1:2:629:A:C8      | 2.52                     | 0.44              |
| 1:2:1014:A:N3     | 1:2:1219:A:H1'    | 2.32                     | 0.44              |
| 1:2:1436:U:H2'    | 1:2:1437:A:C8     | 2.53                     | 0.44              |
| 1:2:1513:A:H2'    | 1:2:1514:G:H8     | 1.82                     | 0.44              |
| 2:g:58:ASN:HB2    | 2:g:220:THR:OG1   | 2.18                     | 0.44              |
| 17:v:19:LYS:HA    | 17:v:51:ASN:HD21  | 1.82                     | 0.44              |
| 24:1:327:G:H2'    | 24:1:328:U:O4'    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:1:422:A:H2'   | 24:1:423:A:C8     | 2.52                     | 0.44              |
| 24:1:1241:A:H3'  | 24:1:1242:U:H6    | 1.83                     | 0.44              |
| 24:1:1526:C:H2'  | 24:1:1527:G:O4'   | 2.18                     | 0.44              |
| 24:1:1726:C:H2'  | 24:1:1727:C:C6    | 2.53                     | 0.44              |
| 24:1:2847:U:H2'  | 24:1:2848:G:O4'   | 2.17                     | 0.44              |
| 1:2:253:A:H2'    | 1:2:254:G:H8      | 1.82                     | 0.44              |
| 1:2:321:A:H2'    | 1:2:322:C:H6      | 1.83                     | 0.44              |
| 1:2:607:A:H2'    | 1:2:608:A:C8      | 2.53                     | 0.44              |
| 1:2:1040:U:H2'   | 1:2:1041:G:H8     | 1.83                     | 0.44              |
| 1:2:1486:G:H2'   | 1:2:1487:G:O4'    | 2.18                     | 0.44              |
| 21:z:24:GLU:OE2  | 22:4:29:A:O2'     | 2.19                     | 0.44              |
| 24:1:279:A:C2    | 24:1:362:A:H5'    | 2.53                     | 0.44              |
| 24:1:359:G:H2'   | 24:1:360:U:H5'    | 1.99                     | 0.44              |
| 24:1:1153:C:OP1  | 38:Q:92:ARG:NH2   | 2.44                     | 0.44              |
| 24:1:1870:C:O2'  | 24:1:1871:A:O4'   | 2.31                     | 0.44              |
| 24:1:2241:A:H2'  | 24:1:2242:G:C8    | 2.53                     | 0.44              |
| 24:1:2494:G:O2'  | 34:M:79:ALA:HA    | 2.17                     | 0.44              |
| 24:1:2794:C:H2'  | 24:1:2795:C:C6    | 2.52                     | 0.44              |
| 26:B:68:LYS:NZ   | 26:B:149:GLY:O    | 2.50                     | 0.44              |
| 34:M:56:ALA:HB2  | 34:M:119:LEU:HD12 | 1.99                     | 0.44              |
| 38:Q:15:LYS:HB3  | 38:Q:15:LYS:HE2   | 1.73                     | 0.44              |
| 44:W:41:ARG:HD3  | 44:W:41:ARG:HA    | 1.70                     | 0.44              |
| 1:2:215:C:H2'    | 1:2:216:U:C6      | 2.53                     | 0.44              |
| 1:2:399:G:H2'    | 1:2:400:C:C6      | 2.52                     | 0.44              |
| 1:2:512:U:H2'    | 1:2:513:C:C6      | 2.52                     | 0.44              |
| 1:2:602:A:H2'    | 1:2:603:U:C6      | 2.53                     | 0.44              |
| 10:o:6:ILE:HD11  | 10:o:84:VAL:HG22  | 2.00                     | 0.44              |
| 24:1:29:U:H2'    | 24:1:30:G:C8      | 2.53                     | 0.44              |
| 24:1:337:C:H2'   | 24:1:338:G:O4'    | 2.18                     | 0.44              |
| 24:1:2813:A:H2'  | 24:1:2814:A:C8    | 2.53                     | 0.44              |
| 30:F:170:ARG:NH1 | 30:F:170:ARG:HA   | 2.33                     | 0.44              |
| 34:M:50:ARG:HA   | 34:M:53:MET:HE3   | 1.99                     | 0.44              |
| 43:V:20:LEU:HD11 | 43:V:41:GLU:HG2   | 2.00                     | 0.44              |
| 1:2:737:C:H2'    | 1:2:738:C:C6      | 2.53                     | 0.44              |
| 5:j:157:ARG:NH1  | 8:m:99:LEU:O      | 2.51                     | 0.44              |
| 6:k:32:ALA:HB2   | 6:k:70:VAL:HG11   | 2.00                     | 0.44              |
| 6:k:38:ARG:HB3   | 6:k:63:ASN:HB2    | 2.00                     | 0.44              |
| 10:o:84:VAL:O    | 10:o:88:MET:HG2   | 2.18                     | 0.44              |
| 24:1:2191:A:H2'  | 24:1:2192:U:H6    | 1.82                     | 0.44              |
| 24:1:2895:G:H2'  | 24:1:2896:C:C6    | 2.53                     | 0.44              |
| 43:V:86:LEU:HD13 | 43:V:89:ILE:HD11  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:2:664:G:OP1      | 18:w:57:ARG:NH2  | 2.41                     | 0.43              |
| 1:2:1121:U:H2'     | 1:2:1122:U:H6    | 1.83                     | 0.43              |
| 1:2:1122:U:H2'     | 1:2:1123:U:C6    | 2.53                     | 0.43              |
| 3:h:135:LYS:HE3    | 3:h:135:LYS:HB2  | 1.83                     | 0.43              |
| 4:i:65:TYR:OH      | 4:i:95:GLU:OE2   | 2.27                     | 0.43              |
| 4:i:85:ASN:HB3     | 4:i:88:GLU:CG    | 2.48                     | 0.43              |
| 24:1:392:U:H2'     | 24:1:393:C:H6    | 1.82                     | 0.43              |
| 24:1:438:G:H2'     | 24:1:439:A:C8    | 2.53                     | 0.43              |
| 24:1:492:A:H2'     | 24:1:493:G:O4'   | 2.17                     | 0.43              |
| 24:1:1915:3TD:H2'  | 24:1:1916:A:O4'  | 2.18                     | 0.43              |
| 25:3:106:G:H2'     | 25:3:107:G:O4'   | 2.18                     | 0.43              |
| 27:C:181:ASP:HB3   | 27:C:186:LEU:HB2 | 1.99                     | 0.43              |
| 56:G:65:ALA:HB1    | 56:G:135:HIS:HB2 | 1.99                     | 0.43              |
| 1:2:859:G:H2'      | 1:2:860:A:H8     | 1.83                     | 0.43              |
| 13:r:34:LEU:HD13   | 13:r:41:GLU:HA   | 2.00                     | 0.43              |
| 24:1:359:G:H2'     | 24:1:359:G:N3    | 2.33                     | 0.43              |
| 24:1:598:U:H2'     | 24:1:599:A:H8    | 1.83                     | 0.43              |
| 24:1:657:U:H2'     | 24:1:658:U:C6    | 2.53                     | 0.43              |
| 24:1:1414:C:H2'    | 24:1:1415:U:O4'  | 2.18                     | 0.43              |
| 24:1:1881:C:H2'    | 24:1:1882:U:O4'  | 2.18                     | 0.43              |
| 24:1:2151:U:H2'    | 24:1:2152:G:H8   | 1.83                     | 0.43              |
| 24:1:2461:A:H2'    | 24:1:2462:C:C6   | 2.54                     | 0.43              |
| 24:1:2838:G:H2'    | 24:1:2839:G:O4'  | 2.18                     | 0.43              |
| 38:Q:87:SER:HB2    | 39:R:51:VAL:HG23 | 1.99                     | 0.43              |
| 55:6:128:CYS:SG    | 55:6:183:ILE:HB  | 2.58                     | 0.43              |
| 1:2:545:C:OP1      | 4:i:58:LYS:NZ    | 2.51                     | 0.43              |
| 1:2:619:U:H3       | 4:i:131:ASN:HD21 | 1.67                     | 0.43              |
| 2:g:112:LYS:HE3    | 2:g:112:LYS:HB3  | 1.82                     | 0.43              |
| 17:v:45:HIS:HB2    | 17:v:70:THR:O    | 2.18                     | 0.43              |
| 17:v:58:VAL:HB     | 17:v:80:GLU:HB2  | 2.00                     | 0.43              |
| 24:1:1683:U:H2'    | 24:1:1684:G:C8   | 2.53                     | 0.43              |
| 24:1:1790:C:H2'    | 24:1:1791:A:C5   | 2.53                     | 0.43              |
| 24:1:2552:OMU:HM23 | 24:1:2554:U:C6   | 2.53                     | 0.43              |
| 25:3:2:G:H2'       | 25:3:3:C:C6      | 2.53                     | 0.43              |
| 45:X:39:TRP:CD1    | 56:G:32:PRO:HA   | 2.54                     | 0.43              |
| 55:6:322:GLN:HE21  | 55:6:322:GLN:HB3 | 1.54                     | 0.43              |
| 1:2:109:A:H5'      | 1:2:110:C:C5     | 2.54                     | 0.43              |
| 1:2:191:G:H2'      | 1:2:192:A:C8     | 2.53                     | 0.43              |
| 1:2:674:G:H21      | 11:p:118:HIS:HB2 | 1.83                     | 0.43              |
| 1:2:1009:U:H2'     | 1:2:1010:U:C6    | 2.54                     | 0.43              |
| 1:2:1017:U:H2'     | 1:2:1018:G:H8    | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:l:110:LYS:HE2  | 7:l:110:LYS:HB3  | 1.75                     | 0.43              |
| 24:1:594:U:H2'   | 24:1:595:C:H6    | 1.83                     | 0.43              |
| 24:1:739:A:N3    | 24:1:740:C:N4    | 2.54                     | 0.43              |
| 24:1:819:A:H5''  | 24:1:973:A:N1    | 2.32                     | 0.43              |
| 24:1:1731:G:C6   | 24:1:1733:G:C5   | 3.06                     | 0.43              |
| 24:1:2071:A:H2'  | 24:1:2072:C:C6   | 2.53                     | 0.43              |
| 24:1:2813:A:H2'  | 24:1:2814:A:H8   | 1.82                     | 0.43              |
| 39:R:41:ILE:HG22 | 39:R:43:ASN:HD21 | 1.84                     | 0.43              |
| 17:v:10:GLY:HA3  | 17:v:25:ILE:HD13 | 2.00                     | 0.43              |
| 22:4:25:A:H2'    | 22:4:26:A:H8     | 1.84                     | 0.43              |
| 24:1:271:G:O2'   | 24:1:272:A:O5'   | 2.34                     | 0.43              |
| 24:1:415:A:H2'   | 24:1:416:U:C6    | 2.53                     | 0.43              |
| 24:1:909:A:H2'   | 24:1:912:C:C5    | 2.53                     | 0.43              |
| 24:1:1278:C:H2'  | 24:1:1279:G:C8   | 2.53                     | 0.43              |
| 24:1:1883:U:H2'  | 24:1:1884:G:O4'  | 2.18                     | 0.43              |
| 24:1:2516:A:O2'  | 24:1:2517:C:H5'  | 2.18                     | 0.43              |
| 24:1:2834:G:H2'  | 24:1:2879:A:H61  | 1.83                     | 0.43              |
| 55:6:221:PHE:HZ  | 55:6:310:MET:HE2 | 1.84                     | 0.43              |
| 1:2:205:A:H2'    | 1:2:206:C:C6     | 2.54                     | 0.43              |
| 1:2:505:G:H2'    | 1:2:506:G:H8     | 1.84                     | 0.43              |
| 1:2:842:U:O3'    | 1:2:844:G:N2     | 2.51                     | 0.43              |
| 23:5:75[B]:C:OP1 | 24:1:2602:A:H5'' | 2.18                     | 0.43              |
| 24:1:6:A:H2'     | 24:1:7:G:H8      | 1.83                     | 0.43              |
| 24:1:477:A:H2'   | 24:1:478:A:C8    | 2.53                     | 0.43              |
| 24:1:1529:G:H2'  | 24:1:1530:G:C8   | 2.54                     | 0.43              |
| 24:1:1614:A:C2   | 40:S:93:ALA:HB2  | 2.54                     | 0.43              |
| 24:1:2897:U:H2'  | 24:1:2898:U:C6   | 2.53                     | 0.43              |
| 26:B:19:VAL:HG23 | 26:B:203:ARG:HB3 | 1.99                     | 0.43              |
| 26:B:145:GLU:HG2 | 26:B:151:GLY:C   | 2.44                     | 0.43              |
| 1:2:224:U:H2'    | 1:2:225:C:C6     | 2.53                     | 0.43              |
| 1:2:350:G:H2'    | 1:2:351:G:C8     | 2.53                     | 0.43              |
| 1:2:381:C:H2'    | 1:2:382:A:O4'    | 2.19                     | 0.43              |
| 1:2:451:A:O2'    | 58:2:1686:SPD:N1 | 2.52                     | 0.43              |
| 1:2:580:C:H2'    | 1:2:581:G:O4'    | 2.18                     | 0.43              |
| 1:2:1009:U:H2'   | 1:2:1010:U:H6    | 1.83                     | 0.43              |
| 1:2:1127:G:H5'   | 1:2:1280:A:O2'   | 2.18                     | 0.43              |
| 2:g:117:LEU:HD21 | 2:g:137:ARG:HB3  | 2.00                     | 0.43              |
| 24:1:191:A:H2'   | 24:1:192:C:H6    | 1.84                     | 0.43              |
| 24:1:227:A:C2    | 24:1:2407:A:H1'  | 2.53                     | 0.43              |
| 24:1:373:U:H2'   | 24:1:374:A:C8    | 2.53                     | 0.43              |
| 24:1:598:U:H2'   | 24:1:599:A:C8    | 2.54                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:1:1433:A:H2'  | 24:1:1434:A:C8    | 2.54                     | 0.43              |
| 24:1:2017:U:H4'  | 48:b:5:GLN:O      | 2.19                     | 0.43              |
| 24:1:2185:U:H2'  | 24:1:2186:G:N7    | 2.34                     | 0.43              |
| 34:M:127:LYS:HE2 | 34:M:127:LYS:HB2  | 1.84                     | 0.43              |
| 56:G:132:PHE:HE1 | 56:G:142:VAL:HB   | 1.83                     | 0.43              |
| 1:2:49:U:O2      | 1:2:362:G:H1'     | 2.19                     | 0.43              |
| 1:2:89:U:H2'     | 1:2:90:C:C6       | 2.54                     | 0.43              |
| 1:2:590:U:H2'    | 1:2:591:U:C6      | 2.53                     | 0.43              |
| 1:2:857:C:H2'    | 1:2:858:G:C8      | 2.52                     | 0.43              |
| 1:2:1326:U:H2'   | 1:2:1327:C:C6     | 2.54                     | 0.43              |
| 13:r:68:ASP:OD1  | 13:r:71:ARG:NH1   | 2.52                     | 0.43              |
| 24:1:413:C:H2'   | 24:1:414:C:C6     | 2.54                     | 0.43              |
| 24:1:967:U:H2'   | 24:1:968:C:C6     | 2.54                     | 0.43              |
| 24:1:1100:C:H2'  | 24:1:1101:U:O4'   | 2.19                     | 0.43              |
| 24:1:1322:A:C5   | 24:1:1323:C:C5    | 3.06                     | 0.43              |
| 25:3:49:C:H2'    | 25:3:50:A:C8      | 2.54                     | 0.43              |
| 48:b:43:ILE:HG22 | 48:b:49:TYR:HB2   | 2.00                     | 0.43              |
| 1:2:513:C:H2'    | 1:2:514:C:C6      | 2.54                     | 0.43              |
| 1:2:1002:G:C6    | 1:2:1039:G:C6     | 3.07                     | 0.43              |
| 24:1:28:A:H1'    | 24:1:513:A:C2     | 2.54                     | 0.43              |
| 24:1:634:C:H2'   | 24:1:635:C:H6     | 1.83                     | 0.43              |
| 24:1:720:U:H2'   | 24:1:721:A:C8     | 2.54                     | 0.43              |
| 24:1:933:A:H5'   | 24:1:934:U:OP2    | 2.19                     | 0.43              |
| 24:1:2705:A:H2'  | 24:1:2706:A:O4'   | 2.19                     | 0.43              |
| 43:V:72:VAL:HB   | 43:V:91:PHE:HB3   | 2.00                     | 0.43              |
| 53:a:12:ILE:HD13 | 53:a:32:LEU:HD23  | 2.01                     | 0.43              |
| 55:6:132:ILE:HB  | 55:6:179:VAL:HG12 | 2.00                     | 0.43              |
| 55:6:167:LYS:HG2 | 55:6:180:THR:HB   | 2.00                     | 0.43              |
| 55:6:202:VAL:HB  | 55:6:327:VAL:HG22 | 2.00                     | 0.43              |
| 56:G:135:HIS:HB3 | 56:G:138:VAL:HG12 | 2.01                     | 0.43              |
| 1:2:389:A:H3'    | 1:2:390:U:H6      | 1.84                     | 0.43              |
| 1:2:502:A:H2'    | 1:2:503:C:O4'     | 2.19                     | 0.43              |
| 1:2:1360:A:H2'   | 1:2:1361:G:C8     | 2.54                     | 0.43              |
| 24:1:297:G:H2'   | 24:1:298:G:O4'    | 2.18                     | 0.43              |
| 24:1:515:A:H1'   | 24:1:581:C:H1'    | 2.00                     | 0.43              |
| 24:1:645:C:H2'   | 24:1:647:G:N7     | 2.34                     | 0.43              |
| 24:1:706:A:H61   | 24:1:725:G:H1'    | 1.84                     | 0.43              |
| 24:1:881:G:H2'   | 24:1:882:G:H8     | 1.82                     | 0.43              |
| 24:1:1651:G:OP1  | 35:N:40:LYS:NZ    | 2.41                     | 0.43              |
| 24:1:2087:G:H2'  | 24:1:2088:A:H8    | 1.83                     | 0.43              |
| 24:1:2257:U:O2'  | 24:1:2258:C:H5'   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:1:2812:G:H2'  | 24:1:2813:A:C8    | 2.54                     | 0.43              |
| 32:K:71:ARG:HD3  | 32:K:71:ARG:HA    | 1.81                     | 0.43              |
| 55:6:206:PRO:HG2 | 55:6:207:PHE:CE1  | 2.54                     | 0.43              |
| 56:G:93:SER:HB2  | 56:G:123:ARG:NE   | 2.34                     | 0.43              |
| 1:2:266:G:H1'    | 1:2:268:U:OP2     | 2.19                     | 0.42              |
| 1:2:996:A:H2'    | 1:2:997:U:C6      | 2.54                     | 0.42              |
| 3:h:77:ILE:HA    | 3:h:84:VAL:CG2    | 2.48                     | 0.42              |
| 5:j:81:LEU:HB2   | 5:j:98:PRO:HG3    | 2.01                     | 0.42              |
| 22:4:30:G:H2'    | 22:4:31:G:H8      | 1.84                     | 0.42              |
| 24:1:639:U:H2'   | 24:1:640:C:H6     | 1.80                     | 0.42              |
| 24:1:766:U:H2'   | 24:1:767:U:C6     | 2.54                     | 0.42              |
| 24:1:1068:G:O6   | 24:1:1069:A:N6    | 2.51                     | 0.42              |
| 24:1:1183:U:H2'  | 24:1:1184:U:C6    | 2.54                     | 0.42              |
| 24:1:1540:G:C6   | 24:1:1541:C:C4    | 3.07                     | 0.42              |
| 1:2:552:U:H2'    | 1:2:553:A:H8      | 1.83                     | 0.42              |
| 1:2:994:A:C4     | 1:2:1216:A:H4'    | 2.53                     | 0.42              |
| 1:2:1010:U:H2'   | 1:2:1011:C:C6     | 2.55                     | 0.42              |
| 1:2:1206:G:C6    | 1:2:1207:2MG:C5   | 3.07                     | 0.42              |
| 1:2:1405:G:O2'   | 1:2:1518:MA6:O2'  | 2.34                     | 0.42              |
| 10:o:52:LEU:HB2  | 14:s:81:ARG:HD2   | 2.00                     | 0.42              |
| 19:x:80:TYR:CZ   | 19:x:82:GLY:HA2   | 2.54                     | 0.42              |
| 24:1:229:C:H2'   | 24:1:230:G:O4'    | 2.19                     | 0.42              |
| 24:1:833:A:H2'   | 24:1:834:G:H8     | 1.83                     | 0.42              |
| 24:1:1055:G:H2'  | 24:1:1056:G:H5'   | 2.00                     | 0.42              |
| 24:1:1428:C:C5   | 24:1:1569:A:H5''  | 2.54                     | 0.42              |
| 24:1:2728:U:O2'  | 24:1:2729:G:H8    | 2.02                     | 0.42              |
| 29:E:52:ASN:CB   | 29:E:150:ARG:HH22 | 2.32                     | 0.42              |
| 39:R:37:GLU:HB3  | 39:R:53:PHE:CE1   | 2.55                     | 0.42              |
| 1:2:646:G:H2'    | 1:2:647:C:C6      | 2.55                     | 0.42              |
| 1:2:1057:G:H2'   | 1:2:1058:G:O4'    | 2.19                     | 0.42              |
| 13:r:71:ARG:NH2  | 29:E:113:ASP:OD1  | 2.51                     | 0.42              |
| 13:r:71:ARG:NH2  | 29:E:115:ARG:HD3  | 2.34                     | 0.42              |
| 22:4:28:G:H2'    | 22:4:29:A:H8      | 1.84                     | 0.42              |
| 24:1:146:A:H2'   | 24:1:147:C:C6     | 2.53                     | 0.42              |
| 24:1:476:G:H4'   | 24:1:502:A:N1     | 2.34                     | 0.42              |
| 24:1:1224:U:H2'  | 24:1:1225:G:C8    | 2.54                     | 0.42              |
| 24:1:1281:G:H2'  | 24:1:1282:U:C6    | 2.55                     | 0.42              |
| 24:1:1365:A:OP1  | 45:X:3:ARG:NH1    | 2.41                     | 0.42              |
| 27:C:105:LYS:HD3 | 27:C:105:LYS:HA   | 1.79                     | 0.42              |
| 37:P:85:SER:OG   | 37:P:87:LYS:NZ    | 2.52                     | 0.42              |
| 1:2:767:A:H2'    | 1:2:768:A:O4'     | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1118:U:H2'   | 1:2:1119:C:C6     | 2.54                     | 0.42              |
| 6:k:44:ARG:HH21  | 6:k:56:LYS:NZ     | 2.18                     | 0.42              |
| 24:1:26:G:H1'    | 24:1:514:A:N6     | 2.34                     | 0.42              |
| 24:1:668:A:H2'   | 24:1:670:A:N6     | 2.34                     | 0.42              |
| 24:1:948:C:H1'   | 24:1:984:A:C8     | 2.54                     | 0.42              |
| 24:1:1263:U:O2'  | 48:b:8:PRO:HD2    | 2.19                     | 0.42              |
| 24:1:1935:G:H1'  | 24:1:1964:G:N2    | 2.34                     | 0.42              |
| 30:F:4:VAL:HG12  | 30:F:69:ARG:HG2   | 2.00                     | 0.42              |
| 32:K:107:LEU:HB2 | 32:K:116:ILE:HD11 | 2.02                     | 0.42              |
| 49:c:11:LEU:HB3  | 49:c:49:TYR:HB3   | 2.02                     | 0.42              |
| 51:e:26:HIS:NE2  | 51:e:48:ALA:HB2   | 2.33                     | 0.42              |
| 1:2:908:A:H2'    | 1:2:909:A:H8      | 1.85                     | 0.42              |
| 1:2:1179:A:H2'   | 1:2:1180:A:O4'    | 2.19                     | 0.42              |
| 1:2:1370:G:C2    | 1:2:1371:G:C8     | 3.07                     | 0.42              |
| 7:l:48:GLU:O     | 7:l:52:GLN:HG2    | 2.19                     | 0.42              |
| 9:n:47:VAL:HG13  | 9:n:80:ARG:HD3    | 2.02                     | 0.42              |
| 16:u:77:GLU:HA   | 16:u:81:ALA:HB2   | 2.01                     | 0.42              |
| 24:1:27:G:N2     | 24:1:512:G:H1'    | 2.35                     | 0.42              |
| 24:1:565:C:H2'   | 24:1:566:U:O4'    | 2.19                     | 0.42              |
| 24:1:948:C:H2'   | 24:1:949:G:H8     | 1.85                     | 0.42              |
| 24:1:1063:G:O2'  | 24:1:1064:C:C6    | 2.73                     | 0.42              |
| 24:1:1668:A:O2'  | 24:1:1674:G:N7    | 2.44                     | 0.42              |
| 24:1:1853:A:N1   | 24:1:2087:G:H1'   | 2.33                     | 0.42              |
| 24:1:2533:U:OP1  | 24:1:2665:A:O2'   | 2.33                     | 0.42              |
| 26:B:71:LYS:NZ   | 26:B:98:ASP:OD2   | 2.45                     | 0.42              |
| 35:N:35:LYS:HE3  | 35:N:100:CYS:SG   | 2.59                     | 0.42              |
| 37:P:53:ARG:HD3  | 37:P:53:ARG:HA    | 1.75                     | 0.42              |
| 55:6:40:GLU:O    | 55:6:46:VAL:HB    | 2.20                     | 0.42              |
| 55:6:154:ARG:NE  | 55:6:350:ASP:O    | 2.36                     | 0.42              |
| 24:1:64:A:H2'    | 24:1:65:U:H6      | 1.83                     | 0.42              |
| 24:1:2405:G:O2'  | 24:1:2411:A:N6    | 2.53                     | 0.42              |
| 55:6:73:MET:HE1  | 55:6:106:LEU:HG   | 2.01                     | 0.42              |
| 1:2:100:G:H2'    | 1:2:101:A:O4'     | 2.19                     | 0.42              |
| 1:2:113:G:H2'    | 1:2:114:U:H6      | 1.85                     | 0.42              |
| 1:2:552:U:C2     | 1:2:553:A:C8      | 3.08                     | 0.42              |
| 7:l:111:ARG:NH1  | 7:l:126:ASP:OD2   | 2.53                     | 0.42              |
| 8:m:90:ASP:OD1   | 8:m:91:GLU:HG3    | 2.20                     | 0.42              |
| 24:1:75:G:N3     | 24:1:75:G:H2'     | 2.33                     | 0.42              |
| 24:1:671:C:H2'   | 24:1:672:C:C6     | 2.54                     | 0.42              |
| 24:1:814:C:H2'   | 24:1:815:C:H6     | 1.84                     | 0.42              |
| 24:1:1636:U:H2'  | 24:1:1637:A:C8    | 2.54                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:1:2636:C:H2'   | 24:1:2637:U:C6     | 2.53                     | 0.42              |
| 24:1:2902:C:H3'   | 24:1:2903:U:H6     | 1.84                     | 0.42              |
| 28:D:46:GLN:O     | 28:D:88:ARG:NH2    | 2.52                     | 0.42              |
| 29:E:123:ASP:OD2  | 29:E:127:ASN:ND2   | 2.53                     | 0.42              |
| 34:M:75:GLU:HB2   | 34:M:90:GLU:HG3    | 2.01                     | 0.42              |
| 1:2:986:U:H2'     | 1:2:987:G:O4'      | 2.20                     | 0.42              |
| 1:2:1000:A:H2'    | 1:2:1001:C:C6      | 2.54                     | 0.42              |
| 1:2:1157:A:C2     | 1:2:1181:G:C4      | 3.08                     | 0.42              |
| 1:2:1323:G:H2'    | 1:2:1324:A:H8      | 1.80                     | 0.42              |
| 5:j:81:LEU:HD11   | 5:j:96:MET:HB3     | 2.00                     | 0.42              |
| 20:y:44:LYS:HD3   | 20:y:87:ALA:HA     | 2.01                     | 0.42              |
| 24:1:25:U:H5''    | 40:S:80:PRO:HD3    | 2.02                     | 0.42              |
| 24:1:1219:U:H2'   | 24:1:1220:G:C8     | 2.55                     | 0.42              |
| 24:1:2469:A:N6    | 24:1:2481:G:O2'    | 2.45                     | 0.42              |
| 24:1:2639:A:H2'   | 24:1:2640:G:O4'    | 2.19                     | 0.42              |
| 24:1:2700:A:H2'   | 24:1:2701:U:H6     | 1.84                     | 0.42              |
| 27:C:46:ARG:NH2   | 27:C:89:GLU:OE1    | 2.53                     | 0.42              |
| 31:J:31:GLU:OE2   | 31:J:34:ARG:NH1    | 2.53                     | 0.42              |
| 1:2:73:C:O2'      | 1:2:74:A:H8        | 2.02                     | 0.42              |
| 1:2:1160:G:C2     | 1:2:1161:C:C6      | 3.07                     | 0.42              |
| 58:2:1687:SPD:H71 | 58:2:1687:SPD:H101 | 1.64                     | 0.42              |
| 3:h:75:ILE:H      | 3:h:75:ILE:HG12    | 1.66                     | 0.42              |
| 6:k:32:ALA:CB     | 6:k:70:VAL:HG11    | 2.50                     | 0.42              |
| 8:m:7:ILE:O       | 8:m:11:LEU:HG      | 2.19                     | 0.42              |
| 8:m:94:LYS:HE2    | 8:m:94:LYS:HB3     | 1.93                     | 0.42              |
| 15:t:29:VAL:HG11  | 15:t:67:LEU:HD21   | 2.01                     | 0.42              |
| 23:5:26:G:H22     | 23:5:44:A:H2       | 1.68                     | 0.42              |
| 24:1:460:A:H2'    | 24:1:461:C:O4'     | 2.20                     | 0.42              |
| 24:1:493:G:O2'    | 40:S:7:HIS:HA      | 2.20                     | 0.42              |
| 24:1:547:A:H4'    | 24:1:548:G:O4'     | 2.20                     | 0.42              |
| 24:1:1932:A:H2'   | 24:1:1933:G:O4'    | 2.18                     | 0.42              |
| 28:D:136:GLN:HA   | 28:D:139:LYS:HE3   | 2.02                     | 0.42              |
| 1:2:466:A:C2      | 1:2:468:A:C4       | 3.08                     | 0.42              |
| 1:2:751:U:H2'     | 1:2:752:G:O4'      | 2.20                     | 0.42              |
| 1:2:864:A:H2'     | 1:2:865:A:C8       | 2.55                     | 0.42              |
| 1:2:901:A:C5      | 1:2:902:G:H1'      | 2.55                     | 0.42              |
| 1:2:1031:C:H4'    | 1:2:1032:G:N1      | 2.34                     | 0.42              |
| 1:2:1102:A:H2'    | 1:2:1103:C:C6      | 2.55                     | 0.42              |
| 1:2:1130:A:H2'    | 1:2:1131:G:C8      | 2.54                     | 0.42              |
| 24:1:208:C:H2'    | 24:1:209:C:C6      | 2.55                     | 0.42              |
| 24:1:1059:G:C2    | 24:1:1080:A:C2     | 3.08                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:1:1853:A:H2'   | 24:1:1854:A:C8    | 2.55                     | 0.42              |
| 24:1:2064:C:H2'   | 24:1:2065:C:H6    | 1.85                     | 0.42              |
| 24:1:2455:G:H2'   | 24:1:2456:C:H6    | 1.83                     | 0.42              |
| 40:S:28:LYS:HE2   | 40:S:28:LYS:HB3   | 1.87                     | 0.42              |
| 41:T:34:VAL:HG21  | 41:T:43:ILE:HD11  | 2.01                     | 0.42              |
| 55:6:166:ILE:HD11 | 55:6:182:LYS:HB2  | 2.01                     | 0.42              |
| 1:2:181:A:N6      | 1:2:195:A:C8      | 2.88                     | 0.41              |
| 1:2:642:A:C5      | 8:m:107:SER:HA    | 2.55                     | 0.41              |
| 1:2:918:A:H2'     | 1:2:919:A:C8      | 2.55                     | 0.41              |
| 1:2:1219:A:H2'    | 1:2:1220:G:C8     | 2.55                     | 0.41              |
| 1:2:1277:C:H1'    | 1:2:1282:C:O2     | 2.20                     | 0.41              |
| 1:2:1315:U:H2'    | 1:2:1316:G:O4'    | 2.19                     | 0.41              |
| 1:2:1402:4OC:H2'  | 1:2:1403:C:O4'    | 2.20                     | 0.41              |
| 2:g:81:LYS:HG3    | 2:g:91:PHE:CZ     | 2.55                     | 0.41              |
| 15:t:88:ARG:NH2   | 24:1:714:U:OP2    | 2.53                     | 0.41              |
| 24:1:282:A:C6     | 24:1:359:G:C6     | 3.08                     | 0.41              |
| 24:1:1588:G:H2'   | 24:1:1589:U:C6    | 2.55                     | 0.41              |
| 1:2:236:A:H2'     | 1:2:237:G:H8      | 1.84                     | 0.41              |
| 1:2:1151:A:O2'    | 1:2:1152:A:H8     | 2.03                     | 0.41              |
| 2:g:184:PHE:HA    | 2:g:198:PHE:HB2   | 2.02                     | 0.41              |
| 3:h:164:ARG:HB3   | 22:4:46:A:H2      | 1.85                     | 0.41              |
| 9:n:27:LYS:HE3    | 9:n:27:LYS:HB3    | 1.91                     | 0.41              |
| 17:v:19:LYS:HG2   | 17:v:47:HIS:CE1   | 2.55                     | 0.41              |
| 23:5:16:C:H3'     | 23:5:17:C:C6      | 2.55                     | 0.41              |
| 23:5:63:G:H2'     | 23:5:64:G:H8      | 1.85                     | 0.41              |
| 24:1:721:A:H2'    | 24:1:722:A:C8     | 2.55                     | 0.41              |
| 24:1:1062:G:C2    | 24:1:1063:G:C5    | 3.08                     | 0.41              |
| 24:1:1316:U:H2'   | 24:1:1317:G:C8    | 2.54                     | 0.41              |
| 24:1:2298:A:H2'   | 24:1:2299:U:O4'   | 2.20                     | 0.41              |
| 42:U:54:GLN:CD    | 42:U:54:GLN:H     | 2.26                     | 0.41              |
| 55:6:151:MET:SD   | 55:6:353:LEU:HD21 | 2.60                     | 0.41              |
| 55:6:333:ILE:HG13 | 55:6:345:THR:HG22 | 2.02                     | 0.41              |
| 1:2:34:C:H2'      | 1:2:35:G:C8       | 2.55                     | 0.41              |
| 1:2:165:G:H2'     | 1:2:166:U:C6      | 2.55                     | 0.41              |
| 1:2:346:G:OP1     | 37:P:39:ARG:NH1   | 2.30                     | 0.41              |
| 1:2:427:U:OP1     | 4:i:13:ARG:NH1    | 2.54                     | 0.41              |
| 1:2:678:U:H2'     | 1:2:679:C:C6      | 2.54                     | 0.41              |
| 1:2:1144:G:N2     | 1:2:1146:A:H62    | 2.18                     | 0.41              |
| 1:2:1326:U:H2'    | 1:2:1327:C:H6     | 1.85                     | 0.41              |
| 1:2:1399:C:O2     | 1:2:1502:A:N6     | 2.54                     | 0.41              |
| 2:g:61:ALA:CB     | 2:g:221:VAL:HG13  | 2.50                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:g:95:ARG:HG2  | 2:g:96:TRP:N     | 2.35                     | 0.41              |
| 3:h:123:GLN:NE2 | 3:h:136:ARG:HH21 | 2.18                     | 0.41              |
| 18:w:57:ARG:O   | 18:w:61:ARG:HG3  | 2.21                     | 0.41              |
| 24:1:56:A:H2'   | 24:1:57:C:O4'    | 2.20                     | 0.41              |
| 24:1:352:A:H2'  | 24:1:353:C:C6    | 2.55                     | 0.41              |
| 24:1:1077:A:N1  | 24:1:1088:A:H2'  | 2.35                     | 0.41              |
| 24:1:2680:U:O2' | 24:1:2681:C:H5'  | 2.20                     | 0.41              |
| 25:3:30:C:H2'   | 25:3:31:C:H5'    | 2.02                     | 0.41              |
| 29:E:33:LYS:HG2 | 29:E:157:THR:HB  | 2.02                     | 0.41              |
| 40:S:31:GLN:O   | 40:S:35:ILE:HG13 | 2.20                     | 0.41              |
| 1:2:66:A:H4'    | 1:2:173:U:C5     | 2.55                     | 0.41              |
| 1:2:458:U:H2'   | 1:2:459:A:H8     | 1.85                     | 0.41              |
| 1:2:459:A:C6    | 1:2:474:G:C6     | 3.08                     | 0.41              |
| 1:2:483:C:H2'   | 1:2:484:G:C8     | 2.56                     | 0.41              |
| 1:2:839:C:H2'   | 1:2:840:C:H6     | 1.86                     | 0.41              |
| 7:l:76:LYS:HE3  | 7:l:89:VAL:HG21  | 2.01                     | 0.41              |
| 8:m:50:LYS:HE3  | 8:m:50:LYS:HB2   | 1.69                     | 0.41              |
| 24:1:36:G:N3    | 24:1:450:G:O2'   | 2.52                     | 0.41              |
| 24:1:749:A:H4'  | 24:1:1271:G:N3   | 2.35                     | 0.41              |
| 24:1:1055:G:C2' | 24:1:1056:G:H5'  | 2.50                     | 0.41              |
| 24:1:1289:C:H2' | 24:1:1290:C:H6   | 1.85                     | 0.41              |
| 24:1:2357:G:N2  | 24:1:2360:G:OP2  | 2.42                     | 0.41              |
| 24:1:2458:G:O2' | 24:1:2460:U:O4   | 2.28                     | 0.41              |
| 25:3:42:C:O2'   | 29:E:63:GLN:HG2  | 2.20                     | 0.41              |
| 29:E:73:SER:OG  | 29:E:81:GLN:N    | 2.49                     | 0.41              |
| 34:M:47:GLU:OE2 | 34:M:50:ARG:NH2  | 2.29                     | 0.41              |
| 56:G:16:GLY:HA3 | 56:G:51:ARG:NH2  | 2.35                     | 0.41              |
| 1:2:159:G:H5'   | 1:2:160:A:OP2    | 2.21                     | 0.41              |
| 1:2:266:G:H3'   | 17:v:69:LYS:HB2  | 2.02                     | 0.41              |
| 1:2:592:G:H2'   | 1:2:593:U:C6     | 2.56                     | 0.41              |
| 1:2:676:A:H2'   | 1:2:677:U:H6     | 1.86                     | 0.41              |
| 1:2:1318:A:O2'  | 19:x:37:ARG:HD2  | 2.19                     | 0.41              |
| 1:2:1330:U:H2'  | 1:2:1331:G:O4'   | 2.21                     | 0.41              |
| 2:g:188:ASP:OD1 | 2:g:189:THR:N    | 2.44                     | 0.41              |
| 24:1:135:U:H5'  | 24:1:136:G:OP2   | 2.21                     | 0.41              |
| 24:1:876:C:H2'  | 24:1:877:A:O4'   | 2.19                     | 0.41              |
| 24:1:975:A:H1'  | 24:1:990:A:C2    | 2.55                     | 0.41              |
| 26:B:232:HIS:CG | 26:B:240:PHE:HE1 | 2.38                     | 0.41              |
| 35:N:24:MET:HE1 | 35:N:40:LYS:HD3  | 2.02                     | 0.41              |
| 35:N:47:VAL:O   | 35:N:51:LEU:HD23 | 2.21                     | 0.41              |
| 55:6:155:TRP:O  | 55:6:158:SER:OG  | 2.30                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2:255:G:C2      | 1:2:272:C:C2       | 3.09                     | 0.41              |
| 1:2:489:C:H2'     | 1:2:490:C:C6       | 2.55                     | 0.41              |
| 1:2:593:U:H3      | 1:2:646:G:H1       | 1.68                     | 0.41              |
| 1:2:790:A:H2'     | 1:2:791:G:C8       | 2.56                     | 0.41              |
| 1:2:1125:U:O2'    | 1:2:1126:U:O5'     | 2.34                     | 0.41              |
| 1:2:1125:U:C2     | 1:2:1127:G:C8      | 3.09                     | 0.41              |
| 1:2:1216:A:H5''   | 14:s:5:SER:HB3     | 2.02                     | 0.41              |
| 5:j:111:MET:HE2   | 5:j:111:MET:HB3    | 1.94                     | 0.41              |
| 22:4:34:U:H4'     | 22:4:35:U:H6       | 1.85                     | 0.41              |
| 23:5:18:G:N2      | 23:5:58:A:OP2      | 2.54                     | 0.41              |
| 24:1:579:G:O2'    | 24:1:2019:A:OP1    | 2.38                     | 0.41              |
| 24:1:1254:A:H5''  | 24:1:1255:U:H5''   | 2.03                     | 0.41              |
| 24:1:1427:A:H4'   | 24:1:1428:C:O4'    | 2.21                     | 0.41              |
| 24:1:2896:C:H2'   | 24:1:2897:U:C6     | 2.56                     | 0.41              |
| 1:2:334:C:H2'     | 1:2:335:C:H6       | 1.85                     | 0.41              |
| 1:2:976:G:OP2     | 1:2:1358:U:O2'     | 2.38                     | 0.41              |
| 1:2:1250:A:H2'    | 1:2:1251:A:C8      | 2.55                     | 0.41              |
| 1:2:1378:C:O2     | 7:l:76:LYS:NZ      | 2.36                     | 0.41              |
| 4:i:99:ASP:OD1    | 4:i:100:ASN:N      | 2.54                     | 0.41              |
| 17:v:19:LYS:HD2   | 17:v:49:GLU:O      | 2.21                     | 0.41              |
| 20:y:4:ILE:O      | 20:y:8:LYS:HG3     | 2.20                     | 0.41              |
| 24:1:930:G:H1'    | 47:Z:25:LEU:HD11   | 2.01                     | 0.41              |
| 24:1:1073:A:C6    | 24:1:1074:G:C5     | 3.08                     | 0.41              |
| 24:1:2226:C:H2'   | 24:1:2227:A:O4'    | 2.20                     | 0.41              |
| 24:1:2230:G:H2'   | 24:1:2231:U:C6     | 2.55                     | 0.41              |
| 24:1:2377:A:O2'   | 36:O:117:PHE:O     | 2.27                     | 0.41              |
| 25:3:111:U:H2'    | 25:3:112:G:H8      | 1.86                     | 0.41              |
| 28:D:168:ASP:HB2  | 28:D:183:PHE:CZ    | 2.56                     | 0.41              |
| 1:2:71:A:C2       | 1:2:72:A:C8        | 3.09                     | 0.41              |
| 1:2:182:A:C4      | 1:2:184:G:C8       | 3.09                     | 0.41              |
| 1:2:204:G:H3'     | 1:2:205:A:C8       | 2.53                     | 0.41              |
| 1:2:1072:G:H2'    | 1:2:1073:U:C6      | 2.55                     | 0.41              |
| 1:2:1352:C:H2'    | 1:2:1353:G:C8      | 2.55                     | 0.41              |
| 1:2:1412:C:H2'    | 1:2:1413:A:C8      | 2.55                     | 0.41              |
| 1:2:1510:C:H2'    | 1:2:1511:G:H8      | 1.86                     | 0.41              |
| 11:p:47:ALA:HB1   | 11:p:62:ALA:HB1    | 2.03                     | 0.41              |
| 24:1:194:G:H2'    | 24:1:195:A:O4'     | 2.20                     | 0.41              |
| 24:1:333:G:H4'    | 58:1:3207:SPD:H22  | 2.03                     | 0.41              |
| 24:1:396:G:OP2    | 45:X:10:LYS:NZ     | 2.45                     | 0.41              |
| 24:1:1231:U:H2'   | 24:1:1232:G:H8     | 1.86                     | 0.41              |
| 24:1:2251:OMG:H1' | 24:1:2251:OMG:HM23 | 1.62                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:K:66:LYS:HB3   | 32:K:66:LYS:HE2   | 1.77                     | 0.41              |
| 34:M:17:ASN:O     | 34:M:38:ARG:HD3   | 2.20                     | 0.41              |
| 36:O:80:GLU:O     | 36:O:84:GLU:HG2   | 2.20                     | 0.41              |
| 1:2:140:U:H2'     | 1:2:141:G:O4'     | 2.20                     | 0.41              |
| 1:2:160:A:H61     | 1:2:347:G:H1'     | 1.86                     | 0.41              |
| 1:2:410:G:H2'     | 1:2:429:U:C5      | 2.56                     | 0.41              |
| 1:2:471:U:H2'     | 1:2:472:U:C6      | 2.56                     | 0.41              |
| 1:2:486:U:H2'     | 1:2:487:A:H8      | 1.86                     | 0.41              |
| 1:2:798:U:H2'     | 1:2:799:G:O4'     | 2.21                     | 0.41              |
| 1:2:977:A:H1'     | 1:2:982:U:O4      | 2.21                     | 0.41              |
| 1:2:1086:U:H3     | 1:2:1099:G:H1     | 1.69                     | 0.41              |
| 1:2:1500:A:H5''   | 1:2:1508:A:H5''   | 2.01                     | 0.41              |
| 2:g:41:ILE:HG21   | 2:g:201:PRO:O     | 2.21                     | 0.41              |
| 4:i:102:VAL:HG13  | 4:i:107:PHE:HB2   | 2.02                     | 0.41              |
| 5:j:38:VAL:HG11   | 5:j:114:VAL:HG22  | 2.03                     | 0.41              |
| 12:q:46:ASN:ND2   | 12:q:89:D2T:SB    | 2.93                     | 0.41              |
| 15:t:3:LEU:HD12   | 15:t:3:LEU:HA     | 1.90                     | 0.41              |
| 23:5:9:G:N2       | 23:5:46:G:OP2     | 2.51                     | 0.41              |
| 24:1:150:U:H2'    | 24:1:151:C:H6     | 1.85                     | 0.41              |
| 24:1:157:C:H2'    | 24:1:158:U:O4'    | 2.21                     | 0.41              |
| 24:1:383:C:H41    | 24:1:386:G:P      | 2.44                     | 0.41              |
| 24:1:491:G:O6     | 40:S:49:LYS:NZ    | 2.44                     | 0.41              |
| 24:1:593:U:H2'    | 24:1:594:U:H6     | 1.82                     | 0.41              |
| 24:1:674:G:H2'    | 24:1:804:A:H61    | 1.85                     | 0.41              |
| 24:1:764:A:H5'    | 26:B:209:GLY:HA2  | 2.03                     | 0.41              |
| 24:1:820:A:H4'    | 24:1:836:G:H22    | 1.86                     | 0.41              |
| 24:1:1048:A:N7    | 24:1:1111:A:C6    | 2.89                     | 0.41              |
| 24:1:1452:G:N3    | 24:1:1452:G:H5''  | 2.36                     | 0.41              |
| 24:1:2063:C:O2    | 24:1:2450:A:N1    | 2.54                     | 0.41              |
| 24:1:2155:U:H2'   | 24:1:2156:G:C8    | 2.56                     | 0.41              |
| 24:1:2345:G:N3    | 24:1:2381:A:H2'   | 2.36                     | 0.41              |
| 24:1:2658:C:OP1   | 30:F:158:LYS:NZ   | 2.47                     | 0.41              |
| 25:3:42:C:C6      | 29:E:66:LEU:HB2   | 2.56                     | 0.41              |
| 26:B:155:ALA:HB2  | 26:B:162:VAL:HG23 | 2.03                     | 0.41              |
| 28:D:118:LEU:HD11 | 28:D:188:MET:SD   | 2.61                     | 0.41              |
| 37:P:29:LYS:HB3   | 37:P:40:LEU:HD23  | 2.03                     | 0.41              |
| 55:6:152:TYR:OH   | 55:6:195:GLU:OE1  | 2.34                     | 0.41              |
| 1:2:79:G:H1       | 1:2:90:C:H42      | 1.69                     | 0.41              |
| 1:2:201:G:H2'     | 1:2:202:G:O4'     | 2.21                     | 0.41              |
| 1:2:276:G:OP1     | 17:v:14:SER:OG    | 2.32                     | 0.41              |
| 1:2:824:G:H2'     | 1:2:825:A:H8      | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1120:C:C2    | 1:2:1121:U:C5    | 3.09                     | 0.41              |
| 1:2:1292:G:H2'   | 1:2:1293:C:C6    | 2.56                     | 0.41              |
| 10:o:10:LEU:HD22 | 10:o:98:VAL:HG22 | 2.02                     | 0.41              |
| 14:s:24:ARG:NH1  | 14:s:55:SER:OG   | 2.54                     | 0.41              |
| 16:u:8:ARG:O     | 16:u:9:HIS:ND1   | 2.54                     | 0.41              |
| 24:1:30:G:H2'    | 24:1:31:C:H6     | 1.84                     | 0.41              |
| 24:1:304:U:H2'   | 24:1:305:C:C6    | 2.56                     | 0.41              |
| 24:1:813:U:H2'   | 24:1:814:C:H6    | 1.86                     | 0.41              |
| 24:1:822:G:H2'   | 24:1:823:C:C6    | 2.56                     | 0.41              |
| 24:1:1064:C:O2'  | 24:1:1065:U:H6   | 2.04                     | 0.41              |
| 24:1:1067:A:N1   | 55:6:54:GLN:HG2  | 2.35                     | 0.41              |
| 24:1:1282:U:H2'  | 24:1:1283:G:O4'  | 2.20                     | 0.41              |
| 24:1:1936:A:H61  | 24:1:1963:U:H3   | 1.68                     | 0.41              |
| 24:1:2323:G:O2'  | 24:1:2324:U:H5'  | 2.20                     | 0.41              |
| 24:1:2820:A:N3   | 24:1:2820:A:H2'  | 2.36                     | 0.41              |
| 25:3:24:G:N7     | 25:3:56:G:H2'    | 2.36                     | 0.41              |
| 25:3:79:G:O6     | 43:V:14:LYS:NZ   | 2.48                     | 0.41              |
| 60:C:301:PUT:H11 | 60:C:301:PUT:H42 | 1.61                     | 0.41              |
| 55:6:153:LEU:O   | 55:6:157:GLU:HG2 | 2.21                     | 0.41              |
| 1:2:1005:A:H8    | 1:2:1005:A:O5'   | 2.05                     | 0.40              |
| 1:2:1478:U:H2'   | 1:2:1479:C:C6    | 2.56                     | 0.40              |
| 2:g:42:ASN:HD22  | 2:g:45:LYS:HG2   | 1.86                     | 0.40              |
| 2:g:101:LEU:HB3  | 2:g:179:LEU:HD12 | 2.03                     | 0.40              |
| 4:i:101:VAL:HG12 | 4:i:105:MET:HE2  | 2.03                     | 0.40              |
| 5:j:77:ASN:HB2   | 5:j:82:GLN:CD    | 2.46                     | 0.40              |
| 16:u:9:HIS:HD2   | 16:u:18:GLN:HG3  | 1.86                     | 0.40              |
| 23:5:58:A:O2'    | 23:5:60:U:OP2    | 2.38                     | 0.40              |
| 24:1:65:U:H2'    | 24:1:66:C:H6     | 1.86                     | 0.40              |
| 24:1:207:A:H2'   | 24:1:208:C:O4'   | 2.21                     | 0.40              |
| 24:1:682:G:H5'   | 50:d:26:ASN:CG   | 2.46                     | 0.40              |
| 24:1:984:A:N3    | 24:1:984:A:H2'   | 2.36                     | 0.40              |
| 24:1:1073:A:N6   | 24:1:1074:G:C6   | 2.89                     | 0.40              |
| 24:1:1558:C:H4'  | 24:1:1559:U:O5'  | 2.20                     | 0.40              |
| 24:1:1993:U:H4'  | 27:C:133:THR:OG1 | 2.21                     | 0.40              |
| 24:1:2047:C:H2'  | 24:1:2048:G:H8   | 1.86                     | 0.40              |
| 24:1:2467:C:H2'  | 24:1:2468:A:O4'  | 2.21                     | 0.40              |
| 33:L:144:GLU:N   | 33:L:144:GLU:OE1 | 2.54                     | 0.40              |
| 42:U:48:PRO:HB3  | 42:U:54:GLN:O    | 2.21                     | 0.40              |
| 49:c:30:LYS:HA   | 49:c:30:LYS:HD3  | 1.89                     | 0.40              |
| 1:2:406:G:H8     | 1:2:406:G:OP2    | 2.05                     | 0.40              |
| 1:2:407:U:H2'    | 1:2:408:A:H8     | 1.87                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:821:G:H2'    | 1:2:822:U:C6      | 2.55                     | 0.40              |
| 2:g:186:ILE:HD13 | 2:g:200:ILE:HB    | 2.03                     | 0.40              |
| 5:j:162:GLU:H    | 5:j:162:GLU:CD    | 2.28                     | 0.40              |
| 7:l:106:GLU:O    | 7:l:110:LYS:HG2   | 2.21                     | 0.40              |
| 24:1:248:G:O5'   | 24:1:249:C:H5''   | 2.21                     | 0.40              |
| 24:1:538:A:H2'   | 24:1:539:G:O4'    | 2.21                     | 0.40              |
| 24:1:1056:G:N2   | 24:1:1104:C:N4    | 2.70                     | 0.40              |
| 24:1:1065:U:O2'  | 24:1:1066:U:O5'   | 2.30                     | 0.40              |
| 24:1:1464:G:H2'  | 24:1:1465:G:C8    | 2.56                     | 0.40              |
| 24:1:2087:G:H2'  | 24:1:2088:A:C8    | 2.55                     | 0.40              |
| 24:1:2602:A:N7   | 55:6:278:ARG:HD3  | 2.36                     | 0.40              |
| 42:U:33:LYS:HB3  | 42:U:64:ALA:HB1   | 2.02                     | 0.40              |
| 51:e:14:PHE:O    | 51:e:15:LYS:HD2   | 2.21                     | 0.40              |
| 1:2:215:C:O2'    | 1:2:465:A:N7      | 2.53                     | 0.40              |
| 1:2:554:A:H2'    | 1:2:555:U:H6      | 1.87                     | 0.40              |
| 1:2:1121:U:H2'   | 1:2:1122:U:C6     | 2.57                     | 0.40              |
| 13:r:27:LYS:HE2  | 13:r:27:LYS:HB2   | 1.88                     | 0.40              |
| 23:5:17:C:H5'    | 23:5:61:C:OP1     | 2.21                     | 0.40              |
| 24:1:27:G:O2'    | 24:1:28:A:OP2     | 2.34                     | 0.40              |
| 24:1:128:C:H2'   | 24:1:129:C:C6     | 2.56                     | 0.40              |
| 24:1:286:U:O2    | 24:1:354:A:H2     | 2.04                     | 0.40              |
| 24:1:493:G:H2'   | 24:1:494:G:O4'    | 2.21                     | 0.40              |
| 24:1:1001:A:H2'  | 24:1:1002:G:O4'   | 2.21                     | 0.40              |
| 24:1:2100:G:H2'  | 24:1:2101:A:O4'   | 2.21                     | 0.40              |
| 24:1:2259:U:OP1  | 60:1:3325:PUT:H42 | 2.22                     | 0.40              |
| 24:1:2314:A:H2'  | 24:1:2315:G:C8    | 2.56                     | 0.40              |
| 26:B:43:ARG:NH2  | 26:B:49:ILE:HD11  | 2.36                     | 0.40              |
| 34:M:54:THR:HG22 | 34:M:59:ARG:HG2   | 2.03                     | 0.40              |
| 36:O:60:GLU:HG3  | 36:O:61:GLN:HG2   | 2.02                     | 0.40              |
| 1:2:76:G:H2'     | 1:2:77:A:H8       | 1.83                     | 0.40              |
| 1:2:1070:U:H2'   | 1:2:1071:C:C6     | 2.56                     | 0.40              |
| 24:1:299:A:H2'   | 24:1:300:A:C8     | 2.57                     | 0.40              |
| 24:1:349:U:H2'   | 24:1:350:G:C8     | 2.56                     | 0.40              |
| 24:1:439:A:H2'   | 24:1:440:C:C6     | 2.56                     | 0.40              |
| 24:1:479:A:N3    | 24:1:481:G:H5''   | 2.36                     | 0.40              |
| 24:1:852:U:H2'   | 24:1:853:C:C6     | 2.56                     | 0.40              |
| 24:1:1197:G:H2'  | 24:1:1198:U:C6    | 2.56                     | 0.40              |
| 24:1:1318:U:H2'  | 24:1:1319:C:C6    | 2.56                     | 0.40              |
| 24:1:1529:G:H2'  | 24:1:1530:G:H8    | 1.87                     | 0.40              |
| 24:1:1599:U:H2'  | 24:1:1600:C:C6    | 2.57                     | 0.40              |
| 24:1:1637:A:H5'  | 24:1:1760:C:O2'   | 2.22                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:1:2070:A:H2'  | 24:1:2071:A:C8    | 2.56                     | 0.40              |
| 24:1:2330:G:H21  | 44:W:42:GLY:HA2   | 1.86                     | 0.40              |
| 24:1:2861:U:H2'  | 24:1:2862:G:H8    | 1.85                     | 0.40              |
| 31:J:36:LEU:O    | 31:J:51:GLY:HA3   | 2.22                     | 0.40              |
| 37:P:31:TRP:CD2  | 37:P:38:LYS:HE2   | 2.56                     | 0.40              |
| 37:P:114:LEU:HA  | 37:P:114:LEU:HD23 | 1.85                     | 0.40              |
| 38:Q:83:LEU:HD23 | 38:Q:83:LEU:HA    | 1.91                     | 0.40              |
| 39:R:29:THR:O    | 39:R:29:THR:HG22  | 2.22                     | 0.40              |
| 39:R:58:VAL:HG12 | 39:R:102:SER:OG   | 2.20                     | 0.40              |
| 1:2:601:G:H2'    | 1:2:602:A:H8      | 1.85                     | 0.40              |
| 1:2:920:U:H2'    | 1:2:921:U:C6      | 2.56                     | 0.40              |
| 1:2:1002:G:C4    | 1:2:1003:G:C8     | 3.10                     | 0.40              |
| 1:2:1414:U:H2'   | 1:2:1415:G:H8     | 1.86                     | 0.40              |
| 1:2:1446:A:H8    | 1:2:1446:A:OP1    | 2.05                     | 0.40              |
| 9:n:7:TYR:CG     | 9:n:8:GLY:N       | 2.90                     | 0.40              |
| 23:5:19:G:N2     | 23:5:57:A:H1'     | 2.37                     | 0.40              |
| 24:1:279:A:H1'   | 24:1:362:A:H4'    | 2.03                     | 0.40              |
| 24:1:601:C:O2'   | 24:1:605:G:H5''   | 2.20                     | 0.40              |
| 24:1:1733:G:H2'  | 24:1:1734:G:H8    | 1.86                     | 0.40              |
| 24:1:1957:C:H5'  | 24:1:1984:G:O2'   | 2.22                     | 0.40              |
| 24:1:2266:A:H4'  | 24:1:2267:A:N3    | 2.36                     | 0.40              |
| 24:1:2282:G:H4'  | 24:1:2389:G:O2'   | 2.22                     | 0.40              |
| 24:1:2305:U:H2'  | 24:1:2306:C:C6    | 2.57                     | 0.40              |
| 24:1:2583:G:H2'  | 24:1:2584:U:O4'   | 2.22                     | 0.40              |
| 31:J:4:PHE:O     | 38:Q:64:ARG:NH1   | 2.53                     | 0.40              |
| 32:K:17:ARG:HA   | 32:K:17:ARG:HD3   | 1.80                     | 0.40              |
| 33:L:78:ARG:HG2  | 33:L:113:ALA:HB3  | 2.03                     | 0.40              |
| 35:N:38:LEU:HB3  | 35:N:39:PRO:HD3   | 2.04                     | 0.40              |
| 54:I:82:ALA:HB2  | 54:I:108:ILE:HD11 | 2.04                     | 0.40              |
| 55:6:137:GLY:H   | 55:6:141:ALA:HB2  | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | g     | 222/241 (92%) | 217 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 3   | h     | 208/233 (89%) | 205 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 4   | i     | 203/206 (98%) | 201 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 5   | j     | 154/167 (92%) | 150 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 6   | k     | 101/135 (75%) | 100 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 7   | l     | 152/179 (85%) | 146 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 8   | m     | 127/130 (98%) | 123 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 9   | n     | 125/130 (96%) | 123 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 10  | o     | 96/103 (93%)  | 93 (97%)  | 2 (2%)  | 1 (1%)   | 12          | 35  |
| 11  | p     | 113/129 (88%) | 111 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 12  | q     | 120/124 (97%) | 116 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 13  | r     | 113/118 (96%) | 108 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 14  | s     | 98/101 (97%)  | 97 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 15  | t     | 86/89 (97%)   | 84 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 16  | u     | 79/82 (96%)   | 76 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 17  | v     | 77/84 (92%)   | 76 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 18  | w     | 64/75 (85%)   | 64 (100%) | 0       | 0        | 100         | 100 |
| 19  | x     | 82/92 (89%)   | 82 (100%) | 0       | 0        | 100         | 100 |
| 20  | y     | 84/87 (97%)   | 84 (100%) | 0       | 0        | 100         | 100 |
| 21  | z     | 68/71 (96%)   | 67 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 26  | B     | 269/273 (98%) | 266 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 27  | C     | 206/209 (99%) | 200 (97%) | 5 (2%)  | 1 (0%)   | 24          | 52  |
| 28  | D     | 199/201 (99%) | 194 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 29  | E     | 175/179 (98%) | 166 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 30  | F     | 173/177 (98%) | 166 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 31  | J     | 140/142 (99%) | 139 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 32  | K     | 121/123 (98%) | 119 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 33  | L     | 142/144 (99%) | 140 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 34  | M     | 132/136 (97%) | 129 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 35  | N     | 116/127 (91%) | 111 (96%) | 5 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 36  | O     | 114/117 (97%)   | 112 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 37  | P     | 112/115 (97%)   | 109 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 38  | Q     | 115/118 (98%)   | 115 (100%) | 0        | 0        | 100         | 100 |
| 39  | R     | 101/103 (98%)   | 98 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 40  | S     | 108/110 (98%)   | 106 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 41  | T     | 91/100 (91%)    | 86 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 42  | U     | 100/104 (96%)   | 98 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 43  | V     | 92/94 (98%)     | 90 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 44  | W     | 74/85 (87%)     | 72 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 45  | X     | 75/78 (96%)     | 75 (100%)  | 0        | 0        | 100         | 100 |
| 46  | Y     | 60/63 (95%)     | 59 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 47  | Z     | 56/59 (95%)     | 53 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 48  | b     | 54/57 (95%)     | 53 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 49  | c     | 49/55 (89%)     | 49 (100%)  | 0        | 0        | 100         | 100 |
| 50  | d     | 44/46 (96%)     | 44 (100%)  | 0        | 0        | 100         | 100 |
| 51  | e     | 62/65 (95%)     | 61 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 52  | f     | 36/38 (95%)     | 36 (100%)  | 0        | 0        | 100         | 100 |
| 53  | a     | 56/70 (80%)     | 54 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 54  | I     | 66/142 (46%)    | 65 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 55  | 6     | 358/365 (98%)   | 352 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 56  | G     | 147/149 (99%)   | 136 (92%)  | 10 (7%)  | 1 (1%)   | 18          | 44  |
| All | All   | 6015/6420 (94%) | 5876 (98%) | 136 (2%) | 3 (0%)   | 100         | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | o     | 57  | VAL  |
| 27  | C     | 149 | ASN  |
| 56  | G     | 76  | GLU  |

### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | g     | 186/199 (94%)  | 180 (97%)  | 6 (3%)   | 34          | 67  |
| 3   | h     | 172/190 (90%)  | 166 (96%)  | 6 (4%)   | 32          | 64  |
| 4   | i     | 172/173 (99%)  | 170 (99%)  | 2 (1%)   | 63          | 84  |
| 5   | j     | 119/126 (94%)  | 118 (99%)  | 1 (1%)   | 73          | 89  |
| 6   | k     | 90/116 (78%)   | 86 (96%)   | 4 (4%)   | 25          | 56  |
| 7   | l     | 127/147 (86%)  | 126 (99%)  | 1 (1%)   | 73          | 89  |
| 8   | m     | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 9   | n     | 105/107 (98%)  | 105 (100%) | 0        | 100         | 100 |
| 10  | o     | 86/90 (96%)    | 85 (99%)   | 1 (1%)   | 63          | 84  |
| 11  | p     | 89/98 (91%)    | 89 (100%)  | 0        | 100         | 100 |
| 12  | q     | 102/103 (99%)  | 101 (99%)  | 1 (1%)   | 68          | 86  |
| 13  | r     | 93/96 (97%)    | 93 (100%)  | 0        | 100         | 100 |
| 14  | s     | 83/84 (99%)    | 83 (100%)  | 0        | 100         | 100 |
| 15  | t     | 76/77 (99%)    | 76 (100%)  | 0        | 100         | 100 |
| 16  | u     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 17  | v     | 73/78 (94%)    | 69 (94%)   | 4 (6%)   | 19          | 47  |
| 18  | w     | 57/65 (88%)    | 57 (100%)  | 0        | 100         | 100 |
| 19  | x     | 72/79 (91%)    | 72 (100%)  | 0        | 100         | 100 |
| 20  | y     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 21  | z     | 60/61 (98%)    | 58 (97%)   | 2 (3%)   | 33          | 66  |
| 26  | B     | 216/218 (99%)  | 213 (99%)  | 3 (1%)   | 59          | 82  |
| 27  | C     | 163/163 (100%) | 160 (98%)  | 3 (2%)   | 51          | 79  |
| 28  | D     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 29  | E     | 148/150 (99%)  | 148 (100%) | 0        | 100         | 100 |
| 30  | F     | 136/138 (99%)  | 133 (98%)  | 3 (2%)   | 45          | 75  |
| 31  | J     | 116/116 (100%) | 115 (99%)  | 1 (1%)   | 70          | 87  |
| 32  | K     | 104/104 (100%) | 103 (99%)  | 1 (1%)   | 68          | 86  |
| 33  | L     | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 68          | 86  |
| 34  | M     | 107/107 (100%) | 103 (96%)  | 4 (4%)   | 30          | 62  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 35  | N     | 98/103 (95%)    | 96 (98%)   | 2 (2%)   | 48          | 77  |
| 36  | O     | 86/87 (99%)     | 85 (99%)   | 1 (1%)   | 63          | 84  |
| 37  | P     | 99/100 (99%)    | 99 (100%)  | 0        | 100         | 100 |
| 38  | Q     | 89/90 (99%)     | 89 (100%)  | 0        | 100         | 100 |
| 39  | R     | 84/84 (100%)    | 80 (95%)   | 4 (5%)   | 23          | 53  |
| 40  | S     | 93/93 (100%)    | 93 (100%)  | 0        | 100         | 100 |
| 41  | T     | 80/84 (95%)     | 78 (98%)   | 2 (2%)   | 42          | 73  |
| 42  | U     | 83/85 (98%)     | 80 (96%)   | 3 (4%)   | 31          | 63  |
| 43  | V     | 78/78 (100%)    | 76 (97%)   | 2 (3%)   | 40          | 72  |
| 44  | W     | 58/63 (92%)     | 56 (97%)   | 2 (3%)   | 32          | 65  |
| 45  | X     | 67/68 (98%)     | 65 (97%)   | 2 (3%)   | 36          | 69  |
| 46  | Y     | 54/55 (98%)     | 53 (98%)   | 1 (2%)   | 50          | 78  |
| 47  | Z     | 48/49 (98%)     | 48 (100%)  | 0        | 100         | 100 |
| 48  | b     | 47/48 (98%)     | 47 (100%)  | 0        | 100         | 100 |
| 49  | c     | 46/49 (94%)     | 45 (98%)   | 1 (2%)   | 45          | 75  |
| 50  | d     | 38/38 (100%)    | 38 (100%)  | 0        | 100         | 100 |
| 51  | e     | 51/52 (98%)     | 50 (98%)   | 1 (2%)   | 48          | 77  |
| 52  | f     | 34/34 (100%)    | 34 (100%)  | 0        | 100         | 100 |
| 53  | a     | 55/62 (89%)     | 54 (98%)   | 1 (2%)   | 51          | 79  |
| 54  | I     | 50/110 (46%)    | 49 (98%)   | 1 (2%)   | 48          | 77  |
| 55  | 6     | 305/310 (98%)   | 299 (98%)  | 6 (2%)   | 48          | 77  |
| 56  | G     | 114/114 (100%)  | 111 (97%)  | 3 (3%)   | 40          | 72  |
| All | All   | 5011/5245 (96%) | 4935 (98%) | 76 (2%)  | 55          | 81  |

All (76) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | g     | 6   | MET  |
| 2   | g     | 117 | LEU  |
| 2   | g     | 129 | LEU  |
| 2   | g     | 135 | LEU  |
| 2   | g     | 152 | LYS  |
| 2   | g     | 203 | ASN  |
| 3   | h     | 75  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | h     | 80  | LYS  |
| 3   | h     | 82  | GLU  |
| 3   | h     | 107 | ARG  |
| 3   | h     | 178 | LEU  |
| 3   | h     | 208 | LEU  |
| 4   | i     | 34  | ILE  |
| 4   | i     | 206 | LYS  |
| 5   | j     | 164 | ILE  |
| 6   | k     | 68  | GLN  |
| 6   | k     | 74  | LEU  |
| 6   | k     | 93  | LYS  |
| 6   | k     | 102 | MET  |
| 7   | l     | 6   | VAL  |
| 10  | o     | 90  | LEU  |
| 12  | q     | 97  | THR  |
| 17  | v     | 19  | LYS  |
| 17  | v     | 42  | THR  |
| 17  | v     | 57  | ASP  |
| 17  | v     | 60  | GLU  |
| 21  | z     | 3   | VAL  |
| 21  | z     | 33  | ARG  |
| 26  | B     | 153 | GLN  |
| 26  | B     | 239 | ASN  |
| 26  | B     | 242 | LYS  |
| 27  | C     | 12  | THR  |
| 27  | C     | 32  | ASN  |
| 27  | C     | 130 | GLN  |
| 30  | F     | 11  | VAL  |
| 30  | F     | 168 | VAL  |
| 30  | F     | 176 | LYS  |
| 31  | J     | 9   | GLU  |
| 32  | K     | 76  | VAL  |
| 33  | L     | 93  | ASN  |
| 34  | M     | 7   | THR  |
| 34  | M     | 14  | LYS  |
| 34  | M     | 51  | ARG  |
| 34  | M     | 135 | VAL  |
| 35  | N     | 65  | LEU  |
| 35  | N     | 72  | ASP  |
| 36  | O     | 85  | LYS  |
| 39  | R     | 6   | GLN  |
| 39  | R     | 47  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | R     | 48  | LYS  |
| 39  | R     | 51  | VAL  |
| 41  | T     | 68  | LYS  |
| 41  | T     | 69  | ARG  |
| 42  | U     | 15  | THR  |
| 42  | U     | 49  | VAL  |
| 42  | U     | 59  | VAL  |
| 43  | V     | 61  | LEU  |
| 43  | V     | 65  | VAL  |
| 44  | W     | 44  | LYS  |
| 44  | W     | 70  | GLU  |
| 45  | X     | 40  | VAL  |
| 45  | X     | 54  | LYS  |
| 46  | Y     | 14  | LEU  |
| 49  | c     | 54  | ILE  |
| 51  | e     | 31  | HIS  |
| 53  | a     | 28  | VAL  |
| 54  | I     | 78  | LEU  |
| 55  | 6     | 114 | GLU  |
| 55  | 6     | 167 | LYS  |
| 55  | 6     | 216 | SER  |
| 55  | 6     | 256 | ARG  |
| 55  | 6     | 273 | GLN  |
| 55  | 6     | 322 | GLN  |
| 56  | G     | 108 | VAL  |
| 56  | G     | 134 | VAL  |
| 56  | G     | 142 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | g     | 109 | GLN  |
| 2   | g     | 203 | ASN  |
| 3   | h     | 100 | GLN  |
| 3   | h     | 102 | ASN  |
| 3   | h     | 139 | GLN  |
| 3   | h     | 176 | HIS  |
| 3   | h     | 190 | HIS  |
| 4   | i     | 131 | ASN  |
| 4   | i     | 198 | HIS  |
| 5   | j     | 146 | ASN  |
| 7   | l     | 68  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | l     | 86  | GLN  |
| 8   | m     | 67  | GLN  |
| 9   | n     | 32  | GLN  |
| 9   | n     | 110 | GLN  |
| 10  | o     | 56  | HIS  |
| 10  | o     | 58  | ASN  |
| 11  | p     | 38  | GLN  |
| 14  | s     | 4   | GLN  |
| 14  | s     | 60  | GLN  |
| 14  | s     | 66  | GLN  |
| 15  | t     | 35  | GLN  |
| 17  | v     | 51  | ASN  |
| 19  | x     | 14  | HIS  |
| 19  | x     | 56  | GLN  |
| 19  | x     | 83  | HIS  |
| 20  | y     | 13  | GLN  |
| 20  | y     | 48  | GLN  |
| 26  | B     | 90  | ASN  |
| 26  | B     | 117 | GLN  |
| 27  | C     | 32  | ASN  |
| 28  | D     | 9   | GLN  |
| 28  | D     | 115 | GLN  |
| 30  | F     | 45  | HIS  |
| 31  | J     | 58  | ASN  |
| 31  | J     | 76  | HIS  |
| 31  | J     | 128 | ASN  |
| 32  | K     | 93  | GLN  |
| 34  | M     | 13  | HIS  |
| 35  | N     | 18  | GLN  |
| 35  | N     | 31  | HIS  |
| 35  | N     | 73  | ASN  |
| 36  | O     | 116 | GLN  |
| 37  | P     | 52  | ASN  |
| 37  | P     | 66  | ASN  |
| 38  | Q     | 44  | GLN  |
| 38  | Q     | 81  | ASN  |
| 39  | R     | 6   | GLN  |
| 39  | R     | 12  | HIS  |
| 39  | R     | 66  | HIS  |
| 40  | S     | 40  | ASN  |
| 42  | U     | 53  | ASN  |
| 43  | V     | 49  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | W     | 12  | ASN  |
| 44  | W     | 57  | HIS  |
| 46  | Y     | 27  | ASN  |
| 46  | Y     | 39  | GLN  |
| 46  | Y     | 58  | ASN  |
| 50  | d     | 26  | ASN  |
| 53  | a     | 30  | HIS  |
| 53  | a     | 33  | ASN  |
| 53  | a     | 65  | ASN  |
| 55  | 6     | 255 | ASN  |
| 55  | 6     | 275 | GLN  |
| 55  | 6     | 280 | GLN  |
| 55  | 6     | 290 | GLN  |
| 55  | 6     | 322 | GLN  |
| 56  | G     | 66  | ASN  |
| 56  | G     | 119 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 2     | 1534/1542 (99%) | 223 (14%)         | 5 (0%)          |
| 22  | 4     | 25/49 (51%)     | 7 (28%)           | 1 (4%)          |
| 23  | 5     | 73/76 (96%)     | 28 (38%)          | 0               |
| 24  | 1     | 2897/2904 (99%) | 470 (16%)         | 7 (0%)          |
| 25  | 3     | 118/120 (98%)   | 14 (11%)          | 0               |
| All | All   | 4647/4691 (99%) | 742 (15%)         | 13 (0%)         |

All (742) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 2   | A    |
| 1   | 2     | 7   | A    |
| 1   | 2     | 9   | G    |
| 1   | 2     | 22  | G    |
| 1   | 2     | 32  | A    |
| 1   | 2     | 39  | G    |
| 1   | 2     | 47  | C    |
| 1   | 2     | 48  | C    |
| 1   | 2     | 50  | A    |
| 1   | 2     | 51  | A    |
| 1   | 2     | 64  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 65  | A    |
| 1   | 2     | 71  | A    |
| 1   | 2     | 74  | A    |
| 1   | 2     | 75  | G    |
| 1   | 2     | 77  | A    |
| 1   | 2     | 80  | A    |
| 1   | 2     | 89  | U    |
| 1   | 2     | 94  | G    |
| 1   | 2     | 95  | C    |
| 1   | 2     | 121 | U    |
| 1   | 2     | 122 | G    |
| 1   | 2     | 131 | A    |
| 1   | 2     | 141 | G    |
| 1   | 2     | 144 | G    |
| 1   | 2     | 163 | C    |
| 1   | 2     | 165 | G    |
| 1   | 2     | 173 | U    |
| 1   | 2     | 182 | A    |
| 1   | 2     | 183 | C    |
| 1   | 2     | 197 | A    |
| 1   | 2     | 201 | G    |
| 1   | 2     | 202 | G    |
| 1   | 2     | 203 | G    |
| 1   | 2     | 204 | G    |
| 1   | 2     | 208 | U    |
| 1   | 2     | 209 | U    |
| 1   | 2     | 210 | C    |
| 1   | 2     | 211 | G    |
| 1   | 2     | 212 | G    |
| 1   | 2     | 226 | G    |
| 1   | 2     | 240 | G    |
| 1   | 2     | 245 | U    |
| 1   | 2     | 247 | G    |
| 1   | 2     | 251 | G    |
| 1   | 2     | 256 | U    |
| 1   | 2     | 257 | G    |
| 1   | 2     | 266 | G    |
| 1   | 2     | 267 | C    |
| 1   | 2     | 280 | C    |
| 1   | 2     | 289 | G    |
| 1   | 2     | 316 | C    |
| 1   | 2     | 321 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 328 | C    |
| 1   | 2     | 330 | C    |
| 1   | 2     | 351 | G    |
| 1   | 2     | 352 | C    |
| 1   | 2     | 354 | G    |
| 1   | 2     | 367 | U    |
| 1   | 2     | 372 | C    |
| 1   | 2     | 373 | A    |
| 1   | 2     | 384 | G    |
| 1   | 2     | 406 | G    |
| 1   | 2     | 412 | A    |
| 1   | 2     | 413 | G    |
| 1   | 2     | 414 | A    |
| 1   | 2     | 415 | A    |
| 1   | 2     | 416 | G    |
| 1   | 2     | 417 | G    |
| 1   | 2     | 421 | U    |
| 1   | 2     | 422 | C    |
| 1   | 2     | 423 | G    |
| 1   | 2     | 424 | G    |
| 1   | 2     | 429 | U    |
| 1   | 2     | 436 | C    |
| 1   | 2     | 446 | G    |
| 1   | 2     | 453 | G    |
| 1   | 2     | 456 | A    |
| 1   | 2     | 457 | G    |
| 1   | 2     | 458 | U    |
| 1   | 2     | 459 | A    |
| 1   | 2     | 463 | U    |
| 1   | 2     | 464 | U    |
| 1   | 2     | 467 | U    |
| 1   | 2     | 468 | A    |
| 1   | 2     | 469 | C    |
| 1   | 2     | 478 | A    |
| 1   | 2     | 479 | U    |
| 1   | 2     | 481 | G    |
| 1   | 2     | 484 | G    |
| 1   | 2     | 486 | U    |
| 1   | 2     | 495 | A    |
| 1   | 2     | 511 | C    |
| 1   | 2     | 518 | C    |
| 1   | 2     | 521 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 524 | G    |
| 1   | 2     | 527 | G7M  |
| 1   | 2     | 531 | U    |
| 1   | 2     | 547 | A    |
| 1   | 2     | 562 | U    |
| 1   | 2     | 572 | A    |
| 1   | 2     | 573 | A    |
| 1   | 2     | 576 | C    |
| 1   | 2     | 577 | G    |
| 1   | 2     | 579 | A    |
| 1   | 2     | 596 | A    |
| 1   | 2     | 607 | A    |
| 1   | 2     | 631 | C    |
| 1   | 2     | 633 | G    |
| 1   | 2     | 648 | A    |
| 1   | 2     | 650 | G    |
| 1   | 2     | 653 | U    |
| 1   | 2     | 665 | A    |
| 1   | 2     | 723 | U    |
| 1   | 2     | 724 | G    |
| 1   | 2     | 746 | A    |
| 1   | 2     | 747 | A    |
| 1   | 2     | 748 | G    |
| 1   | 2     | 755 | G    |
| 1   | 2     | 777 | A    |
| 1   | 2     | 792 | A    |
| 1   | 2     | 793 | U    |
| 1   | 2     | 794 | A    |
| 1   | 2     | 815 | A    |
| 1   | 2     | 817 | C    |
| 1   | 2     | 832 | G    |
| 1   | 2     | 840 | C    |
| 1   | 2     | 841 | C    |
| 1   | 2     | 842 | U    |
| 1   | 2     | 843 | U    |
| 1   | 2     | 844 | G    |
| 1   | 2     | 845 | A    |
| 1   | 2     | 846 | G    |
| 1   | 2     | 847 | G    |
| 1   | 2     | 890 | G    |
| 1   | 2     | 902 | G    |
| 1   | 2     | 914 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 926  | G    |
| 1   | 2     | 934  | C    |
| 1   | 2     | 935  | A    |
| 1   | 2     | 960  | U    |
| 1   | 2     | 963  | G    |
| 1   | 2     | 965  | U    |
| 1   | 2     | 966  | 2MG  |
| 1   | 2     | 969  | A    |
| 1   | 2     | 975  | A    |
| 1   | 2     | 976  | G    |
| 1   | 2     | 977  | A    |
| 1   | 2     | 992  | U    |
| 1   | 2     | 994  | A    |
| 1   | 2     | 1002 | G    |
| 1   | 2     | 1003 | G    |
| 1   | 2     | 1004 | A    |
| 1   | 2     | 1006 | G    |
| 1   | 2     | 1009 | U    |
| 1   | 2     | 1010 | U    |
| 1   | 2     | 1011 | C    |
| 1   | 2     | 1027 | C    |
| 1   | 2     | 1029 | U    |
| 1   | 2     | 1030 | U    |
| 1   | 2     | 1031 | C    |
| 1   | 2     | 1032 | G    |
| 1   | 2     | 1033 | G    |
| 1   | 2     | 1034 | G    |
| 1   | 2     | 1036 | A    |
| 1   | 2     | 1039 | G    |
| 1   | 2     | 1042 | A    |
| 1   | 2     | 1044 | A    |
| 1   | 2     | 1046 | A    |
| 1   | 2     | 1053 | G    |
| 1   | 2     | 1065 | U    |
| 1   | 2     | 1085 | U    |
| 1   | 2     | 1086 | U    |
| 1   | 2     | 1094 | G    |
| 1   | 2     | 1095 | U    |
| 1   | 2     | 1101 | A    |
| 1   | 2     | 1137 | C    |
| 1   | 2     | 1139 | G    |
| 1   | 2     | 1157 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1159 | U    |
| 1   | 2     | 1196 | A    |
| 1   | 2     | 1197 | A    |
| 1   | 2     | 1213 | A    |
| 1   | 2     | 1227 | A    |
| 1   | 2     | 1238 | A    |
| 1   | 2     | 1260 | G    |
| 1   | 2     | 1275 | A    |
| 1   | 2     | 1280 | A    |
| 1   | 2     | 1286 | U    |
| 1   | 2     | 1287 | A    |
| 1   | 2     | 1300 | G    |
| 1   | 2     | 1302 | C    |
| 1   | 2     | 1317 | C    |
| 1   | 2     | 1320 | C    |
| 1   | 2     | 1331 | G    |
| 1   | 2     | 1346 | A    |
| 1   | 2     | 1353 | G    |
| 1   | 2     | 1363 | A    |
| 1   | 2     | 1364 | U    |
| 1   | 2     | 1370 | G    |
| 1   | 2     | 1378 | C    |
| 1   | 2     | 1379 | G    |
| 1   | 2     | 1381 | U    |
| 1   | 2     | 1419 | G    |
| 1   | 2     | 1432 | G    |
| 1   | 2     | 1441 | A    |
| 1   | 2     | 1446 | A    |
| 1   | 2     | 1451 | U    |
| 1   | 2     | 1452 | C    |
| 1   | 2     | 1453 | G    |
| 1   | 2     | 1487 | G    |
| 1   | 2     | 1491 | G    |
| 1   | 2     | 1492 | A    |
| 1   | 2     | 1493 | A    |
| 1   | 2     | 1494 | G    |
| 1   | 2     | 1497 | G    |
| 1   | 2     | 1499 | A    |
| 1   | 2     | 1503 | A    |
| 1   | 2     | 1506 | U    |
| 1   | 2     | 1517 | G    |
| 1   | 2     | 1529 | G    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | 2     | 1530  | G    |
| 1   | 2     | 1536  | C    |
| 22  | 4     | 33    | A    |
| 22  | 4     | 34    | U    |
| 22  | 4     | 35    | U    |
| 22  | 4     | 38    | A    |
| 22  | 4     | 41    | U    |
| 22  | 4     | 44    | G    |
| 22  | 4     | 47    | U    |
| 23  | 5     | 5     | G    |
| 23  | 5     | 6     | G    |
| 23  | 5     | 7     | G    |
| 23  | 5     | 9     | G    |
| 23  | 5     | 13    | C    |
| 23  | 5     | 14    | A    |
| 23  | 5     | 16    | C    |
| 23  | 5     | 17    | C    |
| 23  | 5     | 17(A) | U    |
| 23  | 5     | 18    | G    |
| 23  | 5     | 19    | G    |
| 23  | 5     | 20    | U    |
| 23  | 5     | 21    | A    |
| 23  | 5     | 25    | C    |
| 23  | 5     | 31    | G    |
| 23  | 5     | 42    | G    |
| 23  | 5     | 43    | A    |
| 23  | 5     | 47    | U    |
| 23  | 5     | 48    | C    |
| 23  | 5     | 51    | C    |
| 23  | 5     | 52    | G    |
| 23  | 5     | 53    | G    |
| 23  | 5     | 54    | U    |
| 23  | 5     | 58    | A    |
| 23  | 5     | 65    | C    |
| 23  | 5     | 69    | C    |
| 23  | 5     | 70    | G    |
| 23  | 5     | 71    | C    |
| 24  | 1     | 10    | A    |
| 24  | 1     | 15    | G    |
| 24  | 1     | 23    | G    |
| 24  | 1     | 25    | U    |
| 24  | 1     | 34    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | 1     | 42  | A    |
| 24  | 1     | 45  | G    |
| 24  | 1     | 51  | G    |
| 24  | 1     | 58  | G    |
| 24  | 1     | 61  | C    |
| 24  | 1     | 71  | A    |
| 24  | 1     | 73  | A    |
| 24  | 1     | 74  | A    |
| 24  | 1     | 75  | G    |
| 24  | 1     | 80  | G    |
| 24  | 1     | 101 | A    |
| 24  | 1     | 102 | U    |
| 24  | 1     | 118 | A    |
| 24  | 1     | 119 | A    |
| 24  | 1     | 120 | U    |
| 24  | 1     | 125 | A    |
| 24  | 1     | 134 | G    |
| 24  | 1     | 135 | U    |
| 24  | 1     | 136 | G    |
| 24  | 1     | 139 | U    |
| 24  | 1     | 140 | C    |
| 24  | 1     | 141 | G    |
| 24  | 1     | 142 | A    |
| 24  | 1     | 163 | C    |
| 24  | 1     | 181 | A    |
| 24  | 1     | 196 | A    |
| 24  | 1     | 199 | A    |
| 24  | 1     | 215 | G    |
| 24  | 1     | 216 | A    |
| 24  | 1     | 221 | A    |
| 24  | 1     | 222 | A    |
| 24  | 1     | 231 | A    |
| 24  | 1     | 248 | G    |
| 24  | 1     | 264 | C    |
| 24  | 1     | 265 | A    |
| 24  | 1     | 267 | C    |
| 24  | 1     | 271 | G    |
| 24  | 1     | 272 | A    |
| 24  | 1     | 273 | G    |
| 24  | 1     | 274 | C    |
| 24  | 1     | 276 | U    |
| 24  | 1     | 277 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | 1     | 278 | A    |
| 24  | 1     | 281 | C    |
| 24  | 1     | 282 | A    |
| 24  | 1     | 283 | G    |
| 24  | 1     | 285 | G    |
| 24  | 1     | 287 | G    |
| 24  | 1     | 289 | G    |
| 24  | 1     | 290 | U    |
| 24  | 1     | 291 | G    |
| 24  | 1     | 292 | U    |
| 24  | 1     | 294 | A    |
| 24  | 1     | 303 | G    |
| 24  | 1     | 304 | U    |
| 24  | 1     | 311 | A    |
| 24  | 1     | 312 | G    |
| 24  | 1     | 329 | G    |
| 24  | 1     | 330 | A    |
| 24  | 1     | 331 | C    |
| 24  | 1     | 345 | A    |
| 24  | 1     | 353 | C    |
| 24  | 1     | 356 | G    |
| 24  | 1     | 359 | G    |
| 24  | 1     | 360 | U    |
| 24  | 1     | 361 | G    |
| 24  | 1     | 363 | G    |
| 24  | 1     | 366 | C    |
| 24  | 1     | 370 | G    |
| 24  | 1     | 386 | G    |
| 24  | 1     | 396 | G    |
| 24  | 1     | 405 | U    |
| 24  | 1     | 411 | G    |
| 24  | 1     | 412 | A    |
| 24  | 1     | 447 | A    |
| 24  | 1     | 463 | G    |
| 24  | 1     | 464 | U    |
| 24  | 1     | 475 | C    |
| 24  | 1     | 481 | G    |
| 24  | 1     | 491 | G    |
| 24  | 1     | 504 | A    |
| 24  | 1     | 505 | A    |
| 24  | 1     | 508 | A    |
| 24  | 1     | 509 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | 1     | 513 | A    |
| 24  | 1     | 532 | A    |
| 24  | 1     | 545 | U    |
| 24  | 1     | 546 | U    |
| 24  | 1     | 548 | G    |
| 24  | 1     | 549 | G    |
| 24  | 1     | 563 | A    |
| 24  | 1     | 573 | U    |
| 24  | 1     | 575 | A    |
| 24  | 1     | 603 | A    |
| 24  | 1     | 614 | A    |
| 24  | 1     | 615 | U    |
| 24  | 1     | 627 | A    |
| 24  | 1     | 637 | A    |
| 24  | 1     | 645 | C    |
| 24  | 1     | 646 | U    |
| 24  | 1     | 647 | G    |
| 24  | 1     | 653 | U    |
| 24  | 1     | 654 | A    |
| 24  | 1     | 655 | A    |
| 24  | 1     | 686 | U    |
| 24  | 1     | 717 | C    |
| 24  | 1     | 721 | A    |
| 24  | 1     | 730 | A    |
| 24  | 1     | 738 | G    |
| 24  | 1     | 747 | 5MU  |
| 24  | 1     | 775 | G    |
| 24  | 1     | 776 | G    |
| 24  | 1     | 782 | A    |
| 24  | 1     | 784 | G    |
| 24  | 1     | 785 | G    |
| 24  | 1     | 787 | C    |
| 24  | 1     | 789 | A    |
| 24  | 1     | 791 | C    |
| 24  | 1     | 805 | G    |
| 24  | 1     | 812 | C    |
| 24  | 1     | 827 | U    |
| 24  | 1     | 828 | U    |
| 24  | 1     | 845 | A    |
| 24  | 1     | 846 | U    |
| 24  | 1     | 859 | G    |
| 24  | 1     | 869 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 879  | G    |
| 24  | 1     | 881  | G    |
| 24  | 1     | 882  | G    |
| 24  | 1     | 883  | G    |
| 24  | 1     | 884  | U    |
| 24  | 1     | 885  | C    |
| 24  | 1     | 888  | C    |
| 24  | 1     | 890  | C    |
| 24  | 1     | 891  | G    |
| 24  | 1     | 895  | U    |
| 24  | 1     | 896  | A    |
| 24  | 1     | 897  | C    |
| 24  | 1     | 898  | C    |
| 24  | 1     | 899  | A    |
| 24  | 1     | 909  | A    |
| 24  | 1     | 910  | A    |
| 24  | 1     | 914  | G    |
| 24  | 1     | 915  | C    |
| 24  | 1     | 931  | U    |
| 24  | 1     | 946  | C    |
| 24  | 1     | 958  | U    |
| 24  | 1     | 961  | C    |
| 24  | 1     | 974  | G    |
| 24  | 1     | 983  | A    |
| 24  | 1     | 989  | G    |
| 24  | 1     | 990  | A    |
| 24  | 1     | 996  | A    |
| 24  | 1     | 1012 | U    |
| 24  | 1     | 1013 | C    |
| 24  | 1     | 1022 | G    |
| 24  | 1     | 1026 | G    |
| 24  | 1     | 1033 | U    |
| 24  | 1     | 1041 | G    |
| 24  | 1     | 1042 | G    |
| 24  | 1     | 1047 | G    |
| 24  | 1     | 1051 | G    |
| 24  | 1     | 1054 | A    |
| 24  | 1     | 1055 | G    |
| 24  | 1     | 1056 | G    |
| 24  | 1     | 1057 | A    |
| 24  | 1     | 1062 | G    |
| 24  | 1     | 1064 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 1065 | U    |
| 24  | 1     | 1066 | U    |
| 24  | 1     | 1068 | G    |
| 24  | 1     | 1069 | A    |
| 24  | 1     | 1070 | A    |
| 24  | 1     | 1074 | G    |
| 24  | 1     | 1077 | A    |
| 24  | 1     | 1083 | U    |
| 24  | 1     | 1084 | A    |
| 24  | 1     | 1087 | G    |
| 24  | 1     | 1088 | A    |
| 24  | 1     | 1089 | A    |
| 24  | 1     | 1097 | U    |
| 24  | 1     | 1101 | U    |
| 24  | 1     | 1105 | U    |
| 24  | 1     | 1107 | G    |
| 24  | 1     | 1108 | U    |
| 24  | 1     | 1111 | A    |
| 24  | 1     | 1112 | G    |
| 24  | 1     | 1115 | G    |
| 24  | 1     | 1116 | G    |
| 24  | 1     | 1122 | G    |
| 24  | 1     | 1130 | U    |
| 24  | 1     | 1132 | U    |
| 24  | 1     | 1133 | A    |
| 24  | 1     | 1135 | C    |
| 24  | 1     | 1142 | A    |
| 24  | 1     | 1158 | C    |
| 24  | 1     | 1169 | A    |
| 24  | 1     | 1171 | G    |
| 24  | 1     | 1172 | C    |
| 24  | 1     | 1206 | G    |
| 24  | 1     | 1212 | G    |
| 24  | 1     | 1217 | U    |
| 24  | 1     | 1236 | G    |
| 24  | 1     | 1238 | G    |
| 24  | 1     | 1242 | U    |
| 24  | 1     | 1250 | G    |
| 24  | 1     | 1253 | A    |
| 24  | 1     | 1256 | G    |
| 24  | 1     | 1271 | G    |
| 24  | 1     | 1272 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 1273 | U    |
| 24  | 1     | 1289 | C    |
| 24  | 1     | 1293 | C    |
| 24  | 1     | 1300 | G    |
| 24  | 1     | 1301 | A    |
| 24  | 1     | 1329 | U    |
| 24  | 1     | 1352 | U    |
| 24  | 1     | 1365 | A    |
| 24  | 1     | 1379 | U    |
| 24  | 1     | 1380 | G    |
| 24  | 1     | 1383 | A    |
| 24  | 1     | 1395 | A    |
| 24  | 1     | 1411 | U    |
| 24  | 1     | 1416 | G    |
| 24  | 1     | 1419 | A    |
| 24  | 1     | 1420 | A    |
| 24  | 1     | 1421 | G    |
| 24  | 1     | 1427 | A    |
| 24  | 1     | 1428 | C    |
| 24  | 1     | 1452 | G    |
| 24  | 1     | 1453 | A    |
| 24  | 1     | 1458 | U    |
| 24  | 1     | 1460 | U    |
| 24  | 1     | 1482 | G    |
| 24  | 1     | 1486 | U    |
| 24  | 1     | 1493 | C    |
| 24  | 1     | 1497 | U    |
| 24  | 1     | 1508 | A    |
| 24  | 1     | 1509 | A    |
| 24  | 1     | 1510 | G    |
| 24  | 1     | 1515 | A    |
| 24  | 1     | 1529 | G    |
| 24  | 1     | 1534 | U    |
| 24  | 1     | 1535 | A    |
| 24  | 1     | 1536 | C    |
| 24  | 1     | 1537 | G    |
| 24  | 1     | 1554 | U    |
| 24  | 1     | 1559 | U    |
| 24  | 1     | 1560 | G    |
| 24  | 1     | 1566 | A    |
| 24  | 1     | 1569 | A    |
| 24  | 1     | 1578 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 1583 | A    |
| 24  | 1     | 1584 | U    |
| 24  | 1     | 1585 | C    |
| 24  | 1     | 1586 | A    |
| 24  | 1     | 1607 | C    |
| 24  | 1     | 1608 | A    |
| 24  | 1     | 1613 | G    |
| 24  | 1     | 1634 | A    |
| 24  | 1     | 1647 | U    |
| 24  | 1     | 1648 | U    |
| 24  | 1     | 1649 | G    |
| 24  | 1     | 1667 | G    |
| 24  | 1     | 1674 | G    |
| 24  | 1     | 1715 | G    |
| 24  | 1     | 1729 | U    |
| 24  | 1     | 1730 | C    |
| 24  | 1     | 1731 | G    |
| 24  | 1     | 1732 | C    |
| 24  | 1     | 1738 | G    |
| 24  | 1     | 1764 | C    |
| 24  | 1     | 1773 | A    |
| 24  | 1     | 1782 | U    |
| 24  | 1     | 1786 | A    |
| 24  | 1     | 1800 | C    |
| 24  | 1     | 1801 | A    |
| 24  | 1     | 1808 | A    |
| 24  | 1     | 1816 | C    |
| 24  | 1     | 1829 | A    |
| 24  | 1     | 1847 | A    |
| 24  | 1     | 1857 | G    |
| 24  | 1     | 1858 | A    |
| 24  | 1     | 1868 | C    |
| 24  | 1     | 1870 | C    |
| 24  | 1     | 1871 | A    |
| 24  | 1     | 1873 | G    |
| 24  | 1     | 1905 | C    |
| 24  | 1     | 1906 | G    |
| 24  | 1     | 1910 | G    |
| 24  | 1     | 1913 | A    |
| 24  | 1     | 1914 | C    |
| 24  | 1     | 1915 | 3TD  |
| 24  | 1     | 1916 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 1929 | G    |
| 24  | 1     | 1930 | G    |
| 24  | 1     | 1939 | 5MU  |
| 24  | 1     | 1955 | U    |
| 24  | 1     | 1965 | C    |
| 24  | 1     | 1967 | C    |
| 24  | 1     | 1970 | A    |
| 24  | 1     | 1971 | U    |
| 24  | 1     | 1972 | G    |
| 24  | 1     | 1991 | U    |
| 24  | 1     | 1992 | G    |
| 24  | 1     | 1993 | U    |
| 24  | 1     | 2023 | C    |
| 24  | 1     | 2027 | G    |
| 24  | 1     | 2030 | 6MZ  |
| 24  | 1     | 2031 | A    |
| 24  | 1     | 2033 | A    |
| 24  | 1     | 2036 | C    |
| 24  | 1     | 2043 | C    |
| 24  | 1     | 2049 | G    |
| 24  | 1     | 2055 | C    |
| 24  | 1     | 2056 | G    |
| 24  | 1     | 2060 | A    |
| 24  | 1     | 2061 | G    |
| 24  | 1     | 2062 | A    |
| 24  | 1     | 2069 | G7M  |
| 24  | 1     | 2093 | G    |
| 24  | 1     | 2097 | A    |
| 24  | 1     | 2098 | U    |
| 24  | 1     | 2099 | U    |
| 24  | 1     | 2100 | G    |
| 24  | 1     | 2101 | A    |
| 24  | 1     | 2102 | G    |
| 24  | 1     | 2104 | C    |
| 24  | 1     | 2110 | G    |
| 24  | 1     | 2111 | U    |
| 24  | 1     | 2113 | U    |
| 24  | 1     | 2115 | G    |
| 24  | 1     | 2116 | G    |
| 24  | 1     | 2117 | A    |
| 24  | 1     | 2118 | U    |
| 24  | 1     | 2122 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 2124 | G    |
| 24  | 1     | 2125 | G    |
| 24  | 1     | 2126 | A    |
| 24  | 1     | 2127 | G    |
| 24  | 1     | 2128 | G    |
| 24  | 1     | 2131 | U    |
| 24  | 1     | 2132 | U    |
| 24  | 1     | 2133 | G    |
| 24  | 1     | 2134 | A    |
| 24  | 1     | 2139 | U    |
| 24  | 1     | 2147 | A    |
| 24  | 1     | 2157 | G    |
| 24  | 1     | 2158 | A    |
| 24  | 1     | 2159 | G    |
| 24  | 1     | 2162 | G    |
| 24  | 1     | 2163 | A    |
| 24  | 1     | 2164 | C    |
| 24  | 1     | 2165 | C    |
| 24  | 1     | 2171 | A    |
| 24  | 1     | 2172 | U    |
| 24  | 1     | 2182 | U    |
| 24  | 1     | 2183 | A    |
| 24  | 1     | 2185 | U    |
| 24  | 1     | 2188 | U    |
| 24  | 1     | 2190 | G    |
| 24  | 1     | 2191 | A    |
| 24  | 1     | 2198 | A    |
| 24  | 1     | 2204 | G    |
| 24  | 1     | 2211 | A    |
| 24  | 1     | 2225 | A    |
| 24  | 1     | 2238 | G    |
| 24  | 1     | 2239 | G    |
| 24  | 1     | 2259 | U    |
| 24  | 1     | 2268 | A    |
| 24  | 1     | 2279 | G    |
| 24  | 1     | 2283 | C    |
| 24  | 1     | 2287 | A    |
| 24  | 1     | 2288 | A    |
| 24  | 1     | 2289 | G    |
| 24  | 1     | 2305 | U    |
| 24  | 1     | 2308 | G    |
| 24  | 1     | 2322 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 2325 | G    |
| 24  | 1     | 2333 | A    |
| 24  | 1     | 2335 | A    |
| 24  | 1     | 2337 | G    |
| 24  | 1     | 2340 | A    |
| 24  | 1     | 2345 | G    |
| 24  | 1     | 2347 | C    |
| 24  | 1     | 2350 | C    |
| 24  | 1     | 2361 | G    |
| 24  | 1     | 2383 | G    |
| 24  | 1     | 2385 | C    |
| 24  | 1     | 2402 | U    |
| 24  | 1     | 2406 | A    |
| 24  | 1     | 2408 | U    |
| 24  | 1     | 2410 | G    |
| 24  | 1     | 2425 | A    |
| 24  | 1     | 2429 | G    |
| 24  | 1     | 2430 | A    |
| 24  | 1     | 2435 | A    |
| 24  | 1     | 2441 | U    |
| 24  | 1     | 2448 | A    |
| 24  | 1     | 2476 | A    |
| 24  | 1     | 2478 | A    |
| 24  | 1     | 2491 | U    |
| 24  | 1     | 2494 | G    |
| 24  | 1     | 2498 | OMC  |
| 24  | 1     | 2502 | G    |
| 24  | 1     | 2503 | 2MA  |
| 24  | 1     | 2505 | G    |
| 24  | 1     | 2506 | U    |
| 24  | 1     | 2507 | C    |
| 24  | 1     | 2517 | C    |
| 24  | 1     | 2518 | A    |
| 24  | 1     | 2520 | C    |
| 24  | 1     | 2525 | G    |
| 24  | 1     | 2529 | G    |
| 24  | 1     | 2535 | G    |
| 24  | 1     | 2547 | A    |
| 24  | 1     | 2566 | A    |
| 24  | 1     | 2567 | G    |
| 24  | 1     | 2573 | C    |
| 24  | 1     | 2582 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 2585 | U    |
| 24  | 1     | 2586 | U    |
| 24  | 1     | 2602 | A    |
| 24  | 1     | 2603 | G    |
| 24  | 1     | 2609 | U    |
| 24  | 1     | 2613 | U    |
| 24  | 1     | 2615 | U    |
| 24  | 1     | 2629 | U    |
| 24  | 1     | 2645 | G    |
| 24  | 1     | 2646 | C    |
| 24  | 1     | 2661 | G    |
| 24  | 1     | 2682 | A    |
| 24  | 1     | 2685 | G    |
| 24  | 1     | 2689 | U    |
| 24  | 1     | 2690 | U    |
| 24  | 1     | 2713 | U    |
| 24  | 1     | 2716 | C    |
| 24  | 1     | 2726 | A    |
| 24  | 1     | 2733 | A    |
| 24  | 1     | 2744 | G    |
| 24  | 1     | 2748 | A    |
| 24  | 1     | 2752 | C    |
| 24  | 1     | 2765 | A    |
| 24  | 1     | 2768 | U    |
| 24  | 1     | 2778 | A    |
| 24  | 1     | 2795 | C    |
| 24  | 1     | 2797 | U    |
| 24  | 1     | 2798 | U    |
| 24  | 1     | 2799 | A    |
| 24  | 1     | 2800 | A    |
| 24  | 1     | 2801 | G    |
| 24  | 1     | 2804 | U    |
| 24  | 1     | 2818 | U    |
| 24  | 1     | 2820 | A    |
| 24  | 1     | 2821 | A    |
| 24  | 1     | 2835 | A    |
| 24  | 1     | 2849 | U    |
| 24  | 1     | 2861 | U    |
| 24  | 1     | 2872 | A    |
| 24  | 1     | 2873 | A    |
| 24  | 1     | 2884 | U    |
| 24  | 1     | 2891 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | 1     | 2900 | A    |
| 24  | 1     | 2902 | C    |
| 24  | 1     | 2903 | U    |
| 25  | 3     | 9    | G    |
| 25  | 3     | 13   | G    |
| 25  | 3     | 24   | G    |
| 25  | 3     | 35   | C    |
| 25  | 3     | 36   | C    |
| 25  | 3     | 45   | A    |
| 25  | 3     | 56   | G    |
| 25  | 3     | 57   | A    |
| 25  | 3     | 58   | A    |
| 25  | 3     | 67   | G    |
| 25  | 3     | 89   | U    |
| 25  | 3     | 90   | C    |
| 25  | 3     | 99   | A    |
| 25  | 3     | 109  | A    |

All (13) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 182  | A    |
| 1   | 2     | 209  | U    |
| 1   | 2     | 467  | U    |
| 1   | 2     | 1026 | G    |
| 1   | 2     | 1035 | A    |
| 22  | 4     | 32   | U    |
| 24  | 1     | 277  | G    |
| 24  | 1     | 404  | A    |
| 24  | 1     | 504  | A    |
| 24  | 1     | 784  | G    |
| 24  | 1     | 827  | U    |
| 24  | 1     | 2146 | C    |
| 24  | 1     | 2162 | G    |

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

41 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | PSU  | 1     | 2604 | 24       | 18,21,22     | 0.57 | 0        | 22,30,33    | 0.65 | 0        |
| 24  | 2MA  | 1     | 2503 | 59,57,24 | 22,25,26     | 1.05 | 2 (9%)   | 33,37,40    | 1.30 | 3 (9%)   |
| 27  | MEQ  | C     | 150  | 27       | 8,9,10       | 0.89 | 0        | 5,10,12     | 0.56 | 0        |
| 1   | 2MG  | 2     | 1207 | 59,1     | 23,26,27     | 0.35 | 0        | 32,38,41    | 0.33 | 0        |
| 12  | D2T  | q     | 89   | 12       | 7,9,10       | 0.89 | 0        | 6,11,13     | 1.66 | 2 (33%)  |
| 24  | G7M  | 1     | 2069 | 59,24    | 23,26,27     | 0.41 | 0        | 35,39,42    | 0.52 | 0        |
| 24  | OMG  | 1     | 2251 | 59,23,24 | 23,26,27     | 0.42 | 0        | 33,38,41    | 0.39 | 0        |
| 1   | PSU  | 2     | 516  | 57,1     | 18,21,22     | 0.57 | 1 (5%)   | 22,30,33    | 0.64 | 1 (4%)   |
| 24  | 1MG  | 1     | 745  | 24       | 22,26,27     | 0.44 | 0        | 33,39,42    | 0.66 | 1 (3%)   |
| 24  | PSU  | 1     | 1911 | 24       | 18,21,22     | 0.56 | 0        | 22,30,33    | 0.56 | 0        |
| 1   | 2MG  | 2     | 1516 | 1        | 23,26,27     | 0.39 | 0        | 32,38,41    | 0.46 | 0        |
| 55  | MEQ  | 6     | 252  | 55       | 8,9,10       | 0.93 | 0        | 5,10,12     | 0.91 | 1 (20%)  |
| 24  | PSU  | 1     | 2457 | 24       | 18,21,22     | 0.62 | 0        | 22,30,33    | 0.58 | 0        |
| 24  | 5MU  | 1     | 1939 | 59,24    | 19,22,23     | 0.59 | 0        | 28,32,35    | 0.89 | 3 (10%)  |
| 24  | 6MZ  | 1     | 2030 | 24       | 22,25,26     | 0.36 | 0        | 30,36,39    | 0.41 | 0        |
| 24  | OMC  | 1     | 2498 | 57,24    | 19,22,23     | 0.37 | 0        | 26,31,34    | 0.43 | 0        |
| 1   | MA6  | 2     | 1519 | 1        | 23,26,27     | 0.36 | 0        | 34,38,41    | 0.71 | 1 (2%)   |
| 24  | PSU  | 1     | 746  | 57,24    | 18,21,22     | 0.62 | 0        | 22,30,33    | 0.37 | 0        |
| 24  | PSU  | 1     | 955  | 24       | 18,21,22     | 0.60 | 0        | 22,30,33    | 0.58 | 0        |
| 1   | 5MC  | 2     | 1407 | 1        | 18,22,23     | 0.38 | 0        | 26,32,35    | 0.48 | 0        |
| 34  | 4D4  | M     | 81   | 34       | 9,11,12      | 0.57 | 0        | 8,13,15     | 1.95 | 3 (37%)  |
| 24  | PSU  | 1     | 2504 | 59,24    | 18,21,22     | 0.60 | 0        | 22,30,33    | 0.62 | 0        |
| 24  | 6MZ  | 1     | 1618 | 24       | 22,25,26     | 0.35 | 0        | 30,36,39    | 0.46 | 0        |
| 1   | G7M  | 2     | 527  | 1        | 23,26,27     | 0.38 | 0        | 35,39,42    | 0.51 | 0        |
| 1   | UR3  | 2     | 1498 | 1        | 19,22,23     | 0.37 | 0        | 26,32,35    | 0.35 | 0        |
| 24  | PSU  | 1     | 1917 | 24       | 18,21,22     | 0.57 | 0        | 22,30,33    | 0.57 | 0        |
| 24  | PSU  | 1     | 2580 | 24       | 18,21,22     | 0.69 | 1 (5%)   | 22,30,33    | 0.71 | 1 (4%)   |
| 34  | MS6  | M     | 82   | 34       | 5,7,8        | 0.25 | 0        | 2,7,9       | 0.03 | 0        |
| 11  | IAS  | p     | 119  | 11       | 6,7,8        | 0.94 | 0        | 6,8,10      | 1.25 | 1 (16%)  |
| 24  | 2MG  | 1     | 2445 | 24       | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.31 | 0        |
| 24  | 5MC  | 1     | 1962 | 59,24    | 18,22,23     | 0.35 | 0        | 26,32,35    | 0.43 | 0        |
| 24  | H2U  | 1     | 2449 | 24       | 18,21,22     | 0.34 | 0        | 21,30,33    | 0.48 | 0        |
| 24  | 5MU  | 1     | 747  | 24       | 19,22,23     | 0.38 | 0        | 28,32,35    | 0.32 | 0        |
| 1   | 2MG  | 2     | 966  | 1        | 23,26,27     | 0.31 | 0        | 32,38,41    | 0.34 | 0        |
| 1   | 4OC  | 2     | 1402 | 57,1     | 20,23,24     | 0.38 | 0        | 26,32,35    | 0.62 | 0        |
| 24  | 2MG  | 1     | 1835 | 24       | 23,26,27     | 0.35 | 0        | 32,38,41    | 0.32 | 0        |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | 3TD  | 1     | 1915 | 57,24 | 19,22,23     | 0.56 | 0        | 21,32,35    | 0.83 | 0        |
| 1   | MA6  | 2     | 1518 | 1     | 23,26,27     | 0.35 | 0        | 34,38,41    | 0.68 | 1 (2%)   |
| 24  | OMU  | 1     | 2552 | 57,24 | 19,22,23     | 0.36 | 0        | 26,31,34    | 0.42 | 0        |
| 24  | PSU  | 1     | 2605 | 24    | 18,21,22     | 0.59 | 0        | 22,30,33    | 0.67 | 0        |
| 1   | 5MC  | 2     | 967  | 1     | 18,22,23     | 0.34 | 0        | 26,32,35    | 0.42 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 24  | PSU  | 1     | 2604 | 24       | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | 2MA  | 1     | 2503 | 59,57,24 | -       | 1/7/25/26  | 0/3/3/3 |
| 27  | MEQ  | C     | 150  | 27       | -       | 3/8/9/11   | -       |
| 1   | 2MG  | 2     | 1207 | 59,1     | -       | 0/9/27/28  | 0/3/3/3 |
| 12  | D2T  | q     | 89   | 12       | -       | 1/7/12/14  | -       |
| 24  | G7M  | 1     | 2069 | 59,24    | -       | 1/7/25/26  | 0/3/3/3 |
| 24  | OMG  | 1     | 2251 | 59,23,24 | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 516  | 57,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | 1MG  | 1     | 745  | 24       | -       | 0/7/25/26  | 0/3/3/3 |
| 24  | PSU  | 1     | 1911 | 24       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | 2     | 1516 | 1        | -       | 0/9/27/28  | 0/3/3/3 |
| 55  | MEQ  | 6     | 252  | 55       | -       | 2/8/9/11   | -       |
| 24  | PSU  | 1     | 2457 | 24       | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | 5MU  | 1     | 1939 | 59,24    | -       | 2/7/25/26  | 0/2/2/2 |
| 24  | 6MZ  | 1     | 2030 | 24       | -       | 2/9/27/28  | 0/3/3/3 |
| 24  | OMC  | 1     | 2498 | 57,24    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | MA6  | 2     | 1519 | 1        | -       | 2/11/29/30 | 0/3/3/3 |
| 24  | PSU  | 1     | 746  | 57,24    | -       | 1/7/25/26  | 0/2/2/2 |
| 24  | PSU  | 1     | 955  | 24       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2     | 1407 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 34  | 4D4  | M     | 81   | 34       | -       | 3/11/12/14 | -       |
| 24  | PSU  | 1     | 2504 | 59,24    | -       | 1/7/25/26  | 0/2/2/2 |
| 24  | 6MZ  | 1     | 1618 | 24       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | G7M  | 2     | 527  | 1        | -       | 3/7/25/26  | 0/3/3/3 |
| 1   | UR3  | 2     | 1498 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | PSU  | 1     | 1917 | 24       | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | PSU  | 1     | 2580 | 24       | -       | 0/7/25/26  | 0/2/2/2 |
| 34  | MS6  | M     | 82   | 34       | -       | 1/4/6/8    | -       |
| 11  | IAS  | p     | 119  | 11       | -       | 1/7/7/8    | -       |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 24  | 2MG  | 1     | 2445 | 24    | -       | 1/9/27/28  | 0/3/3/3 |
| 24  | 5MC  | 1     | 1962 | 59,24 | -       | 2/7/25/26  | 0/2/2/2 |
| 24  | H2U  | 1     | 2449 | 24    | -       | 0/7/38/39  | 0/2/2/2 |
| 24  | 5MU  | 1     | 747  | 24    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | 2     | 966  | 1     | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | 4OC  | 2     | 1402 | 57,1  | -       | 0/9/29/30  | 0/2/2/2 |
| 24  | 2MG  | 1     | 1835 | 24    | -       | 0/9/27/28  | 0/3/3/3 |
| 24  | 3TD  | 1     | 1915 | 57,24 | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | MA6  | 2     | 1518 | 1     | -       | 0/11/29/30 | 0/3/3/3 |
| 24  | OMU  | 1     | 2552 | 57,24 | -       | 0/9/27/28  | 0/2/2/2 |
| 24  | PSU  | 1     | 2605 | 24    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2     | 967  | 1     | -       | 0/7/25/26  | 0/2/2/2 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | 1     | 2503 | 2MA  | C6-N6   | -3.78 | 1.24        | 1.34     |
| 24  | 1     | 2580 | PSU  | O4'-C1' | -2.35 | 1.40        | 1.43     |
| 1   | 2     | 516  | PSU  | O4'-C1' | -2.03 | 1.41        | 1.43     |
| 24  | 1     | 2503 | 2MA  | C2-N3   | -2.01 | 1.30        | 1.34     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | 1     | 2503 | 2MA  | N6-C6-N1    | 4.26  | 123.06      | 117.03   |
| 24  | 1     | 2503 | 2MA  | C2-N1-C6    | 3.87  | 124.11      | 118.08   |
| 34  | M     | 81   | 4D4  | NE-CZ-NH2   | 3.66  | 127.12      | 120.70   |
| 24  | 1     | 2503 | 2MA  | C5-C6-N1    | -3.41 | 113.14      | 119.01   |
| 34  | M     | 81   | 4D4  | O-C-CA      | -2.97 | 117.01      | 124.78   |
| 24  | 1     | 745  | 1MG  | C6-C5-C4    | -2.87 | 116.79      | 119.97   |
| 12  | q     | 89   | D2T  | O-C-CA      | -2.83 | 117.36      | 124.78   |
| 34  | M     | 81   | 4D4  | NH1-CZ-NE   | -2.79 | 112.75      | 119.19   |
| 24  | 1     | 1939 | 5MU  | O4'-C1'-N1  | 2.45  | 113.97      | 108.36   |
| 24  | 1     | 2580 | PSU  | O4'-C1'-C2' | 2.45  | 108.60      | 105.14   |
| 11  | p     | 119  | IAS  | OD1-CG-CB   | -2.45 | 118.29      | 125.43   |
| 1   | 2     | 1518 | MA6  | C2-N1-C6    | 2.37  | 117.34      | 111.75   |
| 1   | 2     | 1519 | MA6  | C2-N1-C6    | 2.35  | 117.31      | 111.75   |
| 1   | 2     | 516  | PSU  | O4'-C1'-C2' | 2.26  | 108.33      | 105.14   |
| 12  | q     | 89   | D2T  | OD1-CG-CB   | -2.26 | 117.71      | 122.44   |
| 24  | 1     | 1939 | 5MU  | C1'-N1-C6   | 2.23  | 124.84      | 121.12   |
| 24  | 1     | 1939 | 5MU  | C1'-N1-C2   | -2.09 | 113.79      | 117.57   |
| 55  | 6     | 252  | MEQ  | CB-CG-CD    | -2.03 | 108.51      | 113.04   |

There are no chirality outliers.

All (31) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 27  | C     | 150  | MEQ  | O-C-CA-CB       |
| 24  | 1     | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 24  | 1     | 1939 | 5MU  | O4'-C4'-C5'-O5' |
| 24  | 1     | 2251 | OMG  | C1'-C2'-O2'-CM2 |
| 24  | 1     | 1915 | 3TD  | C3'-C4'-C5'-O5' |
| 24  | 1     | 1939 | 5MU  | C3'-C4'-C5'-O5' |
| 24  | 1     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 1   | 2     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 24  | 1     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 27  | C     | 150  | MEQ  | OE1-CD-CG-CB    |
| 27  | C     | 150  | MEQ  | NE2-CD-CG-CB    |
| 1   | 2     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 34  | M     | 81   | 4D4  | OB-CB-CG-CD     |
| 12  | q     | 89   | D2T  | CG-CB-SB-CB1    |
| 34  | M     | 82   | MS6  | CB-CG-SD-CE     |
| 24  | 1     | 2445 | 2MG  | C3'-C4'-C5'-O5' |
| 1   | 2     | 1519 | MA6  | C5-C6-N6-C10    |
| 55  | 6     | 252  | MEQ  | OE1-CD-CG-CB    |
| 55  | 6     | 252  | MEQ  | NE2-CD-CG-CB    |
| 34  | M     | 81   | 4D4  | CA-CB-CG-CD     |
| 1   | 2     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 24  | 1     | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 24  | 1     | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 24  | 1     | 1962 | 5MC  | C2'-C1'-N1-C6   |
| 1   | 2     | 527  | G7M  | C4'-C5'-O5'-P   |
| 24  | 1     | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 24  | 1     | 1962 | 5MC  | O4'-C1'-N1-C6   |
| 24  | 1     | 746  | PSU  | O4'-C1'-C5-C6   |
| 1   | 2     | 966  | 2MG  | C3'-C4'-C5'-O5' |
| 11  | p     | 119  | IAS  | CA-CB-CG-OD1    |
| 34  | M     | 81   | 4D4  | O-C-CA-CB       |

There are no ring outliers.

10 monomers are involved in 11 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 2     | 1207 | 2MG  | 1       | 0            |
| 12  | q     | 89   | D2T  | 1       | 0            |
| 24  | 1     | 2251 | OMG  | 1       | 0            |
| 1   | 2     | 1516 | 2MG  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24  | 1     | 2030 | 6MZ  | 2       | 0            |
| 1   | 2     | 1519 | MA6  | 1       | 0            |
| 1   | 2     | 1402 | 4OC  | 2       | 0            |
| 24  | 1     | 1915 | 3TD  | 1       | 0            |
| 1   | 2     | 1518 | MA6  | 1       | 0            |
| 24  | 1     | 2552 | OMU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 477 ligands modelled in this entry, 450 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 58  | SPD  | 1     | 3209 | -    | 9,9,9        | 0.08 | 0           | 8,8,8       | 0.29 | 0           |
| 58  | SPD  | 1     | 3210 | -    | 9,9,9        | 0.07 | 0           | 8,8,8       | 0.16 | 0           |
| 58  | SPD  | 1     | 3208 | -    | 9,9,9        | 0.08 | 0           | 8,8,8       | 0.18 | 0           |
| 60  | PUT  | Z     | 101  | -    | 5,5,5        | 0.10 | 0           | 4,4,4       | 0.19 | 0           |
| 58  | SPD  | 1     | 3206 | -    | 9,9,9        | 0.10 | 0           | 8,8,8       | 0.16 | 0           |
| 58  | SPD  | 1     | 3212 | -    | 9,9,9        | 0.09 | 0           | 8,8,8       | 0.12 | 0           |
| 60  | PUT  | 1     | 3325 | -    | 5,5,5        | 0.10 | 0           | 4,4,4       | 0.19 | 0           |
| 60  | PUT  | C     | 301  | -    | 5,5,5        | 0.09 | 0           | 4,4,4       | 0.17 | 0           |
| 60  | PUT  | 1     | 3323 | -    | 5,5,5        | 0.07 | 0           | 4,4,4       | 0.17 | 0           |
| 58  | SPD  | 1     | 3205 | -    | 9,9,9        | 0.12 | 0           | 8,8,8       | 0.11 | 0           |
| 61  | SPM  | 1     | 3213 | -    | 13,13,13     | 0.36 | 0           | 12,12,12    | 0.98 | 0           |
| 60  | PUT  | 1     | 3330 | -    | 5,5,5        | 0.11 | 0           | 4,4,4       | 0.14 | 0           |
| 58  | SPD  | 2     | 1687 | -    | 9,9,9        | 0.10 | 0           | 8,8,8       | 0.16 | 0           |
| 58  | SPD  | 1     | 3204 | -    | 9,9,9        | 0.10 | 0           | 8,8,8       | 0.13 | 0           |
| 60  | PUT  | 1     | 3331 | -    | 5,5,5        | 0.11 | 0           | 4,4,4       | 0.16 | 0           |
| 58  | SPD  | 1     | 3207 | -    | 9,9,9        | 0.09 | 0           | 8,8,8       | 0.15 | 0           |
| 60  | PUT  | 1     | 3329 | -    | 5,5,5        | 0.11 | 0           | 4,4,4       | 0.17 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | SPD  | 1     | 3203 | -    | 9,9,9        | 0.08 | 0        | 8,8,8       | 0.18 | 0        |
| 58  | SPD  | 2     | 1686 | -    | 9,9,9        | 0.12 | 0        | 8,8,8       | 0.10 | 0        |
| 58  | SPD  | 1     | 3211 | -    | 9,9,9        | 0.06 | 0        | 8,8,8       | 0.18 | 0        |
| 60  | PUT  | 1     | 3327 | -    | 5,5,5        | 0.09 | 0        | 4,4,4       | 0.18 | 0        |
| 58  | SPD  | 1     | 3332 | -    | 9,9,9        | 0.10 | 0        | 8,8,8       | 0.13 | 0        |
| 60  | PUT  | 2     | 1727 | -    | 5,5,5        | 0.09 | 0        | 4,4,4       | 0.18 | 0        |
| 60  | PUT  | 1     | 3324 | -    | 5,5,5        | 0.10 | 0        | 4,4,4       | 0.15 | 0        |
| 60  | PUT  | 1     | 3326 | -    | 5,5,5        | 0.06 | 0        | 4,4,4       | 0.20 | 0        |
| 60  | PUT  | 1     | 3328 | -    | 5,5,5        | 0.08 | 0        | 4,4,4       | 0.21 | 0        |
| 60  | PUT  | 2     | 1728 | -    | 5,5,5        | 0.14 | 0        | 4,4,4       | 0.16 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 58  | SPD  | 1     | 3209 | -    | -       | 4/7/7/7    | -     |
| 58  | SPD  | 1     | 3210 | -    | -       | 5/7/7/7    | -     |
| 58  | SPD  | 1     | 3208 | -    | -       | 2/7/7/7    | -     |
| 60  | PUT  | Z     | 101  | -    | -       | 3/3/3/3    | -     |
| 58  | SPD  | 1     | 3206 | -    | -       | 0/7/7/7    | -     |
| 58  | SPD  | 1     | 3212 | -    | -       | 3/7/7/7    | -     |
| 60  | PUT  | 1     | 3325 | -    | -       | 1/3/3/3    | -     |
| 60  | PUT  | C     | 301  | -    | -       | 1/3/3/3    | -     |
| 60  | PUT  | 1     | 3323 | -    | -       | 2/3/3/3    | -     |
| 58  | SPD  | 1     | 3205 | -    | -       | 2/7/7/7    | -     |
| 61  | SPM  | 1     | 3213 | -    | -       | 7/11/11/11 | -     |
| 60  | PUT  | 1     | 3330 | -    | -       | 2/3/3/3    | -     |
| 58  | SPD  | 2     | 1687 | -    | -       | 5/7/7/7    | -     |
| 58  | SPD  | 1     | 3204 | -    | -       | 4/7/7/7    | -     |
| 60  | PUT  | 1     | 3331 | -    | -       | 2/3/3/3    | -     |
| 58  | SPD  | 1     | 3207 | -    | -       | 4/7/7/7    | -     |
| 60  | PUT  | 1     | 3329 | -    | -       | 1/3/3/3    | -     |
| 58  | SPD  | 1     | 3203 | -    | -       | 3/7/7/7    | -     |
| 58  | SPD  | 2     | 1686 | -    | -       | 2/7/7/7    | -     |
| 58  | SPD  | 1     | 3211 | -    | -       | 0/7/7/7    | -     |
| 60  | PUT  | 1     | 3327 | -    | -       | 0/3/3/3    | -     |
| 58  | SPD  | 1     | 3332 | -    | -       | 3/7/7/7    | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 60  | PUT  | 2     | 1727 | -    | -       | 0/3/3/3  | -     |
| 60  | PUT  | 1     | 3324 | -    | -       | 3/3/3/3  | -     |
| 60  | PUT  | 1     | 3326 | -    | -       | 1/3/3/3  | -     |
| 60  | PUT  | 1     | 3328 | -    | -       | 1/3/3/3  | -     |
| 60  | PUT  | 2     | 1728 | -    | -       | 0/3/3/3  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (61) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 60  | C     | 301  | PUT  | C1-C2-C3-C4  |
| 58  | 2     | 1686 | SPD  | C4-C5-N6-C7  |
| 58  | 1     | 3207 | SPD  | C3-C4-C5-N6  |
| 58  | 1     | 3208 | SPD  | N6-C7-C8-C9  |
| 58  | 1     | 3204 | SPD  | C3-C4-C5-N6  |
| 58  | 1     | 3209 | SPD  | C3-C4-C5-N6  |
| 58  | 2     | 1687 | SPD  | C3-C4-C5-N6  |
| 61  | 1     | 3213 | SPM  | C7-C8-C9-N10 |
| 58  | 1     | 3210 | SPD  | C3-C4-C5-N6  |
| 58  | 1     | 3207 | SPD  | N6-C7-C8-C9  |
| 60  | 1     | 3326 | PUT  | C1-C2-C3-C4  |
| 58  | 1     | 3204 | SPD  | C4-C5-N6-C7  |
| 60  | 1     | 3330 | PUT  | C1-C2-C3-C4  |
| 58  | 1     | 3207 | SPD  | C2-C3-C4-C5  |
| 58  | 1     | 3209 | SPD  | C4-C5-N6-C7  |
| 60  | 1     | 3325 | PUT  | N1-C1-C2-C3  |
| 58  | 2     | 1687 | SPD  | C8-C7-N6-C5  |
| 58  | 1     | 3205 | SPD  | C8-C7-N6-C5  |
| 58  | 1     | 3212 | SPD  | C4-C5-N6-C7  |
| 58  | 1     | 3332 | SPD  | C4-C5-N6-C7  |
| 61  | 1     | 3213 | SPM  | C3-C4-N5-C6  |
| 58  | 1     | 3204 | SPD  | N6-C7-C8-C9  |
| 58  | 2     | 1687 | SPD  | C7-C8-C9-N10 |
| 60  | 1     | 3331 | PUT  | C2-C3-C4-N2  |
| 60  | 1     | 3331 | PUT  | N1-C1-C2-C3  |
| 60  | Z     | 101  | PUT  | N1-C1-C2-C3  |
| 60  | 1     | 3329 | PUT  | C1-C2-C3-C4  |
| 58  | 2     | 1687 | SPD  | C2-C3-C4-C5  |
| 60  | 1     | 3324 | PUT  | C1-C2-C3-C4  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 58  | 1     | 3210 | SPD  | C2-C3-C4-C5     |
| 58  | 1     | 3209 | SPD  | C2-C3-C4-C5     |
| 58  | 1     | 3203 | SPD  | C3-C4-C5-N6     |
| 58  | 1     | 3204 | SPD  | C2-C3-C4-C5     |
| 58  | 1     | 3332 | SPD  | C8-C7-N6-C5     |
| 61  | 1     | 3213 | SPM  | C8-C9-N10-C11   |
| 61  | 1     | 3213 | SPM  | C12-C11-N10-C9  |
| 60  | 1     | 3323 | PUT  | N1-C1-C2-C3     |
| 61  | 1     | 3213 | SPM  | C6-C7-C8-C9     |
| 58  | 1     | 3207 | SPD  | C4-C5-N6-C7     |
| 58  | 1     | 3203 | SPD  | N1-C2-C3-C4     |
| 60  | 1     | 3324 | PUT  | C2-C3-C4-N2     |
| 60  | 1     | 3330 | PUT  | C2-C3-C4-N2     |
| 58  | 1     | 3212 | SPD  | C8-C7-N6-C5     |
| 58  | 1     | 3210 | SPD  | N1-C2-C3-C4     |
| 61  | 1     | 3213 | SPM  | C11-C12-C13-N14 |
| 58  | 1     | 3210 | SPD  | C8-C7-N6-C5     |
| 60  | Z     | 101  | PUT  | C1-C2-C3-C4     |
| 58  | 1     | 3212 | SPD  | C2-C3-C4-C5     |
| 58  | 1     | 3203 | SPD  | C8-C7-N6-C5     |
| 60  | 1     | 3324 | PUT  | N1-C1-C2-C3     |
| 60  | 1     | 3328 | PUT  | C1-C2-C3-C4     |
| 58  | 2     | 1687 | SPD  | C4-C5-N6-C7     |
| 61  | 1     | 3213 | SPM  | C7-C6-N5-C4     |
| 58  | 1     | 3208 | SPD  | C7-C8-C9-N10    |
| 58  | 1     | 3205 | SPD  | C4-C5-N6-C7     |
| 58  | 1     | 3209 | SPD  | N1-C2-C3-C4     |
| 58  | 1     | 3210 | SPD  | C4-C5-N6-C7     |
| 60  | 1     | 3323 | PUT  | C1-C2-C3-C4     |
| 58  | 2     | 1686 | SPD  | C2-C3-C4-C5     |
| 58  | 1     | 3332 | SPD  | N1-C2-C3-C4     |
| 60  | Z     | 101  | PUT  | C2-C3-C4-N2     |

There are no ring outliers.

11 monomers are involved in 19 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58  | 1     | 3209 | SPD  | 1       | 0            |
| 60  | 1     | 3325 | PUT  | 1       | 0            |
| 60  | C     | 301  | PUT  | 1       | 0            |
| 60  | 1     | 3330 | PUT  | 2       | 0            |
| 58  | 2     | 1687 | SPD  | 6       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 60  | 1     | 3331 | PUT  | 1       | 0            |
| 58  | 1     | 3207 | SPD  | 1       | 0            |
| 58  | 1     | 3203 | SPD  | 1       | 0            |
| 58  | 2     | 1686 | SPD  | 1       | 0            |
| 60  | 2     | 1727 | PUT  | 1       | 0            |
| 60  | 2     | 1728 | PUT  | 3       | 0            |

## 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.

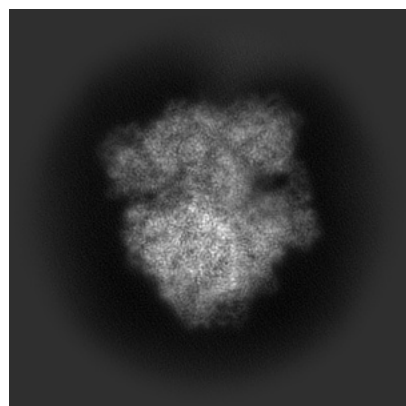
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17348. These allow visual inspection of the internal detail of the map and identification of artifacts.

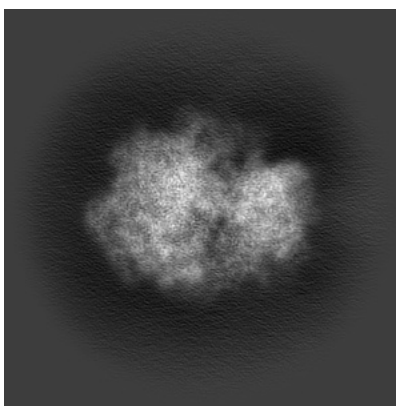
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

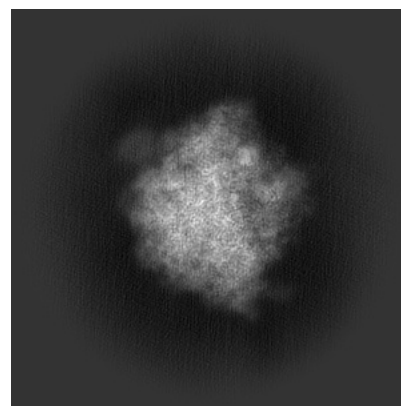
#### 6.1.1 Primary map



X

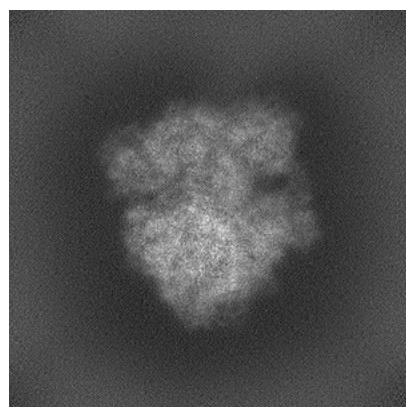


Y

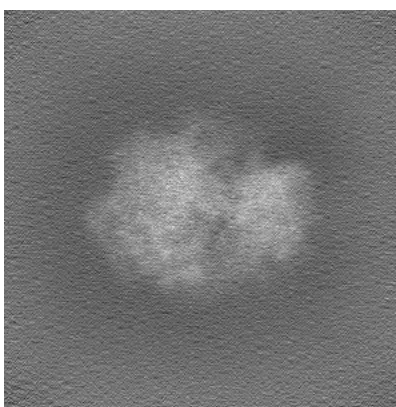


Z

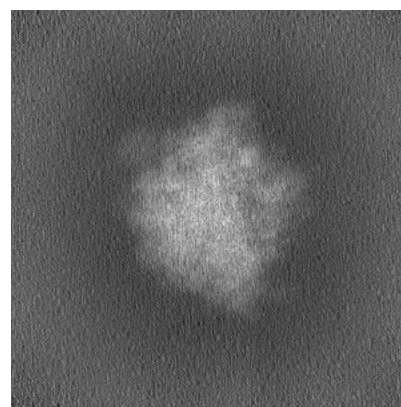
#### 6.1.2 Raw map



X



Y

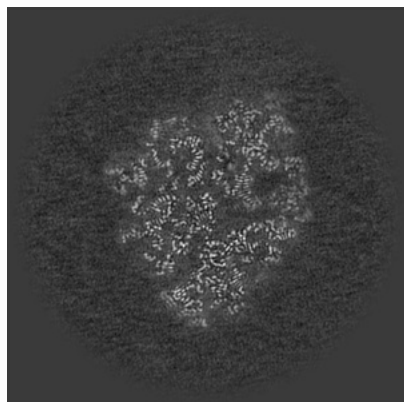


Z

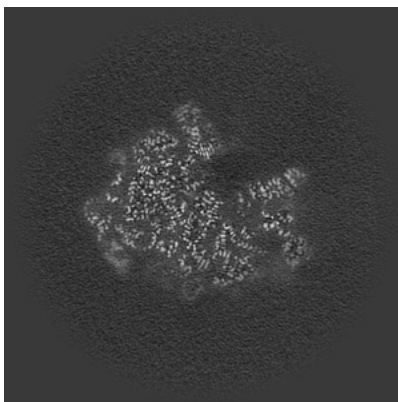
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

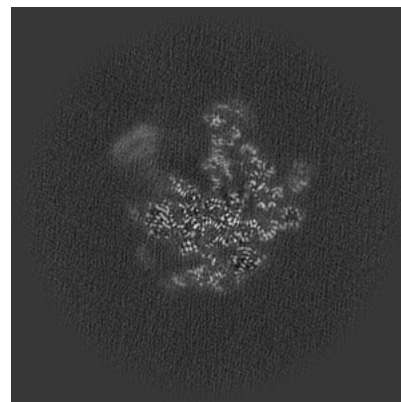
### 6.2.1 Primary map



X Index: 260

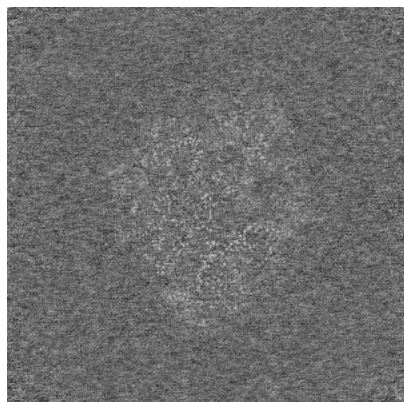


Y Index: 260

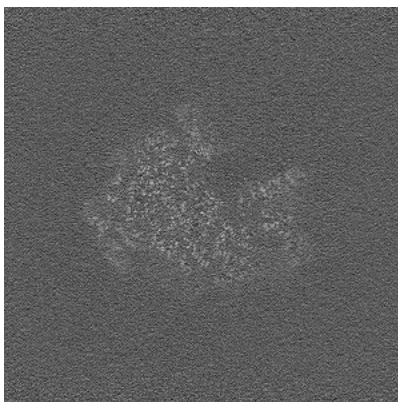


Z Index: 260

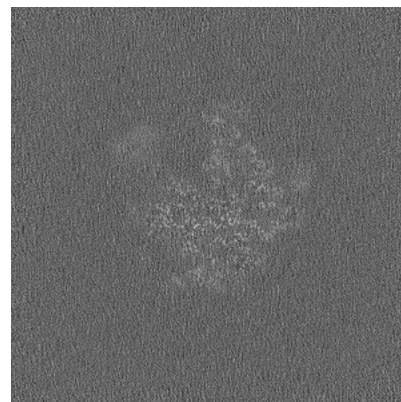
### 6.2.2 Raw map



X Index: 260



Y Index: 260

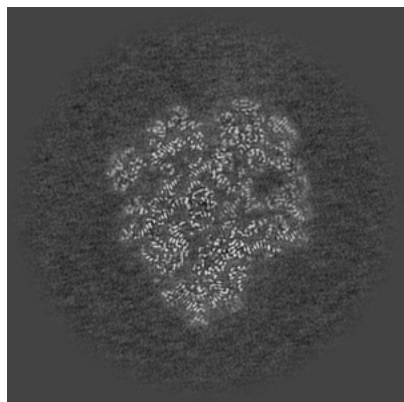


Z Index: 260

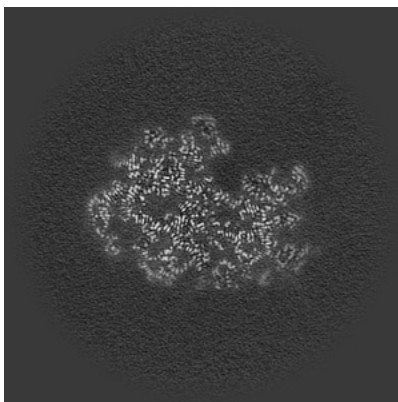
The images above show central slices of the map in three orthogonal directions.

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

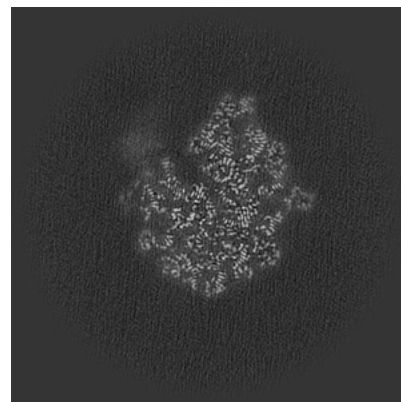
### 6.3.1 Primary map



X Index: 265

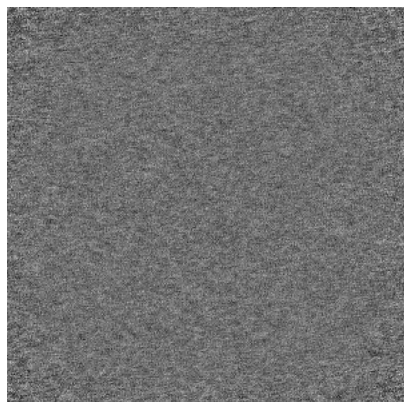


Y Index: 246

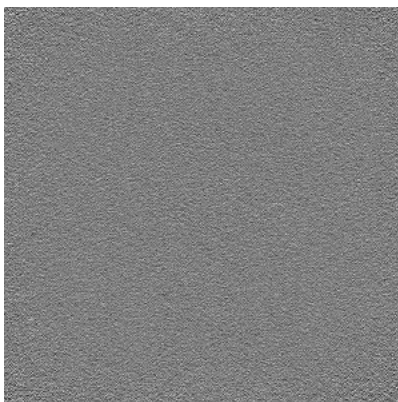


Z Index: 231

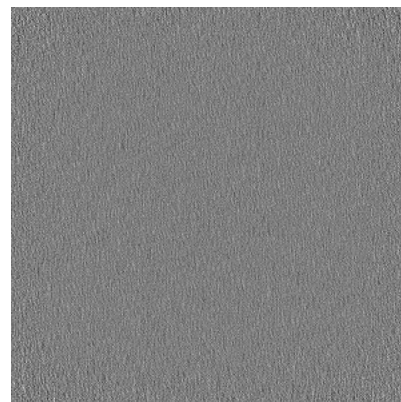
### 6.3.2 Raw map



X Index: 0



Y Index: 0

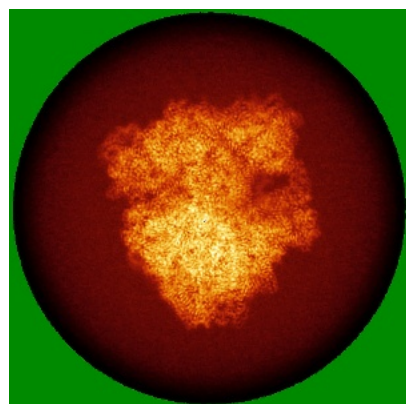


Z Index: 0

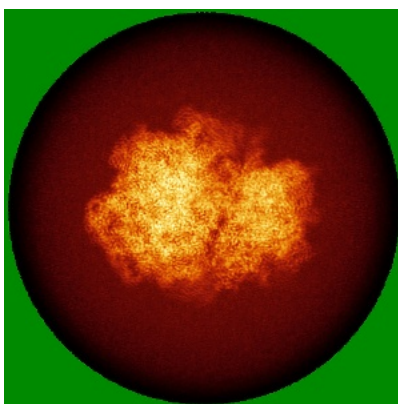
The images above show the largest variance slices of the map in three orthogonal directions.

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

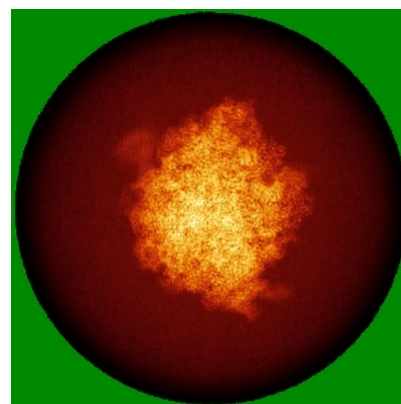
### 6.4.1 Primary map



X

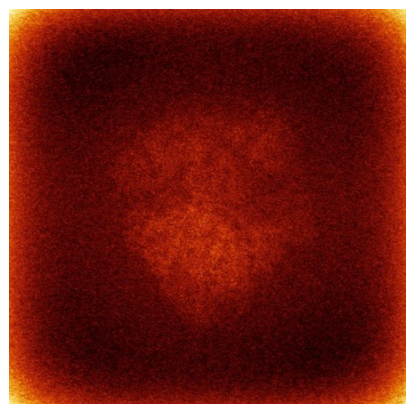


Y

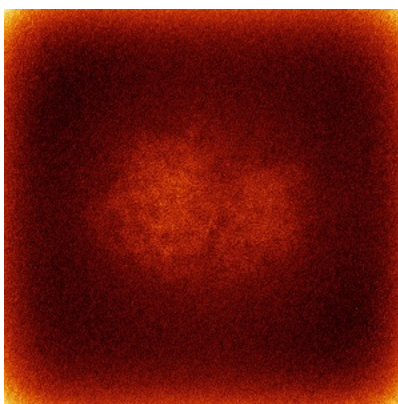


Z

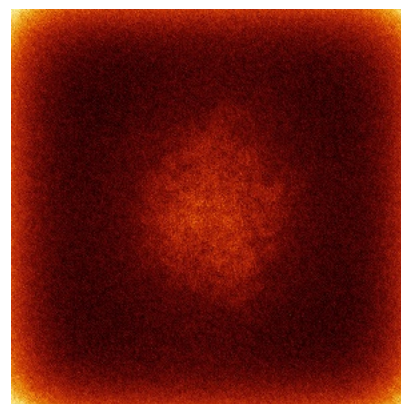
### 6.4.2 Raw map



X



Y



Z

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

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

### 6.5.1 Primary map



X



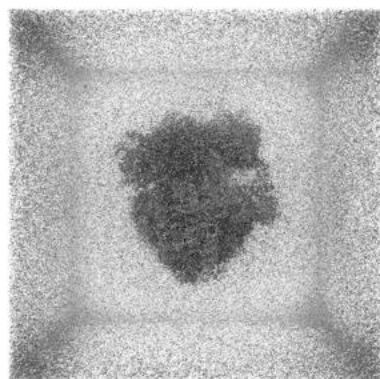
Y



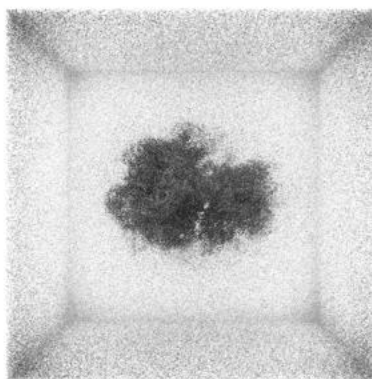
Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

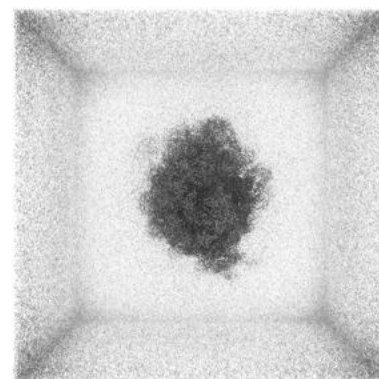
### 6.5.2 Raw map



X



Y



Z

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

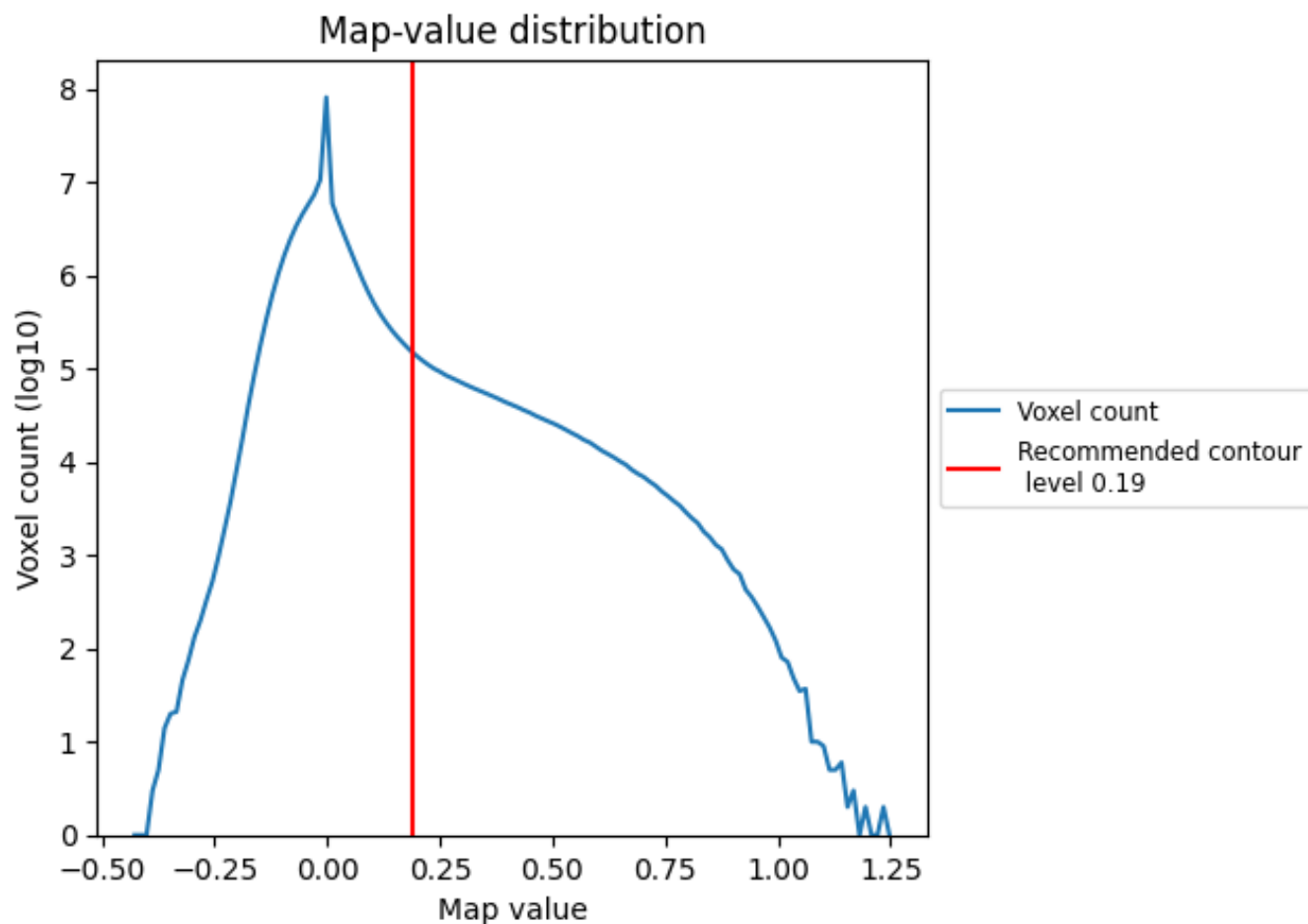
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

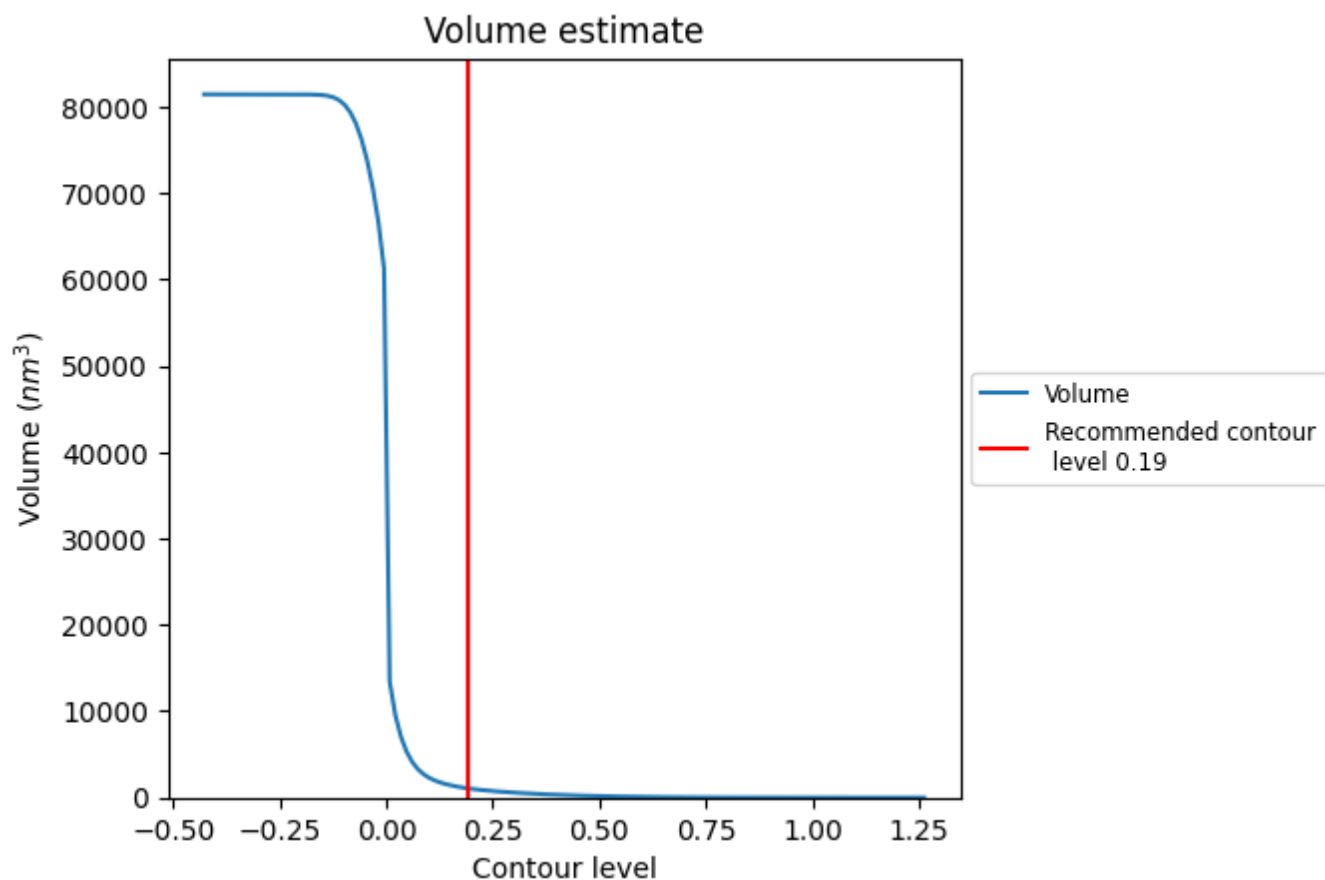
This section contains the results of statistical analysis of the map.

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



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

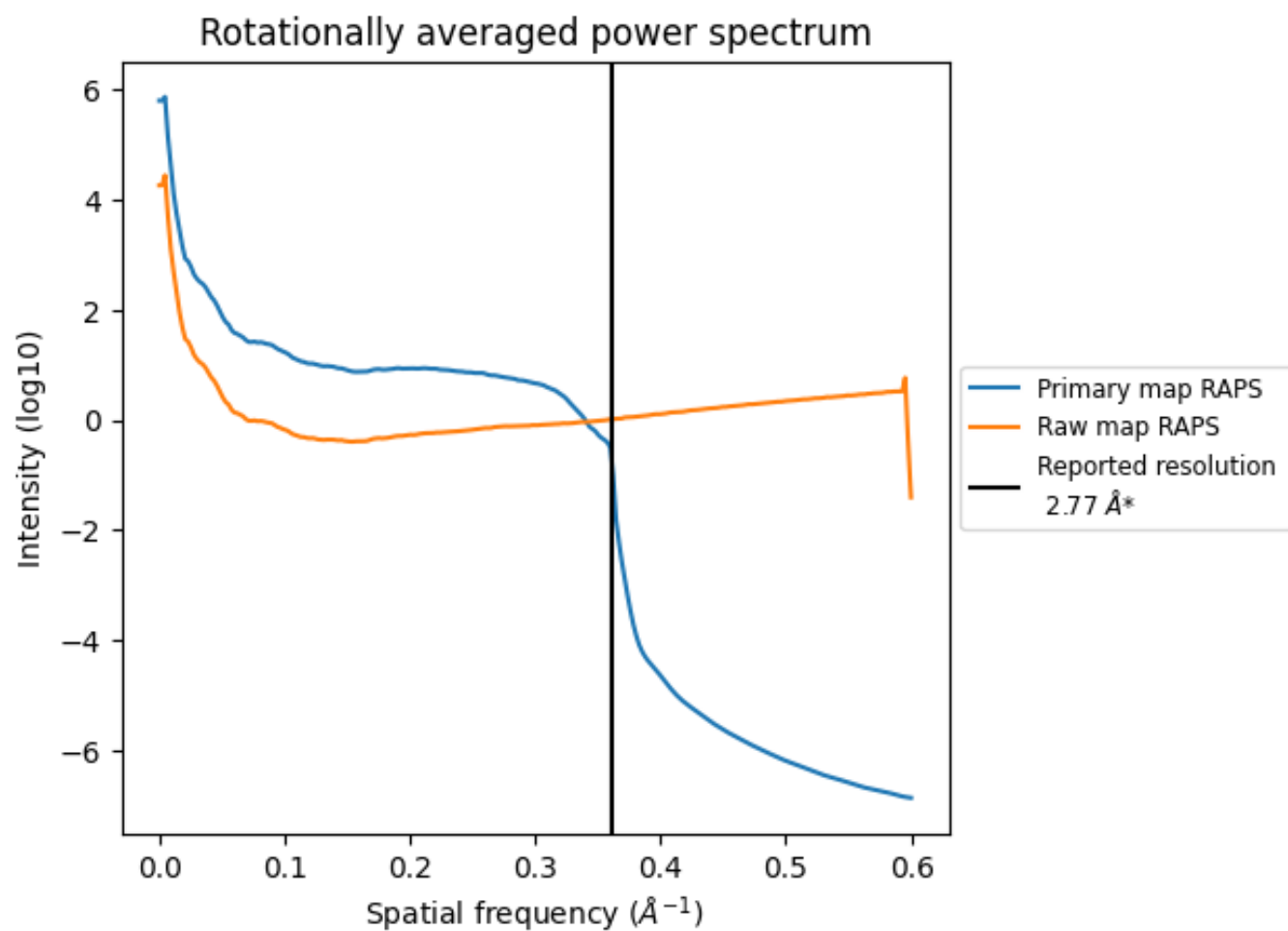
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1074 nm<sup>3</sup>; this corresponds to an approximate mass of 970 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 ⓘ

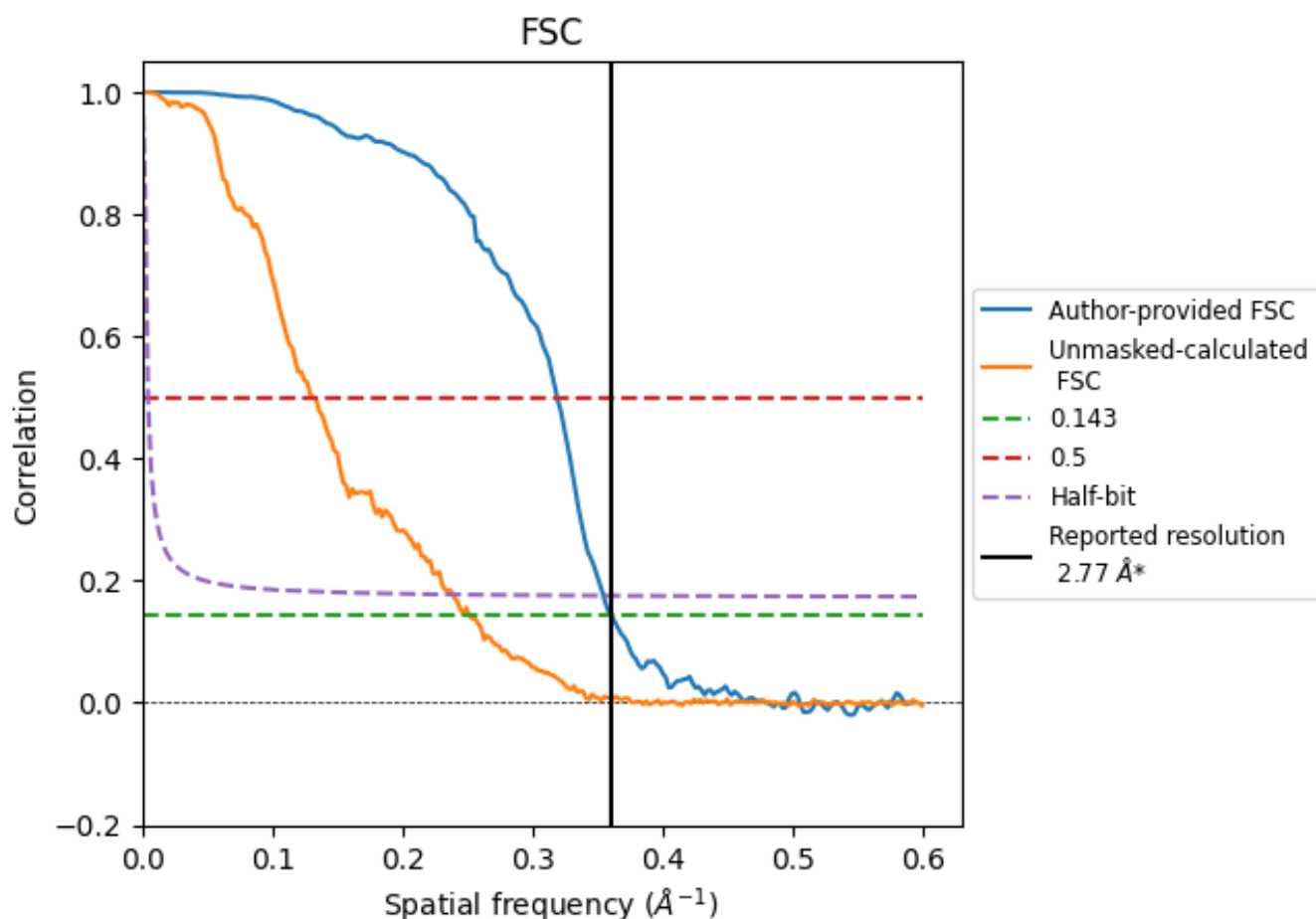


\*Reported resolution corresponds to spatial frequency of 0.361  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.361 Å<sup>-1</sup>

## 8.2 Resolution estimates

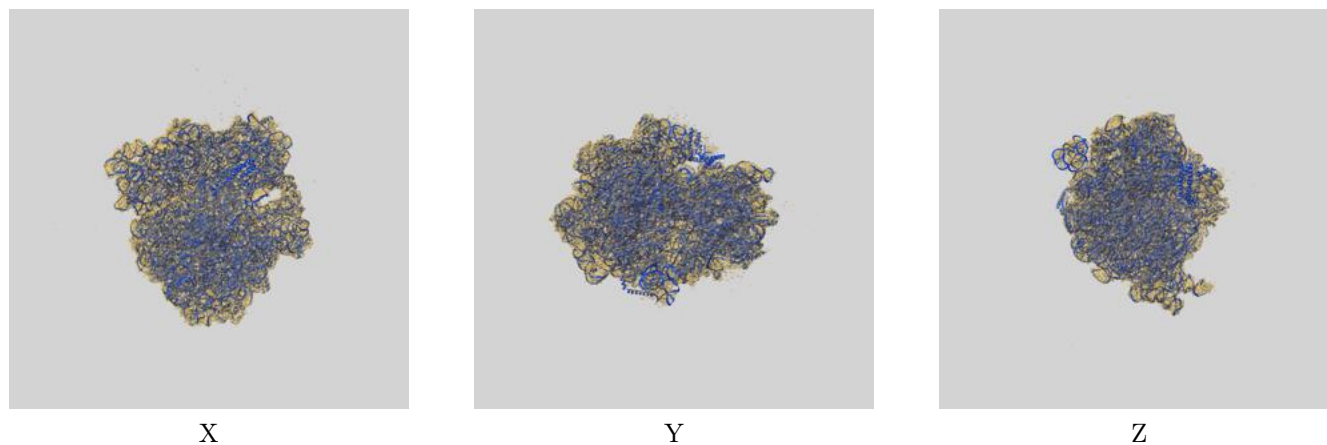
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.77                               | -    | -        |
| Author-provided FSC curve | 2.77                               | 3.13 | 2.82     |
| Unmasked-calculated*      | 3.98                               | 7.59 | 4.19     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.77 by more than 10 %

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

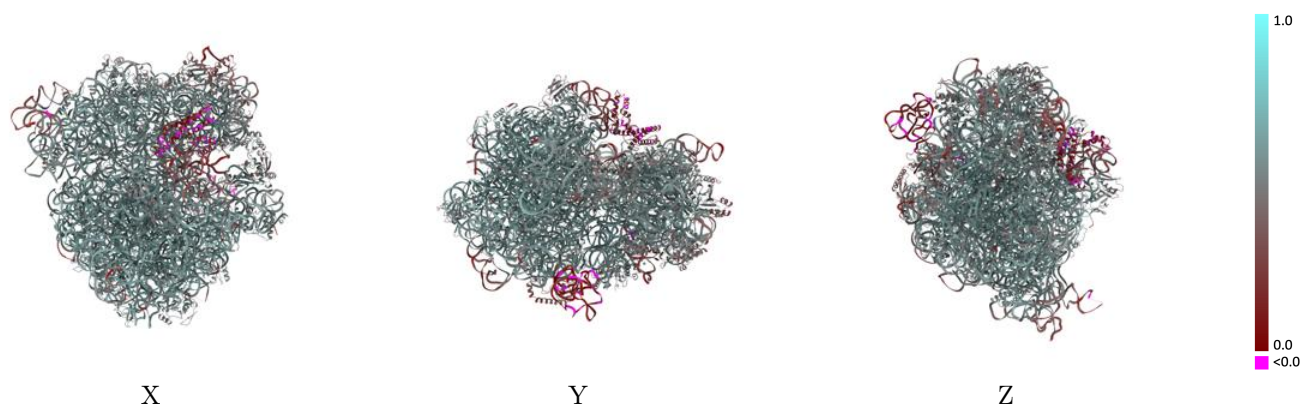
This section contains information regarding the fit between EMDB map EMD-17348 and PDB model 8P18. Per-residue inclusion information can be found in section 3 on page 18.

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



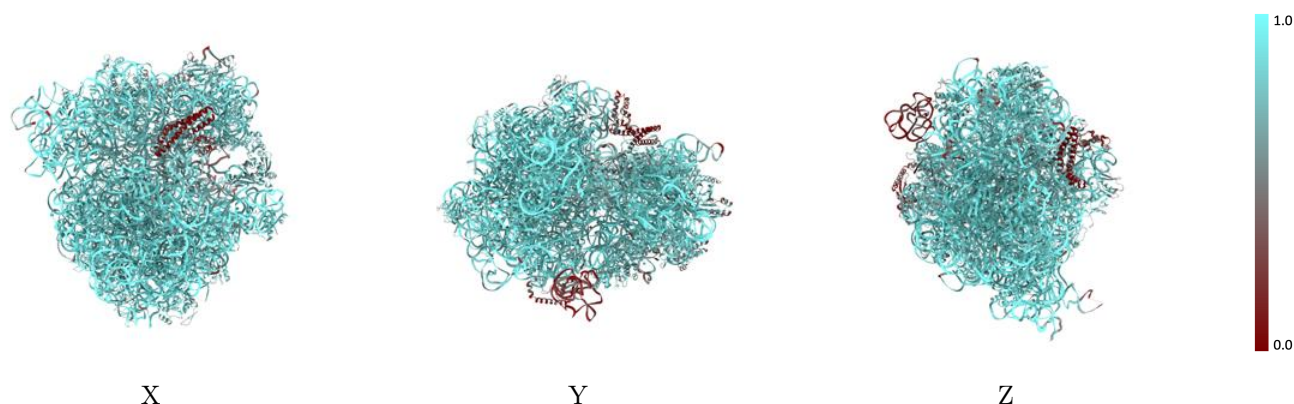
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



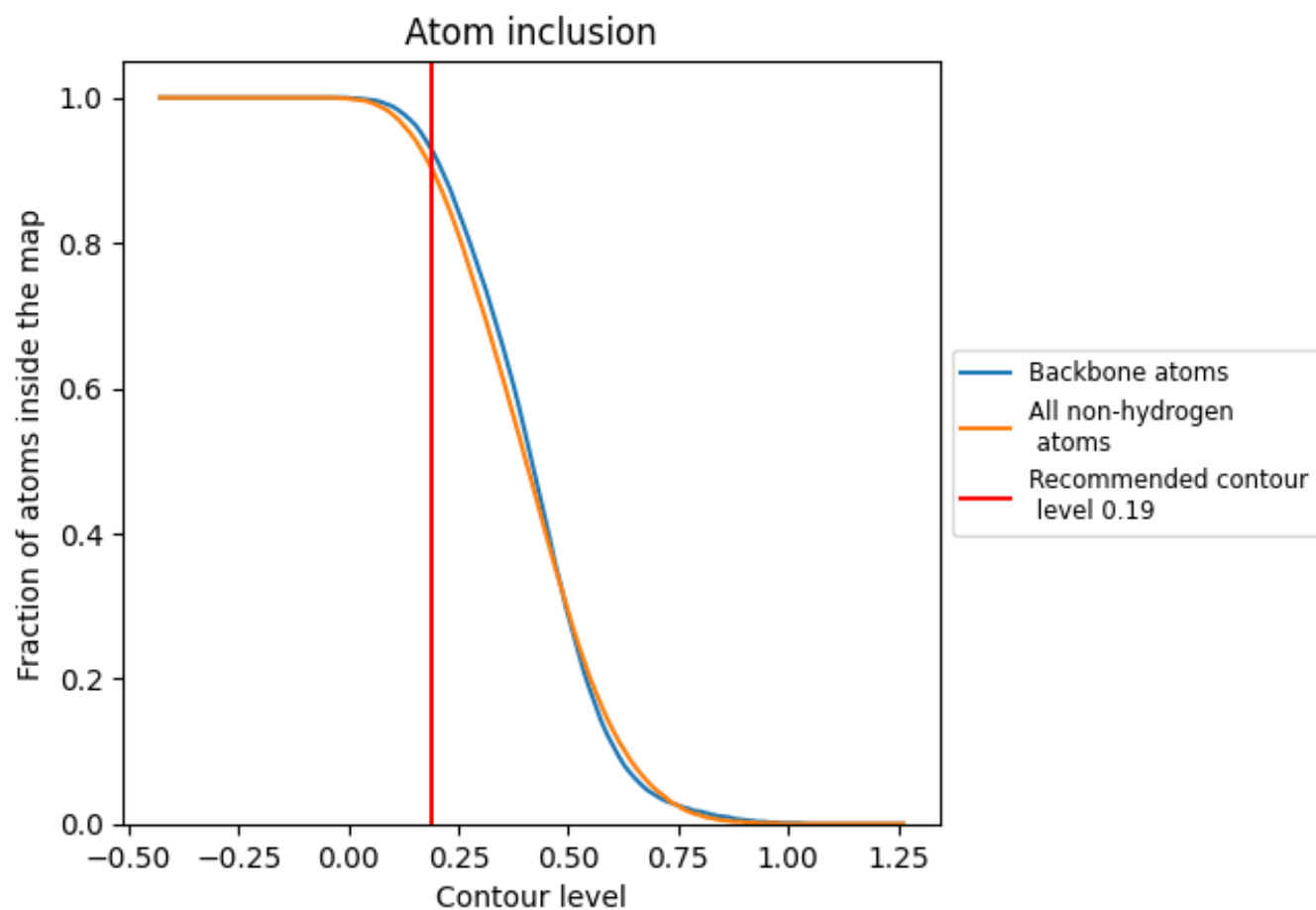
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.19) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9020   |  0.5460   |
| 1     |  0.9440   |  0.5630   |
| 2     |  0.9530   |  0.5520   |
| 3     |  0.9530   |  0.5470   |
| 4     |  0.6740   |  0.3210   |
| 5     |  0.9030   |  0.5440   |
| 6     |  0.5470   |  0.3810   |
| B     |  0.9290   |  0.5990   |
| C     |  0.9050   |  0.5850   |
| D     |  0.8590   |  0.5580   |
| E     |  0.7550   |  0.4960   |
| F     |  0.7560   |  0.4750   |
| G     |  0.3430   |  0.3730   |
| I     |  0.2240   |  0.1380   |
| J     |  0.9220  |  0.5850  |
| K     |  0.8550 |  0.5690 |
| L     |  0.8890 |  0.5710 |
| M     |  0.8750 |  0.5690 |
| N     |  0.9470 |  0.5950 |
| O     |  0.8470 |  0.5280 |
| P     |  0.8570 |  0.5720 |
| Q     |  0.9380 |  0.5990 |
| R     |  0.8920 |  0.5690 |
| S     |  0.9050 |  0.5730 |
| T     |  0.8640 |  0.5380 |
| U     |  0.8420 |  0.5240 |
| V     |  0.8250 |  0.5290 |
| W     |  0.8900 |  0.5560 |
| X     |  0.8970 |  0.5840 |
| Y     |  0.7850 |  0.4950 |
| Z     |  0.8760 |  0.5560 |
| a     |  0.6670 |  0.4290 |
| b     |  0.9040 |  0.5730 |
| c     |  0.8410 |  0.5390 |
| d     |  0.9580 |  0.6150 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| e     |  0.9370   |  0.6080   |
| f     |  0.9040   |  0.5680   |
| g     |  0.6980   |  0.4560   |
| h     |  0.8280   |  0.5140   |
| i     |  0.8570   |  0.5260   |
| j     |  0.8950   |  0.5600   |
| k     |  0.8150   |  0.5170   |
| l     |  0.7710   |  0.4800   |
| m     |  0.8750   |  0.5600   |
| n     |  0.8180   |  0.4930   |
| o     |  0.7360   |  0.4510   |
| p     |  0.8410   |  0.5420   |
| q     |  0.8700   |  0.5660   |
| r     |  0.8250   |  0.5160   |
| s     |  0.8580   |  0.5240   |
| t     |  0.8350   |  0.5380   |
| u     |  0.8860   |  0.5440   |
| v     |  0.8080   |  0.5180   |
| w     |  0.8110   |  0.5280   |
| x     |  0.7940  |  0.5070  |
| y     |  0.8550 |  0.5280 |
| z     |  0.7160 |  0.4530 |