



# Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 11:56 AM JST

PDB ID : 8HU1 / pdb\_00008hu1  
EMDB ID : EMD-35022  
Title : E. coli 70S ribosome complexed with tRNA\_Ile2 bearing L34 and ct6A37 in classical state  
Authors : Akiyama, N.; Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.  
Deposited on : 2022-12-22  
Resolution : 2.69 Å(reported)  
Based on initial model : 7K00

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 : 1.8.5 (274361), 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

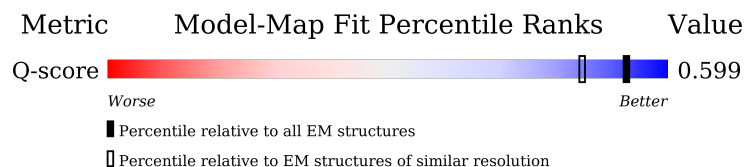
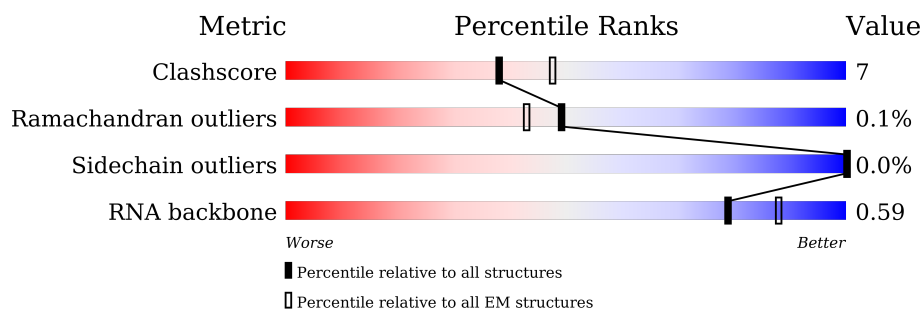
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.69 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                       | 9309 ( 2.19 - 3.19 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1542   |                  |
| 2   | B     | 241    |                  |
| 3   | C     | 233    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | D     | 206    |                  |
| 5   | E     | 167    |                  |
| 6   | F     | 135    |                  |
| 7   | G     | 179    |                  |
| 8   | H     | 130    |                  |
| 9   | I     | 130    |                  |
| 10  | J     | 103    |                  |
| 11  | K     | 129    |                  |
| 12  | L     | 124    |                  |
| 13  | M     | 118    |                  |
| 14  | N     | 101    |                  |
| 15  | O     | 89     |                  |
| 16  | P     | 82     |                  |
| 17  | Q     | 84     |                  |
| 18  | R     | 75     |                  |
| 19  | S     | 92     |                  |
| 20  | T     | 87     |                  |
| 21  | U     | 71     |                  |
| 22  | a     | 2904   |                  |
| 23  | b     | 120    |                  |
| 24  | c     | 273    |                  |
| 25  | d     | 209    |                  |
| 26  | e     | 201    |                  |
| 27  | f     | 179    |                  |
| 28  | g     | 177    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | h     | 149    |                  |
| 30  | i     | 142    |                  |
| 31  | j     | 123    |                  |
| 32  | k     | 144    |                  |
| 33  | l     | 136    |                  |
| 34  | m     | 127    |                  |
| 35  | n     | 117    |                  |
| 36  | o     | 115    |                  |
| 37  | p     | 118    |                  |
| 38  | q     | 103    |                  |
| 39  | r     | 110    |                  |
| 40  | s     | 100    |                  |
| 41  | t     | 104    |                  |
| 42  | u     | 94     |                  |
| 43  | v     | 85     |                  |
| 44  | w     | 78     |                  |
| 45  | x     | 63     |                  |
| 46  | y     | 59     |                  |
| 47  | z     | 57     |                  |
| 48  | 0     | 55     |                  |
| 49  | 1     | 46     |                  |
| 50  | 2     | 65     |                  |
| 51  | 3     | 38     |                  |
| 52  | 4     | 70     |                  |
| 53  | V     | 76     |                  |

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| Mol | Chain | Length | Quality of chain                               |
|-----|-------|--------|------------------------------------------------|
| 54  | W     | 48     | <div><div></div><div>12%6%•77%</div></div>     |
| 55  | X     | 76     | <div><div></div><div>11%50%30%16%•</div></div> |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141875 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   | A     | 1519     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32612 | 14552 | 5986 | 10555 | 1519 |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 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   | G     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 750 | 231 | 218 | 4 |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 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  |
|-------|---------|----------|--------|------------------|------------|
| K     | 119     | IAS      | ASN    | modified residue | UNP P0A7R9 |

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 22  | a     | 2753     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 59130 | 26384 | 10897 | 19096 | 2753 |         |       |

- Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 23  | b     | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2549  | 1135 | 466 | 829 | 119 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | c     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | d     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 980 | 288 | 294 | 4 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | e     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | f     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | g     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | h     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 303   | 194 | 54 | 54 | 1 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | i     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | j     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | k     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | l     | 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  |
|-------|---------|----------|--------|------------------|------------|
| 1     | 82      | MS6      | MET    | modified residue | UNP P0ADY7 |

- Molecule 34 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | m     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 585 | 194 | 161 | 5 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 35  | n     | 116      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | o     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 37  | p     | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | q     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | r     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | s     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | t     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | u     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | v     | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 586   | 362 | 116 | 107 | 1 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | w     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 45  | x     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46  | y     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47  | z     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 48  | 0     | 51       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 417   | 269 | 76 | 72 |  |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | 1     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 50  | 2     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | 3     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52  | 4     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 480   | 299 | 90 | 85 | 6 |         |       |

- Molecule 53 is a RNA chain called P-site tRNA\_Glu.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 53  | V     | 76       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1619  | 724 | 288 | 530 | 76 | 1 |         |       |

- Molecule 54 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 54  | W     | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 236   | 106 | 44 | 75 | 11 |         |       |

- Molecule 55 is a RNA chain called A-site tRNA\_Ile2.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 55  | X     | 76       | Total | C   | N   | O   | P  | S       | 0     | 0 |
|     |       |          | 1646  | 740 | 292 | 537 | 76 | 1       |       |   |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 56  | A     | 92       | Total | Mg  | 0       |
|     |       |          | 92    | 92  |         |
| 56  | E     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 56  | M     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 56  | N     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 56  | a     | 210      | Total | Mg  | 0       |
|     |       |          | 210   | 210 |         |
| 56  | b     | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 56  | d     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 56  | V     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 56  | X     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

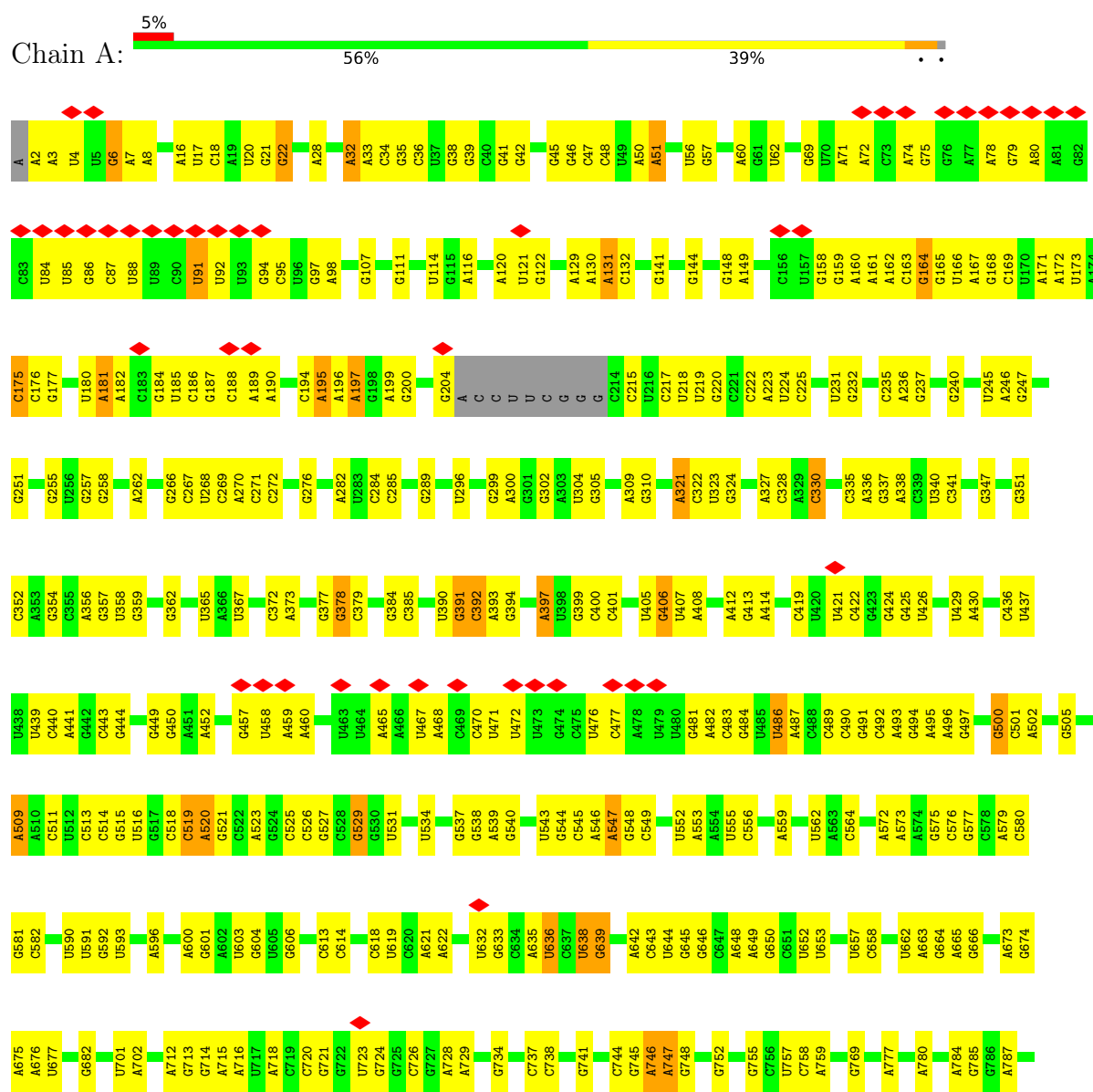
- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

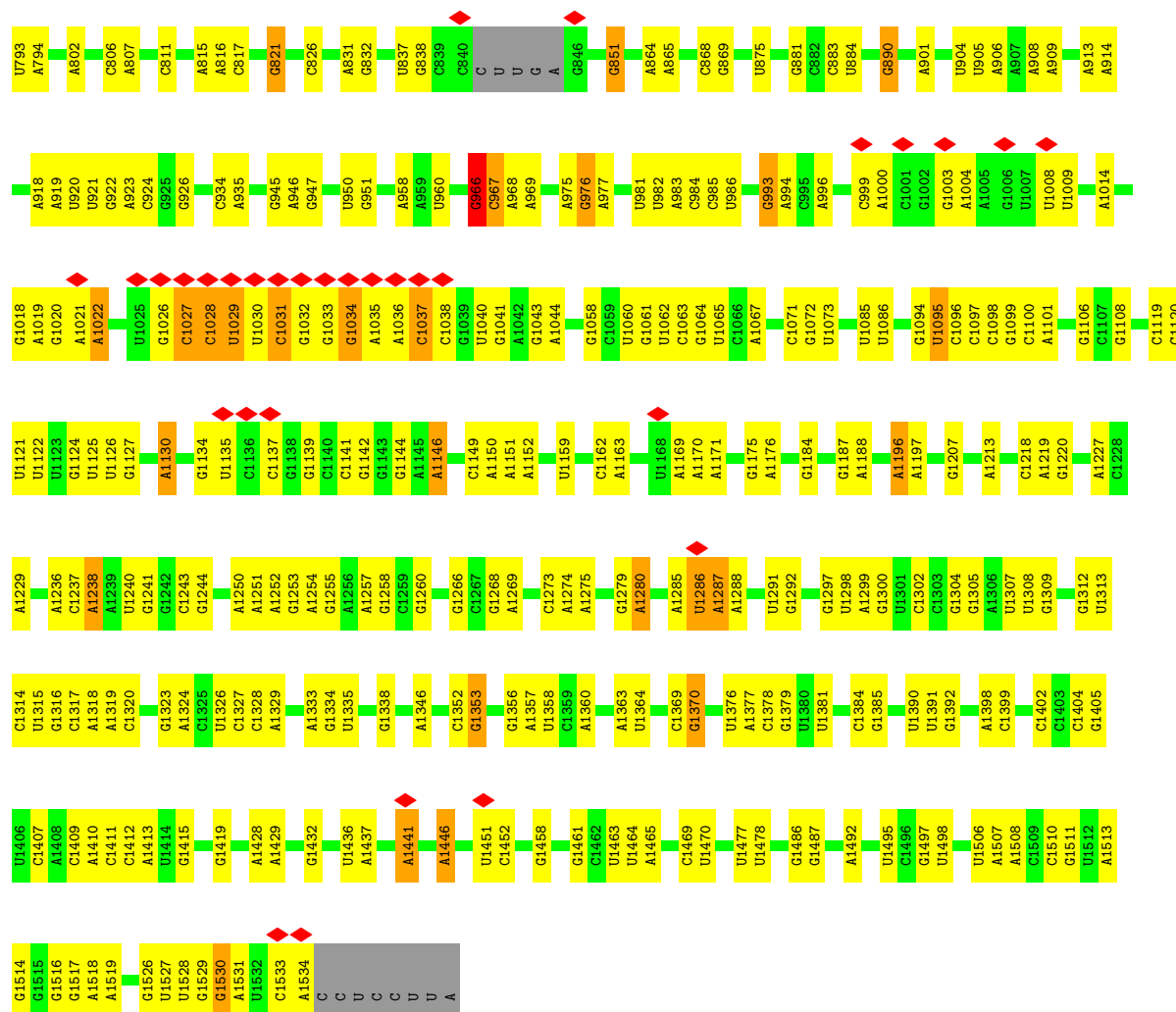
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 57  | A     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

### 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.

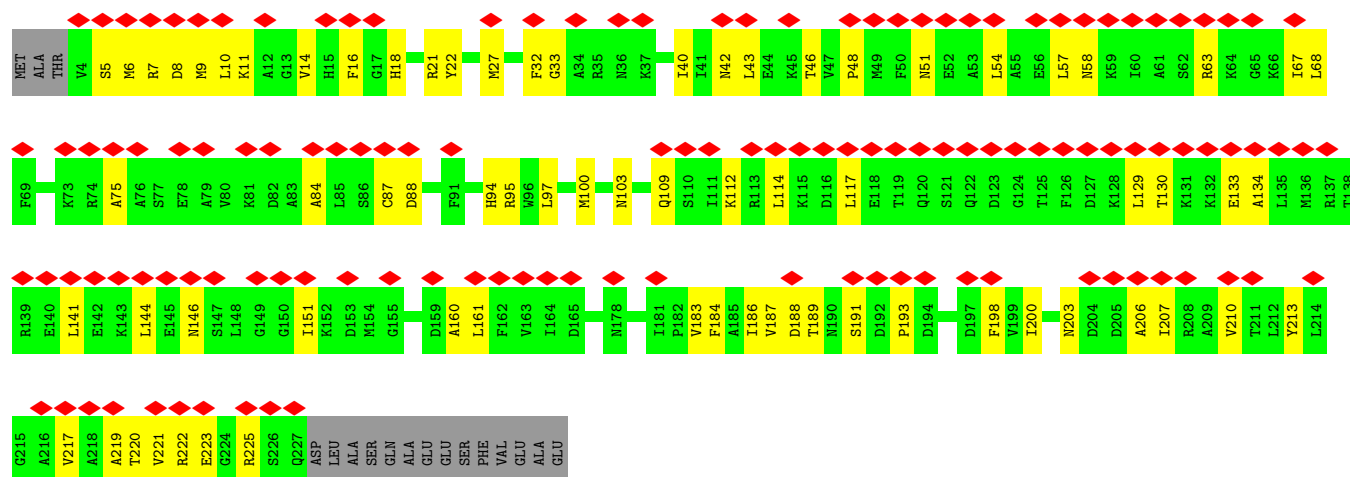
#### • Molecule 1: 16S rRNA



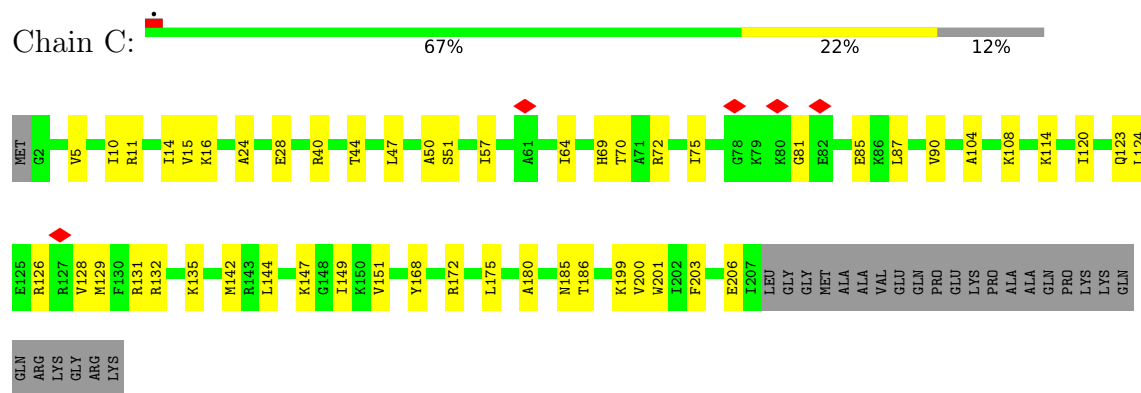


### • Molecule 2: 30S ribosomal protein S2

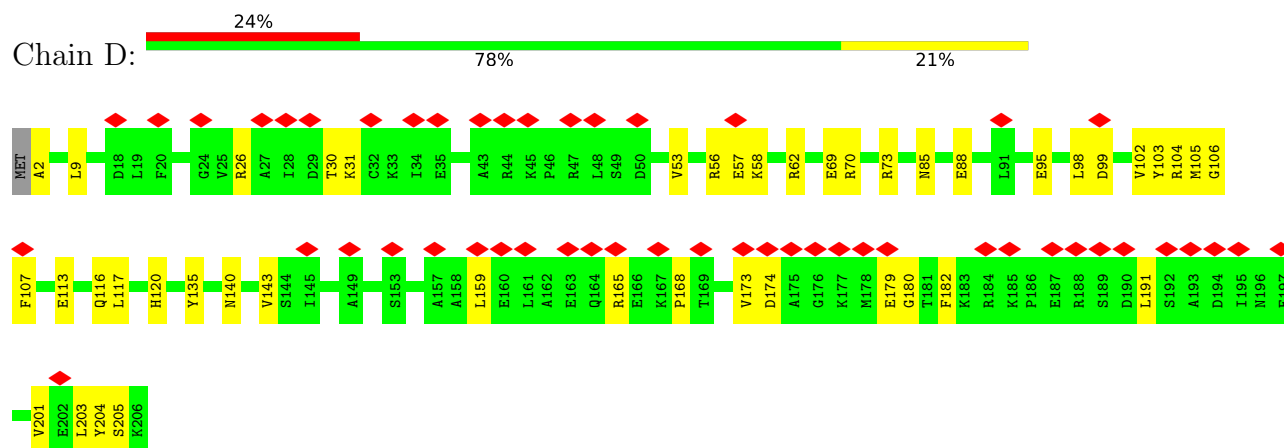
Chain B:



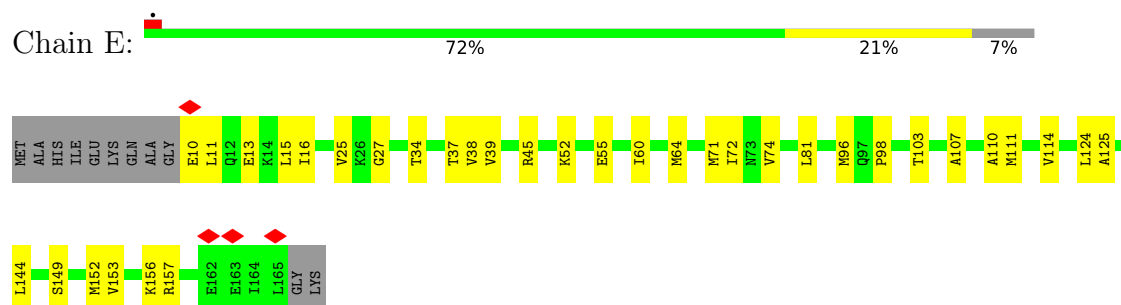
### • Molecule 3: 30S ribosomal protein S3



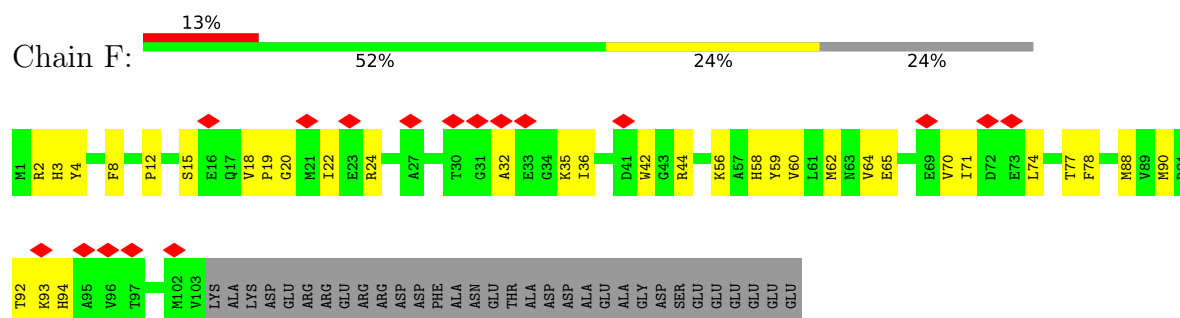
• Molecule 4: 30S ribosomal protein S4



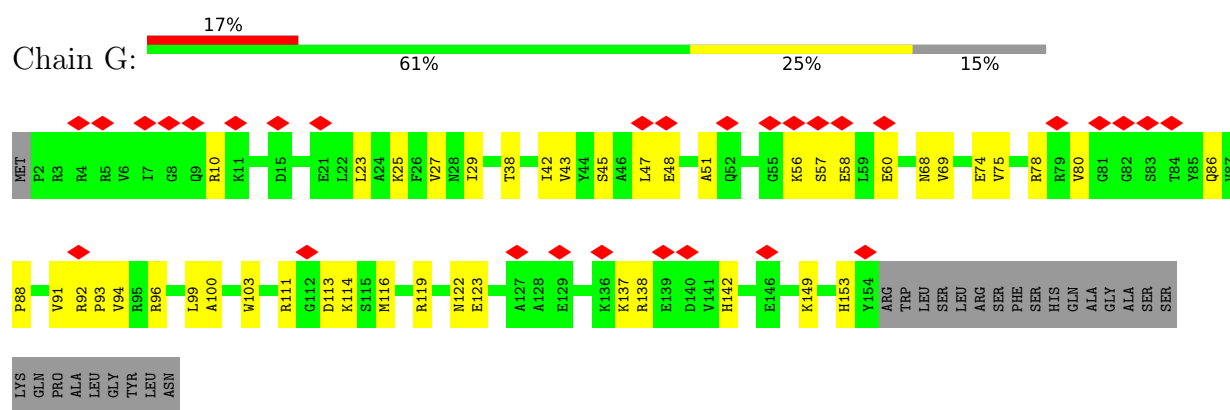
• Molecule 5: 30S ribosomal protein S5



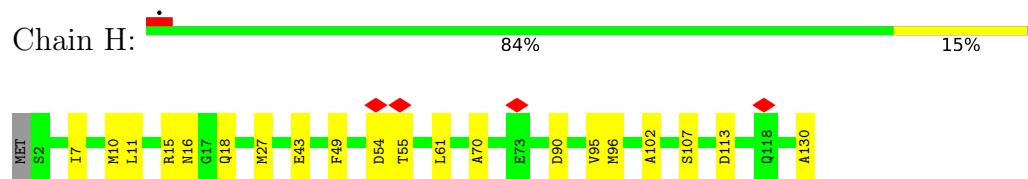
• Molecule 6: 30S ribosomal protein S6, fully modified isoform



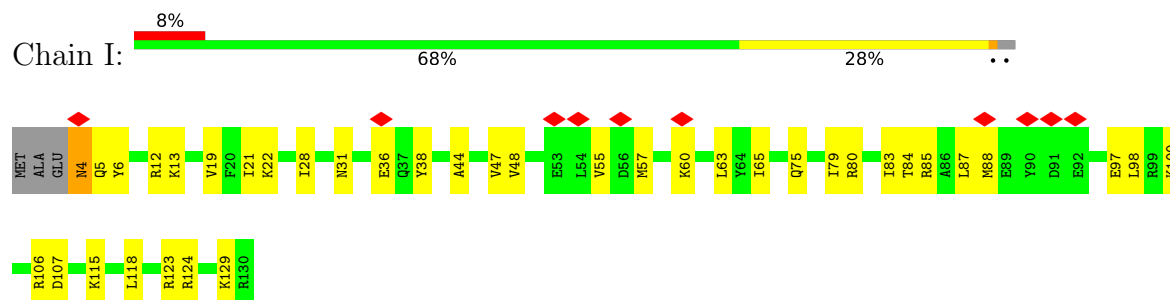
• Molecule 7: 30S ribosomal protein S7



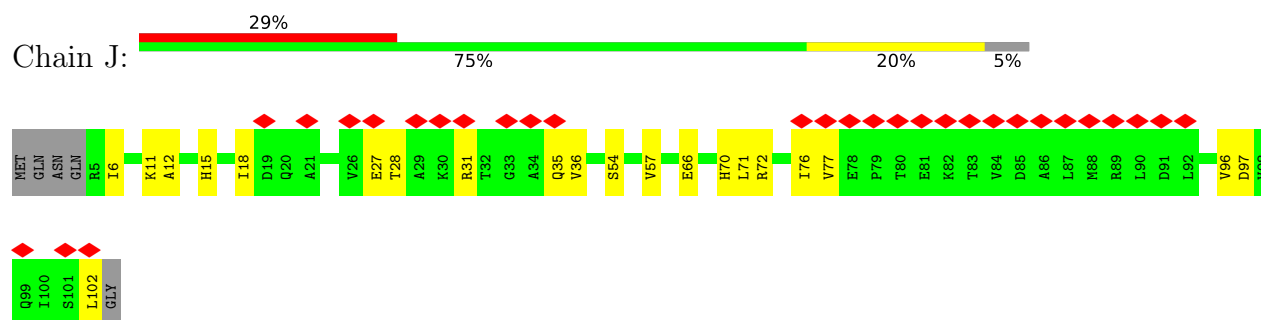
- Molecule 8: 30S ribosomal protein S8



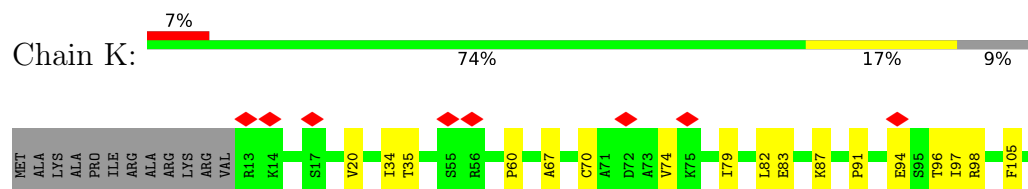
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

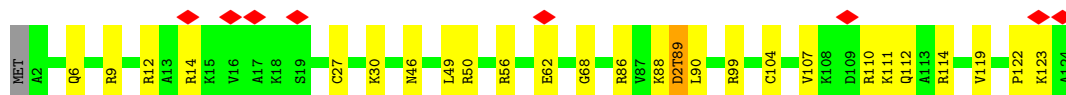
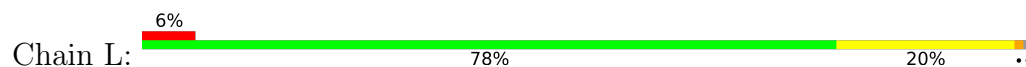


- Molecule 11: 30S ribosomal protein S11

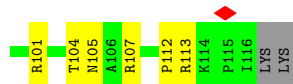




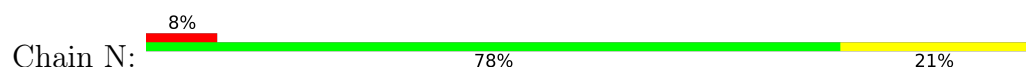
- Molecule 12: 30S ribosomal protein S12



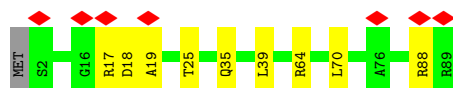
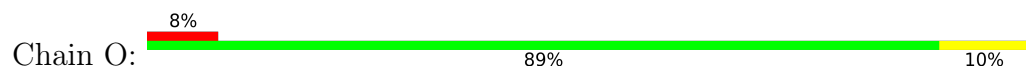
- Molecule 13: 30S ribosomal protein S13



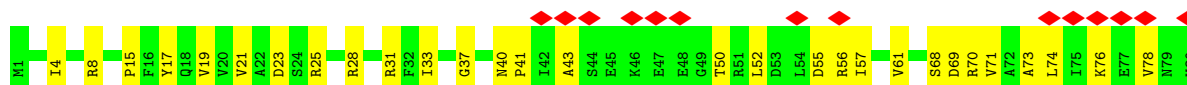
- Molecule 14: 30S ribosomal protein S14



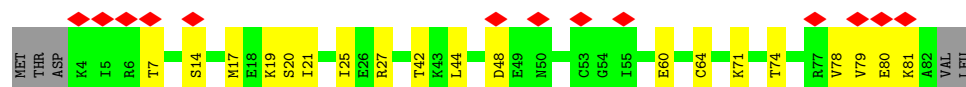
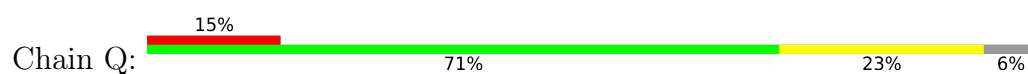
- Molecule 15: 30S ribosomal protein S15



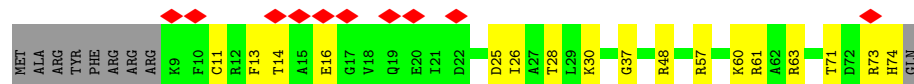
- Molecule 16: 30S ribosomal protein S16



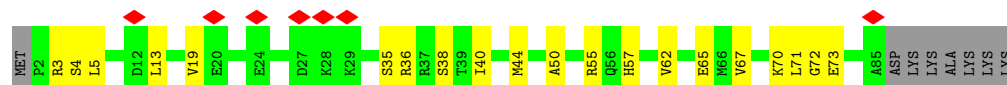
- Molecule 17: 30S ribosomal protein S17



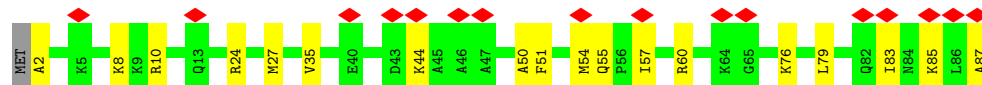
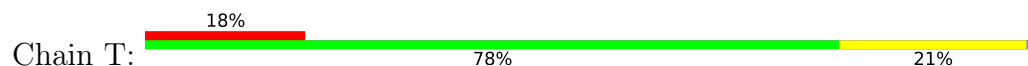
- Molecule 18: 30S ribosomal protein S18



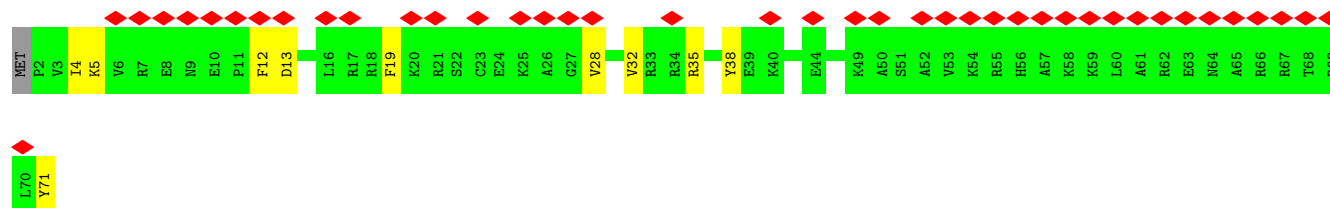
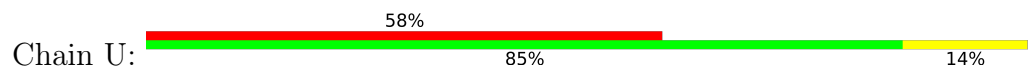
- Molecule 19: 30S ribosomal protein S19



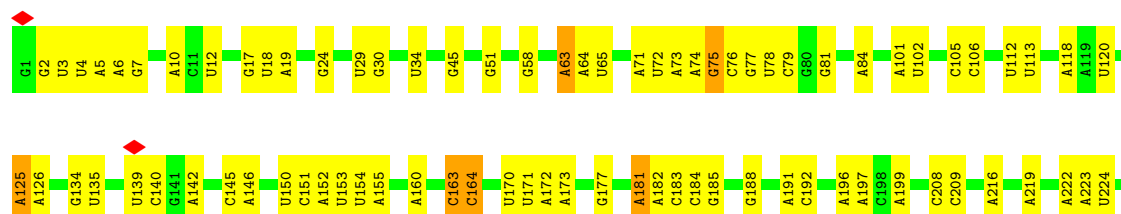
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA

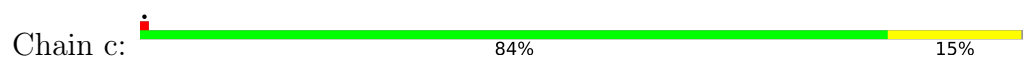




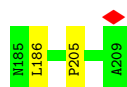
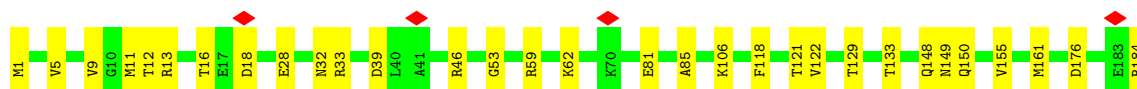
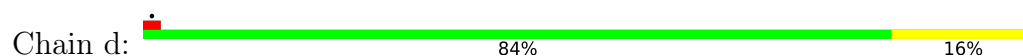




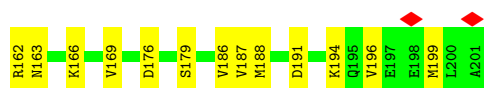
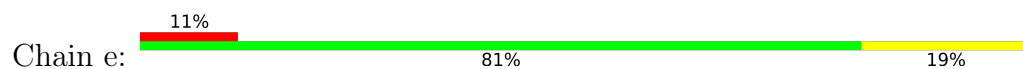
- Molecule 24: 50S ribosomal protein L2



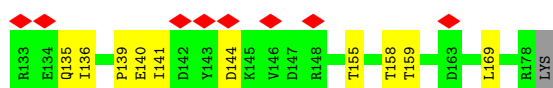
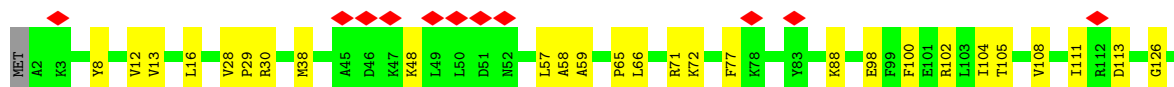
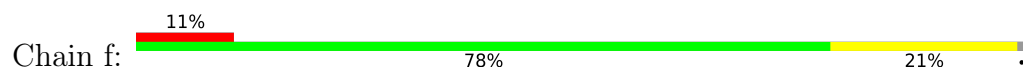
- Molecule 25: 50S ribosomal protein L3



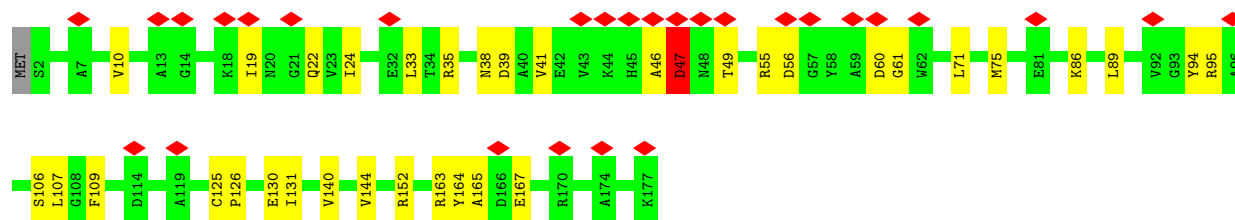
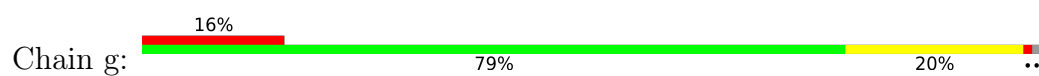
- Molecule 26: 50S ribosomal protein L4



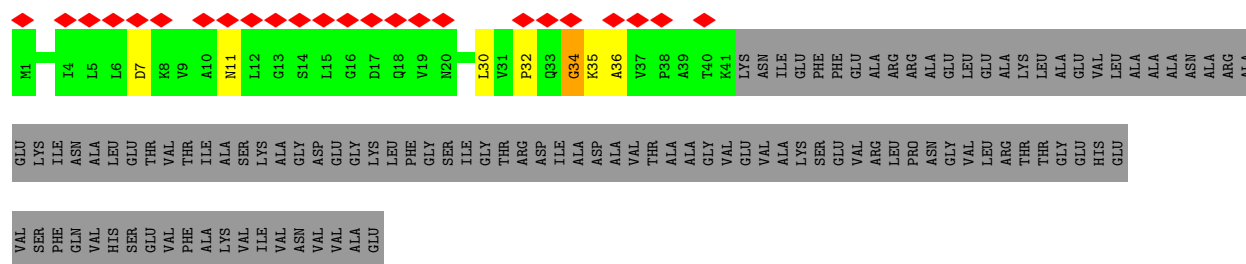
- Molecule 27: 50S ribosomal protein L5



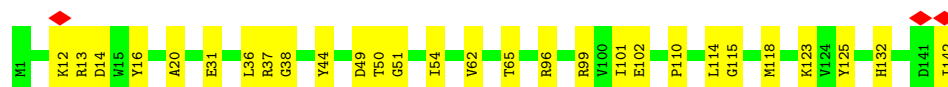
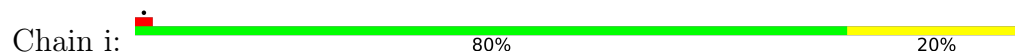
- Molecule 28: 50S ribosomal protein L6



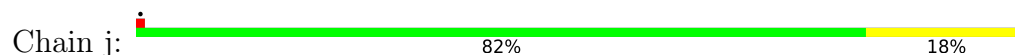
- Molecule 29: 50S ribosomal protein L9



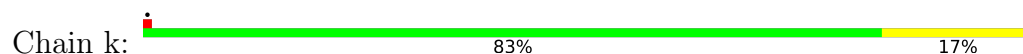
- Molecule 30: 50S ribosomal protein L13



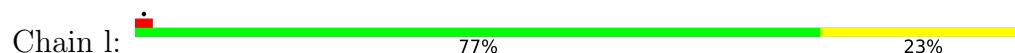
- Molecule 31: 50S ribosomal protein L14



- Molecule 32: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L16





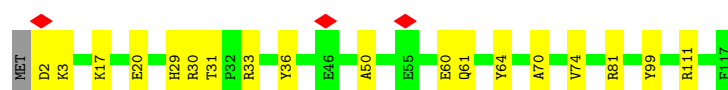
- Molecule 34: 50S ribosomal protein L17

Chain m: 72% 20% 7%



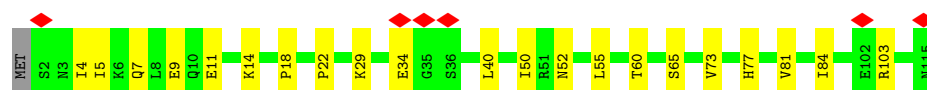
- Molecule 35: 50S ribosomal protein L18

Chain n: 84% 15%



- Molecule 36: 50S ribosomal protein L19

Chain o: 5% 81% 18%



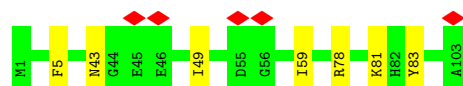
- Molecule 37: 50S ribosomal protein L20

Chain p: 83% 16%



- Molecule 38: 50S ribosomal protein L21

Chain q: 5% 93% 7%

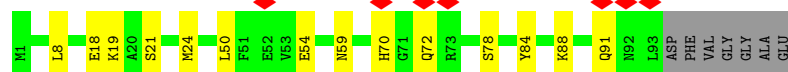
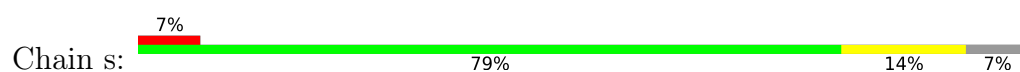


- Molecule 39: 50S ribosomal protein L22

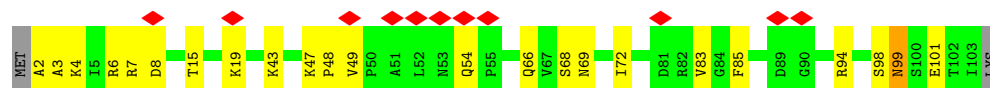
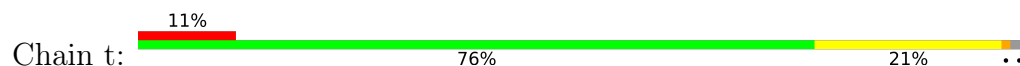
Chain r: 78% 22%



- Molecule 40: 50S ribosomal protein L23



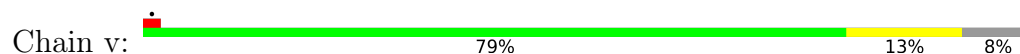
- Molecule 41: 50S ribosomal protein L24



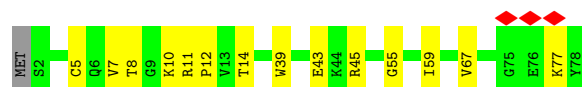
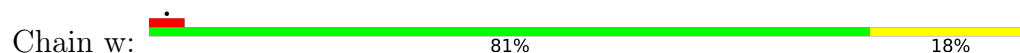
- Molecule 42: 50S ribosomal protein L25



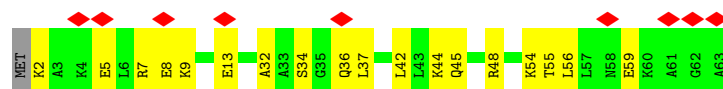
- Molecule 43: 50S ribosomal protein L27



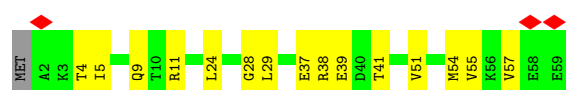
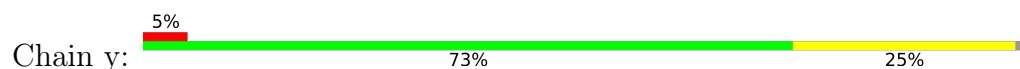
- Molecule 44: 50S ribosomal protein L28



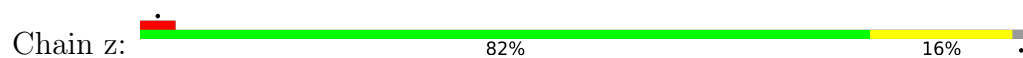
- Molecule 45: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L30



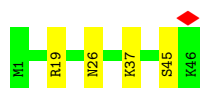
- Molecule 47: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L33



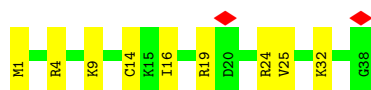
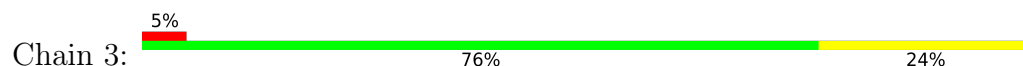
- Molecule 49: 50S ribosomal protein L34



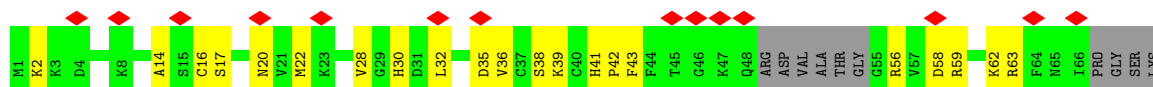
- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36

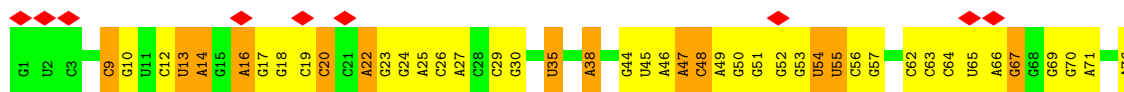


- Molecule 52: 50S ribosomal protein L31



- Molecule 53: P-site tRNA\_Glu

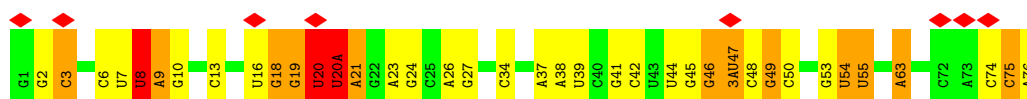




• Molecule 54: mRNA



• Molecule 55: A-site tRNA\_Ile2



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 71561                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.134                                   | Depositor |
| Minimum map value                    | -0.063                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.0156                                  | Depositor |
| Map size (Å)                         | 439.10498, 439.10498, 439.10498         | wwPDB     |
| Map dimensions                       | 530, 530, 530                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.8285, 0.8285, 0.8285                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 3AU, OMG, 5MU, 4OC, 1MG, 2MA, MKX, MEQ, UR3, 4D4, 6MZ, IAS, U8U, 2MG, M3X, MS6, MG, 4SU, 3TD, OMC, K, G7M, PSU, D2T, OMU, H2U, 5MC

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$   |
| 1   | A     | 0.12         | 0/36236     | 0.26        | 0/56520       |
| 2   | B     | 0.14         | 0/1784      | 0.40        | 0/2403        |
| 3   | C     | 0.11         | 0/1651      | 0.29        | 0/2225        |
| 4   | D     | 0.10         | 0/1665      | 0.28        | 0/2227        |
| 5   | E     | 0.13         | 0/1165      | 0.30        | 0/1568        |
| 6   | F     | 0.14         | 0/858       | 0.35        | 0/1160        |
| 7   | G     | 0.13         | 0/1219      | 0.33        | 0/1635        |
| 8   | H     | 0.12         | 0/989       | 0.28        | 0/1326        |
| 9   | I     | 0.12         | 0/1034      | 0.33        | 0/1375        |
| 10  | J     | 0.13         | 0/796       | 0.37        | 0/1077        |
| 11  | K     | 0.11         | 0/884       | 0.29        | 0/1191        |
| 12  | L     | 0.15         | 0/960       | 0.37        | 1/1286 (0.1%) |
| 13  | M     | 0.12         | 0/900       | 0.32        | 0/1204        |
| 14  | N     | 0.15         | 0/817       | 0.32        | 0/1088        |
| 15  | O     | 0.11         | 0/722       | 0.24        | 0/964         |
| 16  | P     | 0.12         | 0/653       | 0.35        | 0/877         |
| 17  | Q     | 0.11         | 0/650       | 0.33        | 0/871         |
| 18  | R     | 0.11         | 0/553       | 0.30        | 0/742         |
| 19  | S     | 0.12         | 0/685       | 0.33        | 0/922         |
| 20  | T     | 0.16         | 0/676       | 0.29        | 0/895         |
| 21  | U     | 0.11         | 0/597       | 0.29        | 0/792         |
| 22  | a     | 0.13         | 0/65651     | 0.27        | 0/102413      |
| 23  | b     | 0.11         | 0/2850      | 0.23        | 0/4444        |
| 24  | c     | 0.11         | 0/2121      | 0.30        | 0/2852        |
| 25  | d     | 0.12         | 0/1576      | 0.32        | 0/2119        |
| 26  | e     | 0.11         | 0/1571      | 0.28        | 0/2113        |
| 27  | f     | 0.13         | 0/1434      | 0.32        | 0/1926        |
| 28  | g     | 0.12         | 0/1343      | 0.40        | 0/1816        |
| 29  | h     | 0.13         | 0/306       | 0.46        | 0/413         |
| 30  | i     | 0.13         | 0/1152      | 0.29        | 0/1551        |
| 31  | j     | 0.13         | 0/955       | 0.31        | 0/1279        |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 32  | k     | 0.12         | 0/1062   | 0.31        | 0/1413          |
| 33  | l     | 0.15         | 0/1073   | 0.32        | 0/1433          |
| 34  | m     | 0.14         | 0/958    | 0.34        | 0/1281          |
| 35  | n     | 0.11         | 0/902    | 0.29        | 0/1209          |
| 36  | o     | 0.11         | 0/929    | 0.28        | 0/1242          |
| 37  | p     | 0.13         | 0/960    | 0.26        | 0/1278          |
| 38  | q     | 0.11         | 0/829    | 0.28        | 0/1107          |
| 39  | r     | 0.13         | 0/864    | 0.30        | 0/1156          |
| 40  | s     | 0.10         | 0/744    | 0.29        | 0/994           |
| 41  | t     | 0.15         | 0/787    | 0.48        | 2/1051 (0.2%)   |
| 42  | u     | 0.10         | 0/766    | 0.27        | 0/1025          |
| 43  | v     | 0.10         | 0/593    | 0.28        | 0/785           |
| 44  | w     | 0.12         | 0/635    | 0.32        | 0/848           |
| 45  | x     | 0.12         | 0/502    | 0.32        | 0/667           |
| 46  | y     | 0.14         | 0/453    | 0.31        | 0/605           |
| 47  | z     | 0.10         | 0/450    | 0.26        | 0/599           |
| 48  | 0     | 0.11         | 0/424    | 0.27        | 0/565           |
| 49  | 1     | 0.09         | 0/380    | 0.26        | 0/498           |
| 50  | 2     | 0.12         | 0/513    | 0.34        | 0/676           |
| 51  | 3     | 0.13         | 0/303    | 0.28        | 0/397           |
| 52  | 4     | 0.10         | 0/488    | 0.30        | 0/649           |
| 53  | V     | 0.11         | 0/1686   | 0.28        | 0/2621          |
| 54  | W     | 0.12         | 0/264    | 0.43        | 0/409           |
| 55  | X     | 0.17         | 0/1551   | 0.27        | 0/2409          |
| All | All   | 0.12         | 0/152569 | 0.28        | 3/228191 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 14  | N     | 0                   | 1                   |
| 28  | g     | 0                   | 1                   |
| 29  | h     | 0                   | 1                   |
| 50  | 2     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 41  | t     | 98  | SER  | CA-C-N  | 6.49  | 133.94      | 121.54   |
| 41  | t     | 98  | SER  | C-N-CA  | 6.49  | 133.94      | 121.54   |
| 12  | L     | 122 | PRO  | CA-N-CD | -5.65 | 104.09      | 112.00   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 50  | 2     | 31  | HIS  | Peptide |
| 14  | N     | 32  | SER  | Peptide |
| 28  | g     | 47  | ASP  | Peptide |
| 29  | h     | 34  | GLY  | Peptide |

## 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   | A     | 32612 | 0        | 16432    | 384     | 0            |
| 2   | B     | 1753  | 0        | 1780     | 53      | 0            |
| 3   | C     | 1624  | 0        | 1696     | 33      | 0            |
| 4   | D     | 1643  | 0        | 1707     | 29      | 0            |
| 5   | E     | 1152  | 0        | 1196     | 22      | 0            |
| 6   | F     | 839   | 0        | 833      | 24      | 0            |
| 7   | G     | 1203  | 0        | 1254     | 34      | 0            |
| 8   | H     | 979   | 0        | 1031     | 14      | 0            |
| 9   | I     | 1022  | 0        | 1070     | 27      | 0            |
| 10  | J     | 786   | 0        | 828      | 14      | 0            |
| 11  | K     | 877   | 0        | 884      | 18      | 0            |
| 12  | L     | 957   | 0        | 1017     | 23      | 0            |
| 13  | M     | 891   | 0        | 952      | 25      | 0            |
| 14  | N     | 805   | 0        | 844      | 20      | 0            |
| 15  | O     | 714   | 0        | 734      | 6       | 0            |
| 16  | P     | 643   | 0        | 661      | 17      | 0            |
| 17  | Q     | 641   | 0        | 682      | 12      | 0            |
| 18  | R     | 544   | 0        | 565      | 11      | 0            |
| 19  | S     | 668   | 0        | 693      | 18      | 0            |
| 20  | T     | 670   | 0        | 719      | 13      | 0            |
| 21  | U     | 589   | 0        | 629      | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | a     | 59130 | 0        | 29768    | 594     | 0            |
| 23  | b     | 2549  | 0        | 1291     | 31      | 0            |
| 24  | c     | 2082  | 0        | 2154     | 29      | 0            |
| 25  | d     | 1566  | 0        | 1618     | 24      | 0            |
| 26  | e     | 1552  | 0        | 1619     | 26      | 0            |
| 27  | f     | 1410  | 0        | 1444     | 24      | 0            |
| 28  | g     | 1323  | 0        | 1371     | 24      | 0            |
| 29  | h     | 303   | 0        | 327      | 9       | 0            |
| 30  | i     | 1129  | 0        | 1162     | 19      | 0            |
| 31  | j     | 946   | 0        | 1023     | 17      | 0            |
| 32  | k     | 1053  | 0        | 1129     | 23      | 0            |
| 33  | l     | 1075  | 0        | 1145     | 22      | 0            |
| 34  | m     | 945   | 0        | 989      | 18      | 0            |
| 35  | n     | 892   | 0        | 923      | 10      | 0            |
| 36  | o     | 917   | 0        | 962      | 15      | 0            |
| 37  | p     | 947   | 0        | 1019     | 15      | 0            |
| 38  | q     | 816   | 0        | 839      | 6       | 0            |
| 39  | r     | 857   | 0        | 922      | 16      | 0            |
| 40  | s     | 738   | 0        | 807      | 13      | 0            |
| 41  | t     | 779   | 0        | 831      | 15      | 0            |
| 42  | u     | 753   | 0        | 780      | 15      | 0            |
| 43  | v     | 586   | 0        | 596      | 7       | 0            |
| 44  | w     | 625   | 0        | 652      | 14      | 0            |
| 45  | x     | 501   | 0        | 531      | 13      | 0            |
| 46  | y     | 449   | 0        | 488      | 8       | 0            |
| 47  | z     | 444   | 0        | 458      | 6       | 0            |
| 48  | 0     | 417   | 0        | 451      | 10      | 0            |
| 49  | 1     | 377   | 0        | 418      | 4       | 0            |
| 50  | 2     | 504   | 0        | 572      | 13      | 0            |
| 51  | 3     | 302   | 0        | 343      | 7       | 0            |
| 52  | 4     | 480   | 0        | 482      | 15      | 0            |
| 53  | V     | 1619  | 0        | 832      | 27      | 0            |
| 54  | W     | 236   | 0        | 119      | 4       | 0            |
| 55  | X     | 1646  | 0        | 816      | 19      | 0            |
| 56  | A     | 92    | 0        | 0        | 0       | 0            |
| 56  | E     | 1     | 0        | 0        | 0       | 0            |
| 56  | M     | 1     | 0        | 0        | 0       | 0            |
| 56  | N     | 1     | 0        | 0        | 0       | 0            |
| 56  | V     | 2     | 0        | 0        | 0       | 0            |
| 56  | X     | 1     | 0        | 0        | 0       | 0            |
| 56  | a     | 210   | 0        | 0        | 0       | 0            |
| 56  | b     | 5     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56  | d     | 1      | 0        | 0        | 0       | 0            |
| 57  | A     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 141875 | 0        | 95088    | 1713    | 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 7.

All (1713) 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:A:539:A:OP2     | 12:L:112:GLN:NE2  | 2.10                     | 0.83              |
| 25:d:5:VAL:H      | 25:d:32:ASN:HD21  | 1.27                     | 0.82              |
| 1:A:664:G:H22     | 1:A:741:G:H1      | 1.28                     | 0.82              |
| 34:m:22:ARG:HG3   | 34:m:70:THR:HA    | 1.61                     | 0.81              |
| 2:B:9:MET:HE2     | 2:B:43:LEU:HD11   | 1.63                     | 0.79              |
| 2:B:43:LEU:HD12   | 2:B:46:THR:HB     | 1.65                     | 0.79              |
| 30:i:62:VAL:HG11  | 30:i:101:ILE:HD11 | 1.64                     | 0.78              |
| 7:G:57:SER:OG     | 7:G:60:GLU:OE1    | 2.02                     | 0.78              |
| 17:Q:27:ARG:NH1   | 17:Q:42:THR:OG1   | 2.17                     | 0.77              |
| 3:C:142:MET:HE3   | 3:C:149:ILE:HG22  | 1.67                     | 0.77              |
| 9:I:106:ARG:NH1   | 9:I:107:ASP:O     | 2.17                     | 0.77              |
| 1:A:310:G:H5''    | 16:P:31:ARG:HG2   | 1.65                     | 0.76              |
| 1:A:6:G:H1        | 5:E:103:THR:HG1   | 1.31                     | 0.76              |
| 4:D:174:ASP:HB3   | 4:D:179:GLU:H     | 1.51                     | 0.76              |
| 42:u:4:ILE:HG12   | 42:u:50:MET:HE1   | 1.69                     | 0.75              |
| 1:A:673:A:H2'     | 1:A:674:G:C8      | 2.22                     | 0.74              |
| 13:M:104:THR:HG22 | 13:M:105:ASN:H    | 1.51                     | 0.74              |
| 22:a:475:C:O2     | 22:a:479:A:N6     | 2.20                     | 0.73              |
| 1:A:187:G:N2      | 1:A:190:A:OP2     | 2.21                     | 0.73              |
| 27:f:136:ILE:HA   | 27:f:141:ILE:HD11 | 1.69                     | 0.73              |
| 1:A:1441:A:H62    | 1:A:1461:G:H21    | 1.37                     | 0.73              |
| 22:a:1869:G:N2    | 22:a:1872:A:OP2   | 2.21                     | 0.73              |
| 1:A:1086:U:H3     | 1:A:1099:G:H22    | 1.35                     | 0.73              |
| 41:t:47:LYS:HD3   | 41:t:48:PRO:HD2   | 1.71                     | 0.73              |
| 3:C:129:MET:HB2   | 3:C:132:ARG:HG3   | 1.70                     | 0.72              |
| 41:t:72:ILE:HD12  | 41:t:83:VAL:HG21  | 1.71                     | 0.72              |
| 1:A:546:A:HO2'    | 1:A:548:G:HO2'    | 1.34                     | 0.72              |
| 3:C:14:ILE:HG22   | 3:C:15:VAL:HG13   | 1.70                     | 0.72              |
| 1:A:405:U:O4      | 4:D:2:ALA:N       | 2.23                     | 0.71              |
| 4:D:85:ASN:ND2    | 4:D:88:GLU:OE1    | 2.18                     | 0.71              |
| 22:a:2450:A:H62   | 22:a:2501:C:H42   | 1.38                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1376:U:O4    | 7:G:10:ARG:NH1    | 2.23                     | 0.71              |
| 22:a:126:A:OP1   | 49:1:45:SER:OG    | 2.09                     | 0.69              |
| 1:A:780:A:H5'    | 11:K:125:LYS:HD3  | 1.75                     | 0.69              |
| 9:I:84:THR:HG22  | 9:I:88:MET:HE1    | 1.74                     | 0.69              |
| 25:d:46:ARG:NH1  | 25:d:85:ALA:O     | 2.25                     | 0.69              |
| 22:a:125:A:OP2   | 49:1:19:ARG:NH1   | 2.25                     | 0.69              |
| 27:f:58:ALA:HB2  | 27:f:65:PRO:HD3   | 1.73                     | 0.69              |
| 47:z:53:LYS:NZ   | 47:z:55:ILE:O     | 2.25                     | 0.69              |
| 1:A:544:G:OP1    | 4:D:56:ARG:NH2    | 2.25                     | 0.69              |
| 1:A:1037:C:H2'   | 1:A:1038:C:H6     | 1.58                     | 0.69              |
| 22:a:995:C:OP2   | 37:p:54:LYS:NZ    | 2.25                     | 0.68              |
| 1:A:28:A:O2'     | 1:A:296:U:OP1     | 2.11                     | 0.68              |
| 1:A:606:G:N2     | 1:A:632:U:OP1     | 2.26                     | 0.68              |
| 33:l:57:VAL:HG21 | 33:l:105:MET:HE1  | 1.75                     | 0.68              |
| 11:K:98:ARG:NH2  | 21:U:13:ASP:OD1   | 2.26                     | 0.68              |
| 46:y:11:ARG:HB2  | 46:y:54:MET:HB2   | 1.75                     | 0.68              |
| 2:B:58:ASN:ND2   | 2:B:223:GLU:OE2   | 2.26                     | 0.68              |
| 22:a:2848:G:O2'  | 22:a:2867:G:N2    | 2.27                     | 0.68              |
| 2:B:18:HIS:ND1   | 2:B:188:ASP:OD2   | 2.26                     | 0.67              |
| 12:L:68:GLY:O    | 12:L:99:ARG:NH2   | 2.22                     | 0.67              |
| 23:b:40:U:H2'    | 52:4:2:LYS:HE3    | 1.76                     | 0.67              |
| 15:O:88:ARG:NH2  | 22:a:714:U:OP2    | 2.22                     | 0.67              |
| 22:a:1649:G:O2'  | 34:m:106:ASP:OD2  | 2.12                     | 0.67              |
| 1:A:1029:U:O2'   | 1:A:1032:G:O6     | 2.13                     | 0.67              |
| 2:B:161:LEU:HB3  | 2:B:183:VAL:HG23  | 1.75                     | 0.66              |
| 1:A:107:G:N7     | 20:T:10:ARG:NH2   | 2.39                     | 0.66              |
| 1:A:881:G:OP2    | 12:L:9:ARG:NH2    | 2.28                     | 0.66              |
| 2:B:67:ILE:HG22  | 2:B:160:ALA:HB3   | 1.77                     | 0.66              |
| 26:e:6:LYS:HD3   | 26:e:119:ILE:HG23 | 1.76                     | 0.66              |
| 1:A:1073:U:O2    | 2:B:103:ASN:ND2   | 2.29                     | 0.66              |
| 22:a:1607:C:N4   | 22:a:1622:G:OP2   | 2.22                     | 0.66              |
| 36:o:29:LYS:HB3  | 36:o:40:LEU:HD11  | 1.76                     | 0.66              |
| 22:a:728:G:H4'   | 24:c:13:ARG:HD3   | 1.78                     | 0.66              |
| 22:a:1539:U:H2'  | 22:a:1540:G:H8    | 1.60                     | 0.66              |
| 1:A:401:C:O2'    | 1:A:621:A:N3      | 2.29                     | 0.66              |
| 10:J:36:VAL:HG22 | 10:J:76:ILE:HG22  | 1.78                     | 0.66              |
| 22:a:1412:U:H2'  | 22:a:1413:A:H8    | 1.59                     | 0.66              |
| 3:C:72:ARG:HD3   | 3:C:75:ILE:HD13   | 1.77                     | 0.66              |
| 22:a:1153:C:OP1  | 37:p:92:ARG:NH2   | 2.22                     | 0.66              |
| 33:l:36:VAL:HG12 | 42:u:82:TYR:HB2   | 1.78                     | 0.66              |
| 22:a:848:C:H2'   | 22:a:849:A:H8     | 1.60                     | 0.65              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 27:f:29:PRO:HB2  | 27:f:169:LEU:HD22  | 1.78                     | 0.65              |
| 2:B:7:ARG:HA     | 2:B:10:LEU:HD12    | 1.78                     | 0.65              |
| 22:a:77:G:O2'    | 45:x:7:ARG:NH2     | 2.29                     | 0.65              |
| 30:i:12:LYS:NZ   | 30:i:14:ASP:OD1    | 2.29                     | 0.65              |
| 2:B:27:MET:HG3   | 2:B:189:THR:HA     | 1.78                     | 0.65              |
| 50:2:16:LYS:HE3  | 50:2:20:GLY:HA2    | 1.77                     | 0.65              |
| 22:a:1141:U:H2'  | 30:i:65:THR:HG21   | 1.78                     | 0.65              |
| 28:g:107:LEU:O   | 28:g:152:ARG:NH1   | 2.29                     | 0.65              |
| 1:A:713:G:H2'    | 1:A:714:G:C8       | 2.31                     | 0.65              |
| 3:C:11:ARG:NH2   | 3:C:175:LEU:O      | 2.30                     | 0.65              |
| 7:G:38:THR:O     | 7:G:42:ILE:HG13    | 1.97                     | 0.65              |
| 2:B:5:SER:OG     | 2:B:6:MET:N        | 2.30                     | 0.65              |
| 22:a:2618:G:H21  | 25:d:155:VAL:HG21  | 1.62                     | 0.65              |
| 3:C:180:ALA:HA   | 3:C:206:GLU:HA     | 1.79                     | 0.64              |
| 22:a:2328:A:H2'  | 22:a:2329:U:C6     | 2.32                     | 0.64              |
| 53:V:16:A:N6     | 53:V:19:C:O2'      | 2.29                     | 0.64              |
| 1:A:677:U:H3     | 1:A:713:G:H22      | 1.43                     | 0.64              |
| 12:L:110:ARG:HB3 | 12:L:119:VAL:HG21  | 1.79                     | 0.64              |
| 22:a:2316:G:H2'  | 22:a:2317:A:H8     | 1.62                     | 0.64              |
| 31:j:58:LEU:HD11 | 31:j:86:LEU:HD23   | 1.79                     | 0.64              |
| 1:A:276:G:OP1    | 17:Q:14:SER:OG     | 2.13                     | 0.64              |
| 4:D:70:ARG:HE    | 4:D:73:ARG:HH21    | 1.45                     | 0.64              |
| 9:I:12:ARG:HG3   | 9:I:13:LYS:H       | 1.62                     | 0.64              |
| 1:A:459:A:H2'    | 1:A:460:A:C8       | 2.32                     | 0.64              |
| 1:A:1119:C:OP1   | 9:I:85:ARG:NH1     | 2.28                     | 0.64              |
| 22:a:2467:C:O2   | 33:l:123:LYS:NZ    | 2.30                     | 0.64              |
| 22:a:2474:U:OP2  | 22:a:2475:C:N4     | 2.27                     | 0.64              |
| 55:X:9:A:O2'     | 55:X:10:G:N7       | 2.29                     | 0.64              |
| 10:J:71:LEU:O    | 10:J:72:ARG:NH1    | 2.28                     | 0.64              |
| 46:y:4:THR:OG1   | 46:y:37:GLU:OE2    | 2.14                     | 0.64              |
| 18:R:25:ASP:HB3  | 18:R:28:THR:HG22   | 1.79                     | 0.64              |
| 3:C:57:ILE:HG23  | 3:C:64:ILE:HD11    | 1.80                     | 0.63              |
| 27:f:139:PRO:HB2 | 52:4:32:LEU:HD11   | 1.80                     | 0.63              |
| 13:M:105:ASN:HB2 | 13:M:107:ARG:HG2   | 1.80                     | 0.63              |
| 1:A:1229:A:OP2   | 13:M:113:ARG:NH1   | 2.31                     | 0.63              |
| 22:a:1245:G:OP1  | 32:k:13:LYS:NZ     | 2.31                     | 0.63              |
| 22:a:2502:G:H5'' | 22:a:2503:2MA:H5'' | 1.79                     | 0.63              |
| 7:G:113:ASP:OD2  | 7:G:122:ASN:ND2    | 2.30                     | 0.63              |
| 22:a:651:G:H5'   | 50:2:19:LYS:HG3    | 1.80                     | 0.63              |
| 22:a:864:G:O2'   | 22:a:914:G:O6      | 2.17                     | 0.63              |
| 53:V:35:U8U:HN3  | 54:W:30:G:H22      | 1.46                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:946:A:H2'    | 1:A:947:G:C8      | 2.32                     | 0.63              |
| 52:4:14:ALA:HB3  | 52:4:22:MET:HB2   | 1.81                     | 0.63              |
| 22:a:2728:U:HO2' | 22:a:2729:G:H8    | 1.46                     | 0.63              |
| 1:A:1071:C:H2'   | 1:A:1072:G:H8     | 1.63                     | 0.62              |
| 7:G:47:LEU:HG    | 7:G:58:GLU:HB3    | 1.81                     | 0.62              |
| 26:e:191:ASP:OD1 | 26:e:194:LYS:NZ   | 2.31                     | 0.62              |
| 11:K:67:ALA:HB2  | 11:K:96:THR:HG23  | 1.81                     | 0.62              |
| 4:D:95:GLU:HG3   | 4:D:191:LEU:HD21  | 1.81                     | 0.62              |
| 22:a:2394:C:H5'' | 32:k:63:LYS:HE2   | 1.81                     | 0.62              |
| 45:x:32:ALA:HB2  | 45:x:37:LEU:HD23  | 1.82                     | 0.62              |
| 39:r:4:ILE:HD13  | 39:r:106:VAL:HG22 | 1.81                     | 0.62              |
| 28:g:94:TYR:HD1  | 28:g:107:LEU:HA   | 1.64                     | 0.62              |
| 42:u:9:ARG:HD3   | 42:u:39:ALA:HB1   | 1.82                     | 0.62              |
| 1:A:1326:U:H2'   | 1:A:1327:C:H6     | 1.65                     | 0.62              |
| 4:D:201:VAL:O    | 4:D:205:SER:N     | 2.33                     | 0.62              |
| 22:a:184:C:H2'   | 22:a:185:G:H8     | 1.65                     | 0.62              |
| 25:d:33:ARG:NH2  | 25:d:53:GLY:O     | 2.32                     | 0.62              |
| 1:A:337:G:H2'    | 1:A:338:A:C8      | 2.35                     | 0.62              |
| 22:a:993:G:OP2   | 37:p:51:ARG:NH2   | 2.33                     | 0.62              |
| 22:a:1405:U:H2'  | 22:a:1406:U:C6    | 2.34                     | 0.62              |
| 22:a:5:A:H2'     | 22:a:6:A:C8       | 2.35                     | 0.61              |
| 39:r:73:LYS:HB2  | 39:r:106:VAL:HB   | 1.82                     | 0.61              |
| 2:B:75:ALA:HB1   | 2:B:207:ILE:HG13  | 1.81                     | 0.61              |
| 26:e:119:ILE:HB  | 26:e:187:VAL:HG12 | 1.82                     | 0.61              |
| 26:e:148:ILE:HB  | 26:e:169:VAL:HG12 | 1.80                     | 0.61              |
| 23:b:1:U:H2'     | 23:b:2:G:H8       | 1.66                     | 0.61              |
| 1:A:1098:C:O2'   | 21:U:71:TYR:O     | 2.18                     | 0.61              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8     | 2.35                     | 0.61              |
| 9:I:85:ARG:HA    | 9:I:88:MET:HE2    | 1.83                     | 0.61              |
| 27:f:108:VAL:HA  | 27:f:111:ILE:HD12 | 1.82                     | 0.61              |
| 30:i:114:LEU:HG  | 30:i:118:MET:HE2  | 1.83                     | 0.61              |
| 3:C:11:ARG:HB2   | 3:C:16:LYS:HD2    | 1.83                     | 0.61              |
| 28:g:89:LEU:HD23 | 28:g:94:TYR:HB3   | 1.83                     | 0.61              |
| 30:i:125:TYR:OH  | 30:i:132:HIS:NE2  | 2.23                     | 0.61              |
| 1:A:335:C:H2'    | 1:A:336:A:H8      | 1.66                     | 0.60              |
| 1:A:1124:G:N2    | 1:A:1125:U:O4     | 2.27                     | 0.60              |
| 13:M:71:ARG:NH1  | 27:f:113:ASP:OD2  | 2.27                     | 0.60              |
| 10:J:12:ALA:HB2  | 10:J:96:VAL:HG22  | 1.83                     | 0.60              |
| 33:l:53:MET:HE1  | 33:l:103:TYR:CD2  | 2.35                     | 0.60              |
| 1:A:714:G:H2'    | 1:A:715:A:C8      | 2.36                     | 0.60              |
| 4:D:58:LYS:NZ    | 4:D:69:GLU:OE2    | 2.25                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:a:172:A:H2'    | 22:a:173:A:C8     | 2.36                     | 0.60              |
| 22:a:396:G:OP2    | 44:w:10:LYS:NZ    | 2.33                     | 0.60              |
| 22:a:1392:A:N6    | 40:s:18:GLU:OE1   | 2.28                     | 0.60              |
| 35:n:99:TYR:OH    | 35:n:111:ARG:NH2  | 2.34                     | 0.60              |
| 22:a:1028:A:H2'   | 22:a:1029:A:C8    | 2.36                     | 0.60              |
| 22:a:1853:A:H2'   | 22:a:1854:A:C8    | 2.36                     | 0.60              |
| 45:x:9:LYS:HD3    | 45:x:13:GLU:HB3   | 1.83                     | 0.60              |
| 18:R:13:PHE:HA    | 18:R:16:GLU:HG2   | 1.83                     | 0.60              |
| 41:t:15:THR:OG1   | 41:t:69:ASN:ND2   | 2.35                     | 0.60              |
| 1:A:662:U:H2'     | 1:A:663:A:C8      | 2.37                     | 0.60              |
| 1:A:1033:G:N2     | 1:A:1033:G:OP2    | 2.32                     | 0.60              |
| 10:J:28:THR:HA    | 10:J:31:ARG:HG2   | 1.83                     | 0.60              |
| 9:I:83:ILE:O      | 9:I:87:LEU:HG     | 2.02                     | 0.60              |
| 10:J:54:SER:O     | 14:N:81:ARG:NH1   | 2.32                     | 0.60              |
| 1:A:545:C:OP1     | 4:D:58:LYS:NZ     | 2.33                     | 0.59              |
| 41:t:99:ASN:ND2   | 41:t:101:GLU:OE2  | 2.35                     | 0.59              |
| 1:A:1033:G:H2'    | 1:A:1034:G:O4'    | 2.02                     | 0.59              |
| 22:a:639:U:H2'    | 22:a:640:C:C6     | 2.37                     | 0.59              |
| 22:a:284:U:O2     | 22:a:356:G:O6     | 2.20                     | 0.59              |
| 22:a:1939:5MU:OP1 | 22:a:2604:PSU:O2' | 2.20                     | 0.59              |
| 26:e:145:ASP:HB3  | 26:e:166:LYS:HE2  | 1.83                     | 0.59              |
| 29:h:30:LEU:HD12  | 29:h:36:ALA:HB2   | 1.85                     | 0.59              |
| 24:c:66:ASP:OD2   | 24:c:102:ARG:NH1  | 2.35                     | 0.59              |
| 42:u:48:MET:HE3   | 42:u:51:GLN:NE2   | 2.18                     | 0.59              |
| 1:A:519:C:O2'     | 1:A:520:A:OP1     | 2.20                     | 0.59              |
| 1:A:746:A:H2'     | 1:A:747:A:C8      | 2.38                     | 0.59              |
| 7:G:25:LYS:O      | 7:G:29:ILE:HG12   | 2.01                     | 0.59              |
| 9:I:31:ASN:ND2    | 9:I:38:TYR:OH     | 2.35                     | 0.59              |
| 22:a:856:G:H2'    | 22:a:857:G:C8     | 2.37                     | 0.59              |
| 22:a:1340:U:OP1   | 40:s:19:LYS:NZ    | 2.35                     | 0.59              |
| 1:A:184:G:H2'     | 1:A:185:U:C6      | 2.38                     | 0.59              |
| 1:A:539:A:H2'     | 1:A:540:G:C8      | 2.37                     | 0.59              |
| 9:I:75:GLN:O      | 9:I:79:ILE:HG12   | 2.03                     | 0.59              |
| 19:S:67:VAL:O     | 52:4:56:ARG:NH1   | 2.36                     | 0.59              |
| 22:a:414:C:H2'    | 22:a:415:A:H8     | 1.68                     | 0.59              |
| 1:A:981:U:OP1     | 14:N:9:ARG:NH1    | 2.35                     | 0.59              |
| 22:a:1548:A:H2'   | 22:a:1549:A:H8    | 1.67                     | 0.59              |
| 22:a:2013:A:O2'   | 39:r:94:ASP:OD2   | 2.19                     | 0.59              |
| 22:a:2547:A:H2'   | 22:a:2548:U:C6    | 2.38                     | 0.59              |
| 1:A:613:C:H2'     | 1:A:614:C:C6      | 2.38                     | 0.59              |
| 11:K:119:IAS:O    | 21:U:35:ARG:NH2   | 2.35                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:a:1141:U:H4'   | 22:a:1142:A:O4'    | 2.03                     | 0.59              |
| 22:a:1539:U:H2'   | 22:a:1540:G:C8     | 2.38                     | 0.59              |
| 44:w:55:GLY:O     | 44:w:59:ILE:HG12   | 2.02                     | 0.59              |
| 53:V:22:A:H61     | 53:V:47:A:H2'      | 1.66                     | 0.59              |
| 14:N:49:GLN:HE22  | 19:S:13:LEU:H      | 1.50                     | 0.58              |
| 28:g:94:TYR:CD1   | 28:g:107:LEU:HA    | 2.38                     | 0.58              |
| 1:A:1404:C:H2'    | 1:A:1405:G:C8      | 2.38                     | 0.58              |
| 22:a:652:U:OP1    | 22:a:654:A:N6      | 2.36                     | 0.58              |
| 22:a:1802:A:H2'   | 22:a:1803:A:C8     | 2.38                     | 0.58              |
| 22:a:2285:C:OP2   | 48:0:6:ARG:NH1     | 2.29                     | 0.58              |
| 26:e:1:MET:N      | 26:e:16:GLU:OE2    | 2.36                     | 0.58              |
| 37:p:112:LYS:HE3  | 38:q:49:ILE:HB     | 1.85                     | 0.58              |
| 1:A:159:G:N2      | 1:A:162:A:OP2      | 2.32                     | 0.58              |
| 16:P:37:GLY:HA3   | 16:P:52:LEU:HD23   | 1.83                     | 0.58              |
| 22:a:568:U:H1'    | 22:a:2030:6MZ:H9C1 | 1.84                     | 0.58              |
| 22:a:1548:A:H2'   | 22:a:1549:A:C8     | 2.38                     | 0.58              |
| 22:a:2469:A:N6    | 22:a:2481:G:O2'    | 2.35                     | 0.58              |
| 31:j:63:VAL:HG23  | 31:j:64:ARG:HG3    | 1.85                     | 0.58              |
| 1:A:1323:G:H2'    | 1:A:1324:A:C8      | 2.38                     | 0.58              |
| 2:B:117:LEU:HB3   | 2:B:141:LEU:HD13   | 1.85                     | 0.58              |
| 5:E:34:THR:HG22   | 5:E:52:LYS:HG2     | 1.85                     | 0.58              |
| 14:N:49:GLN:HE22  | 19:S:13:LEU:HB2    | 1.69                     | 0.58              |
| 22:a:224:U:OP2    | 22:a:408:G:N2      | 2.31                     | 0.58              |
| 22:a:2562:U:OP1   | 31:j:40:LYS:NZ     | 2.32                     | 0.58              |
| 42:u:9:ARG:HG2    | 42:u:41:GLU:HG2    | 1.85                     | 0.58              |
| 1:A:999:C:H2'     | 1:A:1000:A:C8      | 2.39                     | 0.58              |
| 22:a:197:A:N6     | 22:a:2430:A:O2'    | 2.36                     | 0.58              |
| 22:a:279:A:N6     | 22:a:361:G:O2'     | 2.36                     | 0.58              |
| 53:V:24:G:H2'     | 53:V:25:A:C8       | 2.38                     | 0.58              |
| 1:A:1031:C:O3'    | 1:A:1032:G:N2      | 2.36                     | 0.58              |
| 12:L:50:ARG:NH1   | 12:L:89:D2T:OD2    | 2.34                     | 0.58              |
| 22:a:72:U:OP2     | 45:x:54:LYS:NZ     | 2.34                     | 0.58              |
| 22:a:414:C:H2'    | 22:a:415:A:C8      | 2.39                     | 0.58              |
| 2:B:129:LEU:HB2   | 2:B:134:ALA:HB2    | 1.86                     | 0.58              |
| 11:K:113:VAL:HG12 | 18:R:73:ARG:HE     | 1.67                     | 0.58              |
| 12:L:6:GLN:HG2    | 12:L:9:ARG:HH21    | 1.69                     | 0.58              |
| 13:M:11:ASP:HB2   | 13:M:46:SER:HB2    | 1.86                     | 0.58              |
| 53:V:14:A:N1      | 53:V:22:A:O2'      | 2.37                     | 0.58              |
| 1:A:1266:G:N2     | 1:A:1269:A:OP2     | 2.20                     | 0.58              |
| 1:A:1287:A:H2'    | 1:A:1288:A:C8      | 2.39                     | 0.58              |
| 22:a:833:A:H2'    | 22:a:834:G:C8      | 2.39                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:a:2291:U:H2'   | 22:a:2292:U:C6    | 2.39                     | 0.58              |
| 26:e:2:GLU:HB3    | 26:e:11:ALA:HB1   | 1.86                     | 0.58              |
| 4:D:105:MET:HE1   | 4:D:143:VAL:HB    | 1.86                     | 0.58              |
| 22:a:639:U:H2'    | 22:a:640:C:H6     | 1.67                     | 0.58              |
| 22:a:359:G:H2'    | 22:a:360:U:C6     | 2.39                     | 0.58              |
| 22:a:967:U:H2'    | 22:a:968:C:C6     | 2.39                     | 0.58              |
| 22:a:2000:C:OP1   | 34:m:5:LYS:NZ     | 2.31                     | 0.58              |
| 1:A:1149:C:H2'    | 1:A:1150:A:C8     | 2.39                     | 0.57              |
| 16:P:8:ARG:H      | 16:P:28:ARG:HD3   | 1.69                     | 0.57              |
| 22:a:1704:C:H2'   | 22:a:1705:A:H8    | 1.69                     | 0.57              |
| 28:g:19:ILE:HG23  | 28:g:24:ILE:HG22  | 1.86                     | 0.57              |
| 33:l:33:LEU:HD13  | 33:l:117:PHE:HB3  | 1.85                     | 0.57              |
| 1:A:340:U:OP2     | 31:j:98:ARG:NE    | 2.36                     | 0.57              |
| 2:B:54:LEU:HA     | 2:B:57:LEU:HD12   | 1.86                     | 0.57              |
| 1:A:946:A:H2'     | 1:A:947:G:H8      | 1.67                     | 0.57              |
| 6:F:44:ARG:HE     | 6:F:56:LYS:HZ1    | 1.50                     | 0.57              |
| 30:i:96:ARG:HG2   | 30:i:99:ARG:HG2   | 1.85                     | 0.57              |
| 1:A:674:G:H2'     | 1:A:675:A:H8      | 1.68                     | 0.57              |
| 11:K:20:VAL:N     | 11:K:35:THR:O     | 2.25                     | 0.57              |
| 23:b:52:A:N7      | 35:n:64:TYR:OH    | 2.27                     | 0.57              |
| 31:j:121:GLU:OE1  | 36:o:65:SER:OG    | 2.19                     | 0.57              |
| 32:k:108:ALA:HB3  | 32:k:125:LEU:HD22 | 1.85                     | 0.57              |
| 9:I:28:ILE:HG12   | 9:I:63:LEU:HD12   | 1.84                     | 0.57              |
| 9:I:115:LYS:HB2   | 9:I:118:LEU:HD12  | 1.85                     | 0.57              |
| 22:a:347:A:H2'    | 22:a:348:A:C8     | 2.39                     | 0.57              |
| 22:a:1353:A:H2'   | 22:a:1354:A:C8    | 2.39                     | 0.57              |
| 22:a:1412:U:H2'   | 22:a:1413:A:C8    | 2.39                     | 0.57              |
| 1:A:1175:G:H2'    | 1:A:1176:A:H8     | 1.68                     | 0.57              |
| 14:N:49:GLN:NE2   | 19:S:13:LEU:HB2   | 2.20                     | 0.57              |
| 20:T:79:LEU:O     | 20:T:83:ILE:HG12  | 2.05                     | 0.57              |
| 22:a:581:C:H2'    | 22:a:582:A:H8     | 1.70                     | 0.57              |
| 22:a:742:A:H2'    | 22:a:743:A:C8     | 2.40                     | 0.57              |
| 22:a:2522:U:O2'   | 22:a:2647:U:OP1   | 2.17                     | 0.57              |
| 25:d:121:THR:HG22 | 25:d:161:MET:HA   | 1.85                     | 0.57              |
| 52:4:35:ASP:OD1   | 52:4:36:VAL:N     | 2.38                     | 0.57              |
| 22:a:299:A:N1     | 22:a:322:A:O2'    | 2.31                     | 0.57              |
| 1:A:56:U:H2'      | 1:A:57:G:H8       | 1.70                     | 0.57              |
| 1:A:304:U:H2'     | 1:A:305:G:C8      | 2.40                     | 0.57              |
| 17:Q:79:VAL:HG12  | 17:Q:80:GLU:HG3   | 1.87                     | 0.57              |
| 22:a:81:G:HO2'    | 22:a:295:G:HO2'   | 1.51                     | 0.57              |
| 22:a:84:A:OP1     | 41:t:6:ARG:NH2    | 2.37                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:2646:C:OP2  | 22:a:2732:G:O2'  | 2.23                     | 0.57              |
| 40:s:54:GLU:OE1  | 40:s:91:GLN:NE2  | 2.37                     | 0.57              |
| 1:A:471:U:H2'    | 1:A:472:U:C6     | 2.39                     | 0.57              |
| 22:a:499:U:H5''  | 41:t:43:LYS:HE3  | 1.85                     | 0.57              |
| 26:e:5:LEU:HD11  | 26:e:12:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:745:G:OP1    | 1:A:851:G:O2'    | 2.22                     | 0.57              |
| 1:A:1268:G:H2'   | 1:A:1269:A:C8    | 2.39                     | 0.57              |
| 22:a:1278:C:H2'  | 22:a:1279:G:H8   | 1.70                     | 0.57              |
| 22:a:2756:U:OP2  | 51:3:19:ARG:NH2  | 2.36                     | 0.57              |
| 51:3:16:ILE:HD13 | 51:3:25:VAL:HG22 | 1.87                     | 0.57              |
| 11:K:34:ILE:HD12 | 11:K:74:VAL:HG11 | 1.87                     | 0.56              |
| 2:B:114:LEU:HD12 | 2:B:144:LEU:HB3  | 1.86                     | 0.56              |
| 22:a:320:A:OP1   | 26:e:130:LYS:NZ  | 2.38                     | 0.56              |
| 1:A:131:A:H2'    | 1:A:132:C:C6     | 2.40                     | 0.56              |
| 1:A:459:A:H2'    | 1:A:460:A:H8     | 1.69                     | 0.56              |
| 1:A:492:C:H2'    | 1:A:493:A:C8     | 2.40                     | 0.56              |
| 4:D:98:LEU:HB2   | 4:D:135:TYR:HB3  | 1.87                     | 0.56              |
| 9:I:123:ARG:NH1  | 9:I:124:ARG:O    | 2.38                     | 0.56              |
| 22:a:721:A:H2'   | 22:a:722:A:H8    | 1.70                     | 0.56              |
| 22:a:1636:U:H2'  | 22:a:1637:A:C8   | 2.41                     | 0.56              |
| 1:A:486:U:H2'    | 1:A:487:A:H8     | 1.70                     | 0.56              |
| 1:A:1273:C:H2'   | 1:A:1274:A:O4'   | 2.06                     | 0.56              |
| 4:D:173:VAL:HA   | 4:D:180:GLY:HA2  | 1.86                     | 0.56              |
| 16:P:55:ASP:OD1  | 16:P:56:ARG:N    | 2.38                     | 0.56              |
| 22:a:463:G:N2    | 22:a:466:A:OP2   | 2.30                     | 0.56              |
| 22:a:581:C:H2'   | 22:a:582:A:C8    | 2.40                     | 0.56              |
| 22:a:1315:C:O2'  | 22:a:1392:A:N3   | 2.34                     | 0.56              |
| 22:a:1901:A:OP2  | 24:c:253:LYS:NZ  | 2.39                     | 0.56              |
| 1:A:38:G:H22     | 1:A:397:A:H5'    | 1.69                     | 0.56              |
| 7:G:88:PRO:HG3   | 7:G:149:LYS:HA   | 1.86                     | 0.56              |
| 9:I:84:THR:HG23  | 9:I:98:LEU:HD13  | 1.88                     | 0.56              |
| 22:a:151:C:H2'   | 22:a:152:A:H8    | 1.71                     | 0.56              |
| 22:a:2635:A:O2'  | 25:d:81:GLU:OE2  | 2.20                     | 0.56              |
| 2:B:54:LEU:HD23  | 2:B:220:THR:HB   | 1.87                     | 0.56              |
| 22:a:1149:G:H2'  | 22:a:1150:C:C6   | 2.40                     | 0.56              |
| 34:m:30:ARG:NH2  | 34:m:74:GLU:OE2  | 2.39                     | 0.56              |
| 2:B:187:VAL:HG13 | 2:B:191:SER:HB3  | 1.87                     | 0.56              |
| 1:A:182:A:N1     | 1:A:223:A:O2'    | 2.38                     | 0.56              |
| 1:A:362:G:N1     | 1:A:365:U:OP2    | 2.38                     | 0.56              |
| 6:F:42:TRP:HB2   | 6:F:59:TYR:HB2   | 1.87                     | 0.56              |
| 22:a:1720:U:H2'  | 22:a:1721:G:O4'  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:1754:A:O2'  | 36:o:103:ARG:NH2  | 2.39                     | 0.56              |
| 45:x:34:SER:OG   | 45:x:36:GLN:OE1   | 2.21                     | 0.56              |
| 1:A:309:A:H2'    | 1:A:310:G:H8      | 1.70                     | 0.56              |
| 1:A:718:A:OP2    | 1:A:720:C:N4      | 2.38                     | 0.56              |
| 20:T:35:VAL:HG21 | 20:T:54:MET:SD    | 2.45                     | 0.56              |
| 22:a:172:A:H2'   | 22:a:173:A:H8     | 1.71                     | 0.56              |
| 22:a:291:G:O6    | 22:a:349:U:O2     | 2.24                     | 0.56              |
| 23:b:1:U:H2'     | 23:b:2:G:C8       | 2.41                     | 0.56              |
| 40:s:59:ASN:HB2  | 40:s:84:TYR:HB2   | 1.87                     | 0.55              |
| 1:A:34:C:H2'     | 1:A:35:G:H8       | 1.70                     | 0.55              |
| 33:l:25:ASP:O    | 33:l:66:ARG:NH1   | 2.39                     | 0.55              |
| 1:A:1071:C:H2'   | 1:A:1072:G:C8     | 2.40                     | 0.55              |
| 5:E:45:ARG:HG2   | 5:E:71:MET:HE3    | 1.88                     | 0.55              |
| 22:a:2273:A:H2'  | 22:a:2274:A:C8    | 2.41                     | 0.55              |
| 28:g:55:ARG:HG2  | 28:g:56:ASP:H     | 1.69                     | 0.55              |
| 32:k:85:VAL:HG21 | 32:k:90:VAL:HG13  | 1.88                     | 0.55              |
| 16:P:50:THR:HG21 | 16:P:74:LEU:HD12  | 1.89                     | 0.55              |
| 22:a:729:G:H5'   | 22:a:730:A:H5''   | 1.87                     | 0.55              |
| 1:A:490:C:H2'    | 1:A:491:G:C8      | 2.41                     | 0.55              |
| 1:A:1152:A:OP1   | 10:J:70:HIS:ND1   | 2.34                     | 0.55              |
| 40:s:54:GLU:HB3  | 40:s:88:LYS:NZ    | 2.21                     | 0.55              |
| 43:v:59:LEU:HD12 | 43:v:80:ILE:HD12  | 1.87                     | 0.55              |
| 1:A:1106:G:H5''  | 3:C:172:ARG:HG2   | 1.88                     | 0.55              |
| 1:A:1326:U:H2'   | 1:A:1327:C:C6     | 2.42                     | 0.55              |
| 11:K:79:ILE:HB   | 11:K:105:PHE:HE1  | 1.72                     | 0.55              |
| 14:N:27:LEU:HD22 | 14:N:48:LEU:HD13  | 1.88                     | 0.55              |
| 18:R:57:ARG:O    | 18:R:61:ARG:HG3   | 2.07                     | 0.55              |
| 30:i:31:GLU:HG2  | 30:i:142:ILE:HG12 | 1.89                     | 0.55              |
| 1:A:302:G:O2'    | 12:L:14:ARG:NH1   | 2.39                     | 0.55              |
| 12:L:56:ARG:NE   | 12:L:62:GLU:OE2   | 2.39                     | 0.55              |
| 22:a:177:G:OP2   | 22:a:177:G:N2     | 2.30                     | 0.55              |
| 22:a:1000:A:H2'  | 22:a:1001:A:C8    | 2.42                     | 0.55              |
| 1:A:490:C:H2'    | 1:A:491:G:H8      | 1.72                     | 0.55              |
| 22:a:1484:U:H2'  | 22:a:1485:U:C6    | 2.41                     | 0.55              |
| 22:a:1590:A:H2'  | 22:a:1591:A:C8    | 2.42                     | 0.55              |
| 22:a:1597:A:H5'' | 22:a:1598:A:H5'   | 1.89                     | 0.55              |
| 22:a:1799:G:OP1  | 24:c:258:ARG:NH1  | 2.33                     | 0.55              |
| 26:e:1:MET:HG3   | 26:e:14:VAL:HG23  | 1.89                     | 0.55              |
| 40:s:54:GLU:H    | 40:s:91:GLN:HG2   | 1.72                     | 0.55              |
| 1:A:235:C:H2'    | 1:A:236:A:H8      | 1.71                     | 0.54              |
| 1:A:1279:G:OP2   | 10:J:11:LYS:NZ    | 2.27                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:69:VAL:HG23  | 7:G:100:ALA:HB1   | 1.88                     | 0.54              |
| 22:a:272:A:H2'   | 22:a:273:G:C8     | 2.42                     | 0.54              |
| 22:a:2581:G:N2   | 22:a:2581:G:OP2   | 2.35                     | 0.54              |
| 23:b:48:U:H2'    | 23:b:49:C:C6      | 2.41                     | 0.54              |
| 33:l:42:THR:HG22 | 33:l:93:VAL:HG12  | 1.89                     | 0.54              |
| 38:q:43:ASN:O    | 38:q:43:ASN:ND2   | 2.40                     | 0.54              |
| 1:A:407:U:H2'    | 1:A:408:A:C8      | 2.42                     | 0.54              |
| 22:a:1864:U:OP1  | 22:a:2410:G:O2'   | 2.20                     | 0.54              |
| 23:b:66:A:N6     | 23:b:107:G:H2'    | 2.23                     | 0.54              |
| 1:A:950:U:O4     | 13:M:104:THR:HG21 | 2.07                     | 0.54              |
| 22:a:2246:G:H2'  | 22:a:2247:A:H8    | 1.72                     | 0.54              |
| 53:V:63:C:H2'    | 53:V:64:C:C6      | 2.43                     | 0.54              |
| 1:A:1162:C:H2'   | 1:A:1163:A:H8     | 1.72                     | 0.54              |
| 5:E:15:LEU:HD12  | 5:E:37:THR:HG22   | 1.89                     | 0.54              |
| 6:F:3:HIS:ND1    | 6:F:65:GLU:OE2    | 2.38                     | 0.54              |
| 22:a:323:C:H2'   | 26:e:163:ASN:OD1  | 2.06                     | 0.54              |
| 22:a:1754:A:N1   | 22:a:2716:C:O2'   | 2.36                     | 0.54              |
| 55:X:23:A:H2'    | 55:X:24:G:H8      | 1.73                     | 0.54              |
| 1:A:1314:C:H2'   | 1:A:1315:U:C6     | 2.43                     | 0.54              |
| 11:K:87:LYS:HB2  | 11:K:113:VAL:HG23 | 1.88                     | 0.54              |
| 13:M:3:ARG:O     | 13:M:57:ARG:NH2   | 2.39                     | 0.54              |
| 22:a:851:C:H2'   | 22:a:852:U:H6     | 1.73                     | 0.54              |
| 34:m:98:LEU:HG   | 47:z:54:VAL:HG11  | 1.90                     | 0.54              |
| 1:A:1120:C:H2'   | 1:A:1121:U:H6     | 1.72                     | 0.54              |
| 33:l:35:ALA:HB2  | 33:l:102:LEU:HD11 | 1.88                     | 0.54              |
| 1:A:993:G:O2'    | 1:A:994:A:N7      | 2.38                     | 0.54              |
| 1:A:1314:C:H2'   | 1:A:1315:U:H6     | 1.72                     | 0.54              |
| 3:C:5:VAL:HG21   | 3:C:10:ILE:HD11   | 1.90                     | 0.54              |
| 22:a:721:A:H2'   | 22:a:722:A:C8     | 2.43                     | 0.54              |
| 22:a:5:A:H2'     | 22:a:6:A:H8       | 1.73                     | 0.54              |
| 1:A:1291:U:H2'   | 1:A:1292:G:H8     | 1.73                     | 0.54              |
| 4:D:140:ASN:N    | 4:D:182:PHE:O     | 2.41                     | 0.54              |
| 8:H:90:ASP:OD1   | 8:H:90:ASP:N      | 2.41                     | 0.54              |
| 29:h:30:LEU:HD13 | 29:h:35:LYS:HG3   | 1.88                     | 0.54              |
| 42:u:77:VAL:HG23 | 42:u:89:ILE:HG12  | 1.90                     | 0.54              |
| 7:G:75:VAL:HB    | 7:G:86:GLN:HB3    | 1.90                     | 0.54              |
| 22:a:1476:U:H2'  | 22:a:1477:A:H8    | 1.73                     | 0.54              |
| 22:a:2071:A:H2'  | 22:a:2072:C:C6    | 2.42                     | 0.54              |
| 1:A:269:C:H2'    | 1:A:270:A:C8      | 2.44                     | 0.53              |
| 1:A:945:G:C2     | 1:A:946:A:C8      | 2.96                     | 0.53              |
| 1:A:1021:A:H2'   | 1:A:1022:A:C8     | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1250:A:H2'   | 1:A:1251:A:C8    | 2.42                     | 0.53              |
| 13:M:17:ILE:O    | 13:M:20:THR:OG1  | 2.26                     | 0.53              |
| 22:a:1432:G:H2'  | 22:a:1433:A:C8   | 2.43                     | 0.53              |
| 22:a:1475:G:O2'  | 22:a:1514:G:O6   | 2.26                     | 0.53              |
| 22:a:2097:A:H2'  | 22:a:2098:U:C6   | 2.43                     | 0.53              |
| 33:l:55:ARG:NE   | 55:X:54:5MU:OP1  | 2.39                     | 0.53              |
| 33:l:106:ASP:OD1 | 33:l:107:GLY:N   | 2.38                     | 0.53              |
| 1:A:720:C:O2     | 18:R:60:LYS:NZ   | 2.37                     | 0.53              |
| 22:a:580:U:H2'   | 22:a:581:C:C6    | 2.43                     | 0.53              |
| 22:a:2419:U:H4'  | 48:0:22:THR:HG21 | 1.89                     | 0.53              |
| 35:n:70:ALA:O    | 35:n:74:VAL:HG23 | 2.09                     | 0.53              |
| 1:A:384:G:H2'    | 1:A:385:C:H6     | 1.72                     | 0.53              |
| 22:a:2283:C:OP1  | 48:0:4:GLY:N     | 2.42                     | 0.53              |
| 1:A:1238:A:OP1   | 1:A:1335:U:O2'   | 2.16                     | 0.53              |
| 5:E:110:ALA:O    | 5:E:114:VAL:HG23 | 2.09                     | 0.53              |
| 22:a:1636:U:H2'  | 22:a:1637:A:H8   | 1.73                     | 0.53              |
| 22:a:1856:U:H2'  | 22:a:1857:G:O4'  | 2.09                     | 0.53              |
| 22:a:1913:A:N1   | 55:X:37:MKX:O2'  | 2.42                     | 0.53              |
| 33:l:28:PHE:N    | 33:l:104:GLU:OE2 | 2.39                     | 0.53              |
| 55:X:49:G:H2'    | 55:X:50:C:C6     | 2.44                     | 0.53              |
| 1:A:1063:C:OP2   | 1:A:1064:G:O2'   | 2.26                     | 0.53              |
| 22:a:703:U:H2'   | 22:a:704:G:O4'   | 2.09                     | 0.53              |
| 22:a:1190:G:OP1  | 32:k:30:THR:OG1  | 2.21                     | 0.53              |
| 22:a:1433:A:H2'  | 22:a:1434:A:C8   | 2.44                     | 0.53              |
| 23:b:66:A:H61    | 23:b:107:G:H2'   | 1.73                     | 0.53              |
| 1:A:111:G:H1     | 1:A:330:C:H41    | 1.55                     | 0.53              |
| 2:B:8:ASP:OD1    | 2:B:9:MET:N      | 2.41                     | 0.53              |
| 18:R:37:GLY:O    | 18:R:63:ARG:NH2  | 2.42                     | 0.53              |
| 1:A:222:C:H2'    | 1:A:223:A:H8     | 1.73                     | 0.53              |
| 1:A:324:G:N1     | 1:A:327:A:OP2    | 2.41                     | 0.53              |
| 1:A:1391:U:H2'   | 1:A:1392:G:C8    | 2.43                     | 0.53              |
| 3:C:69:HIS:HA    | 3:C:104:ALA:HB3  | 1.91                     | 0.53              |
| 7:G:74:GLU:HG2   | 7:G:91:VAL:HG22  | 1.91                     | 0.53              |
| 13:M:89:LEU:HD22 | 13:M:93:ARG:NH2  | 2.24                     | 0.53              |
| 22:a:296:U:H2'   | 22:a:297:G:H8    | 1.74                     | 0.53              |
| 26:e:83:VAL:HB   | 26:e:86:ALA:HB2  | 1.91                     | 0.53              |
| 1:A:384:G:H2'    | 1:A:385:C:C6     | 2.44                     | 0.53              |
| 13:M:7:ILE:HD11  | 13:M:22:ILE:HG13 | 1.90                     | 0.53              |
| 39:r:18:ARG:HG3  | 39:r:76:VAL:HB   | 1.89                     | 0.53              |
| 40:s:54:GLU:HB3  | 40:s:88:LYS:HZ1  | 1.74                     | 0.53              |
| 2:B:129:LEU:HB3  | 2:B:133:GLU:HG2  | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:15:SER:OG    | 6:F:44:ARG:NH1    | 2.41                     | 0.53              |
| 22:a:171:U:H2'   | 22:a:172:A:H8     | 1.74                     | 0.53              |
| 23:b:14:U:OP2    | 23:b:70:C:O2'     | 2.27                     | 0.53              |
| 50:2:15:LYS:HB2  | 50:2:23:LYS:HE2   | 1.91                     | 0.53              |
| 1:A:519:C:HO2'   | 1:A:520:A:P       | 2.32                     | 0.52              |
| 1:A:976:G:OP2    | 1:A:1358:U:O2'    | 2.27                     | 0.52              |
| 22:a:64:A:H2'    | 22:a:65:U:C6      | 2.43                     | 0.52              |
| 22:a:281:C:N4    | 22:a:282:A:H62    | 2.08                     | 0.52              |
| 46:y:24:LEU:HD21 | 46:y:54:MET:HE3   | 1.91                     | 0.52              |
| 1:A:579:A:H2'    | 1:A:580:C:C6      | 2.44                     | 0.52              |
| 2:B:27:MET:HE1   | 2:B:193:PRO:HG3   | 1.91                     | 0.52              |
| 4:D:102:VAL:HG13 | 4:D:107:PHE:HB2   | 1.91                     | 0.52              |
| 22:a:2246:G:H2'  | 22:a:2247:A:C8    | 2.45                     | 0.52              |
| 44:w:11:ARG:HD3  | 44:w:12:PRO:HD2   | 1.90                     | 0.52              |
| 1:A:407:U:O2'    | 4:D:113:GLU:OE1   | 2.27                     | 0.52              |
| 14:N:27:LEU:CD2  | 14:N:48:LEU:HB2   | 2.38                     | 0.52              |
| 19:S:38:SER:HB2  | 19:S:71:LEU:HD12  | 1.91                     | 0.52              |
| 22:a:219:A:N3    | 22:a:234:U:O2'    | 2.35                     | 0.52              |
| 22:a:871:U:H2'   | 22:a:872:U:C6     | 2.45                     | 0.52              |
| 22:a:1353:A:H2'  | 22:a:1354:A:H8    | 1.74                     | 0.52              |
| 22:a:1794:A:H2'  | 22:a:1795:C:C6    | 2.44                     | 0.52              |
| 22:a:2025:C:H2'  | 22:a:2026:U:C6    | 2.44                     | 0.52              |
| 22:a:2505:G:N2   | 22:a:2506:U:O4    | 2.41                     | 0.52              |
| 24:c:107:PRO:HD2 | 24:c:110:LEU:HD22 | 1.90                     | 0.52              |
| 26:e:147:LEU:HB3 | 26:e:186:VAL:HG23 | 1.91                     | 0.52              |
| 1:A:745:G:H2'    | 1:A:746:A:C8      | 2.44                     | 0.52              |
| 1:A:1376:U:OP2   | 7:G:25:LYS:NZ     | 2.40                     | 0.52              |
| 2:B:217:VAL:HA   | 2:B:220:THR:HG22  | 1.91                     | 0.52              |
| 5:E:25:VAL:HG23  | 5:E:27:GLY:H      | 1.73                     | 0.52              |
| 13:M:107:ARG:NH2 | 13:M:112:PRO:O    | 2.43                     | 0.52              |
| 22:a:720:U:H2'   | 22:a:721:A:C8     | 2.44                     | 0.52              |
| 23:b:115:A:H2'   | 23:b:116:G:H8     | 1.74                     | 0.52              |
| 41:t:66:GLN:HB2  | 41:t:69:ASN:OD1   | 2.10                     | 0.52              |
| 48:0:11:LEU:N    | 48:0:21:TYR:O     | 2.42                     | 0.52              |
| 6:F:8:PHE:CE1    | 6:F:62:MET:HE2    | 2.44                     | 0.52              |
| 7:G:68:ASN:O     | 7:G:138:ARG:NE    | 2.41                     | 0.52              |
| 22:a:1199:U:H1'  | 37:p:4:VAL:HG22   | 1.92                     | 0.52              |
| 23:b:48:U:OP1    | 35:n:30:ARG:NH2   | 2.39                     | 0.52              |
| 36:o:5:ILE:O     | 36:o:9:GLU:HG2    | 2.09                     | 0.52              |
| 1:A:148:G:O2'    | 1:A:1446:A:N3     | 2.38                     | 0.52              |
| 7:G:27:VAL:HG22  | 7:G:43:VAL:HG21   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:577:G:O2'   | 22:a:1254:A:OP1   | 2.26                     | 0.52              |
| 22:a:1434:A:H2'  | 22:a:1435:G:C8    | 2.45                     | 0.52              |
| 22:a:589:U:H2'   | 22:a:590:A:C8     | 2.45                     | 0.52              |
| 22:a:2788:C:H2'  | 22:a:2789:C:C6    | 2.45                     | 0.52              |
| 33:l:64:TRP:HB2  | 33:l:104:GLU:HB3  | 1.91                     | 0.52              |
| 53:V:47:A:O2'    | 53:V:48:C:OP1     | 2.25                     | 0.52              |
| 5:E:81:LEU:HB2   | 5:E:98:PRO:HG3    | 1.90                     | 0.52              |
| 7:G:138:ARG:HG2  | 7:G:142:HIS:CE1   | 2.44                     | 0.52              |
| 22:a:1703:G:H2'  | 22:a:1704:C:C6    | 2.45                     | 0.52              |
| 27:f:16:LEU:HD13 | 27:f:29:PRO:HD2   | 1.91                     | 0.52              |
| 22:a:1386:C:H2'  | 22:a:1387:A:C8    | 2.45                     | 0.52              |
| 22:a:1443:U:H2'  | 22:a:1444:G:H8    | 1.75                     | 0.52              |
| 23:b:111:U:H2'   | 23:b:112:G:H8     | 1.75                     | 0.52              |
| 24:c:155:ALA:HB2 | 24:c:162:VAL:HG23 | 1.91                     | 0.52              |
| 1:A:501:C:H2'    | 1:A:502:A:C8      | 2.45                     | 0.52              |
| 1:A:1318:A:H5''  | 19:S:3:ARG:HH12   | 1.75                     | 0.52              |
| 27:f:126:GLY:O   | 27:f:158:THR:OG1  | 2.24                     | 0.52              |
| 1:A:1507:A:H2'   | 1:A:1508:A:C8     | 2.46                     | 0.51              |
| 6:F:32:ALA:HB2   | 6:F:70:VAL:HG11   | 1.92                     | 0.51              |
| 20:T:35:VAL:HG22 | 20:T:50:ALA:HB1   | 1.91                     | 0.51              |
| 22:a:153:U:OP1   | 44:w:77:LYS:NZ    | 2.44                     | 0.51              |
| 22:a:608:A:H2'   | 22:a:609:A:C8     | 2.45                     | 0.51              |
| 22:a:668:A:H2'   | 22:a:670:A:H62    | 1.76                     | 0.51              |
| 22:a:2809:A:H2'  | 22:a:2810:A:C8    | 2.45                     | 0.51              |
| 22:a:2845:U:H5'' | 36:o:52:ASN:O     | 2.09                     | 0.51              |
| 29:h:7:ASP:OD1   | 29:h:7:ASP:N      | 2.42                     | 0.51              |
| 36:o:7:GLN:NE2   | 36:o:11:GLU:OE2   | 2.39                     | 0.51              |
| 1:A:56:U:H2'     | 1:A:57:G:C8       | 2.45                     | 0.51              |
| 1:A:181:A:N6     | 1:A:195:A:OP2     | 2.40                     | 0.51              |
| 1:A:1032:G:H2'   | 1:A:1033:G:O4'    | 2.09                     | 0.51              |
| 22:a:296:U:H2'   | 22:a:297:G:C8     | 2.44                     | 0.51              |
| 22:a:576:U:H2'   | 22:a:577:G:C8     | 2.44                     | 0.51              |
| 22:a:1198:U:H2'  | 22:a:1199:U:C6    | 2.46                     | 0.51              |
| 28:g:35:ARG:HD3  | 28:g:71:LEU:HD13  | 1.93                     | 0.51              |
| 1:A:1513:A:H2'   | 1:A:1514:G:C8     | 2.46                     | 0.51              |
| 14:N:27:LEU:O    | 14:N:31:ILE:HD12  | 2.11                     | 0.51              |
| 22:a:181:A:H1'   | 22:a:435:C:H5'    | 1.93                     | 0.51              |
| 22:a:593:U:H2'   | 22:a:594:U:C6     | 2.45                     | 0.51              |
| 22:a:1296:G:OP1  | 22:a:2709:G:O2'   | 2.22                     | 0.51              |
| 26:e:7:ASP:OD1   | 26:e:7:ASP:N      | 2.43                     | 0.51              |
| 1:A:1464:U:H2'   | 1:A:1465:A:H8     | 1.76                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:103:TRP:CE2  | 7:G:137:LYS:HE2   | 2.46                     | 0.51              |
| 15:O:18:ASP:OD1  | 15:O:19:ALA:N     | 2.43                     | 0.51              |
| 17:Q:21:ILE:HG12 | 17:Q:48:ASP:HB2   | 1.91                     | 0.51              |
| 22:a:657:U:H2'   | 22:a:658:U:C6     | 2.45                     | 0.51              |
| 22:a:881:G:H2'   | 22:a:882:G:C8     | 2.46                     | 0.51              |
| 22:a:1508:A:O2'  | 22:a:1509:A:O4'   | 2.27                     | 0.51              |
| 22:a:2818:U:H2'  | 22:a:2819:G:H8    | 1.76                     | 0.51              |
| 3:C:185:ASN:OD1  | 3:C:186:THR:N     | 2.40                     | 0.51              |
| 22:a:704:G:O2'   | 22:a:726:G:N2     | 2.40                     | 0.51              |
| 22:a:1645:G:H5'' | 22:a:1646:C:H5'   | 1.91                     | 0.51              |
| 22:a:2392:A:OP2  | 50:2:31:HIS:NE2   | 2.43                     | 0.51              |
| 22:a:2799:A:O2'  | 22:a:2800:A:H5''  | 2.10                     | 0.51              |
| 50:2:52:LYS:HA   | 50:2:55:LEU:HD13  | 1.92                     | 0.51              |
| 1:A:17:U:H2'     | 1:A:18:C:C6       | 2.45                     | 0.51              |
| 1:A:160:A:H2'    | 1:A:161:A:O4'     | 2.10                     | 0.51              |
| 34:m:72:ASP:OD2  | 34:m:75:ILE:HG12  | 2.11                     | 0.51              |
| 1:A:129:A:H2     | 1:A:232:G:H22     | 1.57                     | 0.51              |
| 1:A:715:A:H2'    | 1:A:716:A:C8      | 2.45                     | 0.51              |
| 22:a:347:A:H2'   | 22:a:348:A:H8     | 1.74                     | 0.51              |
| 22:a:1429:G:H2'  | 22:a:1430:G:H8    | 1.76                     | 0.51              |
| 22:a:1478:G:H1   | 22:a:1513:U:H3    | 1.56                     | 0.51              |
| 22:a:2591:C:H2'  | 22:a:2592:G:C8    | 2.45                     | 0.51              |
| 55:X:23:A:H2'    | 55:X:24:G:C8      | 2.46                     | 0.51              |
| 10:J:66:GLU:HB2  | 14:N:99:ALA:HB2   | 1.92                     | 0.51              |
| 22:a:851:C:H2'   | 22:a:852:U:C6     | 2.45                     | 0.51              |
| 22:a:1796:U:H2'  | 22:a:1797:G:H8    | 1.76                     | 0.51              |
| 23:b:106:G:H2'   | 23:b:107:G:O4'    | 2.11                     | 0.51              |
| 53:V:16:A:N6     | 53:V:19:C:HO2'    | 2.07                     | 0.51              |
| 3:C:203:PHE:HZ   | 3:C:206:GLU:HG3   | 1.76                     | 0.51              |
| 22:a:797:G:OP1   | 26:e:55:SER:OG    | 2.25                     | 0.51              |
| 22:a:1469:A:H2'  | 22:a:1470:A:C8    | 2.46                     | 0.51              |
| 22:a:1704:C:H2'  | 22:a:1705:A:C8    | 2.45                     | 0.51              |
| 53:V:65:U:H2'    | 53:V:66:A:H8      | 1.76                     | 0.51              |
| 53:V:69:G:H2'    | 53:V:70:G:H8      | 1.75                     | 0.51              |
| 1:A:79:G:N1      | 1:A:91:U:O4       | 2.44                     | 0.51              |
| 1:A:470:C:H2'    | 1:A:471:U:C6      | 2.46                     | 0.51              |
| 5:E:10:GLU:HG2   | 5:E:11:LEU:HD23   | 1.94                     | 0.51              |
| 6:F:4:TYR:CE2    | 6:F:71:ILE:HG13   | 2.47                     | 0.51              |
| 22:a:1820:U:H5   | 24:c:177:ARG:HH12 | 1.57                     | 0.51              |
| 22:a:2241:A:H2'  | 22:a:2242:G:C8    | 2.46                     | 0.51              |
| 22:a:2243:U:H2'  | 22:a:2244:U:C6    | 2.45                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:k:70:LYS:O    | 32:k:74:THR:OG1   | 2.19                     | 0.51              |
| 1:A:399:G:H2'    | 1:A:400:C:C6      | 2.46                     | 0.50              |
| 3:C:72:ARG:HB2   | 3:C:75:ILE:HD13   | 1.93                     | 0.50              |
| 14:N:27:LEU:HD21 | 14:N:48:LEU:HB2   | 1.92                     | 0.50              |
| 22:a:832:U:H2'   | 22:a:833:A:H8     | 1.75                     | 0.50              |
| 11:K:109:ASN:HB3 | 21:U:5:LYS:HA     | 1.93                     | 0.50              |
| 17:Q:20:SER:HB3  | 17:Q:71:LYS:NZ    | 2.26                     | 0.50              |
| 22:a:160:A:N3    | 22:a:2208:C:O2'   | 2.43                     | 0.50              |
| 22:a:364:C:H2'   | 22:a:365:U:C6     | 2.47                     | 0.50              |
| 22:a:848:C:H2'   | 22:a:849:A:C8     | 2.44                     | 0.50              |
| 22:a:1019:U:OP1  | 22:a:1035:U:O2'   | 2.20                     | 0.50              |
| 46:y:39:GLU:HG3  | 46:y:41:THR:HG23  | 1.92                     | 0.50              |
| 1:A:35:G:H2'     | 1:A:36:C:C6       | 2.46                     | 0.50              |
| 1:A:436:C:H2'    | 1:A:437:U:C6      | 2.46                     | 0.50              |
| 22:a:987:C:O2'   | 22:a:1000:A:N3    | 2.37                     | 0.50              |
| 22:a:2064:C:H2'  | 22:a:2065:C:C6    | 2.46                     | 0.50              |
| 41:t:4:LYS:O     | 41:t:94:ARG:NH1   | 2.45                     | 0.50              |
| 41:t:7:ARG:HD2   | 41:t:8:ASP:CG     | 2.36                     | 0.50              |
| 1:A:2:A:H2'      | 1:A:3:A:C8        | 2.46                     | 0.50              |
| 1:A:167:A:H2'    | 1:A:168:G:C8      | 2.46                     | 0.50              |
| 1:A:1458:G:H5'   | 20:T:27:MET:HB3   | 1.92                     | 0.50              |
| 22:a:2649:C:H2'  | 22:a:2650:U:H6    | 1.76                     | 0.50              |
| 30:i:13:ARG:NH1  | 30:i:49:ASP:O     | 2.44                     | 0.50              |
| 1:A:575:G:O2'    | 1:A:821:G:OP2     | 2.28                     | 0.50              |
| 1:A:652:U:O4     | 1:A:752:G:O2'     | 2.22                     | 0.50              |
| 1:A:1120:C:H2'   | 1:A:1121:U:C6     | 2.45                     | 0.50              |
| 1:A:1218:C:H2'   | 1:A:1219:A:C8     | 2.47                     | 0.50              |
| 8:H:96:MET:SD    | 8:H:130:ALA:HB1   | 2.52                     | 0.50              |
| 22:a:645:C:H2'   | 22:a:647:G:C8     | 2.47                     | 0.50              |
| 22:a:2300:C:H2'  | 22:a:2301:C:H6    | 1.76                     | 0.50              |
| 25:d:184:ARG:HB2 | 25:d:186:LEU:HD13 | 1.94                     | 0.50              |
| 55:X:8:4SU:O2'   | 55:X:21:A:N1      | 2.43                     | 0.50              |
| 1:A:643:C:H2'    | 1:A:644:U:H6      | 1.77                     | 0.50              |
| 3:C:24:ALA:HB1   | 3:C:28:GLU:HG2    | 1.93                     | 0.50              |
| 6:F:44:ARG:HB3   | 6:F:56:LYS:HE3    | 1.93                     | 0.50              |
| 22:a:1746:A:H2'  | 22:a:1747:U:C6    | 2.47                     | 0.50              |
| 25:d:5:VAL:H     | 25:d:32:ASN:ND2   | 2.02                     | 0.50              |
| 33:l:53:MET:HG3  | 33:l:120:ALA:HB2  | 1.92                     | 0.50              |
| 2:B:57:LEU:HG    | 2:B:184:PHE:HE2   | 1.77                     | 0.50              |
| 10:J:27:GLU:HB3  | 10:J:31:ARG:NH2   | 2.27                     | 0.50              |
| 22:a:306:U:H2'   | 22:a:307:G:O4'    | 2.12                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:1443:U:H2'  | 22:a:1444:G:C8    | 2.46                     | 0.50              |
| 22:a:2300:C:H2'  | 22:a:2301:C:C6    | 2.47                     | 0.50              |
| 1:A:34:C:H2'     | 1:A:35:G:C8       | 2.47                     | 0.50              |
| 1:A:666:G:H5'    | 1:A:726:C:H1'     | 1.92                     | 0.50              |
| 2:B:16:PHE:O     | 2:B:203:ASN:ND2   | 2.45                     | 0.50              |
| 8:H:18:GLN:HE21  | 8:H:70:ALA:HB1    | 1.77                     | 0.50              |
| 22:a:17:G:H2'    | 22:a:18:U:C6      | 2.46                     | 0.50              |
| 22:a:191:A:H2'   | 22:a:192:C:C6     | 2.46                     | 0.50              |
| 22:a:191:A:H2'   | 22:a:192:C:H6     | 1.75                     | 0.50              |
| 22:a:875:G:H2'   | 22:a:876:C:C6     | 2.47                     | 0.50              |
| 22:a:2515:C:H2'  | 22:a:2516:A:H8    | 1.77                     | 0.50              |
| 24:c:232:HIS:HA  | 24:c:242:LYS:HE3  | 1.92                     | 0.50              |
| 28:g:140:VAL:O   | 28:g:144:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:648:A:H2'    | 1:A:649:A:C8      | 2.47                     | 0.50              |
| 1:A:728:A:H2'    | 1:A:729:A:C8      | 2.47                     | 0.50              |
| 22:a:1540:G:H2'  | 22:a:1541:C:C6    | 2.47                     | 0.50              |
| 55:X:2:G:H2'     | 55:X:3:C:C6       | 2.47                     | 0.50              |
| 1:A:673:A:H2'    | 1:A:674:G:H8      | 1.74                     | 0.49              |
| 22:a:494:G:H4'   | 39:r:6:LYS:HG3    | 1.93                     | 0.49              |
| 1:A:493:A:H2'    | 1:A:494:G:C8      | 2.47                     | 0.49              |
| 22:a:278:A:N6    | 22:a:362:A:N7     | 2.60                     | 0.49              |
| 22:a:582:A:H2'   | 22:a:583:G:C8     | 2.46                     | 0.49              |
| 22:a:909:A:H2'   | 22:a:912:C:H5     | 1.77                     | 0.49              |
| 22:a:1571:A:H2'  | 22:a:1572:A:C8    | 2.46                     | 0.49              |
| 22:a:1667:G:O2'  | 22:a:1991:U:O4    | 2.27                     | 0.49              |
| 22:a:2392:A:C2   | 32:k:55:MET:HE3   | 2.47                     | 0.49              |
| 27:f:105:THR:HA  | 52:4:38:SER:HB3   | 1.93                     | 0.49              |
| 30:i:115:GLY:HA2 | 30:i:118:MET:HE3  | 1.93                     | 0.49              |
| 6:F:74:LEU:HG    | 6:F:78:PHE:CE2    | 2.46                     | 0.49              |
| 7:G:92:ARG:NH1   | 7:G:94:VAL:HB     | 2.26                     | 0.49              |
| 9:I:44:ALA:O     | 9:I:48:VAL:HG23   | 2.12                     | 0.49              |
| 13:M:83:LEU:HD21 | 19:S:65:GLU:HB3   | 1.94                     | 0.49              |
| 19:S:50:ALA:HB1  | 19:S:57:HIS:HB3   | 1.92                     | 0.49              |
| 23:b:95:U:H2'    | 23:b:96:G:H8      | 1.77                     | 0.49              |
| 28:g:164:TYR:HB2 | 28:g:167:GLU:HB2  | 1.94                     | 0.49              |
| 32:k:57:LEU:HD22 | 50:2:54:ASP:HB3   | 1.95                     | 0.49              |
| 37:p:86:ALA:HB2  | 37:p:116:ALA:HB2  | 1.94                     | 0.49              |
| 53:V:50:G:H2'    | 53:V:51:G:C8      | 2.47                     | 0.49              |
| 8:H:49:PHE:HB3   | 8:H:61:LEU:HD23   | 1.94                     | 0.49              |
| 18:R:26:ILE:O    | 18:R:30:LYS:HG2   | 2.12                     | 0.49              |
| 22:a:278:A:H2'   | 22:a:278:A:N3     | 2.26                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:534:U:O2'   | 37:p:49:ASP:OD1  | 2.15                     | 0.49              |
| 22:a:742:A:H2'   | 22:a:743:A:H8    | 1.78                     | 0.49              |
| 22:a:1281:G:H2'  | 22:a:1282:U:C6   | 2.47                     | 0.49              |
| 27:f:30:ARG:H    | 27:f:159:THR:HB  | 1.77                     | 0.49              |
| 31:j:105:ARG:NH1 | 36:o:34:GLU:OE2  | 2.44                     | 0.49              |
| 40:s:72:GLN:O    | 40:s:72:GLN:HG2  | 2.11                     | 0.49              |
| 1:A:195:A:O2'    | 1:A:196:A:O4'    | 2.16                     | 0.49              |
| 1:A:236:A:H2'    | 1:A:237:G:C8     | 2.47                     | 0.49              |
| 3:C:120:ILE:O    | 3:C:124:LEU:HG   | 2.13                     | 0.49              |
| 22:a:495:G:H21   | 39:r:61:ASN:HD21 | 1.60                     | 0.49              |
| 22:a:2327:A:H2'  | 22:a:2328:A:C8   | 2.47                     | 0.49              |
| 23:b:48:U:H2'    | 23:b:49:C:H6     | 1.76                     | 0.49              |
| 36:o:22:PRO:HD3  | 36:o:50:ILE:HD12 | 1.93                     | 0.49              |
| 53:V:16:A:N6     | 53:V:20:C:OP1    | 2.45                     | 0.49              |
| 1:A:171:A:H2'    | 1:A:172:A:C8     | 2.47                     | 0.49              |
| 6:F:3:HIS:O      | 6:F:92:THR:N     | 2.43                     | 0.49              |
| 10:J:6:ILE:HD12  | 10:J:76:ILE:HD11 | 1.95                     | 0.49              |
| 22:a:357:C:H2'   | 22:a:358:U:C6    | 2.48                     | 0.49              |
| 22:a:1187:G:H5'' | 38:q:83:TYR:CE1  | 2.48                     | 0.49              |
| 22:a:1689:A:H2'  | 22:a:1690:A:C8   | 2.47                     | 0.49              |
| 34:m:57:THR:HG23 | 34:m:62:ASN:ND2  | 2.27                     | 0.49              |
| 42:u:9:ARG:NE    | 42:u:27:PRO:HB3  | 2.28                     | 0.49              |
| 1:A:920:U:H2'    | 1:A:921:U:C6     | 2.48                     | 0.49              |
| 22:a:24:G:O2'    | 39:r:78:GLU:O    | 2.27                     | 0.49              |
| 22:a:589:U:H2'   | 22:a:590:A:H8    | 1.77                     | 0.49              |
| 22:a:2328:A:H2'  | 22:a:2329:U:H6   | 1.75                     | 0.49              |
| 32:k:49:GLY:HA3  | 32:k:58:TYR:HE2  | 1.75                     | 0.49              |
| 39:r:23:LEU:HD22 | 47:z:24:ALA:HB2  | 1.95                     | 0.49              |
| 44:w:59:ILE:HD12 | 44:w:67:VAL:HG21 | 1.94                     | 0.49              |
| 1:A:737:C:H2'    | 1:A:738:C:H6     | 1.78                     | 0.49              |
| 3:C:10:ILE:HD13  | 14:N:98:LYS:HG3  | 1.95                     | 0.49              |
| 4:D:103:TYR:OH   | 4:D:165:ARG:NH1  | 2.45                     | 0.49              |
| 15:O:64:ARG:O    | 15:O:64:ARG:HD3  | 2.13                     | 0.49              |
| 22:a:112:U:H2'   | 22:a:113:U:O4'   | 2.13                     | 0.49              |
| 22:a:287:G:H2'   | 22:a:288:U:C6    | 2.48                     | 0.49              |
| 22:a:550:C:H2'   | 22:a:551:G:H8    | 1.78                     | 0.49              |
| 12:L:86:ARG:HH12 | 12:L:88:LYS:HD3  | 1.78                     | 0.49              |
| 15:O:35:GLN:HE21 | 15:O:39:LEU:HG   | 1.78                     | 0.49              |
| 22:a:411:G:OP2   | 22:a:2406:A:O2'  | 2.30                     | 0.49              |
| 22:a:1748:C:H2'  | 22:a:1749:A:C8   | 2.48                     | 0.49              |
| 22:a:2557:G:H2'  | 22:a:2558:C:C6   | 2.48                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:c:72:ASP:OD1   | 24:c:189:ARG:NH2  | 2.45                     | 0.49              |
| 27:f:8:TYR:HA     | 27:f:12:VAL:HB    | 1.95                     | 0.49              |
| 1:A:1095:U:H2'    | 1:A:1096:C:C6     | 2.47                     | 0.49              |
| 1:A:1463:U:H2'    | 1:A:1464:U:H6     | 1.78                     | 0.49              |
| 6:F:93:LYS:HG3    | 6:F:94:HIS:ND1    | 2.28                     | 0.49              |
| 9:I:6:TYR:HB2     | 9:I:21:ILE:HB     | 1.95                     | 0.49              |
| 22:a:151:C:H2'    | 22:a:152:A:C8     | 2.48                     | 0.49              |
| 22:a:2074:U:H2'   | 22:a:2075:U:C6    | 2.48                     | 0.49              |
| 22:a:2421:G:OP2   | 50:2:32:ILE:HG22  | 2.13                     | 0.49              |
| 24:c:225:MET:SD   | 24:c:230:HIS:HB2  | 2.53                     | 0.49              |
| 25:d:122:VAL:HG21 | 25:d:129:THR:HG22 | 1.94                     | 0.49              |
| 28:g:126:PRO:HG2  | 28:g:130:GLU:OE2  | 2.12                     | 0.49              |
| 37:p:94:ILE:O     | 37:p:98:ILE:HG12  | 2.13                     | 0.49              |
| 1:A:168:G:H2'     | 1:A:169:C:H6      | 1.78                     | 0.48              |
| 1:A:1020:G:H2'    | 1:A:1021:A:H8     | 1.77                     | 0.48              |
| 1:A:1021:A:H2'    | 1:A:1022:A:H8     | 1.77                     | 0.48              |
| 1:A:1412:C:H2'    | 1:A:1413:A:C8     | 2.48                     | 0.48              |
| 6:F:20:GLY:O      | 6:F:24:ARG:HG3    | 2.13                     | 0.48              |
| 9:I:4:ASN:N       | 9:I:4:ASN:ND2     | 2.60                     | 0.48              |
| 16:P:4:ILE:HG13   | 16:P:21:VAL:HG22  | 1.94                     | 0.48              |
| 21:U:28:VAL:O     | 21:U:32:VAL:HG23  | 2.13                     | 0.48              |
| 22:a:184:C:H2'    | 22:a:185:G:C8     | 2.46                     | 0.48              |
| 24:c:98:ASP:N     | 24:c:98:ASP:OD1   | 2.46                     | 0.48              |
| 24:c:133:ARG:NH2  | 24:c:187:ASP:OD1  | 2.38                     | 0.48              |
| 27:f:38:MET:SD    | 27:f:57:LEU:HB2   | 2.52                     | 0.48              |
| 27:f:135:GLN:OE1  | 27:f:141:ILE:HD13 | 2.12                     | 0.48              |
| 1:A:131:A:H2'     | 1:A:132:C:H6      | 1.78                     | 0.48              |
| 1:A:235:C:H2'     | 1:A:236:A:C8      | 2.48                     | 0.48              |
| 1:A:335:C:H2'     | 1:A:336:A:C8      | 2.47                     | 0.48              |
| 1:A:1062:U:H2'    | 1:A:1063:C:C6     | 2.48                     | 0.48              |
| 1:A:1377:A:OP1    | 7:G:92:ARG:NH2    | 2.46                     | 0.48              |
| 2:B:32:PHE:N      | 2:B:40:ILE:O      | 2.46                     | 0.48              |
| 22:a:282:A:H2'    | 22:a:283:G:H8     | 1.79                     | 0.48              |
| 22:a:1744:A:H3'   | 22:a:1745:A:H8    | 1.79                     | 0.48              |
| 1:A:501:C:H2'     | 1:A:502:A:H8      | 1.77                     | 0.48              |
| 1:A:1018:G:H2'    | 1:A:1019:A:H8     | 1.78                     | 0.48              |
| 13:M:34:LEU:HD13  | 13:M:41:GLU:HA    | 1.94                     | 0.48              |
| 21:U:4:ILE:HD13   | 21:U:19:PHE:HD1   | 1.77                     | 0.48              |
| 22:a:276:U:O2'    | 22:a:278:A:N7     | 2.45                     | 0.48              |
| 22:a:1292:G:H2'   | 22:a:1293:C:C6    | 2.47                     | 0.48              |
| 22:a:2287:A:OP1   | 48:0:30:LYS:NZ    | 2.31                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:2740:A:H2'  | 22:a:2741:A:C8    | 2.49                     | 0.48              |
| 24:c:145:GLU:HB2 | 24:c:188:CYS:HB3  | 1.95                     | 0.48              |
| 27:f:71:ARG:HH21 | 27:f:72:LYS:HD3   | 1.79                     | 0.48              |
| 44:w:43:GLU:OE1  | 44:w:45:ARG:NH1   | 2.42                     | 0.48              |
| 1:A:958:A:C5     | 19:S:55:ARG:HD3   | 2.48                     | 0.48              |
| 1:A:1436:U:H2'   | 1:A:1437:A:C8     | 2.48                     | 0.48              |
| 2:B:57:LEU:HG    | 2:B:184:PHE:CE2   | 2.49                     | 0.48              |
| 7:G:111:ARG:HH21 | 7:G:123:GLU:HA    | 1.77                     | 0.48              |
| 8:H:7:ILE:O      | 8:H:11:LEU:HG     | 2.14                     | 0.48              |
| 19:S:35:SER:OG   | 19:S:38:SER:OG    | 2.30                     | 0.48              |
| 22:a:1434:A:H2'  | 22:a:1435:G:H8    | 1.77                     | 0.48              |
| 22:a:1871:A:H2'  | 22:a:1872:A:C8    | 2.48                     | 0.48              |
| 22:a:2482:A:O2'  | 55:X:63:A:O2'     | 2.21                     | 0.48              |
| 22:a:2682:A:C8   | 25:d:11:MET:HG2   | 2.48                     | 0.48              |
| 34:m:95:THR:HG22 | 34:m:115:LEU:HD23 | 1.94                     | 0.48              |
| 1:A:674:G:H2'    | 1:A:675:A:C8      | 2.48                     | 0.48              |
| 22:a:2818:U:H2'  | 22:a:2819:G:C8    | 2.49                     | 0.48              |
| 31:j:71:ARG:HA   | 31:j:71:ARG:HD3   | 1.70                     | 0.48              |
| 35:n:50:ALA:O    | 35:n:81:ARG:NH1   | 2.47                     | 0.48              |
| 5:E:107:ALA:HB2  | 5:E:125:ALA:HB3   | 1.96                     | 0.48              |
| 19:S:40:ILE:HG21 | 19:S:62:VAL:HG21  | 1.95                     | 0.48              |
| 22:a:612:G:C2    | 22:a:614:A:H5''   | 2.48                     | 0.48              |
| 22:a:1278:C:H2'  | 22:a:1279:G:C8    | 2.49                     | 0.48              |
| 22:a:1716:U:H2'  | 22:a:1717:A:H8    | 1.78                     | 0.48              |
| 22:a:2687:U:H2'  | 22:a:2688:G:O4'   | 2.13                     | 0.48              |
| 28:g:60:ASP:OD1  | 28:g:61:GLY:N     | 2.44                     | 0.48              |
| 31:j:92:GLU:HB2  | 31:j:111:LYS:HE3  | 1.96                     | 0.48              |
| 1:A:51:A:N7      | 1:A:114:U:O2'     | 2.46                     | 0.48              |
| 1:A:269:C:H2'    | 1:A:270:A:H8      | 1.76                     | 0.48              |
| 2:B:186:ILE:HD12 | 2:B:200:ILE:O     | 2.14                     | 0.48              |
| 8:H:10:MET:HG3   | 8:H:27:MET:SD     | 2.54                     | 0.48              |
| 22:a:1809:A:H2'  | 22:a:1810:A:C8    | 2.49                     | 0.48              |
| 22:a:2728:U:O2'  | 22:a:2729:G:H8    | 1.97                     | 0.48              |
| 22:a:2849:U:H4'  | 22:a:2868:A:C2    | 2.48                     | 0.48              |
| 28:g:95:ARG:HG2  | 28:g:106:SER:HB3  | 1.96                     | 0.48              |
| 55:X:44:U:H2'    | 55:X:45:G:C8      | 2.49                     | 0.48              |
| 1:A:323:U:H2'    | 1:A:324:G:O4'     | 2.13                     | 0.48              |
| 6:F:18:VAL:HG11  | 6:F:58:HIS:CE1    | 2.49                     | 0.48              |
| 22:a:1385:A:O2'  | 22:a:1396:U:O2    | 2.31                     | 0.48              |
| 22:a:1794:A:H2'  | 22:a:1795:C:H6    | 1.77                     | 0.48              |
| 32:k:85:VAL:HG11 | 32:k:90:VAL:HG22  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 52:4:28:VAL:HG22 | 52:4:30:HIS:CE1   | 2.49                     | 0.48              |
| 1:A:7:A:H2'      | 5:E:124:LEU:HD22  | 1.95                     | 0.48              |
| 1:A:1285:A:H4'   | 1:A:1286:U:H5''   | 1.96                     | 0.48              |
| 1:A:1360:A:OP2   | 14:N:75:ARG:NH2   | 2.47                     | 0.48              |
| 6:F:36:ILE:HG12  | 6:F:64:VAL:HG12   | 1.95                     | 0.48              |
| 17:Q:78:VAL:HG11 | 17:Q:81:LYS:HE2   | 1.94                     | 0.48              |
| 22:a:1563:U:H2'  | 22:a:1564:C:C6    | 2.49                     | 0.48              |
| 22:a:1572:A:H2'  | 22:a:1573:G:H8    | 1.79                     | 0.48              |
| 23:b:5:U:H2'     | 23:b:6:G:H8       | 1.79                     | 0.48              |
| 52:4:16:CYS:SG   | 52:4:17:SER:N     | 2.87                     | 0.48              |
| 54:W:32:U:H2'    | 54:W:33:A:C8      | 2.49                     | 0.48              |
| 1:A:246:A:C2     | 1:A:282:A:C5      | 3.02                     | 0.48              |
| 1:A:299:G:H2'    | 1:A:300:A:C8      | 2.49                     | 0.48              |
| 1:A:918:A:H2'    | 1:A:919:A:C8      | 2.49                     | 0.48              |
| 22:a:271:G:O2'   | 22:a:272:A:O5'    | 2.29                     | 0.48              |
| 22:a:577:G:H2'   | 22:a:578:G:C8     | 2.48                     | 0.48              |
| 22:a:784:G:H5'   | 22:a:785:G:OP1    | 2.13                     | 0.48              |
| 22:a:832:U:H2'   | 22:a:833:A:C8     | 2.48                     | 0.48              |
| 22:a:876:C:H2'   | 22:a:877:A:O4'    | 2.14                     | 0.48              |
| 22:a:1570:A:H2'  | 22:a:1571:A:C8    | 2.49                     | 0.48              |
| 22:a:1796:U:H2'  | 22:a:1797:G:C8    | 2.48                     | 0.48              |
| 22:a:1830:C:H2'  | 22:a:1831:G:H8    | 1.79                     | 0.48              |
| 22:a:2459:A:N3   | 33:l:78:LEU:HD11  | 2.29                     | 0.48              |
| 33:l:51:ARG:O    | 33:l:55:ARG:HG2   | 2.13                     | 0.48              |
| 33:l:57:VAL:HG13 | 33:l:108:VAL:HG11 | 1.95                     | 0.48              |
| 41:t:3:ALA:O     | 41:t:6:ARG:NE     | 2.46                     | 0.48              |
| 1:A:45:G:H2'     | 1:A:46:G:C8       | 2.49                     | 0.47              |
| 1:A:999:C:H2'    | 1:A:1000:A:H8     | 1.77                     | 0.47              |
| 4:D:53:VAL:O     | 4:D:57:GLU:HG2    | 2.14                     | 0.47              |
| 22:a:3:U:H2'     | 22:a:4:U:C6       | 2.49                     | 0.47              |
| 22:a:363:G:H2'   | 22:a:364:C:H6     | 1.78                     | 0.47              |
| 22:a:1779:U:OP2  | 22:a:1784:A:N6    | 2.33                     | 0.47              |
| 22:a:2014:A:H2'  | 22:a:2015:A:C8    | 2.49                     | 0.47              |
| 32:k:82:LEU:HD13 | 32:k:120:VAL:HG21 | 1.96                     | 0.47              |
| 20:T:35:VAL:HG12 | 20:T:79:LEU:HD22  | 1.96                     | 0.47              |
| 22:a:2636:C:H2'  | 22:a:2637:U:H6    | 1.79                     | 0.47              |
| 26:e:109:LEU:O   | 26:e:113:VAL:HG23 | 2.13                     | 0.47              |
| 1:A:337:G:H2'    | 1:A:338:A:H8      | 1.77                     | 0.47              |
| 1:A:1127:G:H5'   | 1:A:1280:A:O2'    | 2.14                     | 0.47              |
| 1:A:1527:U:H2'   | 1:A:1528:U:C6     | 2.48                     | 0.47              |
| 2:B:186:ILE:HG12 | 2:B:213:TYR:CE2   | 2.50                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:M:104:THR:HG22 | 13:M:105:ASN:N     | 2.26                     | 0.47              |
| 22:a:1231:U:H2'   | 22:a:1232:G:H8     | 1.78                     | 0.47              |
| 22:a:1361:G:H2'   | 22:a:1362:C:C6     | 2.49                     | 0.47              |
| 22:a:1923:U:OP1   | 53:V:25:A:O2'      | 2.31                     | 0.47              |
| 22:a:2086:U:H2'   | 22:a:2087:G:C8     | 2.49                     | 0.47              |
| 44:w:5:CYS:HB3    | 44:w:10:LYS:H      | 1.79                     | 0.47              |
| 52:4:58:ASP:OD1   | 52:4:59:ARG:N      | 2.48                     | 0.47              |
| 1:A:120:A:H1'     | 1:A:122:G:N7       | 2.29                     | 0.47              |
| 1:A:185:U:H2'     | 1:A:186:C:C6       | 2.48                     | 0.47              |
| 1:A:185:U:H2'     | 1:A:186:C:H6       | 1.79                     | 0.47              |
| 1:A:538:G:H5''    | 12:L:111:LYS:HB2   | 1.96                     | 0.47              |
| 1:A:545:C:H5'     | 4:D:69:GLU:HG3     | 1.97                     | 0.47              |
| 1:A:712:A:H2'     | 1:A:713:G:C8       | 2.50                     | 0.47              |
| 22:a:1047:G:O2'   | 22:a:1110:G:N1     | 2.44                     | 0.47              |
| 22:a:2064:C:H2'   | 22:a:2065:C:H6     | 1.77                     | 0.47              |
| 22:a:2302:U:H2'   | 22:a:2303:G:H8     | 1.80                     | 0.47              |
| 27:f:13:VAL:HG13  | 27:f:28:VAL:HG21   | 1.97                     | 0.47              |
| 55:X:20:H2U:H4'   | 55:X:20(A):H2U:H3' | 1.96                     | 0.47              |
| 1:A:1313:U:H2'    | 1:A:1314:C:C6      | 2.48                     | 0.47              |
| 2:B:6:MET:HE3     | 2:B:10:LEU:HD21    | 1.95                     | 0.47              |
| 3:C:147:LYS:HA    | 3:C:147:LYS:HD2    | 1.76                     | 0.47              |
| 5:E:153:VAL:HA    | 5:E:156:LYS:HG2    | 1.97                     | 0.47              |
| 22:a:78:U:H2'     | 22:a:79:C:C6       | 2.49                     | 0.47              |
| 22:a:1159:U:C2    | 22:a:1160:G:C8     | 3.03                     | 0.47              |
| 22:a:1799:G:N7    | 24:c:178:SER:OG    | 2.40                     | 0.47              |
| 22:a:2636:C:H2'   | 22:a:2637:U:C6     | 2.49                     | 0.47              |
| 29:h:30:LEU:HB3   | 29:h:36:ALA:HB3    | 1.96                     | 0.47              |
| 32:k:85:VAL:HG13  | 32:k:94:THR:HG21   | 1.96                     | 0.47              |
| 33:l:20:LEU:HD13  | 42:u:81:PRO:HG2    | 1.96                     | 0.47              |
| 35:n:2:ASP:OD1    | 35:n:3:LYS:N       | 2.46                     | 0.47              |
| 1:A:966:2MG:HM21  | 9:I:129:LYS:HG2    | 1.96                     | 0.47              |
| 12:L:50:ARG:HG3   | 12:L:90:LEU:HD21   | 1.96                     | 0.47              |
| 22:a:1038:G:H2'   | 22:a:1039:A:C8     | 2.50                     | 0.47              |
| 22:a:1683:U:H2'   | 22:a:1684:G:H8     | 1.80                     | 0.47              |
| 1:A:22:G:O2'      | 1:A:913:A:N1       | 2.43                     | 0.47              |
| 1:A:97:G:H2'      | 1:A:98:A:O4'       | 2.15                     | 0.47              |
| 1:A:701:U:OP1     | 1:A:702:A:O2'      | 2.29                     | 0.47              |
| 1:A:1495:U:O2'    | 22:a:1919:A:N1     | 2.44                     | 0.47              |
| 1:A:1530:G:H2'    | 1:A:1531:A:C8      | 2.49                     | 0.47              |
| 2:B:33:GLY:O      | 2:B:40:ILE:N       | 2.47                     | 0.47              |
| 2:B:151:ILE:O     | 2:B:151:ILE:HG22   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:15:HIS:HA   | 10:J:18:ILE:HG12 | 1.96                     | 0.47              |
| 17:Q:7:THR:HG23  | 17:Q:60:GLU:HG3  | 1.97                     | 0.47              |
| 22:a:181:A:H2'   | 22:a:182:A:H8    | 1.79                     | 0.47              |
| 22:a:641:U:O2'   | 22:a:2350:C:OP1  | 2.33                     | 0.47              |
| 22:a:1179:G:H2'  | 22:a:1180:U:C6   | 2.49                     | 0.47              |
| 22:a:1541:C:H2'  | 22:a:1542:U:C6   | 2.49                     | 0.47              |
| 22:a:2372:U:H2'  | 22:a:2373:G:H8   | 1.79                     | 0.47              |
| 22:a:2450:A:H62  | 22:a:2501:C:N4   | 2.09                     | 0.47              |
| 22:a:2834:G:H2'  | 22:a:2879:A:H61  | 1.79                     | 0.47              |
| 34:m:69:ARG:O    | 34:m:70:THR:OG1  | 2.29                     | 0.47              |
| 53:V:44:G:H2'    | 53:V:45:U:C6     | 2.50                     | 0.47              |
| 1:A:219:U:H2'    | 1:A:220:G:H8     | 1.79                     | 0.47              |
| 4:D:104:ARG:HD2  | 4:D:168:PRO:HG3  | 1.97                     | 0.47              |
| 13:M:24:GLY:O    | 13:M:29:ARG:NH1  | 2.47                     | 0.47              |
| 13:M:87:ARG:HG3  | 13:M:97:VAL:HG13 | 1.97                     | 0.47              |
| 13:M:101:ARG:NH2 | 13:M:104:THR:OG1 | 2.34                     | 0.47              |
| 22:a:419:U:H2'   | 22:a:420:C:C6    | 2.50                     | 0.47              |
| 22:a:1269:A:H2'  | 22:a:1270:C:C6   | 2.50                     | 0.47              |
| 22:a:2329:U:H2'  | 22:a:2330:G:C8   | 2.50                     | 0.47              |
| 36:o:9:GLU:OE1   | 36:o:55:LEU:HB3  | 2.15                     | 0.47              |
| 44:w:8:THR:OG1   | 44:w:10:LYS:HG3  | 2.14                     | 0.47              |
| 55:X:75:C:H2'    | 55:X:76:A:C8     | 2.50                     | 0.47              |
| 1:A:967:5MC:OP2  | 1:A:968:A:O2'    | 2.29                     | 0.47              |
| 6:F:4:TYR:HE2    | 6:F:71:ILE:HG13  | 1.79                     | 0.47              |
| 22:a:250:G:H2'   | 22:a:251:A:C8    | 2.50                     | 0.47              |
| 22:a:598:U:H2'   | 22:a:599:A:C8    | 2.49                     | 0.47              |
| 22:a:1274:A:N1   | 22:a:1644:C:O2'  | 2.45                     | 0.47              |
| 22:a:1683:U:H2'  | 22:a:1684:G:C8   | 2.49                     | 0.47              |
| 29:h:34:GLY:O    | 29:h:36:ALA:N    | 2.47                     | 0.47              |
| 30:i:38:GLY:HA3  | 30:i:50:THR:HG23 | 1.95                     | 0.47              |
| 32:k:29:LYS:O    | 32:k:29:LYS:HG2  | 2.14                     | 0.47              |
| 1:A:1063:C:H3'   | 1:A:1064:G:H2'   | 1.97                     | 0.47              |
| 1:A:1219:A:H2'   | 1:A:1220:G:C8    | 2.50                     | 0.47              |
| 7:G:113:ASP:HB3  | 7:G:119:ARG:HG2  | 1.97                     | 0.47              |
| 22:a:675:A:N3    | 22:a:2443:C:O2'  | 2.45                     | 0.47              |
| 22:a:729:G:O2'   | 22:a:763:G:H4'   | 2.15                     | 0.47              |
| 22:a:1716:U:H2'  | 22:a:1717:A:C8   | 2.50                     | 0.47              |
| 22:a:2430:A:N3   | 22:a:2430:A:H2'  | 2.29                     | 0.47              |
| 24:c:180:GLU:HB2 | 24:c:269:ARG:O   | 2.15                     | 0.47              |
| 31:j:35:VAL:HA   | 31:j:62:VAL:HG23 | 1.97                     | 0.47              |
| 1:A:837:U:H2'    | 1:A:838:G:H8     | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1169:A:H2'   | 1:A:1170:A:C8    | 2.50                     | 0.46              |
| 6:F:44:ARG:HE    | 6:F:56:LYS:NZ    | 2.12                     | 0.46              |
| 7:G:138:ARG:CG   | 7:G:142:HIS:CE1  | 2.99                     | 0.46              |
| 16:P:40:ASN:HB3  | 16:P:43:ALA:HB2  | 1.96                     | 0.46              |
| 16:P:73:ALA:O    | 16:P:76:LYS:HG2  | 2.15                     | 0.46              |
| 22:a:1007:C:OP1  | 30:i:37:ARG:NH1  | 2.49                     | 0.46              |
| 22:a:1995:U:O2   | 31:j:3:GLN:NE2   | 2.47                     | 0.46              |
| 22:a:2466:C:OP1  | 51:3:4:ARG:HB2   | 2.15                     | 0.46              |
| 53:V:45:U:H2'    | 53:V:46:A:O4'    | 2.15                     | 0.46              |
| 22:a:1902:C:H4'  | 24:c:242:LYS:O   | 2.15                     | 0.46              |
| 26:e:130:LYS:HE3 | 26:e:130:LYS:HB3 | 1.71                     | 0.46              |
| 48:0:33:LYS:HA   | 48:0:51:GLU:OE2  | 2.14                     | 0.46              |
| 2:B:94:HIS:ND1   | 2:B:146:ASN:O    | 2.48                     | 0.46              |
| 2:B:207:ILE:H    | 2:B:207:ILE:HD12 | 1.80                     | 0.46              |
| 9:I:4:ASN:N      | 9:I:4:ASN:HD22   | 2.12                     | 0.46              |
| 9:I:47:VAL:HG13  | 9:I:80:ARG:HD3   | 1.98                     | 0.46              |
| 22:a:468:G:H5''  | 26:e:55:SER:HB2  | 1.96                     | 0.46              |
| 22:a:910:A:H2'   | 22:a:911:A:C8    | 2.50                     | 0.46              |
| 22:a:2070:A:H2'  | 22:a:2071:A:C8   | 2.50                     | 0.46              |
| 22:a:2514:U:H2'  | 22:a:2515:C:C6   | 2.50                     | 0.46              |
| 25:d:9:VAL:CG2   | 25:d:28:GLU:HG2  | 2.44                     | 0.46              |
| 1:A:148:G:N3     | 1:A:1446:A:H2    | 2.13                     | 0.46              |
| 1:A:186:C:H2'    | 1:A:187:G:H8     | 1.81                     | 0.46              |
| 1:A:1196:A:H5''  | 54:W:35:A:H61    | 1.79                     | 0.46              |
| 11:K:34:ILE:HG13 | 11:K:70:CYS:SG   | 2.56                     | 0.46              |
| 22:a:2567:G:H2'  | 22:a:2568:U:C6   | 2.51                     | 0.46              |
| 22:a:2634:A:H2'  | 22:a:2635:A:C8   | 2.50                     | 0.46              |
| 22:a:2847:U:H2'  | 22:a:2848:G:O4'  | 2.15                     | 0.46              |
| 46:y:5:ILE:HD11  | 46:y:57:VAL:HG11 | 1.97                     | 0.46              |
| 1:A:257:G:H2'    | 1:A:258:G:H8     | 1.80                     | 0.46              |
| 1:A:514:C:H2'    | 1:A:515:G:H8     | 1.79                     | 0.46              |
| 1:A:784:A:H2'    | 1:A:785:G:C8     | 2.51                     | 0.46              |
| 1:A:1020:G:H2'   | 1:A:1021:A:C8    | 2.51                     | 0.46              |
| 1:A:1318:A:H5''  | 19:S:3:ARG:NH1   | 2.30                     | 0.46              |
| 4:D:58:LYS:HD2   | 4:D:204:TYR:OH   | 2.15                     | 0.46              |
| 22:a:363:G:H2'   | 22:a:364:C:C6    | 2.50                     | 0.46              |
| 22:a:1590:A:H2'  | 22:a:1591:A:H8   | 1.78                     | 0.46              |
| 22:a:1654:A:O2'  | 25:d:118:PHE:O   | 2.30                     | 0.46              |
| 1:A:555:U:H2'    | 1:A:556:C:C6     | 2.49                     | 0.46              |
| 2:B:97:LEU:H     | 2:B:100:MET:HE3  | 1.80                     | 0.46              |
| 22:a:170:U:H2'   | 22:a:171:U:H6    | 1.81                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:1593:A:H2'  | 22:a:1594:U:C6    | 2.50                     | 0.46              |
| 25:d:9:VAL:HG21  | 25:d:28:GLU:HG2   | 1.98                     | 0.46              |
| 25:d:13:ARG:NH2  | 31:j:73:ASP:O     | 2.48                     | 0.46              |
| 40:s:21:SER:HA   | 40:s:24:MET:HE2   | 1.98                     | 0.46              |
| 45:x:5:GLU:HA    | 45:x:8:GLU:CD     | 2.41                     | 0.46              |
| 1:A:482:A:H2'    | 1:A:483:C:O4'     | 2.15                     | 0.46              |
| 1:A:501:C:OP1    | 12:L:114:ARG:NH2  | 2.34                     | 0.46              |
| 1:A:985:C:H2'    | 1:A:986:U:C6      | 2.51                     | 0.46              |
| 1:A:1328:C:C2    | 1:A:1329:A:C8     | 3.04                     | 0.46              |
| 6:F:12:PRO:O     | 6:F:44:ARG:NH1    | 2.42                     | 0.46              |
| 14:N:37:SER:OG   | 14:N:40:ASP:OD2   | 2.33                     | 0.46              |
| 22:a:282:A:N6    | 22:a:359:G:O6     | 2.49                     | 0.46              |
| 22:a:1413:A:H2'  | 22:a:1414:C:C6    | 2.50                     | 0.46              |
| 22:a:2812:G:H2'  | 22:a:2813:A:C8    | 2.50                     | 0.46              |
| 31:j:40:LYS:HD3  | 31:j:58:LEU:O     | 2.15                     | 0.46              |
| 34:m:71:ARG:HD2  | 34:m:71:ARG:HA    | 1.77                     | 0.46              |
| 39:r:17:VAL:HG11 | 39:r:103:ILE:HG12 | 1.96                     | 0.46              |
| 1:A:582:C:O2     | 1:A:759:A:N6      | 2.49                     | 0.46              |
| 1:A:618:C:O2     | 1:A:622:A:N6      | 2.49                     | 0.46              |
| 1:A:908:A:H2'    | 1:A:909:A:C8      | 2.51                     | 0.46              |
| 3:C:149:ILE:HG13 | 3:C:201:TRP:O     | 2.15                     | 0.46              |
| 22:a:636:G:N1    | 32:k:76:GLU:OE1   | 2.38                     | 0.46              |
| 22:a:1637:A:H5'  | 22:a:1760:C:O2'   | 2.16                     | 0.46              |
| 40:s:8:LEU:HD23  | 40:s:50:LEU:HD11  | 1.97                     | 0.46              |
| 48:0:11:LEU:HB2  | 48:0:21:TYR:HB2   | 1.97                     | 0.46              |
| 50:2:62:LEU:HB3  | 50:2:65:ALA:HB3   | 1.97                     | 0.46              |
| 1:A:525:C:OP1    | 12:L:86:ARG:NH1   | 2.47                     | 0.46              |
| 1:A:744:C:H2'    | 1:A:745:G:C8      | 2.50                     | 0.46              |
| 1:A:744:C:H2'    | 1:A:745:G:H8      | 1.81                     | 0.46              |
| 2:B:63:ARG:O     | 2:B:63:ARG:HD3    | 2.15                     | 0.46              |
| 3:C:50:ALA:O     | 3:C:70:THR:OG1    | 2.34                     | 0.46              |
| 17:Q:64:CYS:SG   | 17:Q:74:THR:HG23  | 2.56                     | 0.46              |
| 22:a:1203:U:OP2  | 22:a:1204:A:O2'   | 2.31                     | 0.46              |
| 22:a:1357:C:H2'  | 22:a:1358:G:O4'   | 2.16                     | 0.46              |
| 22:a:1571:A:H2'  | 22:a:1572:A:H8    | 1.80                     | 0.46              |
| 22:a:2364:C:H2'  | 22:a:2365:G:O4'   | 2.16                     | 0.46              |
| 23:b:42:C:C6     | 27:f:66:LEU:HB2   | 2.51                     | 0.46              |
| 23:b:49:C:H2'    | 23:b:50:A:H8      | 1.81                     | 0.46              |
| 39:r:52:GLU:HA   | 39:r:55:ILE:HD12  | 1.97                     | 0.46              |
| 1:A:2:A:H1'      | 1:A:613:C:O2'     | 2.16                     | 0.46              |
| 1:A:392:C:C2     | 1:A:393:A:C8      | 3.03                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 5:E:96:MET:HE1   | 5:E:144:LEU:HG  | 1.97                     | 0.46              |
| 14:N:6:MET:O     | 14:N:10:GLU:HG2 | 2.15                     | 0.46              |
| 22:a:272:A:H2'   | 22:a:273:G:H8   | 1.80                     | 0.46              |
| 22:a:624:C:O2'   | 22:a:657:U:OP1  | 2.33                     | 0.46              |
| 22:a:1712:U:OP2  | 22:a:1713:A:O2' | 2.28                     | 0.46              |
| 22:a:1746:A:H2'  | 22:a:1747:U:H6  | 1.81                     | 0.46              |
| 22:a:2339:C:O3'  | 23:b:41:G:N2    | 2.48                     | 0.46              |
| 22:a:2645:G:OP2  | 22:a:2645:G:N2  | 2.29                     | 0.46              |
| 1:A:1175:G:H2'   | 1:A:1176:A:C8   | 2.49                     | 0.45              |
| 2:B:84:ALA:HA    | 2:B:87:CYS:SG   | 2.57                     | 0.45              |
| 6:F:19:PRO:HA    | 6:F:22:ILE:HG22 | 1.98                     | 0.45              |
| 6:F:22:ILE:HD12  | 6:F:60:VAL:HG11 | 1.98                     | 0.45              |
| 6:F:74:LEU:O     | 6:F:77:THR:OG1  | 2.26                     | 0.45              |
| 11:K:20:VAL:HG22 | 11:K:83:GLU:HB2 | 1.98                     | 0.45              |
| 22:a:145:C:H2'   | 22:a:146:A:C8   | 2.51                     | 0.45              |
| 22:a:552:U:H2'   | 22:a:553:G:H8   | 1.81                     | 0.45              |
| 22:a:2070:A:H2'  | 22:a:2071:A:H8  | 1.81                     | 0.45              |
| 22:a:2419:U:OP1  | 50:2:41:LYS:NZ  | 2.47                     | 0.45              |
| 22:a:2478:A:H5'  | 51:3:32:LYS:HD3 | 1.96                     | 0.45              |
| 23:b:95:U:H2'    | 23:b:96:G:C8    | 2.51                     | 0.45              |
| 3:C:47:LEU:HB3   | 3:C:50:ALA:HB3  | 1.98                     | 0.45              |
| 16:P:8:ARG:NE    | 16:P:15:PRO:HB3 | 2.31                     | 0.45              |
| 22:a:569:U:O2'   | 22:a:983:A:N1   | 2.45                     | 0.45              |
| 22:a:1487:U:H2'  | 22:a:1488:C:H6  | 1.81                     | 0.45              |
| 22:a:2266:A:H4'  | 22:a:2267:A:N3  | 2.31                     | 0.45              |
| 43:v:52:GLY:HA3  | 43:v:62:LYS:HE3 | 1.98                     | 0.45              |
| 53:V:70:G:H2'    | 53:V:71:A:H8    | 1.81                     | 0.45              |
| 1:A:440:C:C2     | 1:A:441:A:C8    | 3.04                     | 0.45              |
| 1:A:868:C:H2'    | 1:A:869:G:O4'   | 2.15                     | 0.45              |
| 2:B:48:PRO:O     | 2:B:51:ASN:N    | 2.49                     | 0.45              |
| 6:F:35:LYS:O     | 6:F:65:GLU:N    | 2.47                     | 0.45              |
| 7:G:153:HIS:ND1  | 7:G:153:HIS:O   | 2.48                     | 0.45              |
| 22:a:282:A:H2'   | 22:a:283:G:C8   | 2.51                     | 0.45              |
| 22:a:594:U:H2'   | 22:a:595:C:C6   | 2.52                     | 0.45              |
| 22:a:1487:U:H2'  | 22:a:1488:C:C6  | 2.51                     | 0.45              |
| 22:a:2047:C:H2'  | 22:a:2048:G:H8  | 1.80                     | 0.45              |
| 22:a:2591:C:H2'  | 22:a:2592:G:H8  | 1.81                     | 0.45              |
| 22:a:2649:C:H2'  | 22:a:2650:U:C6  | 2.50                     | 0.45              |
| 42:u:20:LEU:HD23 | 42:u:27:PRO:HD3 | 1.99                     | 0.45              |
| 2:B:184:PHE:HE1  | 2:B:198:PHE:CD1 | 2.35                     | 0.45              |
| 5:E:60:ILE:O     | 5:E:64:MET:HG2  | 2.16                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:P:21:VAL:HG12   | 16:P:33:ILE:HD13  | 1.99                     | 0.45              |
| 22:a:76:C:O2'      | 45:x:55:THR:HG21  | 2.16                     | 0.45              |
| 22:a:182:A:H2'     | 22:a:183:C:H6     | 1.80                     | 0.45              |
| 22:a:598:U:H2'     | 22:a:599:A:H8     | 1.82                     | 0.45              |
| 22:a:2602:A:N7     | 53:V:76:A:H4'     | 2.32                     | 0.45              |
| 22:a:2615:U:C2     | 47:z:4:GLN:HA     | 2.51                     | 0.45              |
| 22:a:2784:U:H2'    | 22:a:2785:C:H6    | 1.81                     | 0.45              |
| 1:A:175:C:H2'      | 1:A:176:C:C6      | 2.52                     | 0.45              |
| 1:A:1097:C:H2'     | 1:A:1098:C:C6     | 2.52                     | 0.45              |
| 1:A:1463:U:H2'     | 1:A:1464:U:C6     | 2.52                     | 0.45              |
| 6:F:2:ARG:HB3      | 6:F:4:TYR:CE1     | 2.51                     | 0.45              |
| 9:I:55:VAL:HG13    | 9:I:57:MET:H      | 1.80                     | 0.45              |
| 11:K:94:GLU:HA     | 11:K:97:ILE:HD12  | 1.99                     | 0.45              |
| 21:U:4:ILE:HD13    | 21:U:19:PHE:CD1   | 2.50                     | 0.45              |
| 22:a:1883:U:H2'    | 22:a:1884:G:O4'   | 2.16                     | 0.45              |
| 28:g:86:LYS:HB3    | 28:g:165:ALA:HB2  | 1.98                     | 0.45              |
| 44:w:7:VAL:HG21    | 44:w:59:ILE:HD11  | 1.99                     | 0.45              |
| 1:A:486:U:H2'      | 1:A:487:A:C8      | 2.52                     | 0.45              |
| 1:A:642:A:C8       | 8:H:107:SER:HA    | 2.52                     | 0.45              |
| 2:B:217:VAL:O      | 2:B:221:VAL:HG13  | 2.16                     | 0.45              |
| 4:D:58:LYS:HD3     | 4:D:203:LEU:HD23  | 1.98                     | 0.45              |
| 14:N:49:GLN:HE22   | 19:S:13:LEU:N     | 2.12                     | 0.45              |
| 22:a:1386:C:H2'    | 22:a:1387:A:H8    | 1.80                     | 0.45              |
| 22:a:1425:G:H2'    | 22:a:1426:G:C8    | 2.52                     | 0.45              |
| 22:a:2030:6MZ:C2   | 22:a:2499:C:H5''  | 2.47                     | 0.45              |
| 22:a:2469:A:H2'    | 22:a:2470:G:O4'   | 2.17                     | 0.45              |
| 24:c:31:ALA:HA     | 24:c:34:LEU:HD12  | 1.97                     | 0.45              |
| 24:c:146:MET:HE3   | 24:c:154:LEU:HD21 | 1.99                     | 0.45              |
| 1:A:271:C:H2'      | 1:A:272:C:C6      | 2.51                     | 0.45              |
| 1:A:950:U:H2'      | 1:A:951:G:C8      | 2.51                     | 0.45              |
| 2:B:88:ASP:OD2     | 2:B:225:ARG:NH2   | 2.49                     | 0.45              |
| 20:T:44:LYS:HE3    | 20:T:87:ALA:HB2   | 1.98                     | 0.45              |
| 22:a:580:U:H2'     | 22:a:581:C:H6     | 1.80                     | 0.45              |
| 22:a:1295:C:C2     | 22:a:1296:G:C8    | 3.05                     | 0.45              |
| 22:a:1709:U:H2'    | 22:a:1710:G:C8    | 2.52                     | 0.45              |
| 22:a:2230:G:H2'    | 22:a:2231:U:C6    | 2.52                     | 0.45              |
| 22:a:2251:OMG:HM23 | 22:a:2251:OMG:H1' | 1.77                     | 0.45              |
| 52:4:41:HIS:CG     | 52:4:42:PRO:HD2   | 2.52                     | 0.45              |
| 1:A:405:U:OP1      | 1:A:406:G:O2'     | 2.20                     | 0.45              |
| 1:A:1187:G:H2'     | 1:A:1188:A:C8     | 2.51                     | 0.45              |
| 1:A:1236:A:H2'     | 1:A:1237:C:C6     | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1477:U:H2'    | 1:A:1478:U:C6     | 2.52                     | 0.45              |
| 1:A:1513:A:H2'    | 1:A:1514:G:H8     | 1.81                     | 0.45              |
| 7:G:138:ARG:CG    | 7:G:142:HIS:HE1   | 2.29                     | 0.45              |
| 19:S:36:ARG:NH2   | 19:S:72:GLY:O     | 2.50                     | 0.45              |
| 20:T:57:ILE:HA    | 20:T:60:ARG:HG2   | 1.97                     | 0.45              |
| 22:a:29:U:H2'     | 22:a:30:G:C8      | 2.51                     | 0.45              |
| 22:a:793:A:OP2    | 22:a:2071:A:O2'   | 2.35                     | 0.45              |
| 22:a:2836:U:H2'   | 22:a:2837:A:C8    | 2.52                     | 0.45              |
| 23:b:104:A:H2'    | 23:b:105:G:O4'    | 2.17                     | 0.45              |
| 26:e:153:LEU:HD11 | 26:e:158:PHE:HB2  | 1.98                     | 0.45              |
| 27:f:100:PHE:CZ   | 27:f:104:ILE:HD11 | 2.52                     | 0.45              |
| 35:n:29:HIS:HB3   | 35:n:36:TYR:HB2   | 1.98                     | 0.45              |
| 38:q:5:PHE:HB3    | 38:q:59:ILE:HD12  | 1.99                     | 0.45              |
| 39:r:82:MET:HE3   | 39:r:98:LYS:HD2   | 1.99                     | 0.45              |
| 53:V:62:C:H2'     | 53:V:63:C:C6      | 2.52                     | 0.45              |
| 1:A:407:U:H2'     | 1:A:408:A:H8      | 1.80                     | 0.45              |
| 1:A:983:A:H5'     | 1:A:984:C:OP2     | 2.17                     | 0.45              |
| 2:B:32:PHE:HB2    | 2:B:42:ASN:HA     | 1.99                     | 0.45              |
| 3:C:87:LEU:HA     | 3:C:90:VAL:HG12   | 1.99                     | 0.45              |
| 4:D:116:GLN:OE1   | 4:D:120:HIS:NE2   | 2.50                     | 0.45              |
| 24:c:29:PRO:HG2   | 24:c:34:LEU:HD11  | 1.99                     | 0.45              |
| 28:g:47:ASP:OD1   | 28:g:47:ASP:N     | 2.49                     | 0.45              |
| 53:V:66:A:H2'     | 53:V:67:G:O4'     | 2.17                     | 0.45              |
| 1:A:111:G:H1      | 1:A:330:C:N4      | 2.15                     | 0.45              |
| 1:A:580:C:H2'     | 1:A:581:G:O4'     | 2.17                     | 0.45              |
| 1:A:1410:A:H2'    | 1:A:1411:C:C6     | 2.52                     | 0.45              |
| 3:C:123:GLN:HA    | 3:C:126:ARG:HH11  | 1.82                     | 0.45              |
| 22:a:181:A:H2'    | 22:a:182:A:C8     | 2.52                     | 0.45              |
| 22:a:682:G:H5'    | 49:1:26:ASN:CG    | 2.42                     | 0.45              |
| 22:a:1326:U:H2'   | 22:a:1327:A:H8    | 1.81                     | 0.45              |
| 22:a:2804:U:H2'   | 22:a:2805:C:C6    | 2.51                     | 0.45              |
| 33:l:55:ARG:NH2   | 55:X:53:G:O3'     | 2.50                     | 0.45              |
| 34:m:29:VAL:HG11  | 34:m:75:ILE:HG23  | 1.99                     | 0.45              |
| 1:A:188:C:H2'     | 1:A:189:A:C8      | 2.52                     | 0.44              |
| 1:A:443:C:H2'     | 1:A:444:G:C8      | 2.52                     | 0.44              |
| 9:I:22:LYS:HB2    | 9:I:22:LYS:HE3    | 1.82                     | 0.44              |
| 22:a:720:U:H2'    | 22:a:721:A:H8     | 1.80                     | 0.44              |
| 22:a:917:A:H5''   | 22:a:2268:A:H61   | 1.82                     | 0.44              |
| 22:a:974:G:O5'    | 38:q:78:ARG:NH1   | 2.50                     | 0.44              |
| 22:a:1359:A:OP2   | 22:a:1371:G:N1    | 2.38                     | 0.44              |
| 22:a:2372:U:H2'   | 22:a:2373:G:C8    | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:2698:U:H2'  | 22:a:2699:C:C6   | 2.52                     | 0.44              |
| 23:b:5:U:OP1     | 23:b:61:G:O2'    | 2.29                     | 0.44              |
| 28:g:33:LEU:HD12 | 28:g:75:MET:HB2  | 1.99                     | 0.44              |
| 31:j:7:MET:HA    | 31:j:7:MET:HE3   | 1.99                     | 0.44              |
| 35:n:17:LYS:HD2  | 35:n:20:GLU:OE2  | 2.17                     | 0.44              |
| 42:u:72:VAL:HG12 | 42:u:93:ARG:HA   | 1.97                     | 0.44              |
| 47:z:43:ILE:HG22 | 47:z:49:TYR:HB2  | 1.99                     | 0.44              |
| 51:3:19:ARG:HD2  | 51:3:24:ARG:HD2  | 1.98                     | 0.44              |
| 1:A:62:U:O2'     | 1:A:379:C:O2     | 2.32                     | 0.44              |
| 1:A:816:A:OP1    | 1:A:1526:G:O2'   | 2.29                     | 0.44              |
| 1:A:1130:A:O2'   | 9:I:5:GLN:OE1    | 2.35                     | 0.44              |
| 4:D:31:LYS:HE2   | 4:D:31:LYS:HB3   | 1.75                     | 0.44              |
| 7:G:51:ALA:HB2   | 7:G:58:GLU:HG3   | 1.98                     | 0.44              |
| 7:G:99:LEU:HG    | 7:G:103:TRP:CE2  | 2.52                     | 0.44              |
| 9:I:57:MET:SD    | 9:I:60:LYS:HD2   | 2.57                     | 0.44              |
| 11:K:20:VAL:HA   | 11:K:83:GLU:HB2  | 2.00                     | 0.44              |
| 18:R:11:CYS:HB3  | 18:R:14:THR:HG22 | 1.98                     | 0.44              |
| 19:S:19:VAL:HG21 | 19:S:44:MET:HG2  | 1.99                     | 0.44              |
| 22:a:1383:A:H2'  | 22:a:1384:A:C8   | 2.52                     | 0.44              |
| 22:a:1446:C:H2'  | 22:a:1447:C:C6   | 2.52                     | 0.44              |
| 31:j:79:PHE:HE2  | 31:j:102:PRO:HG2 | 1.81                     | 0.44              |
| 34:m:28:LEU:HD23 | 34:m:48:VAL:HG21 | 1.98                     | 0.44              |
| 45:x:42:LEU:HA   | 45:x:45:GLN:HG3  | 1.99                     | 0.44              |
| 53:V:65:U:H2'    | 53:V:66:A:C8     | 2.53                     | 0.44              |
| 1:A:393:A:C2     | 1:A:394:G:C8     | 3.05                     | 0.44              |
| 8:H:54:ASP:OD1   | 8:H:55:THR:N     | 2.47                     | 0.44              |
| 14:N:27:LEU:HD21 | 14:N:44:ALA:O    | 2.18                     | 0.44              |
| 22:a:227:A:C2    | 22:a:2407:A:H1'  | 2.52                     | 0.44              |
| 22:a:922:C:O2'   | 43:v:29:GLU:OE2  | 2.19                     | 0.44              |
| 22:a:1338:G:O2'  | 22:a:1393:A:N1   | 2.50                     | 0.44              |
| 22:a:2667:C:H1'  | 28:g:109:PHE:HD1 | 1.82                     | 0.44              |
| 22:a:2700:A:H2'  | 22:a:2701:U:C6   | 2.53                     | 0.44              |
| 25:d:1:MET:HG3   | 25:d:205:PRO:HG2 | 1.99                     | 0.44              |
| 30:i:20:ALA:HB1  | 30:i:62:VAL:HG12 | 2.00                     | 0.44              |
| 34:m:114:GLU:OE1 | 34:m:118:ARG:NE  | 2.33                     | 0.44              |
| 40:s:54:GLU:HB2  | 40:s:91:GLN:NE2  | 2.32                     | 0.44              |
| 1:A:158:G:C6     | 1:A:164:G:C5     | 3.06                     | 0.44              |
| 1:A:922:G:H4'    | 5:E:25:VAL:HA    | 1.99                     | 0.44              |
| 1:A:1428:A:H2'   | 1:A:1429:A:O4'   | 2.17                     | 0.44              |
| 4:D:26:ARG:HH21  | 4:D:30:THR:HB    | 1.81                     | 0.44              |
| 8:H:95:VAL:HG12  | 8:H:96:MET:HG2   | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:T:24:ARG:O      | 20:T:27:MET:HG3    | 2.17                     | 0.44              |
| 22:a:2:G:H2'       | 22:a:3:U:C6        | 2.53                     | 0.44              |
| 22:a:163:C:H2'     | 22:a:164:C:C6      | 2.52                     | 0.44              |
| 33:l:108:VAL:HB    | 33:l:112:LEU:HD23  | 1.98                     | 0.44              |
| 1:A:590:U:H2'      | 1:A:591:U:C6       | 2.53                     | 0.44              |
| 1:A:645:G:C2       | 1:A:646:G:C8       | 3.05                     | 0.44              |
| 1:A:1067:A:N1      | 1:A:1108:G:O2'     | 2.43                     | 0.44              |
| 1:A:1268:G:H1'     | 1:A:1326:U:O2'     | 2.18                     | 0.44              |
| 22:a:365:U:H2'     | 22:a:366:C:C6      | 2.52                     | 0.44              |
| 22:a:760:G:H2'     | 22:a:761:A:O4'     | 2.18                     | 0.44              |
| 22:a:1012:U:OP2    | 37:p:70:ARG:NH2    | 2.48                     | 0.44              |
| 23:b:112:G:H2'     | 23:b:113:C:C6      | 2.53                     | 0.44              |
| 24:c:270:ARG:HA    | 24:c:270:ARG:HD2   | 1.82                     | 0.44              |
| 30:i:49:ASP:OD1    | 30:i:118:MET:HG2   | 2.17                     | 0.44              |
| 34:m:79:LEU:HD23   | 34:m:83:LEU:HD12   | 1.99                     | 0.44              |
| 52:4:41:HIS:CD2    | 52:4:43:PHE:HB3    | 2.52                     | 0.44              |
| 52:4:59:ARG:HA     | 52:4:62:LYS:HG2    | 2.00                     | 0.44              |
| 1:A:811:C:O2'      | 1:A:901:A:N1       | 2.49                     | 0.44              |
| 22:a:820:A:H4'     | 22:a:836:G:H22     | 1.82                     | 0.44              |
| 22:a:894:U:H2'     | 22:a:895:U:C6      | 2.53                     | 0.44              |
| 24:c:8:PRO:HB3     | 24:c:14:ARG:HG3    | 2.00                     | 0.44              |
| 29:h:7:ASP:OD1     | 29:h:35:LYS:HD3    | 2.17                     | 0.44              |
| 35:n:31:THR:HG22   | 35:n:33:ARG:H      | 1.82                     | 0.44              |
| 1:A:397:A:N7       | 1:A:547:A:O2'      | 2.43                     | 0.44              |
| 1:A:1058:G:OP1     | 3:C:199:LYS:HE3    | 2.17                     | 0.44              |
| 5:E:16:ILE:HD11    | 5:E:38:VAL:HG22    | 1.98                     | 0.44              |
| 7:G:56:LYS:HG3     | 7:G:57:SER:H       | 1.82                     | 0.44              |
| 9:I:98:LEU:HD23    | 9:I:98:LEU:HA      | 1.89                     | 0.44              |
| 22:a:171:U:C2      | 22:a:172:A:C8      | 3.05                     | 0.44              |
| 22:a:499:U:H2'     | 22:a:500:G:O4'     | 2.18                     | 0.44              |
| 22:a:1239:G:H2'    | 22:a:1240:U:O4'    | 2.17                     | 0.44              |
| 22:a:1252:G:N2     | 37:p:33:ARG:HB3    | 2.33                     | 0.44              |
| 22:a:1549:A:H2'    | 22:a:1550:C:C6     | 2.52                     | 0.44              |
| 22:a:1689:A:H2'    | 22:a:1690:A:H8     | 1.81                     | 0.44              |
| 22:a:1703:G:H2'    | 22:a:1704:C:H6     | 1.80                     | 0.44              |
| 23:b:2:G:H2'       | 23:b:3:C:H6        | 1.83                     | 0.44              |
| 28:g:163:ARG:HG2   | 28:g:164:TYR:O     | 2.18                     | 0.44              |
| 30:i:44:TYR:HA     | 30:i:50:THR:HG21   | 2.00                     | 0.44              |
| 52:4:41:HIS:HD2    | 52:4:43:PHE:HB3    | 1.83                     | 0.44              |
| 55:X:20(A):H2U:H61 | 55:X:20(A):H2U:H2' | 1.75                     | 0.44              |
| 1:A:642:A:N7       | 8:H:107:SER:HA     | 2.32                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1014:A:C2    | 1:A:1219:A:H1'    | 2.53                     | 0.44              |
| 22:a:188:G:H5'   | 44:w:14:THR:HG21  | 2.00                     | 0.44              |
| 22:a:1604:C:H2'  | 22:a:1605:C:C6    | 2.53                     | 0.44              |
| 22:a:1980:G:O2'  | 22:a:1982:U:OP2   | 2.34                     | 0.44              |
| 22:a:2420:C:H4'  | 48:0:54:ILE:HG21  | 2.00                     | 0.44              |
| 33:l:105:MET:HE2 | 33:l:108:VAL:HG21 | 2.00                     | 0.44              |
| 36:o:14:LYS:NZ   | 36:o:81:VAL:O     | 2.51                     | 0.44              |
| 46:y:9:GLN:HB2   | 46:y:29:LEU:HD13  | 2.00                     | 0.44              |
| 53:V:26:C:H2'    | 53:V:27:A:O4'     | 2.18                     | 0.44              |
| 1:A:1253:G:H2'   | 1:A:1254:A:C8     | 2.53                     | 0.44              |
| 22:a:134:G:H2'   | 22:a:135:U:C6     | 2.52                     | 0.44              |
| 22:a:723:C:H2'   | 22:a:724:U:O4'    | 2.18                     | 0.44              |
| 22:a:1275:A:N1   | 22:a:1295:C:O2'   | 2.48                     | 0.44              |
| 22:a:1316:U:H2'  | 22:a:1317:G:C8    | 2.53                     | 0.44              |
| 22:a:1476:U:H2'  | 22:a:1477:A:C8    | 2.52                     | 0.44              |
| 22:a:1710:G:H4'  | 22:a:2858:C:O2    | 2.18                     | 0.44              |
| 24:c:133:ARG:HA  | 24:c:167:ARG:NH1  | 2.32                     | 0.44              |
| 24:c:142:HIS:ND1 | 24:c:193:GLY:O    | 2.31                     | 0.44              |
| 46:y:28:GLY:HA3  | 46:y:38:ARG:HH21  | 1.82                     | 0.44              |
| 1:A:390:U:H2'    | 1:A:391:G:H8      | 1.82                     | 0.43              |
| 5:E:13:GLU:HG2   | 5:E:39:VAL:HG12   | 2.00                     | 0.43              |
| 14:N:20:TYR:O    | 14:N:24:ARG:HG2   | 2.18                     | 0.43              |
| 22:a:1438:U:H2'  | 22:a:1439:A:H8    | 1.83                     | 0.43              |
| 22:a:1747:U:H2'  | 22:a:1748:C:C6    | 2.53                     | 0.43              |
| 22:a:2292:U:H2'  | 22:a:2293:G:H8    | 1.83                     | 0.43              |
| 22:a:2804:U:H2'  | 22:a:2805:C:H6    | 1.82                     | 0.43              |
| 43:v:10:THR:HG22 | 43:v:12:ASN:H     | 1.82                     | 0.43              |
| 1:A:613:C:H2'    | 1:A:614:C:H6      | 1.80                     | 0.43              |
| 10:J:6:ILE:HG12  | 10:J:102:LEU:HD13 | 2.00                     | 0.43              |
| 22:a:154:U:H2'   | 22:a:155:A:H8     | 1.83                     | 0.43              |
| 22:a:807:U:OP2   | 32:k:41:ARG:NH2   | 2.46                     | 0.43              |
| 22:a:1013:C:H2'  | 22:a:1014:A:H8    | 1.83                     | 0.43              |
| 22:a:1167:C:H2'  | 22:a:1168:G:H8    | 1.83                     | 0.43              |
| 22:a:1405:U:H2'  | 22:a:1406:U:H6    | 1.81                     | 0.43              |
| 22:a:1728:C:H2'  | 22:a:1729:U:H5''  | 2.01                     | 0.43              |
| 32:k:143:GLU:N   | 32:k:143:GLU:OE1  | 2.51                     | 0.43              |
| 52:4:20:ASN:ND2  | 52:4:39:LYS:HD2   | 2.32                     | 0.43              |
| 1:A:489:C:H2'    | 1:A:490:C:H6      | 1.84                     | 0.43              |
| 1:A:890:G:O2'    | 1:A:906:A:N6      | 2.51                     | 0.43              |
| 11:K:60:PRO:HD3  | 11:K:91:PRO:HB2   | 2.00                     | 0.43              |
| 13:M:90:ARG:HD2  | 13:M:90:ARG:HA    | 1.73                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:a:18:U:H2'     | 22:a:19:A:C8      | 2.53                     | 0.43              |
| 22:a:1748:C:H2'   | 22:a:1749:A:H8    | 1.84                     | 0.43              |
| 22:a:2700:A:H2'   | 22:a:2701:U:H6    | 1.82                     | 0.43              |
| 26:e:196:VAL:HA   | 26:e:199:MET:HG2  | 2.00                     | 0.43              |
| 28:g:22:GLN:NE2   | 28:g:38:ASN:O     | 2.51                     | 0.43              |
| 29:h:32:PRO:HA    | 44:w:39:TRP:CD1   | 2.54                     | 0.43              |
| 31:j:75:SER:HB2   | 36:o:73:VAL:O     | 2.18                     | 0.43              |
| 32:k:63:LYS:HB2   | 32:k:63:LYS:HE3   | 1.71                     | 0.43              |
| 1:A:904:U:H2'     | 1:A:905:U:C6      | 2.52                     | 0.43              |
| 1:A:1298:U:H4'    | 1:A:1299:A:O4'    | 2.19                     | 0.43              |
| 2:B:21:ARG:HD2    | 2:B:22:TYR:CE1    | 2.53                     | 0.43              |
| 22:a:1039:A:H2    | 22:a:1116:G:H22   | 1.67                     | 0.43              |
| 22:a:2096:C:H2'   | 22:a:2097:A:C8    | 2.53                     | 0.43              |
| 22:a:2605:PSU:C4  | 22:a:2606:C:C5    | 3.05                     | 0.43              |
| 22:a:2605:PSU:H2' | 22:a:2606:C:C6    | 2.53                     | 0.43              |
| 24:c:145:GLU:HG2  | 24:c:151:GLY:C    | 2.43                     | 0.43              |
| 30:i:110:PRO:O    | 30:i:115:GLY:HA3  | 2.19                     | 0.43              |
| 32:k:123:ARG:HG2  | 32:k:123:ARG:HH11 | 1.82                     | 0.43              |
| 1:A:1510:C:H2'    | 1:A:1511:G:C8     | 2.54                     | 0.43              |
| 2:B:68:LEU:HB3    | 2:B:161:LEU:HD12  | 2.01                     | 0.43              |
| 7:G:23:LEU:HD12   | 7:G:23:LEU:HA     | 1.85                     | 0.43              |
| 22:a:1003:G:O2'   | 22:a:1010:A:N1    | 2.48                     | 0.43              |
| 25:d:12:THR:OG1   | 25:d:13:ARG:N     | 2.46                     | 0.43              |
| 27:f:144:ASP:OD1  | 27:f:144:ASP:N    | 2.50                     | 0.43              |
| 32:k:62:PRO:HG2   | 50:2:25:LYS:HB3   | 2.00                     | 0.43              |
| 42:u:55:GLU:O     | 42:u:59:GLU:HG3   | 2.17                     | 0.43              |
| 1:A:908:A:H2'     | 1:A:909:A:H8      | 1.83                     | 0.43              |
| 1:A:1060:U:H2'    | 1:A:1061:G:H8     | 1.83                     | 0.43              |
| 1:A:1121:U:H2'    | 1:A:1122:U:H6     | 1.82                     | 0.43              |
| 1:A:1384:C:H2'    | 1:A:1385:G:C8     | 2.54                     | 0.43              |
| 3:C:131:ARG:O     | 3:C:135:LYS:HG2   | 2.19                     | 0.43              |
| 22:a:18:U:H2'     | 22:a:19:A:H8      | 1.84                     | 0.43              |
| 22:a:588:U:H2'    | 22:a:589:U:C6     | 2.53                     | 0.43              |
| 22:a:675:A:OP1    | 26:e:58:LYS:NZ    | 2.46                     | 0.43              |
| 22:a:2854:G:H2'   | 22:a:2855:C:H6    | 1.84                     | 0.43              |
| 25:d:106:LYS:NZ   | 25:d:176:ASP:OD1  | 2.48                     | 0.43              |
| 39:r:70:LYS:N     | 39:r:108:SER:O    | 2.34                     | 0.43              |
| 44:w:5:CYS:SG     | 44:w:8:THR:OG1    | 2.70                     | 0.43              |
| 1:A:224:U:H2'     | 1:A:225:C:C6      | 2.53                     | 0.43              |
| 1:A:501:C:H1'     | 1:A:549:C:H1'     | 2.01                     | 0.43              |
| 1:A:1040:U:H2'    | 1:A:1041:G:C8     | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1121:U:H2'   | 1:A:1122:U:C6     | 2.54                     | 0.43              |
| 1:A:1255:G:O2'   | 1:A:1258:G:N3     | 2.46                     | 0.43              |
| 1:A:1314:C:OP2   | 19:S:4:SER:OG     | 2.25                     | 0.43              |
| 2:B:109:GLN:HA   | 2:B:112:LYS:HD2   | 2.01                     | 0.43              |
| 22:a:645:C:H2'   | 22:a:647:G:N7     | 2.34                     | 0.43              |
| 22:a:966:G:C5    | 22:a:967:U:C4     | 3.07                     | 0.43              |
| 22:a:1494:A:H2'  | 22:a:1495:A:C8    | 2.54                     | 0.43              |
| 22:a:1518:C:H2'  | 22:a:1519:G:H8    | 1.84                     | 0.43              |
| 22:a:1783:A:H5'  | 22:a:2608:G:H4'   | 2.00                     | 0.43              |
| 22:a:1843:C:H2'  | 22:a:1844:C:C6    | 2.54                     | 0.43              |
| 1:A:231:U:H2'    | 1:A:232:G:H8      | 1.84                     | 0.43              |
| 1:A:676:A:H2'    | 1:A:677:U:H6      | 1.83                     | 0.43              |
| 1:A:806:C:H2'    | 1:A:807:A:H8      | 1.84                     | 0.43              |
| 1:A:875:U:O2'    | 8:H:15:ARG:HD2    | 2.19                     | 0.43              |
| 1:A:1309:G:H5'   | 13:M:77:ILE:HD11  | 2.01                     | 0.43              |
| 22:a:468:G:OP2   | 49:1:37:LYS:NZ    | 2.51                     | 0.43              |
| 22:a:833:A:H2'   | 22:a:834:G:H8     | 1.81                     | 0.43              |
| 22:a:2094:A:O3'  | 29:h:11:ASN:ND2   | 2.43                     | 0.43              |
| 22:a:2854:G:H2'  | 22:a:2855:C:C6    | 2.53                     | 0.43              |
| 32:k:85:VAL:HG13 | 32:k:94:THR:CG2   | 2.49                     | 0.43              |
| 53:V:62:C:H2'    | 53:V:63:C:H6      | 1.84                     | 0.43              |
| 1:A:182:A:C4     | 1:A:184:G:C8      | 3.07                     | 0.43              |
| 1:A:430:A:OP1    | 4:D:9:LEU:HB2     | 2.19                     | 0.43              |
| 1:A:1162:C:H2'   | 1:A:1163:A:C8     | 2.52                     | 0.43              |
| 15:O:25:THR:HG21 | 15:O:70:LEU:HB2   | 2.01                     | 0.43              |
| 22:a:361:G:H8    | 22:a:361:G:OP2    | 2.01                     | 0.43              |
| 22:a:2308:G:H2'  | 22:a:2308:G:N3    | 2.34                     | 0.43              |
| 22:a:2408:U:H2'  | 22:a:2409:G:C8    | 2.54                     | 0.43              |
| 23:b:62:C:H2'    | 23:b:63:C:C6      | 2.54                     | 0.43              |
| 37:p:72:ASN:HD21 | 37:p:107:THR:HG22 | 1.83                     | 0.43              |
| 45:x:56:LEU:HD13 | 45:x:59:GLU:OE2   | 2.18                     | 0.43              |
| 51:3:9:LYS:HE3   | 51:3:14:CYS:O     | 2.18                     | 0.43              |
| 1:A:1236:A:H4'   | 1:A:1304:G:H4'    | 2.01                     | 0.43              |
| 2:B:130:THR:OG1  | 2:B:133:GLU:OE2   | 2.35                     | 0.43              |
| 13:M:105:ASN:O   | 13:M:107:ARG:HD2  | 2.19                     | 0.43              |
| 18:R:48:ARG:HA   | 18:R:48:ARG:HD2   | 1.82                     | 0.43              |
| 22:a:596:U:H2'   | 22:a:597:G:H8     | 1.83                     | 0.43              |
| 31:j:109:SER:C   | 31:j:113:MET:HE2  | 2.43                     | 0.43              |
| 42:u:80:HIS:HD2  | 42:u:83:LYS:H     | 1.66                     | 0.43              |
| 44:w:59:ILE:CD1  | 44:w:67:VAL:HG21  | 2.49                     | 0.43              |
| 1:A:769:G:H4'    | 1:A:1513:A:H4'    | 2.00                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:45:ARG:HG3    | 5:E:72:ILE:O     | 2.18                     | 0.42              |
| 8:H:102:ALA:HB3   | 8:H:113:ASP:HB3  | 2.01                     | 0.42              |
| 18:R:26:ILE:HG22  | 18:R:30:LYS:HE3  | 2.01                     | 0.42              |
| 22:a:150:U:H2'    | 22:a:151:C:C6    | 2.54                     | 0.42              |
| 22:a:744:U:H2'    | 22:a:745:1MG:O4' | 2.18                     | 0.42              |
| 22:a:814:C:H1'    | 22:a:1225:G:N2   | 2.34                     | 0.42              |
| 22:a:2308:G:C6    | 27:f:77:PHE:HE2  | 2.37                     | 0.42              |
| 22:a:2646:C:H2'   | 22:a:2647:U:O4'  | 2.19                     | 0.42              |
| 28:g:10:VAL:HG13  | 28:g:10:VAL:O    | 2.19                     | 0.42              |
| 45:x:44:LYS:O     | 45:x:48:ARG:HG2  | 2.19                     | 0.42              |
| 48:0:40:ASP:HA    | 48:0:41:PRO:HD3  | 1.87                     | 0.42              |
| 1:A:831:A:H5'     | 2:B:21:ARG:HG3   | 2.02                     | 0.42              |
| 6:F:88:MET:HE2    | 6:F:90:MET:SD    | 2.60                     | 0.42              |
| 20:T:55:GLN:HG3   | 20:T:76:LYS:HE3  | 2.01                     | 0.42              |
| 22:a:327:G:N2     | 41:t:68:SER:OG   | 2.52                     | 0.42              |
| 22:a:476:G:N1     | 22:a:479:A:OP2   | 2.45                     | 0.42              |
| 22:a:1332:G:N7    | 22:a:1609:A:O2'  | 2.45                     | 0.42              |
| 22:a:1469:A:H2'   | 22:a:1470:A:H8   | 1.83                     | 0.42              |
| 22:a:1821:A:H2'   | 22:a:1822:C:C6   | 2.54                     | 0.42              |
| 22:a:1957:C:H2'   | 22:a:1958:C:C6   | 2.54                     | 0.42              |
| 34:m:24:MET:SD    | 34:m:44:LEU:HD22 | 2.59                     | 0.42              |
| 43:v:23:VAL:HA    | 43:v:38:VAL:HG23 | 2.00                     | 0.42              |
| 50:2:50:VAL:HG12  | 50:2:55:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:537:G:H2'     | 1:A:538:G:H8     | 1.84                     | 0.42              |
| 1:A:600:A:H2'     | 1:A:601:G:C8     | 2.55                     | 0.42              |
| 1:A:1384:C:H2'    | 1:A:1385:G:H8    | 1.84                     | 0.42              |
| 2:B:32:PHE:HB3    | 2:B:40:ILE:HG22  | 2.01                     | 0.42              |
| 2:B:184:PHE:HE1   | 2:B:198:PHE:HD1  | 1.67                     | 0.42              |
| 9:I:19:VAL:HG13   | 9:I:65:ILE:HG12  | 2.01                     | 0.42              |
| 13:M:89:LEU:O     | 13:M:93:ARG:HG2  | 2.19                     | 0.42              |
| 17:Q:20:SER:HB3   | 17:Q:71:LYS:HZ1  | 1.83                     | 0.42              |
| 20:T:2:ALA:HB3    | 20:T:8:LYS:HG3   | 2.01                     | 0.42              |
| 22:a:302:C:H2'    | 22:a:303:G:H8    | 1.82                     | 0.42              |
| 22:a:304:U:H2'    | 22:a:305:C:C6    | 2.53                     | 0.42              |
| 22:a:640:C:H2'    | 22:a:641:U:H6    | 1.85                     | 0.42              |
| 22:a:813:U:H2'    | 22:a:814:C:C6    | 2.54                     | 0.42              |
| 22:a:969:G:H2'    | 22:a:970:U:C6    | 2.54                     | 0.42              |
| 22:a:1533:C:H2'   | 22:a:1534:U:O4'  | 2.18                     | 0.42              |
| 23:b:40:U:N3      | 23:b:44:G:OP2    | 2.30                     | 0.42              |
| 26:e:108:ILE:HG23 | 32:k:1:MET:HE1   | 2.00                     | 0.42              |
| 28:g:38:ASN:O     | 28:g:41:VAL:HG12 | 2.20                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 28:g:55:ARG:HG2 | 28:g:56:ASP:N   | 2.34                     | 0.42              |
| 1:A:167:A:H2'   | 1:A:168:G:H8    | 1.82                     | 0.42              |
| 1:A:168:G:H2'   | 1:A:169:C:C6    | 2.54                     | 0.42              |
| 1:A:255:G:H4'   | 17:Q:19:LYS:HD2 | 2.02                     | 0.42              |
| 5:E:149:SER:H   | 5:E:152:MET:HE3 | 1.84                     | 0.42              |
| 7:G:113:ASP:OD1 | 7:G:114:LYS:N   | 2.39                     | 0.42              |
| 10:J:11:LYS:HB2 | 10:J:97:ASP:OD1 | 2.19                     | 0.42              |
| 17:Q:17:MET:HG3 | 17:Q:20:SER:OG  | 2.19                     | 0.42              |
| 18:R:71:THR:H   | 18:R:74:HIS:CE1 | 2.38                     | 0.42              |
| 22:a:599:A:H2'  | 22:a:600:G:H8   | 1.84                     | 0.42              |
| 22:a:722:A:H2'  | 22:a:723:C:C6   | 2.55                     | 0.42              |
| 22:a:948:C:H2'  | 22:a:949:G:C8   | 2.54                     | 0.42              |
| 22:a:1433:A:H2' | 22:a:1434:A:H8  | 1.82                     | 0.42              |
| 22:a:1672:A:C2  | 22:a:2582:G:H5' | 2.54                     | 0.42              |
| 42:u:73:LYS:HZ3 | 42:u:94:ALA:HA  | 1.85                     | 0.42              |
| 55:X:6:C:H2'    | 55:X:7:U:C6     | 2.55                     | 0.42              |
| 1:A:33:A:H2'    | 1:A:34:C:C6     | 2.53                     | 0.42              |
| 1:A:449:G:H2'   | 1:A:450:G:C8    | 2.55                     | 0.42              |
| 1:A:562:U:H1'   | 12:L:12:ARG:HB3 | 2.02                     | 0.42              |
| 1:A:923:A:O2'   | 1:A:1399:C:OP2  | 2.35                     | 0.42              |
| 12:L:27:CYS:SG  | 12:L:30:LYS:HE2 | 2.60                     | 0.42              |
| 13:M:27:LYS:HA  | 13:M:27:LYS:HD2 | 1.87                     | 0.42              |
| 22:a:12:U:O2    | 22:a:2626:C:H4' | 2.18                     | 0.42              |
| 22:a:739:A:H1'  | 22:a:740:C:H5   | 1.85                     | 0.42              |
| 22:a:2052:A:O2' | 25:d:148:GLN:O  | 2.35                     | 0.42              |
| 23:b:49:C:H2'   | 23:b:50:A:C8    | 2.54                     | 0.42              |
| 23:b:115:A:H2'  | 23:b:116:G:C8   | 2.52                     | 0.42              |
| 24:c:30:PHE:CE2 | 24:c:32:PRO:HG2 | 2.54                     | 0.42              |
| 25:d:16:THR:OG1 | 25:d:18:ASP:OD1 | 2.30                     | 0.42              |
| 25:d:39:ASP:HA  | 25:d:46:ARG:HG2 | 2.01                     | 0.42              |
| 1:A:509:A:N3    | 1:A:543:U:O2'   | 2.49                     | 0.42              |
| 1:A:523:A:C2    | 12:L:88:LYS:HB3 | 2.55                     | 0.42              |
| 1:A:603:U:H2'   | 1:A:604:G:H8    | 1.85                     | 0.42              |
| 1:A:638:U:C2    | 1:A:639:G:C8    | 3.08                     | 0.42              |
| 1:A:644:U:C2    | 1:A:645:G:C8    | 3.08                     | 0.42              |
| 1:A:883:C:O2'   | 1:A:884:U:H5'   | 2.20                     | 0.42              |
| 1:A:1251:A:H2'  | 1:A:1252:A:C8   | 2.55                     | 0.42              |
| 22:a:543:G:H2'  | 22:a:544:C:C6   | 2.55                     | 0.42              |
| 22:a:568:U:O4   | 38:q:81:LYS:NZ  | 2.53                     | 0.42              |
| 22:a:749:A:H4'  | 22:a:1271:G:N3  | 2.34                     | 0.42              |
| 22:a:959:A:H2'  | 22:a:960:A:C8   | 2.54                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:1715:G:O2'  | 22:a:1743:G:O6    | 2.34                     | 0.42              |
| 22:a:2408:U:H2'  | 22:a:2409:G:H8    | 1.85                     | 0.42              |
| 22:a:2642:G:H2'  | 22:a:2643:G:H8    | 1.85                     | 0.42              |
| 27:f:59:ALA:HB1  | 27:f:140:GLU:CD   | 2.44                     | 0.42              |
| 28:g:125:CYS:SG  | 28:g:131:ILE:HG12 | 2.60                     | 0.42              |
| 1:A:321:A:H2'    | 1:A:322:C:H6      | 1.85                     | 0.42              |
| 1:A:399:G:H2'    | 1:A:400:C:H6      | 1.84                     | 0.42              |
| 1:A:537:G:H2'    | 1:A:538:G:C8      | 2.54                     | 0.42              |
| 1:A:657:U:H2'    | 1:A:658:C:H6      | 1.85                     | 0.42              |
| 1:A:1297:G:N3    | 7:G:114:LYS:HD2   | 2.34                     | 0.42              |
| 15:O:17:ARG:O    | 15:O:17:ARG:HD2   | 2.20                     | 0.42              |
| 16:P:68:SER:OG   | 16:P:71:VAL:HG12  | 2.19                     | 0.42              |
| 22:a:277:G:H4'   | 22:a:278:A:C4     | 2.53                     | 0.42              |
| 22:a:558:U:H2'   | 22:a:559:G:H8     | 1.84                     | 0.42              |
| 22:a:839:U:H2'   | 22:a:840:C:C6     | 2.55                     | 0.42              |
| 22:a:1414:C:H2'  | 22:a:1415:U:O4'   | 2.19                     | 0.42              |
| 22:a:1604:C:H2'  | 22:a:1605:C:H6    | 1.85                     | 0.42              |
| 22:a:2815:C:C2   | 22:a:2816:G:C8    | 3.07                     | 0.42              |
| 26:e:136:GLN:NE2 | 26:e:140:ASP:OD2  | 2.52                     | 0.42              |
| 34:m:32:GLU:OE2  | 34:m:115:LEU:HB2  | 2.20                     | 0.42              |
| 53:V:70:G:H2'    | 53:V:71:A:C8      | 2.55                     | 0.42              |
| 1:A:32:A:H2'     | 1:A:33:A:C8       | 2.54                     | 0.42              |
| 12:L:99:ARG:NH1  | 12:L:104:CYS:SG   | 2.92                     | 0.42              |
| 22:a:582:A:H2'   | 22:a:583:G:H8     | 1.84                     | 0.42              |
| 22:a:1028:A:H2'  | 22:a:1029:A:H8    | 1.80                     | 0.42              |
| 22:a:2292:U:H2'  | 22:a:2293:G:C8    | 2.55                     | 0.42              |
| 22:a:2405:G:O2'  | 22:a:2411:A:N6    | 2.49                     | 0.42              |
| 22:a:2526:G:O2'  | 51:3:1:MET:N      | 2.35                     | 0.42              |
| 33:l:29:GLY:N    | 33:l:104:GLU:OE2  | 2.52                     | 0.42              |
| 41:t:2:ALA:HB1   | 41:t:6:ARG:HH21   | 1.85                     | 0.42              |
| 1:A:16:A:N1      | 1:A:919:A:H2      | 2.18                     | 0.42              |
| 1:A:164:G:C2     | 1:A:165:G:C8      | 3.08                     | 0.42              |
| 1:A:1027:C:H2'   | 1:A:1028:C:C6     | 2.55                     | 0.42              |
| 1:A:1352:C:H2'   | 1:A:1353:G:C8     | 2.55                     | 0.42              |
| 1:A:1469:C:H2'   | 1:A:1470:U:O4'    | 2.20                     | 0.42              |
| 2:B:206:ALA:O    | 2:B:210:VAL:HG23  | 2.20                     | 0.42              |
| 2:B:219:ALA:HA   | 2:B:222:ARG:HG2   | 2.02                     | 0.42              |
| 3:C:114:LYS:HD3  | 3:C:185:ASN:ND2   | 2.35                     | 0.42              |
| 3:C:168:TYR:OH   | 5:E:55:GLU:OE2    | 2.25                     | 0.42              |
| 17:Q:25:ILE:HD13 | 17:Q:44:LEU:HD13  | 2.00                     | 0.42              |
| 20:T:51:PHE:HA   | 20:T:54:MET:HG2   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:78:U:H2'    | 22:a:79:C:H6     | 1.85                     | 0.42              |
| 22:a:105:C:C2    | 22:a:106:C:C5    | 3.08                     | 0.42              |
| 22:a:417:C:H2'   | 22:a:418:C:C6    | 2.54                     | 0.42              |
| 22:a:1153:C:H2'  | 22:a:1154:G:O4'  | 2.20                     | 0.42              |
| 22:a:1224:U:H2'  | 22:a:1225:G:C8   | 2.55                     | 0.42              |
| 22:a:1361:G:H2'  | 22:a:1362:C:H6   | 1.84                     | 0.42              |
| 22:a:1592:C:H2'  | 22:a:1593:A:C8   | 2.55                     | 0.42              |
| 22:a:2247:A:H2'  | 22:a:2248:C:H6   | 1.84                     | 0.42              |
| 22:a:2313:C:H5'' | 27:f:88:LYS:HD3  | 2.01                     | 0.42              |
| 22:a:2896:C:H2'  | 22:a:2897:U:C6   | 2.55                     | 0.42              |
| 24:c:265:LYS:HE3 | 24:c:265:LYS:HB3 | 1.79                     | 0.42              |
| 27:f:98:GLU:O    | 27:f:102:ARG:HG3 | 2.20                     | 0.42              |
| 28:g:22:GLN:HE21 | 28:g:39:ASP:HA   | 1.84                     | 0.42              |
| 41:t:49:VAL:O    | 41:t:54:GLN:HA   | 2.20                     | 0.42              |
| 50:2:31:HIS:O    | 50:2:33:LEU:HG   | 2.19                     | 0.42              |
| 53:V:69:G:H2'    | 53:V:70:G:C8     | 2.53                     | 0.42              |
| 1:A:20:U:H2'     | 1:A:21:G:O4'     | 2.19                     | 0.42              |
| 1:A:197:A:N1     | 1:A:220:G:O2'    | 2.41                     | 0.42              |
| 1:A:270:A:H2'    | 1:A:271:C:C6     | 2.55                     | 0.42              |
| 1:A:513:C:H2'    | 1:A:514:C:C6     | 2.55                     | 0.42              |
| 1:A:529:G:O6     | 12:L:46:ASN:HB2  | 2.19                     | 0.42              |
| 1:A:826:C:O2     | 8:H:16:ASN:ND2   | 2.53                     | 0.42              |
| 1:A:1238:A:H2    | 1:A:1241:G:N3    | 2.18                     | 0.42              |
| 1:A:1240:U:C5    | 7:G:116:MET:HG2  | 2.55                     | 0.42              |
| 3:C:123:GLN:O    | 3:C:128:VAL:HG22 | 2.19                     | 0.42              |
| 11:K:123:PRO:HD2 | 21:U:38:TYR:HB2  | 2.01                     | 0.42              |
| 22:a:492:A:H2'   | 22:a:493:G:O4'   | 2.20                     | 0.42              |
| 22:a:1155:A:OP1  | 37:p:55:ARG:HG2  | 2.20                     | 0.42              |
| 22:a:1564:C:H2'  | 22:a:1565:C:C6   | 2.55                     | 0.42              |
| 22:a:2302:U:H2'  | 22:a:2303:G:C8   | 2.54                     | 0.42              |
| 22:a:2812:G:H2'  | 22:a:2813:A:H8   | 1.84                     | 0.42              |
| 23:b:2:G:H2'     | 23:b:3:C:C6      | 2.55                     | 0.42              |
| 41:t:85:PHE:CE1  | 41:t:94:ARG:HG2  | 2.55                     | 0.42              |
| 55:X:26:A:H2'    | 55:X:27:G:H8     | 1.85                     | 0.42              |
| 1:A:539:A:H2'    | 1:A:540:G:H8     | 1.82                     | 0.41              |
| 1:A:1130:A:C8    | 1:A:1146:A:C2    | 3.07                     | 0.41              |
| 1:A:1415:G:C6    | 1:A:1486:G:C6    | 3.08                     | 0.41              |
| 4:D:106:GLY:O    | 4:D:159:LEU:HD22 | 2.20                     | 0.41              |
| 11:K:82:LEU:HD23 | 11:K:82:LEU:HA   | 1.93                     | 0.41              |
| 13:M:79:ARG:NH1  | 13:M:83:LEU:HD11 | 2.35                     | 0.41              |
| 20:T:85:LYS:HA   | 20:T:85:LYS:HD2  | 1.91                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 22:a:134:G:H2'    | 22:a:135:U:H6    | 1.85                     | 0.41              |
| 22:a:315:G:H2'    | 22:a:316:C:C6    | 2.55                     | 0.41              |
| 22:a:754:U:H2'    | 22:a:755:U:C6    | 2.55                     | 0.41              |
| 22:a:1199:U:H2'   | 22:a:1200:C:H6   | 1.85                     | 0.41              |
| 22:a:1416:G:O2'   | 22:a:1417:C:OP2  | 2.32                     | 0.41              |
| 24:c:245:VAL:HG12 | 24:c:251:GLN:HA  | 2.02                     | 0.41              |
| 26:e:176:ASP:OD1  | 26:e:179:SER:N   | 2.46                     | 0.41              |
| 39:r:46:LEU:O     | 39:r:50:VAL:HG23 | 2.20                     | 0.41              |
| 43:v:26:PHE:N     | 43:v:29:GLU:OE1  | 2.52                     | 0.41              |
| 55:X:41:G:H2'     | 55:X:42:C:C6     | 2.54                     | 0.41              |
| 1:A:425:G:H2'     | 1:A:426:U:C6     | 2.55                     | 0.41              |
| 1:A:520:A:OP2     | 12:L:49:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:745:G:H2'     | 1:A:746:A:H8     | 1.85                     | 0.41              |
| 1:A:1043:G:O2'    | 1:A:1044:A:H5''  | 2.21                     | 0.41              |
| 1:A:1119:C:H2'    | 1:A:1120:C:H6    | 1.84                     | 0.41              |
| 6:F:74:LEU:HG     | 6:F:78:PHE:HE2   | 1.85                     | 0.41              |
| 22:a:646:U:C4     | 22:a:2368:C:H1'  | 2.54                     | 0.41              |
| 22:a:1047:G:HO2'  | 22:a:1110:G:H1   | 1.65                     | 0.41              |
| 22:a:1199:U:H2'   | 22:a:1200:C:C6   | 2.56                     | 0.41              |
| 22:a:2347:C:H2'   | 22:a:2348:U:C6   | 2.55                     | 0.41              |
| 28:g:46:ALA:O     | 28:g:49:THR:HG22 | 2.20                     | 0.41              |
| 30:i:16:TYR:HB2   | 30:i:54:ILE:HD13 | 2.03                     | 0.41              |
| 30:i:36:LEU:O     | 30:i:51:GLY:HA3  | 2.20                     | 0.41              |
| 30:i:99:ARG:HD2   | 30:i:102:GLU:OE1 | 2.21                     | 0.41              |
| 55:X:19:G:H4'     | 55:X:20:H2U:H5'  | 2.01                     | 0.41              |
| 1:A:166:U:H2'     | 1:A:167:A:C8     | 2.56                     | 0.41              |
| 1:A:505:G:H4'     | 1:A:534:U:C4     | 2.55                     | 0.41              |
| 1:A:635:A:H2'     | 1:A:636:U:H6     | 1.84                     | 0.41              |
| 1:A:1125:U:HO2'   | 1:A:1126:U:P     | 2.43                     | 0.41              |
| 1:A:1319:A:C8     | 1:A:1323:G:C6    | 3.08                     | 0.41              |
| 2:B:11:LYS:HE2    | 2:B:11:LYS:HB2   | 1.83                     | 0.41              |
| 3:C:51:SER:HB3    | 3:C:72:ARG:NH1   | 2.36                     | 0.41              |
| 4:D:99:ASP:OD1    | 4:D:99:ASP:N     | 2.53                     | 0.41              |
| 22:a:58:G:O2'     | 22:a:73:A:N1     | 2.47                     | 0.41              |
| 22:a:395:U:O2'    | 22:a:396:G:N7    | 2.50                     | 0.41              |
| 22:a:404:A:H1'    | 22:a:405:U:OP2   | 2.20                     | 0.41              |
| 22:a:549:G:H2'    | 22:a:550:C:O4'   | 2.19                     | 0.41              |
| 22:a:948:C:H2'    | 22:a:949:G:H8    | 1.85                     | 0.41              |
| 22:a:1838:C:H4'   | 22:a:1839:G:H8   | 1.85                     | 0.41              |
| 23:b:17:C:C2      | 23:b:18:G:C8     | 3.08                     | 0.41              |
| 23:b:45:A:C4      | 23:b:46:A:C8     | 3.09                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:r:36:LEU:HD23  | 39:r:36:LEU:HA    | 1.91                     | 0.41              |
| 45:x:2:LYS:HA     | 45:x:5:GLU:OE2    | 2.21                     | 0.41              |
| 1:A:1170:A:H2'    | 1:A:1171:A:O4'    | 2.20                     | 0.41              |
| 1:A:1390:U:H2'    | 1:A:1391:U:C6     | 2.56                     | 0.41              |
| 3:C:40:ARG:O      | 3:C:44:THR:HG23   | 2.20                     | 0.41              |
| 13:M:39:ILE:HD12  | 13:M:56:LEU:HD21  | 2.01                     | 0.41              |
| 16:P:23:ASP:OD1   | 16:P:25:ARG:N     | 2.42                     | 0.41              |
| 22:a:63:A:H2      | 40:s:70:HIS:CE1   | 2.38                     | 0.41              |
| 22:a:553:G:H2'    | 22:a:554:U:H6     | 1.86                     | 0.41              |
| 22:a:1197:G:H2'   | 22:a:1198:U:H6    | 1.86                     | 0.41              |
| 22:a:1913:A:C6    | 55:X:38:A:H5'     | 2.55                     | 0.41              |
| 22:a:1932:A:H2'   | 22:a:1933:G:O4'   | 2.20                     | 0.41              |
| 22:a:2051:A:H8    | 22:a:2051:A:OP2   | 2.03                     | 0.41              |
| 26:e:158:PHE:O    | 26:e:162:ARG:HG3  | 2.20                     | 0.41              |
| 53:V:9:C:O2'      | 53:V:10:G:N7      | 2.45                     | 0.41              |
| 1:A:35:G:H2'      | 1:A:36:C:H6       | 1.85                     | 0.41              |
| 1:A:271:C:H2'     | 1:A:272:C:H6      | 1.85                     | 0.41              |
| 1:A:881:G:P       | 12:L:9:ARG:HH22   | 2.42                     | 0.41              |
| 1:A:1121:U:C2     | 1:A:1122:U:C5     | 3.09                     | 0.41              |
| 1:A:1141:C:H2'    | 1:A:1142:G:C8     | 2.55                     | 0.41              |
| 1:A:1313:U:H2'    | 1:A:1314:C:H6     | 1.85                     | 0.41              |
| 16:P:17:TYR:HE2   | 16:P:41:PRO:HG3   | 1.86                     | 0.41              |
| 16:P:69:ASP:OD1   | 16:P:70:ARG:N     | 2.54                     | 0.41              |
| 22:a:78:U:H5'     | 45:x:7:ARG:NH2    | 2.36                     | 0.41              |
| 22:a:1149:G:H2'   | 22:a:1150:C:H6    | 1.85                     | 0.41              |
| 22:a:1316:U:H2'   | 22:a:1317:G:H8    | 1.85                     | 0.41              |
| 22:a:1394:U:H2'   | 22:a:1395:A:O4'   | 2.20                     | 0.41              |
| 22:a:1447:C:H2'   | 22:a:1448:G:H8    | 1.86                     | 0.41              |
| 22:a:1808:A:H3'   | 22:a:1809:A:C8    | 2.55                     | 0.41              |
| 22:a:2096:C:H2'   | 22:a:2097:A:H8    | 1.85                     | 0.41              |
| 22:a:2290:G:H2'   | 22:a:2291:U:C6    | 2.55                     | 0.41              |
| 22:a:2314:A:H1'   | 27:f:155:THR:HG21 | 2.02                     | 0.41              |
| 22:a:2547:A:H4'   | 31:j:29:HIS:NE2   | 2.36                     | 0.41              |
| 22:a:2552:OMU:O5' | 22:a:2552:OMU:H6  | 2.20                     | 0.41              |
| 25:d:62:LYS:HB3   | 25:d:62:LYS:HE3   | 1.80                     | 0.41              |
| 35:n:60:GLU:HG3   | 35:n:61:GLN:HG3   | 2.02                     | 0.41              |
| 44:w:59:ILE:HD13  | 44:w:67:VAL:HG11  | 2.00                     | 0.41              |
| 1:A:321:A:H2'     | 1:A:322:C:C6      | 2.55                     | 0.41              |
| 1:A:1240:U:OP1    | 7:G:116:MET:HB2   | 2.21                     | 0.41              |
| 1:A:1307:U:H2'    | 1:A:1308:U:C6     | 2.56                     | 0.41              |
| 5:E:74:VAL:HG11   | 5:E:144:LEU:HB3   | 2.01                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:G:93:PRO:O    | 7:G:96:ARG:HB2   | 2.20                     | 0.41              |
| 14:N:57:PRO:O   | 14:N:60:GLN:HG2  | 2.20                     | 0.41              |
| 19:S:70:LYS:O   | 19:S:73:GLU:HG2  | 2.20                     | 0.41              |
| 22:a:310:A:OP1  | 41:t:19:LYS:HD2  | 2.20                     | 0.41              |
| 22:a:987:C:H2'  | 22:a:988:A:O4'   | 2.21                     | 0.41              |
| 22:a:1411:U:H2' | 22:a:1412:U:C6   | 2.56                     | 0.41              |
| 22:a:1993:U:H4' | 25:d:133:THR:OG1 | 2.21                     | 0.41              |
| 22:a:2228:G:H2' | 22:a:2229:U:C6   | 2.55                     | 0.41              |
| 46:y:51:VAL:O   | 46:y:55:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:41:G:H2'    | 1:A:42:G:H8      | 1.85                     | 0.41              |
| 1:A:600:A:H2'   | 1:A:601:G:H8     | 1.85                     | 0.41              |
| 1:A:618:C:H5'   | 1:A:619:U:H5''   | 2.03                     | 0.41              |
| 2:B:9:MET:O     | 2:B:14:VAL:HG12  | 2.21                     | 0.41              |
| 3:C:81:GLY:O    | 3:C:85:GLU:HG2   | 2.21                     | 0.41              |
| 7:G:111:ARG:HB3 | 7:G:119:ARG:HD2  | 2.02                     | 0.41              |
| 22:a:274:C:H2'  | 22:a:275:C:C1'   | 2.51                     | 0.41              |
| 22:a:857:G:H2'  | 22:a:858:G:O4'   | 2.20                     | 0.41              |
| 22:a:1682:G:C4  | 22:a:1757:A:H1'  | 2.56                     | 0.41              |
| 22:a:2229:U:H2' | 22:a:2230:G:H8   | 1.85                     | 0.41              |
| 22:a:2282:G:H4' | 22:a:2389:G:O2'  | 2.21                     | 0.41              |
| 22:a:2595:G:N2  | 22:a:2598:A:OP2  | 2.40                     | 0.41              |
| 22:a:2637:U:H2' | 22:a:2638:G:O4'  | 2.20                     | 0.41              |
| 22:a:2795:C:H2' | 22:a:2796:U:C6   | 2.56                     | 0.41              |
| 36:o:14:LYS:HE3 | 36:o:77:HIS:HA   | 2.02                     | 0.41              |
| 42:u:45:ASP:OD1 | 42:u:46:LYS:N    | 2.52                     | 0.41              |
| 1:A:476:U:H2'   | 1:A:477:C:C6     | 2.55                     | 0.41              |
| 1:A:490:C:C2    | 1:A:491:G:C8     | 3.09                     | 0.41              |
| 1:A:526:C:OP2   | 12:L:88:LYS:HE3  | 2.21                     | 0.41              |
| 1:A:757:U:H2'   | 1:A:758:C:O4'    | 2.20                     | 0.41              |
| 1:A:1124:G:H1'  | 1:A:1125:U:H5    | 1.85                     | 0.41              |
| 1:A:1315:U:H2'  | 1:A:1316:G:O4'   | 2.21                     | 0.41              |
| 7:G:78:ARG:NH1  | 7:G:80:VAL:HG22  | 2.36                     | 0.41              |
| 9:I:36:GLU:OE1  | 9:I:36:GLU:N     | 2.54                     | 0.41              |
| 10:J:35:GLN:HB3 | 10:J:77:VAL:HB   | 2.03                     | 0.41              |
| 13:M:5:ALA:HB2  | 13:M:60:VAL:HG11 | 2.02                     | 0.41              |
| 22:a:7:G:H5''   | 30:i:123:LYS:HE2 | 2.03                     | 0.41              |
| 22:a:208:C:H2'  | 22:a:209:C:C6    | 2.56                     | 0.41              |
| 22:a:559:G:H1'  | 37:p:56:GLN:NE2  | 2.36                     | 0.41              |
| 22:a:1360:G:N7  | 22:a:1361:G:C8   | 2.89                     | 0.41              |
| 22:a:1410:G:H2' | 22:a:1411:U:C6   | 2.56                     | 0.41              |
| 22:a:1441:G:H2' | 22:a:1442:U:C6   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:1472:C:C2   | 22:a:1473:G:C8    | 3.09                     | 0.41              |
| 22:a:1496:A:H2'  | 22:a:1498:C:C5    | 2.55                     | 0.41              |
| 22:a:1831:G:H2'  | 22:a:1832:C:C6    | 2.56                     | 0.41              |
| 22:a:2757:A:C2   | 22:a:2758:A:C8    | 3.08                     | 0.41              |
| 26:e:149:ILE:HB  | 26:e:188:MET:HG2  | 2.02                     | 0.41              |
| 34:m:32:GLU:OE1  | 34:m:115:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:217:C:H2'    | 1:A:218:U:C6      | 2.55                     | 0.41              |
| 1:A:284:C:H2'    | 1:A:285:C:H6      | 1.86                     | 0.41              |
| 1:A:356:A:H2'    | 1:A:357:G:O4'     | 2.20                     | 0.41              |
| 1:A:592:G:H2'    | 1:A:593:U:C6      | 2.56                     | 0.41              |
| 1:A:648:A:H2'    | 1:A:649:A:H8      | 1.86                     | 0.41              |
| 1:A:864:A:H2'    | 1:A:865:A:C8      | 2.56                     | 0.41              |
| 1:A:923:A:H2'    | 1:A:924:C:C6      | 2.56                     | 0.41              |
| 1:A:1100:C:OP2   | 2:B:95:ARG:HD2    | 2.20                     | 0.41              |
| 1:A:1533:C:H4'   | 1:A:1534:A:C8     | 2.56                     | 0.41              |
| 5:E:111:MET:HE2  | 5:E:125:ALA:HB1   | 2.02                     | 0.41              |
| 9:I:97:GLU:HA    | 9:I:100:LYS:HG2   | 2.02                     | 0.41              |
| 12:L:107:VAL:O   | 12:L:119:VAL:HG11 | 2.21                     | 0.41              |
| 12:L:123:LYS:HE3 | 12:L:123:LYS:HB3  | 1.94                     | 0.41              |
| 14:N:82:ILE:H    | 14:N:82:ILE:HD12  | 1.85                     | 0.41              |
| 16:P:19:VAL:HG21 | 16:P:52:LEU:HD21  | 2.03                     | 0.41              |
| 16:P:57:ILE:O    | 16:P:61:VAL:HG23  | 2.21                     | 0.41              |
| 19:S:5:LEU:HD21  | 52:4:63:ARG:HH21  | 1.85                     | 0.41              |
| 22:a:170:U:H2'   | 22:a:171:U:C6     | 2.55                     | 0.41              |
| 22:a:283:G:H2'   | 22:a:284:U:O4'    | 2.21                     | 0.41              |
| 22:a:360:U:H2'   | 22:a:361:G:O4'    | 2.19                     | 0.41              |
| 22:a:362:A:C6    | 22:a:363:G:C5     | 3.09                     | 0.41              |
| 22:a:550:C:H2'   | 22:a:551:G:C8     | 2.56                     | 0.41              |
| 22:a:704:G:H1'   | 22:a:727:A:N6     | 2.35                     | 0.41              |
| 22:a:820:A:H4'   | 22:a:836:G:N2     | 2.36                     | 0.41              |
| 22:a:934:U:H2'   | 22:a:935:C:C6     | 2.55                     | 0.41              |
| 22:a:1219:U:H2'  | 22:a:1220:G:C8    | 2.55                     | 0.41              |
| 33:l:74:THR:HG22 | 33:l:89:VAL:HG22  | 2.02                     | 0.41              |
| 36:o:60:THR:HG23 | 36:o:73:VAL:HG22  | 2.02                     | 0.41              |
| 39:r:85:ILE:HD13 | 39:r:85:ILE:HA    | 1.92                     | 0.41              |
| 42:u:21:ARG:HA   | 42:u:25:LYS:O     | 2.20                     | 0.41              |
| 43:v:9:SER:OG    | 43:v:10:THR:N     | 2.54                     | 0.41              |
| 53:V:35:U8U:HN3  | 54:W:30:G:H1      | 1.69                     | 0.41              |
| 1:A:166:U:C2     | 1:A:167:A:N7      | 2.88                     | 0.41              |
| 1:A:358:U:H2'    | 1:A:359:G:H8      | 1.85                     | 0.41              |
| 1:A:377:G:H2'    | 1:A:378:G:H8      | 1.86                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:982:U:H4'    | 1:A:983:A:O4'     | 2.21                     | 0.41              |
| 3:C:108:LYS:HD3  | 3:C:144:LEU:HD13  | 2.03                     | 0.41              |
| 4:D:62:ARG:CZ    | 4:D:69:GLU:HG2    | 2.51                     | 0.41              |
| 22:a:58:G:OP1    | 40:s:78:SER:OG    | 2.28                     | 0.41              |
| 22:a:404:A:H4'   | 22:a:405:U:O5'    | 2.21                     | 0.41              |
| 22:a:487:C:H2'   | 22:a:488:G:O4'    | 2.21                     | 0.41              |
| 22:a:546:U:H2'   | 22:a:548:G:N2     | 2.36                     | 0.41              |
| 22:a:596:U:H2'   | 22:a:597:G:C8     | 2.56                     | 0.41              |
| 22:a:891:G:C4    | 22:a:892:A:C8     | 3.09                     | 0.41              |
| 22:a:909:A:H2'   | 22:a:912:C:C5     | 2.56                     | 0.41              |
| 22:a:963:U:C2    | 22:a:964:C:C5     | 3.09                     | 0.41              |
| 22:a:1526:C:H2'  | 22:a:1527:G:O4'   | 2.21                     | 0.41              |
| 22:a:1824:G:O3'  | 24:c:247:PRO:HD3  | 2.21                     | 0.41              |
| 36:o:18:PRO:HG3  | 36:o:84:ILE:O     | 2.20                     | 0.41              |
| 48:0:11:LEU:HD23 | 48:0:51:GLU:HA    | 2.03                     | 0.41              |
| 1:A:500:G:H2'    | 1:A:501:C:C6      | 2.55                     | 0.40              |
| 1:A:552:U:H2'    | 1:A:553:A:H8      | 1.86                     | 0.40              |
| 1:A:649:A:H2'    | 1:A:650:G:O4'     | 2.21                     | 0.40              |
| 7:G:45:SER:O     | 7:G:48:GLU:HG3    | 2.21                     | 0.40              |
| 14:N:16:LEU:HD12 | 14:N:16:LEU:HA    | 1.84                     | 0.40              |
| 16:P:74:LEU:O    | 16:P:78:VAL:HG23  | 2.20                     | 0.40              |
| 22:a:1243:C:H1'  | 32:k:4:ASN:O      | 2.20                     | 0.40              |
| 23:b:5:U:H2'     | 23:b:6:G:C8       | 2.55                     | 0.40              |
| 24:c:146:MET:CE  | 24:c:154:LEU:HD21 | 2.51                     | 0.40              |
| 29:h:30:LEU:O    | 29:h:35:LYS:HB3   | 2.21                     | 0.40              |
| 37:p:49:ASP:HA   | 37:p:52:GLN:HB2   | 2.02                     | 0.40              |
| 37:p:66:ASN:HA   | 37:p:76:TYR:HB2   | 2.03                     | 0.40              |
| 50:2:32:ILE:HG13 | 50:2:32:ILE:O     | 2.20                     | 0.40              |
| 1:A:78:A:N6      | 1:A:92:U:O4       | 2.54                     | 0.40              |
| 1:A:236:A:H2'    | 1:A:237:G:H8      | 1.86                     | 0.40              |
| 1:A:322:C:H2'    | 1:A:323:U:C6      | 2.56                     | 0.40              |
| 1:A:1144:G:N2    | 1:A:1146:A:H62    | 2.19                     | 0.40              |
| 1:A:1356:G:H2'   | 1:A:1357:A:H8     | 1.82                     | 0.40              |
| 1:A:1409:C:H2'   | 1:A:1410:A:H8     | 1.86                     | 0.40              |
| 5:E:157:ARG:NH2  | 8:H:43:GLU:OE2    | 2.54                     | 0.40              |
| 22:a:248:G:O5'   | 22:a:249:C:H5''   | 2.20                     | 0.40              |
| 22:a:278:A:N6    | 22:a:362:A:C5     | 2.90                     | 0.40              |
| 22:a:634:C:H2'   | 22:a:635:C:C6     | 2.56                     | 0.40              |
| 22:a:2329:U:H2'  | 22:a:2330:G:H8    | 1.85                     | 0.40              |
| 22:a:2626:C:H2'  | 22:a:2627:G:C8    | 2.56                     | 0.40              |
| 47:z:29:SER:O    | 47:z:37:LYS:HA    | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:603:U:H2'    | 1:A:604:G:C8     | 2.56                     | 0.40              |
| 1:A:1243:C:H2'   | 1:A:1244:G:H8    | 1.85                     | 0.40              |
| 1:A:1327:C:H2'   | 1:A:1328:C:H6    | 1.85                     | 0.40              |
| 1:A:1369:C:H2'   | 1:A:1370:G:C8    | 2.56                     | 0.40              |
| 3:C:151:VAL:HG22 | 3:C:200:VAL:HG12 | 2.04                     | 0.40              |
| 4:D:117:LEU:HA   | 4:D:117:LEU:HD23 | 1.84                     | 0.40              |
| 22:a:3:U:H2'     | 22:a:4:U:H6      | 1.86                     | 0.40              |
| 22:a:579:G:H2'   | 22:a:580:U:C6    | 2.56                     | 0.40              |
| 22:a:1599:U:C2   | 22:a:1600:C:C5   | 3.10                     | 0.40              |
| 22:a:2265:U:OP2  | 22:a:2266:A:O2'  | 2.27                     | 0.40              |
| 22:a:2784:U:H2'  | 22:a:2785:C:C6   | 2.56                     | 0.40              |
| 27:f:48:LYS:HE3  | 27:f:48:LYS:HB3  | 1.86                     | 0.40              |
| 32:k:49:GLY:HA3  | 32:k:58:TYR:CE2  | 2.55                     | 0.40              |
| 53:V:29:C:H2'    | 53:V:30:G:H8     | 1.86                     | 0.40              |
| 1:A:268:U:H2'    | 1:A:269:C:C6     | 2.57                     | 0.40              |
| 1:A:419:C:OP1    | 1:A:513:C:O2'    | 2.36                     | 0.40              |
| 1:A:1436:U:H2'   | 1:A:1437:A:H8    | 1.86                     | 0.40              |
| 2:B:219:ALA:O    | 2:B:222:ARG:HG2  | 2.21                     | 0.40              |
| 9:I:28:ILE:HA    | 9:I:63:LEU:HB2   | 2.03                     | 0.40              |
| 11:K:97:ILE:HG22 | 21:U:12:PHE:CZ   | 2.56                     | 0.40              |
| 22:a:154:U:H2'   | 22:a:155:A:C8    | 2.56                     | 0.40              |
| 22:a:171:U:H2'   | 22:a:172:A:C8    | 2.55                     | 0.40              |
| 22:a:546:U:H2'   | 22:a:548:G:H21   | 1.87                     | 0.40              |
| 22:a:1464:G:H2'  | 22:a:1465:G:C8   | 2.57                     | 0.40              |
| 22:a:1599:U:H2'  | 22:a:1600:C:H6   | 1.86                     | 0.40              |
| 22:a:1843:C:H2'  | 22:a:1844:C:H6   | 1.87                     | 0.40              |
| 22:a:2316:G:H2'  | 22:a:2317:A:C8   | 2.48                     | 0.40              |
| 22:a:2723:C:H2'  | 22:a:2724:U:O4'  | 2.21                     | 0.40              |
| 22:a:2831:G:OP2  | 25:d:59:ARG:NE   | 2.47                     | 0.40              |
| 1:A:1120:C:C2    | 1:A:1121:U:C5    | 3.10                     | 0.40              |
| 1:A:1333:A:H2'   | 1:A:1334:G:O4'   | 2.22                     | 0.40              |
| 22:a:75:G:H4'    | 45:x:48:ARG:NH2  | 2.37                     | 0.40              |
| 22:a:150:U:H2'   | 22:a:151:C:H6    | 1.87                     | 0.40              |
| 22:a:302:C:H2'   | 22:a:303:G:C8    | 2.56                     | 0.40              |
| 22:a:965:C:C2    | 22:a:966:G:C8    | 3.09                     | 0.40              |
| 22:a:1219:U:H2'  | 22:a:1220:G:H8   | 1.86                     | 0.40              |
| 22:a:1989:G:H2'  | 22:a:1990:C:O4'  | 2.22                     | 0.40              |
| 22:a:2088:A:H2'  | 22:a:2089:C:C6   | 2.56                     | 0.40              |
| 22:a:2745:C:H2'  | 22:a:2746:U:C6   | 2.57                     | 0.40              |
| 25:d:28:GLU:OE2  | 36:o:4:ILE:HD13  | 2.22                     | 0.40              |
| 34:m:45:ARG:HE   | 34:m:45:ARG:HB2  | 1.69                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 39:r:83:LYS:HG2 | 39:r:95:ARG:HD3 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | B     | 222/241 (92%) | 204 (92%) | 18 (8%) | 0        | 100         | 100 |
| 3   | C     | 204/233 (88%) | 194 (95%) | 10 (5%) | 0        | 100         | 100 |
| 4   | D     | 203/206 (98%) | 193 (95%) | 10 (5%) | 0        | 100         | 100 |
| 5   | E     | 154/167 (92%) | 148 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 6   | F     | 101/135 (75%) | 95 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 7   | G     | 151/179 (84%) | 140 (93%) | 11 (7%) | 0        | 100         | 100 |
| 8   | H     | 127/130 (98%) | 123 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 9   | I     | 125/130 (96%) | 121 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 10  | J     | 96/103 (93%)  | 86 (90%)  | 9 (9%)  | 1 (1%)   | 12          | 32  |
| 11  | K     | 113/129 (88%) | 105 (93%) | 8 (7%)  | 0        | 100         | 100 |
| 12  | L     | 120/124 (97%) | 115 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 13  | M     | 113/118 (96%) | 105 (93%) | 8 (7%)  | 0        | 100         | 100 |
| 14  | N     | 98/101 (97%)  | 95 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 15  | O     | 86/89 (97%)   | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 16  | P     | 79/82 (96%)   | 75 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 17  | Q     | 77/84 (92%)   | 74 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 18  | R     | 64/75 (85%)   | 58 (91%)  | 6 (9%)  | 0        | 100         | 100 |
| 19  | S     | 82/92 (89%)   | 81 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 20  | T     | 84/87 (97%)   | 82 (98%)  | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 21  | U     | 68/71 (96%)     | 67 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 24  | c     | 269/273 (98%)   | 262 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 25  | d     | 206/209 (99%)   | 199 (97%)  | 6 (3%)   | 1 (0%)   | 24          | 48  |
| 26  | e     | 199/201 (99%)   | 194 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 27  | f     | 175/179 (98%)   | 164 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 28  | g     | 174/177 (98%)   | 158 (91%)  | 15 (9%)  | 1 (1%)   | 21          | 44  |
| 29  | h     | 39/149 (26%)    | 32 (82%)   | 7 (18%)  | 0        | 100         | 100 |
| 30  | i     | 140/142 (99%)   | 138 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 31  | j     | 121/123 (98%)   | 116 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 32  | k     | 142/144 (99%)   | 135 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 33  | l     | 132/136 (97%)   | 130 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 34  | m     | 116/127 (91%)   | 111 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 35  | n     | 114/117 (97%)   | 108 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 36  | o     | 112/115 (97%)   | 110 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 37  | p     | 115/118 (98%)   | 114 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 38  | q     | 101/103 (98%)   | 97 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 39  | r     | 108/110 (98%)   | 107 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 40  | s     | 91/100 (91%)    | 83 (91%)   | 8 (9%)   | 0        | 100         | 100 |
| 41  | t     | 100/104 (96%)   | 94 (94%)   | 5 (5%)   | 1 (1%)   | 12          | 32  |
| 42  | u     | 92/94 (98%)     | 91 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 43  | v     | 76/85 (89%)     | 74 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 44  | w     | 75/78 (96%)     | 75 (100%)  | 0        | 0        | 100         | 100 |
| 45  | x     | 60/63 (95%)     | 56 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 46  | y     | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 47  | z     | 54/57 (95%)     | 54 (100%)  | 0        | 0        | 100         | 100 |
| 48  | 0     | 49/55 (89%)     | 49 (100%)  | 0        | 0        | 100         | 100 |
| 49  | 1     | 44/46 (96%)     | 43 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 50  | 2     | 62/65 (95%)     | 59 (95%)   | 2 (3%)   | 1 (2%)   | 7           | 20  |
| 51  | 3     | 36/38 (95%)     | 36 (100%)  | 0        | 0        | 100         | 100 |
| 52  | 4     | 56/70 (80%)     | 52 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| All | All   | 5481/5913 (93%) | 5240 (96%) | 236 (4%) | 5 (0%)   | 49          | 73  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | d     | 149 | ASN  |
| 28  | g     | 47  | ASP  |
| 41  | t     | 99  | ASN  |
| 50  | 2     | 32  | ILE  |
| 10  | J     | 57  | VAL  |

### 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   | B     | 186/199 (94%) | 186 (100%) | 0        | 100         | 100 |
| 3   | C     | 170/190 (90%) | 170 (100%) | 0        | 100         | 100 |
| 4   | D     | 172/173 (99%) | 172 (100%) | 0        | 100         | 100 |
| 5   | E     | 119/126 (94%) | 119 (100%) | 0        | 100         | 100 |
| 6   | F     | 90/116 (78%)  | 90 (100%)  | 0        | 100         | 100 |
| 7   | G     | 126/147 (86%) | 126 (100%) | 0        | 100         | 100 |
| 8   | H     | 104/105 (99%) | 104 (100%) | 0        | 100         | 100 |
| 9   | I     | 105/107 (98%) | 104 (99%)  | 1 (1%)   | 68          | 86  |
| 10  | J     | 86/90 (96%)   | 86 (100%)  | 0        | 100         | 100 |
| 11  | K     | 89/98 (91%)   | 89 (100%)  | 0        | 100         | 100 |
| 12  | L     | 102/103 (99%) | 102 (100%) | 0        | 100         | 100 |
| 13  | M     | 93/96 (97%)   | 93 (100%)  | 0        | 100         | 100 |
| 14  | N     | 83/84 (99%)   | 83 (100%)  | 0        | 100         | 100 |
| 15  | O     | 76/77 (99%)   | 76 (100%)  | 0        | 100         | 100 |
| 16  | P     | 65/65 (100%)  | 65 (100%)  | 0        | 100         | 100 |
| 17  | Q     | 73/78 (94%)   | 73 (100%)  | 0        | 100         | 100 |
| 18  | R     | 57/65 (88%)   | 57 (100%)  | 0        | 100         | 100 |
| 19  | S     | 72/79 (91%)   | 72 (100%)  | 0        | 100         | 100 |
| 20  | T     | 65/66 (98%)   | 65 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 21  | U     | 60/61 (98%)     | 60 (100%)   | 0        | 100         | 100 |
| 24  | c     | 216/218 (99%)   | 216 (100%)  | 0        | 100         | 100 |
| 25  | d     | 163/163 (100%)  | 163 (100%)  | 0        | 100         | 100 |
| 26  | e     | 165/165 (100%)  | 165 (100%)  | 0        | 100         | 100 |
| 27  | f     | 148/150 (99%)   | 148 (100%)  | 0        | 100         | 100 |
| 28  | g     | 137/138 (99%)   | 137 (100%)  | 0        | 100         | 100 |
| 29  | h     | 32/114 (28%)    | 32 (100%)   | 0        | 100         | 100 |
| 30  | i     | 116/116 (100%)  | 116 (100%)  | 0        | 100         | 100 |
| 31  | j     | 104/104 (100%)  | 104 (100%)  | 0        | 100         | 100 |
| 32  | k     | 103/103 (100%)  | 103 (100%)  | 0        | 100         | 100 |
| 33  | l     | 107/107 (100%)  | 107 (100%)  | 0        | 100         | 100 |
| 34  | m     | 98/103 (95%)    | 98 (100%)   | 0        | 100         | 100 |
| 35  | n     | 86/87 (99%)     | 86 (100%)   | 0        | 100         | 100 |
| 36  | o     | 99/100 (99%)    | 99 (100%)   | 0        | 100         | 100 |
| 37  | p     | 89/90 (99%)     | 89 (100%)   | 0        | 100         | 100 |
| 38  | q     | 84/84 (100%)    | 84 (100%)   | 0        | 100         | 100 |
| 39  | r     | 93/93 (100%)    | 93 (100%)   | 0        | 100         | 100 |
| 40  | s     | 80/84 (95%)     | 80 (100%)   | 0        | 100         | 100 |
| 41  | t     | 83/85 (98%)     | 83 (100%)   | 0        | 100         | 100 |
| 42  | u     | 78/78 (100%)    | 78 (100%)   | 0        | 100         | 100 |
| 43  | v     | 58/63 (92%)     | 58 (100%)   | 0        | 100         | 100 |
| 44  | w     | 67/68 (98%)     | 67 (100%)   | 0        | 100         | 100 |
| 45  | x     | 54/55 (98%)     | 54 (100%)   | 0        | 100         | 100 |
| 46  | y     | 48/49 (98%)     | 48 (100%)   | 0        | 100         | 100 |
| 47  | z     | 47/48 (98%)     | 47 (100%)   | 0        | 100         | 100 |
| 48  | 0     | 46/49 (94%)     | 46 (100%)   | 0        | 100         | 100 |
| 49  | 1     | 38/38 (100%)    | 38 (100%)   | 0        | 100         | 100 |
| 50  | 2     | 51/52 (98%)     | 51 (100%)   | 0        | 100         | 100 |
| 51  | 3     | 34/34 (100%)    | 34 (100%)   | 0        | 100         | 100 |
| 52  | 4     | 55/62 (89%)     | 55 (100%)   | 0        | 100         | 100 |
| All | All   | 4572/4825 (95%) | 4571 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 4   | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 203 | ASN  |
| 3   | C     | 139 | GLN  |
| 3   | C     | 176 | HIS  |
| 4   | D     | 54  | GLN  |
| 4   | D     | 152 | GLN  |
| 5   | E     | 61  | GLN  |
| 5   | E     | 122 | ASN  |
| 5   | E     | 132 | ASN  |
| 7   | G     | 86  | GLN  |
| 8   | H     | 4   | GLN  |
| 8   | H     | 118 | GLN  |
| 9   | I     | 110 | GLN  |
| 11  | K     | 101 | ASN  |
| 12  | L     | 5   | ASN  |
| 12  | L     | 96  | HIS  |
| 14  | N     | 49  | GLN  |
| 15  | O     | 35  | GLN  |
| 16  | P     | 18  | GLN  |
| 16  | P     | 63  | GLN  |
| 19  | S     | 56  | GLN  |
| 20  | T     | 48  | GLN  |
| 20  | T     | 52  | ASN  |
| 20  | T     | 61  | GLN  |
| 21  | U     | 9   | ASN  |
| 24  | c     | 53  | HIS  |
| 24  | c     | 117 | GLN  |
| 24  | c     | 134 | ASN  |
| 24  | c     | 226 | ASN  |
| 25  | d     | 32  | ASN  |
| 25  | d     | 94  | GLN  |
| 25  | d     | 130 | GLN  |
| 30  | i     | 76  | HIS  |
| 30  | i     | 136 | GLN  |
| 33  | l     | 60  | GLN  |
| 35  | n     | 38  | GLN  |
| 37  | p     | 66  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | r     | 7   | HIS  |
| 39  | r     | 61  | ASN  |
| 41  | t     | 27  | ASN  |
| 41  | t     | 74  | ASN  |
| 44  | w     | 17  | ASN  |
| 45  | x     | 25  | GLN  |
| 45  | x     | 31  | GLN  |
| 48  | 0     | 26  | ASN  |
| 49  | 1     | 6   | GLN  |
| 49  | 1     | 29  | GLN  |
| 52  | 4     | 30  | HIS  |
| 52  | 4     | 61  | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1516/1542 (98%) | 212 (13%)         | 3 (0%)          |
| 22  | a     | 2749/2904 (94%) | 299 (10%)         | 0               |
| 23  | b     | 118/120 (98%)   | 13 (11%)          | 0               |
| 53  | V     | 75/76 (98%)     | 20 (26%)          | 1 (1%)          |
| 54  | W     | 10/48 (20%)     | 2 (20%)           | 1 (10%)         |
| 55  | X     | 73/76 (96%)     | 18 (24%)          | 0               |
| All | All   | 4541/4766 (95%) | 564 (12%)         | 5 (0%)          |

All (564) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | U    |
| 1   | A     | 6   | G    |
| 1   | A     | 8   | A    |
| 1   | A     | 22  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 39  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 60  | A    |
| 1   | A     | 69  | G    |
| 1   | A     | 71  | A    |
| 1   | A     | 72  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 74  | A    |
| 1   | A     | 75  | G    |
| 1   | A     | 80  | A    |
| 1   | A     | 84  | U    |
| 1   | A     | 85  | U    |
| 1   | A     | 86  | G    |
| 1   | A     | 87  | C    |
| 1   | A     | 88  | U    |
| 1   | A     | 91  | U    |
| 1   | A     | 94  | G    |
| 1   | A     | 95  | C    |
| 1   | A     | 116 | A    |
| 1   | A     | 121 | U    |
| 1   | A     | 130 | A    |
| 1   | A     | 131 | A    |
| 1   | A     | 141 | G    |
| 1   | A     | 144 | G    |
| 1   | A     | 149 | A    |
| 1   | A     | 163 | C    |
| 1   | A     | 164 | G    |
| 1   | A     | 173 | U    |
| 1   | A     | 175 | C    |
| 1   | A     | 177 | G    |
| 1   | A     | 180 | U    |
| 1   | A     | 181 | A    |
| 1   | A     | 194 | C    |
| 1   | A     | 195 | A    |
| 1   | A     | 197 | A    |
| 1   | A     | 199 | A    |
| 1   | A     | 200 | G    |
| 1   | A     | 204 | G    |
| 1   | A     | 215 | C    |
| 1   | A     | 240 | G    |
| 1   | A     | 245 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |
| 1   | A     | 262 | A    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 289 | G    |
| 1   | A     | 321 | A    |
| 1   | A     | 328 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 330 | C    |
| 1   | A     | 341 | C    |
| 1   | A     | 347 | G    |
| 1   | A     | 351 | G    |
| 1   | A     | 352 | C    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 372 | C    |
| 1   | A     | 373 | A    |
| 1   | A     | 378 | G    |
| 1   | A     | 391 | G    |
| 1   | A     | 392 | C    |
| 1   | A     | 397 | A    |
| 1   | A     | 406 | G    |
| 1   | A     | 412 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 421 | U    |
| 1   | A     | 422 | C    |
| 1   | A     | 424 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 439 | U    |
| 1   | A     | 452 | A    |
| 1   | A     | 457 | G    |
| 1   | A     | 458 | U    |
| 1   | A     | 465 | A    |
| 1   | A     | 467 | U    |
| 1   | A     | 468 | A    |
| 1   | A     | 481 | G    |
| 1   | A     | 484 | G    |
| 1   | A     | 486 | U    |
| 1   | A     | 495 | A    |
| 1   | A     | 496 | A    |
| 1   | A     | 497 | G    |
| 1   | A     | 500 | G    |
| 1   | A     | 509 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 520 | A    |
| 1   | A     | 521 | G    |
| 1   | A     | 529 | G    |
| 1   | A     | 531 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 564 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 576 | C    |
| 1   | A     | 577 | G    |
| 1   | A     | 596 | A    |
| 1   | A     | 633 | G    |
| 1   | A     | 636 | U    |
| 1   | A     | 638 | U    |
| 1   | A     | 639 | G    |
| 1   | A     | 653 | U    |
| 1   | A     | 665 | A    |
| 1   | A     | 682 | G    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |
| 1   | A     | 734 | G    |
| 1   | A     | 746 | A    |
| 1   | A     | 747 | A    |
| 1   | A     | 748 | G    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 787 | A    |
| 1   | A     | 793 | U    |
| 1   | A     | 794 | A    |
| 1   | A     | 802 | A    |
| 1   | A     | 815 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 821 | G    |
| 1   | A     | 832 | G    |
| 1   | A     | 851 | G    |
| 1   | A     | 890 | G    |
| 1   | A     | 914 | A    |
| 1   | A     | 926 | G    |
| 1   | A     | 934 | C    |
| 1   | A     | 935 | A    |
| 1   | A     | 960 | U    |
| 1   | A     | 966 | 2MG  |
| 1   | A     | 969 | A    |
| 1   | A     | 975 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 993  | G    |
| 1   | A     | 996  | A    |
| 1   | A     | 1003 | G    |
| 1   | A     | 1004 | A    |
| 1   | A     | 1008 | U    |
| 1   | A     | 1009 | U    |
| 1   | A     | 1022 | A    |
| 1   | A     | 1027 | C    |
| 1   | A     | 1028 | C    |
| 1   | A     | 1029 | U    |
| 1   | A     | 1030 | U    |
| 1   | A     | 1031 | C    |
| 1   | A     | 1034 | G    |
| 1   | A     | 1035 | A    |
| 1   | A     | 1036 | A    |
| 1   | A     | 1037 | C    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1085 | U    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1134 | G    |
| 1   | A     | 1135 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1146 | A    |
| 1   | A     | 1151 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1196 | A    |
| 1   | A     | 1197 | A    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1257 | A    |
| 1   | A     | 1260 | G    |
| 1   | A     | 1275 | A    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1286 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1287 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1302 | C    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1312 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1364 | U    |
| 1   | A     | 1370 | G    |
| 1   | A     | 1378 | C    |
| 1   | A     | 1379 | G    |
| 1   | A     | 1381 | U    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1419 | G    |
| 1   | A     | 1432 | G    |
| 1   | A     | 1441 | A    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1451 | U    |
| 1   | A     | 1452 | C    |
| 1   | A     | 1487 | G    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 22  | a     | 10   | A    |
| 22  | a     | 34   | U    |
| 22  | a     | 45   | G    |
| 22  | a     | 51   | G    |
| 22  | a     | 63   | A    |
| 22  | a     | 71   | A    |
| 22  | a     | 74   | A    |
| 22  | a     | 75   | G    |
| 22  | a     | 101  | A    |
| 22  | a     | 102  | U    |
| 22  | a     | 118  | A    |
| 22  | a     | 120  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | a     | 125 | A    |
| 22  | a     | 139 | U    |
| 22  | a     | 140 | C    |
| 22  | a     | 142 | A    |
| 22  | a     | 163 | C    |
| 22  | a     | 164 | C    |
| 22  | a     | 181 | A    |
| 22  | a     | 196 | A    |
| 22  | a     | 199 | A    |
| 22  | a     | 216 | A    |
| 22  | a     | 222 | A    |
| 22  | a     | 223 | A    |
| 22  | a     | 233 | A    |
| 22  | a     | 248 | G    |
| 22  | a     | 272 | A    |
| 22  | a     | 275 | C    |
| 22  | a     | 278 | A    |
| 22  | a     | 279 | A    |
| 22  | a     | 281 | C    |
| 22  | a     | 285 | G    |
| 22  | a     | 311 | A    |
| 22  | a     | 329 | G    |
| 22  | a     | 330 | A    |
| 22  | a     | 346 | A    |
| 22  | a     | 353 | C    |
| 22  | a     | 356 | G    |
| 22  | a     | 362 | A    |
| 22  | a     | 386 | G    |
| 22  | a     | 396 | G    |
| 22  | a     | 405 | U    |
| 22  | a     | 411 | G    |
| 22  | a     | 473 | G    |
| 22  | a     | 481 | G    |
| 22  | a     | 491 | G    |
| 22  | a     | 504 | A    |
| 22  | a     | 505 | A    |
| 22  | a     | 509 | C    |
| 22  | a     | 529 | A    |
| 22  | a     | 530 | G    |
| 22  | a     | 531 | C    |
| 22  | a     | 532 | A    |
| 22  | a     | 545 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | a     | 546 | U    |
| 22  | a     | 547 | A    |
| 22  | a     | 549 | G    |
| 22  | a     | 563 | A    |
| 22  | a     | 573 | U    |
| 22  | a     | 575 | A    |
| 22  | a     | 603 | A    |
| 22  | a     | 614 | A    |
| 22  | a     | 615 | U    |
| 22  | a     | 627 | A    |
| 22  | a     | 637 | A    |
| 22  | a     | 645 | C    |
| 22  | a     | 646 | U    |
| 22  | a     | 647 | G    |
| 22  | a     | 654 | A    |
| 22  | a     | 655 | A    |
| 22  | a     | 686 | U    |
| 22  | a     | 717 | C    |
| 22  | a     | 726 | G    |
| 22  | a     | 730 | A    |
| 22  | a     | 738 | G    |
| 22  | a     | 747 | 5MU  |
| 22  | a     | 764 | A    |
| 22  | a     | 765 | C    |
| 22  | a     | 775 | G    |
| 22  | a     | 776 | G    |
| 22  | a     | 782 | A    |
| 22  | a     | 784 | G    |
| 22  | a     | 785 | G    |
| 22  | a     | 789 | A    |
| 22  | a     | 792 | A    |
| 22  | a     | 805 | G    |
| 22  | a     | 812 | C    |
| 22  | a     | 827 | U    |
| 22  | a     | 828 | U    |
| 22  | a     | 846 | U    |
| 22  | a     | 847 | U    |
| 22  | a     | 859 | G    |
| 22  | a     | 883 | G    |
| 22  | a     | 884 | U    |
| 22  | a     | 888 | C    |
| 22  | a     | 890 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 893  | C    |
| 22  | a     | 896  | A    |
| 22  | a     | 899  | A    |
| 22  | a     | 907  | G    |
| 22  | a     | 910  | A    |
| 22  | a     | 927  | A    |
| 22  | a     | 931  | U    |
| 22  | a     | 932  | U    |
| 22  | a     | 946  | C    |
| 22  | a     | 958  | U    |
| 22  | a     | 961  | C    |
| 22  | a     | 974  | G    |
| 22  | a     | 983  | A    |
| 22  | a     | 984  | A    |
| 22  | a     | 996  | A    |
| 22  | a     | 1009 | A    |
| 22  | a     | 1012 | U    |
| 22  | a     | 1013 | C    |
| 22  | a     | 1025 | G    |
| 22  | a     | 1026 | G    |
| 22  | a     | 1033 | U    |
| 22  | a     | 1046 | A    |
| 22  | a     | 1047 | G    |
| 22  | a     | 1110 | G    |
| 22  | a     | 1111 | A    |
| 22  | a     | 1112 | G    |
| 22  | a     | 1116 | G    |
| 22  | a     | 1132 | U    |
| 22  | a     | 1133 | A    |
| 22  | a     | 1135 | C    |
| 22  | a     | 1142 | A    |
| 22  | a     | 1186 | G    |
| 22  | a     | 1206 | G    |
| 22  | a     | 1236 | G    |
| 22  | a     | 1250 | G    |
| 22  | a     | 1253 | A    |
| 22  | a     | 1256 | G    |
| 22  | a     | 1271 | G    |
| 22  | a     | 1272 | A    |
| 22  | a     | 1275 | A    |
| 22  | a     | 1300 | G    |
| 22  | a     | 1301 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 1325 | U    |
| 22  | a     | 1329 | U    |
| 22  | a     | 1352 | U    |
| 22  | a     | 1365 | A    |
| 22  | a     | 1378 | A    |
| 22  | a     | 1379 | U    |
| 22  | a     | 1383 | A    |
| 22  | a     | 1416 | G    |
| 22  | a     | 1417 | C    |
| 22  | a     | 1427 | A    |
| 22  | a     | 1428 | C    |
| 22  | a     | 1452 | G    |
| 22  | a     | 1453 | A    |
| 22  | a     | 1482 | G    |
| 22  | a     | 1485 | U    |
| 22  | a     | 1493 | C    |
| 22  | a     | 1497 | U    |
| 22  | a     | 1509 | A    |
| 22  | a     | 1510 | G    |
| 22  | a     | 1515 | A    |
| 22  | a     | 1524 | G    |
| 22  | a     | 1529 | G    |
| 22  | a     | 1535 | A    |
| 22  | a     | 1536 | C    |
| 22  | a     | 1537 | G    |
| 22  | a     | 1560 | G    |
| 22  | a     | 1566 | A    |
| 22  | a     | 1569 | A    |
| 22  | a     | 1578 | U    |
| 22  | a     | 1583 | A    |
| 22  | a     | 1584 | U    |
| 22  | a     | 1608 | A    |
| 22  | a     | 1626 | A    |
| 22  | a     | 1634 | A    |
| 22  | a     | 1647 | U    |
| 22  | a     | 1648 | U    |
| 22  | a     | 1649 | G    |
| 22  | a     | 1674 | G    |
| 22  | a     | 1675 | C    |
| 22  | a     | 1715 | G    |
| 22  | a     | 1730 | C    |
| 22  | a     | 1733 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 1738 | G    |
| 22  | a     | 1744 | A    |
| 22  | a     | 1756 | G    |
| 22  | a     | 1757 | A    |
| 22  | a     | 1758 | U    |
| 22  | a     | 1764 | C    |
| 22  | a     | 1773 | A    |
| 22  | a     | 1782 | U    |
| 22  | a     | 1800 | C    |
| 22  | a     | 1801 | A    |
| 22  | a     | 1808 | A    |
| 22  | a     | 1816 | C    |
| 22  | a     | 1829 | A    |
| 22  | a     | 1848 | A    |
| 22  | a     | 1858 | A    |
| 22  | a     | 1906 | G    |
| 22  | a     | 1913 | A    |
| 22  | a     | 1915 | 3TD  |
| 22  | a     | 1929 | G    |
| 22  | a     | 1930 | G    |
| 22  | a     | 1937 | A    |
| 22  | a     | 1938 | A    |
| 22  | a     | 1955 | U    |
| 22  | a     | 1966 | A    |
| 22  | a     | 1967 | C    |
| 22  | a     | 1970 | A    |
| 22  | a     | 1971 | U    |
| 22  | a     | 1972 | G    |
| 22  | a     | 1991 | U    |
| 22  | a     | 1993 | U    |
| 22  | a     | 2023 | C    |
| 22  | a     | 2030 | 6MZ  |
| 22  | a     | 2031 | A    |
| 22  | a     | 2032 | G    |
| 22  | a     | 2033 | A    |
| 22  | a     | 2043 | C    |
| 22  | a     | 2055 | C    |
| 22  | a     | 2056 | G    |
| 22  | a     | 2060 | A    |
| 22  | a     | 2061 | G    |
| 22  | a     | 2062 | A    |
| 22  | a     | 2069 | G7M  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 2093 | G    |
| 22  | a     | 2198 | A    |
| 22  | a     | 2204 | G    |
| 22  | a     | 2211 | A    |
| 22  | a     | 2212 | A    |
| 22  | a     | 2225 | A    |
| 22  | a     | 2238 | G    |
| 22  | a     | 2239 | G    |
| 22  | a     | 2279 | G    |
| 22  | a     | 2283 | C    |
| 22  | a     | 2287 | A    |
| 22  | a     | 2305 | U    |
| 22  | a     | 2308 | G    |
| 22  | a     | 2319 | G    |
| 22  | a     | 2322 | A    |
| 22  | a     | 2325 | G    |
| 22  | a     | 2333 | A    |
| 22  | a     | 2336 | A    |
| 22  | a     | 2345 | G    |
| 22  | a     | 2347 | C    |
| 22  | a     | 2350 | C    |
| 22  | a     | 2361 | G    |
| 22  | a     | 2377 | A    |
| 22  | a     | 2383 | G    |
| 22  | a     | 2385 | C    |
| 22  | a     | 2396 | G    |
| 22  | a     | 2402 | U    |
| 22  | a     | 2403 | C    |
| 22  | a     | 2424 | C    |
| 22  | a     | 2425 | A    |
| 22  | a     | 2426 | A    |
| 22  | a     | 2429 | G    |
| 22  | a     | 2430 | A    |
| 22  | a     | 2435 | A    |
| 22  | a     | 2441 | U    |
| 22  | a     | 2448 | A    |
| 22  | a     | 2475 | C    |
| 22  | a     | 2476 | A    |
| 22  | a     | 2491 | U    |
| 22  | a     | 2502 | G    |
| 22  | a     | 2505 | G    |
| 22  | a     | 2518 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 2529 | G    |
| 22  | a     | 2547 | A    |
| 22  | a     | 2566 | A    |
| 22  | a     | 2567 | G    |
| 22  | a     | 2585 | U    |
| 22  | a     | 2586 | U    |
| 22  | a     | 2602 | A    |
| 22  | a     | 2609 | U    |
| 22  | a     | 2613 | U    |
| 22  | a     | 2615 | U    |
| 22  | a     | 2629 | U    |
| 22  | a     | 2638 | G    |
| 22  | a     | 2689 | U    |
| 22  | a     | 2690 | U    |
| 22  | a     | 2714 | G    |
| 22  | a     | 2726 | A    |
| 22  | a     | 2733 | A    |
| 22  | a     | 2744 | G    |
| 22  | a     | 2748 | A    |
| 22  | a     | 2757 | A    |
| 22  | a     | 2778 | A    |
| 22  | a     | 2780 | G    |
| 22  | a     | 2791 | G    |
| 22  | a     | 2797 | U    |
| 22  | a     | 2818 | U    |
| 22  | a     | 2820 | A    |
| 22  | a     | 2821 | A    |
| 22  | a     | 2849 | U    |
| 22  | a     | 2872 | A    |
| 22  | a     | 2873 | A    |
| 22  | a     | 2880 | C    |
| 22  | a     | 2884 | U    |
| 22  | a     | 2891 | U    |
| 22  | a     | 2895 | G    |
| 22  | a     | 2900 | A    |
| 23  | b     | 13   | G    |
| 23  | b     | 24   | G    |
| 23  | b     | 35   | C    |
| 23  | b     | 36   | C    |
| 23  | b     | 45   | A    |
| 23  | b     | 53   | A    |
| 23  | b     | 56   | G    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 23  | b     | 58    | A    |
| 23  | b     | 67    | G    |
| 23  | b     | 89    | U    |
| 23  | b     | 90    | C    |
| 23  | b     | 99    | A    |
| 23  | b     | 109   | A    |
| 53  | V     | 9     | C    |
| 53  | V     | 12    | C    |
| 53  | V     | 13    | PSU  |
| 53  | V     | 14    | A    |
| 53  | V     | 16    | A    |
| 53  | V     | 17    | G    |
| 53  | V     | 18    | G    |
| 53  | V     | 20    | C    |
| 53  | V     | 22    | A    |
| 53  | V     | 23    | G    |
| 53  | V     | 38    | 2MA  |
| 53  | V     | 48    | C    |
| 53  | V     | 49    | A    |
| 53  | V     | 52    | G    |
| 53  | V     | 53    | G    |
| 53  | V     | 54    | 5MU  |
| 53  | V     | 55    | PSU  |
| 53  | V     | 56    | C    |
| 53  | V     | 57    | G    |
| 53  | V     | 67    | G    |
| 54  | W     | 31    | A    |
| 54  | W     | 35    | A    |
| 55  | X     | 3     | C    |
| 55  | X     | 8     | 4SU  |
| 55  | X     | 9     | A    |
| 55  | X     | 13    | C    |
| 55  | X     | 16    | U    |
| 55  | X     | 18    | OMG  |
| 55  | X     | 19    | G    |
| 55  | X     | 20    | H2U  |
| 55  | X     | 20(A) | H2U  |
| 55  | X     | 21    | A    |
| 55  | X     | 46    | G7M  |
| 55  | X     | 47    | 3AU  |
| 55  | X     | 48    | C    |
| 55  | X     | 49    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | X     | 55  | PSU  |
| 55  | X     | 63  | A    |
| 55  | X     | 74  | C    |
| 55  | X     | 75  | C    |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 519  | C    |
| 1   | A     | 1026 | G    |
| 1   | A     | 1035 | A    |
| 53  | V     | 47   | A    |
| 54  | W     | 30   | G    |

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

55 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$ |
| 22  | 2MA  | a     | 2503 | 56,22 | 22,25,26     | 3.88 | 8 (36%)     | 33,37,40    | 2.84 | 8 (24%)     |
| 22  | PSU  | a     | 2605 | 22    | 18,21,22     | 3.85 | 6 (33%)     | 22,30,33    | 1.84 | 5 (22%)     |
| 22  | 6MZ  | a     | 2030 | 22    | 22,25,26     | 2.75 | 4 (18%)     | 30,36,39    | 2.34 | 11 (36%)    |
| 53  | U8U  | V     | 35   | 54,53 | 19,24,25     | 2.63 | 6 (31%)     | 23,34,37    | 1.28 | 3 (13%)     |
| 1   | PSU  | A     | 516  | 1,56  | 18,21,22     | 3.93 | 7 (38%)     | 22,30,33    | 1.85 | 6 (27%)     |
| 1   | 5MC  | A     | 967  | 1     | 18,22,23     | 3.84 | 8 (44%)     | 26,32,35    | 0.99 | 1 (3%)      |
| 55  | G7M  | X     | 46   | 55    | 23,26,27     | 2.83 | 9 (39%)     | 35,39,42    | 1.74 | 9 (25%)     |
| 25  | MEQ  | d     | 150  | 25    | 8,9,10       | 0.86 | 0           | 5,10,12     | 1.53 | 2 (40%)     |
| 55  | 5MU  | X     | 54   | 55    | 19,22,23     | 4.72 | 6 (31%)     | 28,32,35    | 3.83 | 12 (42%)    |
| 22  | 5MU  | a     | 747  | 22    | 19,22,23     | 4.74 | 6 (31%)     | 28,32,35    | 3.62 | 9 (32%)     |
| 55  | H2U  | X     | 20   | 55    | 18,21,22     | 1.07 | 2 (11%)     | 21,30,33    | 1.61 | 2 (9%)      |
| 22  | PSU  | a     | 2457 | 22    | 18,21,22     | 3.88 | 6 (33%)     | 22,30,33    | 1.91 | 6 (27%)     |

| Mol | Type | Chain | Res   | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |       |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | G7M  | A     | 527   | 1     | 23,26,27     | 2.83 | 9 (39%)  | 35,39,42    | 1.71 | 7 (20%)  |
| 53  | PSU  | V     | 55    | 53    | 18,21,22     | 3.97 | 5 (27%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 22  | PSU  | a     | 2504  | 22    | 18,21,22     | 3.92 | 5 (27%)  | 22,30,33    | 1.76 | 5 (22%)  |
| 55  | 3AU  | X     | 47    | 55    | 24,28,29     | 2.73 | 9 (37%)  | 33,40,43    | 1.33 | 2 (6%)   |
| 12  | D2T  | L     | 89    | 12    | 7,9,10       | 1.56 | 1 (14%)  | 6,11,13     | 2.12 | 3 (50%)  |
| 1   | 2MG  | A     | 1516  | 1     | 23,26,27     | 2.64 | 8 (34%)  | 32,38,41    | 2.12 | 10 (31%) |
| 33  | 4D4  | l     | 81    | 33    | 9,11,12      | 1.46 | 1 (11%)  | 8,13,15     | 2.02 | 3 (37%)  |
| 55  | 4SU  | X     | 8     | 55    | 18,21,22     | 3.75 | 8 (44%)  | 26,30,33    | 2.26 | 4 (15%)  |
| 1   | MA6  | A     | 1519  | 1     | 23,26,27     | 1.25 | 4 (17%)  | 34,38,41    | 2.29 | 11 (32%) |
| 22  | 3TD  | a     | 1915  | 22    | 19,22,23     | 4.04 | 6 (31%)  | 21,32,35    | 1.77 | 3 (14%)  |
| 22  | 2MG  | a     | 2445  | 22    | 23,26,27     | 2.65 | 7 (30%)  | 32,38,41    | 2.18 | 10 (31%) |
| 22  | OMG  | a     | 2251  | 22,53 | 23,26,27     | 2.62 | 8 (34%)  | 33,38,41    | 1.92 | 9 (27%)  |
| 22  | PSU  | a     | 955   | 22    | 18,21,22     | 3.93 | 6 (33%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 33  | MS6  | l     | 82    | 33    | 5,7,8        | 1.97 | 1 (20%)  | 2,7,9       | 2.15 | 1 (50%)  |
| 55  | OMG  | X     | 18    | 55    | 23,26,27     | 2.62 | 8 (34%)  | 33,38,41    | 1.94 | 10 (30%) |
| 55  | M3X  | X     | 34    | 55,54 | 24,30,31     | 2.02 | 3 (12%)  | 26,41,44    | 1.18 | 3 (11%)  |
| 22  | PSU  | a     | 746   | 56,22 | 18,21,22     | 3.92 | 6 (33%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 53  | PSU  | V     | 13    | 53    | 18,21,22     | 3.98 | 7 (38%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 53  | 5MU  | V     | 54    | 53    | 19,22,23     | 4.76 | 5 (26%)  | 28,32,35    | 3.57 | 9 (32%)  |
| 22  | 5MC  | a     | 1962  | 22    | 18,22,23     | 3.81 | 8 (44%)  | 26,32,35    | 1.01 | 2 (7%)   |
| 55  | PSU  | X     | 39    | 55    | 18,21,22     | 3.92 | 6 (33%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 22  | OMU  | a     | 2552  | 22    | 19,22,23     | 2.90 | 8 (42%)  | 26,31,34    | 1.73 | 5 (19%)  |
| 1   | 5MC  | A     | 1407  | 1     | 18,22,23     | 3.81 | 8 (44%)  | 26,32,35    | 1.00 | 2 (7%)   |
| 22  | PSU  | a     | 2604  | 22    | 18,21,22     | 3.89 | 6 (33%)  | 22,30,33    | 1.77 | 5 (22%)  |
| 22  | OMC  | a     | 2498  | 56,22 | 19,22,23     | 2.98 | 8 (42%)  | 26,31,34    | 0.80 | 0        |
| 55  | H2U  | X     | 20(A) | 55    | 18,21,22     | 1.03 | 2 (11%)  | 21,30,33    | 1.03 | 2 (9%)   |
| 22  | 1MG  | a     | 745   | 22    | 22,26,27     | 2.63 | 7 (31%)  | 33,39,42    | 1.69 | 7 (21%)  |
| 22  | G7M  | a     | 2069  | 22    | 23,26,27     | 2.80 | 9 (39%)  | 35,39,42    | 1.73 | 9 (25%)  |
| 55  | PSU  | X     | 55    | 55    | 18,21,22     | 3.99 | 6 (33%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 11  | IAS  | K     | 119   | 11    | 6,7,8        | 1.06 | 0        | 6,8,10      | 1.30 | 0        |
| 53  | 2MA  | V     | 38    | 53    | 22,25,26     | 3.89 | 8 (36%)  | 33,37,40    | 2.83 | 8 (24%)  |
| 1   | MA6  | A     | 1518  | 1     | 23,26,27     | 1.24 | 4 (17%)  | 34,38,41    | 2.28 | 11 (32%) |
| 1   | 2MG  | A     | 966   | 1     | 23,26,27     | 2.67 | 7 (30%)  | 32,38,41    | 2.20 | 9 (28%)  |
| 1   | UR3  | A     | 1498  | 1     | 19,22,23     | 2.79 | 8 (42%)  | 26,32,35    | 1.33 | 2 (7%)   |
| 22  | 5MU  | a     | 1939  | 22    | 19,22,23     | 4.71 | 6 (31%)  | 28,32,35    | 3.64 | 9 (32%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 4OC  | A     | 1402 | 1,56 | 20,23,24     | 3.13 | 8 (40%)  | 26,32,35    | 0.91 | 1 (3%)   |
| 1   | 2MG  | A     | 1207 | 1    | 23,26,27     | 2.67 | 7 (30%)  | 32,38,41    | 2.13 | 9 (28%)  |
| 22  | PSU  | a     | 1917 | 22   | 18,21,22     | 3.91 | 6 (33%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 22  | PSU  | a     | 2580 | 22   | 18,21,22     | 3.89 | 7 (38%)  | 22,30,33    | 1.89 | 6 (27%)  |
| 22  | H2U  | a     | 2449 | 22   | 18,21,22     | 1.06 | 2 (11%)  | 21,30,33    | 0.87 | 0        |
| 22  | 6MZ  | a     | 1618 | 22   | 22,25,26     | 2.75 | 4 (18%)  | 30,36,39    | 2.32 | 10 (33%) |
| 22  | 2MG  | a     | 1835 | 22   | 23,26,27     | 2.64 | 7 (30%)  | 32,38,41    | 2.19 | 9 (28%)  |
| 22  | PSU  | a     | 1911 | 22   | 18,21,22     | 3.92 | 6 (33%)  | 22,30,33    | 1.80 | 5 (22%)  |

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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 22  | 2MA  | a     | 2503 | 56,22 | -       | 2/7/25/26  | 0/3/3/3 |
| 22  | PSU  | a     | 2605 | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 6MZ  | a     | 2030 | 22    | -       | 2/9/27/28  | 0/3/3/3 |
| 53  | U8U  | V     | 35   | 54,53 | -       | 1/9/28/29  | 0/2/2/2 |
| 1   | PSU  | A     | 516  | 1,56  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 967  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | G7M  | X     | 46   | 55    | -       | 3/7/25/26  | 0/3/3/3 |
| 25  | MEQ  | d     | 150  | 25    | -       | 2/8/9/11   | -       |
| 55  | 5MU  | X     | 54   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 5MU  | a     | 747  | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | H2U  | X     | 20   | 55    | -       | 1/7/38/39  | 0/2/2/2 |
| 22  | PSU  | a     | 2457 | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | G7M  | A     | 527  | 1     | -       | 2/7/25/26  | 0/3/3/3 |
| 53  | PSU  | V     | 55   | 53    | -       | 2/7/25/26  | 0/2/2/2 |
| 22  | PSU  | a     | 2504 | 22    | -       | 2/7/25/26  | 0/2/2/2 |
| 55  | 3AU  | X     | 47   | 55    | -       | 5/16/34/35 | 0/2/2/2 |
| 12  | D2T  | L     | 89   | 12    | -       | 1/7/12/14  | -       |
| 1   | 2MG  | A     | 1516 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 33  | 4D4  | l     | 81   | 33    | -       | 2/11/12/14 | -       |
| 55  | 4SU  | X     | 8    | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | A     | 1519 | 1     | -       | 3/11/29/30 | 0/3/3/3 |
| 22  | 3TD  | a     | 1915 | 22    | -       | 2/7/25/26  | 0/2/2/2 |
| 22  | 2MG  | a     | 2445 | 22    | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res   | Link  | Chirals | Torsions    | Rings   |
|-----|------|-------|-------|-------|---------|-------------|---------|
| 22  | OMG  | a     | 2251  | 22,53 | -       | 1/9/27/28   | 0/3/3/3 |
| 22  | PSU  | a     | 955   | 22    | -       | 0/7/25/26   | 0/2/2/2 |
| 33  | MS6  | l     | 82    | 33    | -       | 1/4/6/8     | -       |
| 55  | OMG  | X     | 18    | 55    | -       | 3/9/27/28   | 0/3/3/3 |
| 55  | M3X  | X     | 34    | 55,54 | -       | 12/17/37/38 | 0/2/2/2 |
| 22  | PSU  | a     | 746   | 56,22 | -       | 1/7/25/26   | 0/2/2/2 |
| 53  | PSU  | V     | 13    | 53    | -       | 3/7/25/26   | 0/2/2/2 |
| 53  | 5MU  | V     | 54    | 53    | -       | 2/7/25/26   | 0/2/2/2 |
| 22  | 5MC  | a     | 1962  | 22    | -       | 0/7/25/26   | 0/2/2/2 |
| 55  | PSU  | X     | 39    | 55    | -       | 0/7/25/26   | 0/2/2/2 |
| 22  | OMU  | a     | 2552  | 22    | -       | 0/9/27/28   | 0/2/2/2 |
| 1   | 5MC  | A     | 1407  | 1     | -       | 0/7/25/26   | 0/2/2/2 |
| 22  | PSU  | a     | 2604  | 22    | -       | 0/7/25/26   | 0/2/2/2 |
| 22  | OMC  | a     | 2498  | 56,22 | -       | 0/9/27/28   | 0/2/2/2 |
| 55  | H2U  | X     | 20(A) | 55    | -       | 4/7/38/39   | 0/2/2/2 |
| 22  | 1MG  | a     | 745   | 22    | -       | 0/7/25/26   | 0/3/3/3 |
| 22  | G7M  | a     | 2069  | 22    | -       | 1/7/25/26   | 0/3/3/3 |
| 55  | PSU  | X     | 55    | 55    | -       | 2/7/25/26   | 0/2/2/2 |
| 11  | IAS  | K     | 119   | 11    | -       | 1/7/7/8     | -       |
| 53  | 2MA  | V     | 38    | 53    | -       | 0/7/25/26   | 0/3/3/3 |
| 1   | MA6  | A     | 1518  | 1     | -       | 0/11/29/30  | 0/3/3/3 |
| 1   | 2MG  | A     | 966   | 1     | -       | 1/9/27/28   | 0/3/3/3 |
| 1   | UR3  | A     | 1498  | 1     | -       | 0/7/25/26   | 0/2/2/2 |
| 22  | 5MU  | a     | 1939  | 22    | -       | 0/7/25/26   | 0/2/2/2 |
| 1   | 4OC  | A     | 1402  | 1,56  | -       | 2/9/29/30   | 0/2/2/2 |
| 1   | 2MG  | A     | 1207  | 1     | -       | 0/9/27/28   | 0/3/3/3 |
| 22  | PSU  | a     | 1917  | 22    | -       | 0/7/25/26   | 0/2/2/2 |
| 22  | PSU  | a     | 2580  | 22    | -       | 0/7/25/26   | 0/2/2/2 |
| 22  | H2U  | a     | 2449  | 22    | -       | 0/7/38/39   | 0/2/2/2 |
| 22  | 6MZ  | a     | 1618  | 22    | -       | 1/9/27/28   | 0/3/3/3 |
| 22  | 2MG  | a     | 1835  | 22    | -       | 0/9/27/28   | 0/3/3/3 |
| 22  | PSU  | a     | 1911  | 22    | -       | 0/7/25/26   | 0/2/2/2 |

All (323) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | a     | 1915 | 3TD  | C6-C5 | 12.46 | 1.49        | 1.35     |
| 22  | a     | 2503 | 2MA  | C4-N3 | 12.09 | 1.49        | 1.34     |
| 53  | V     | 38   | 2MA  | C4-N3 | 11.91 | 1.49        | 1.34     |
| 22  | a     | 1618 | 6MZ  | C6-N6 | 11.83 | 1.47        | 1.34     |
| 22  | a     | 2030 | 6MZ  | C6-N6 | 11.80 | 1.47        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 55  | X     | 54   | 5MU  | C2-N1 | 11.28 | 1.56        | 1.38     |
| 53  | V     | 54   | 5MU  | C6-N1 | 10.96 | 1.56        | 1.38     |
| 53  | V     | 54   | 5MU  | C2-N1 | 10.90 | 1.55        | 1.38     |
| 22  | a     | 747  | 5MU  | C2-N1 | 10.85 | 1.55        | 1.38     |
| 22  | a     | 747  | 5MU  | C6-N1 | 10.76 | 1.56        | 1.38     |
| 22  | a     | 1939 | 5MU  | C6-N1 | 10.76 | 1.56        | 1.38     |
| 22  | a     | 1939 | 5MU  | C2-N1 | 10.61 | 1.55        | 1.38     |
| 55  | X     | 54   | 5MU  | C6-N1 | 10.29 | 1.55        | 1.38     |
| 55  | X     | 55   | PSU  | C6-C5 | 9.99  | 1.47        | 1.35     |
| 53  | V     | 55   | PSU  | C6-C5 | 9.82  | 1.46        | 1.35     |
| 53  | V     | 13   | PSU  | C6-C5 | 9.77  | 1.46        | 1.35     |
| 22  | a     | 2504 | PSU  | C6-C5 | 9.70  | 1.46        | 1.35     |
| 1   | A     | 516  | PSU  | C6-C5 | 9.67  | 1.46        | 1.35     |
| 55  | X     | 39   | PSU  | C6-C5 | 9.65  | 1.46        | 1.35     |
| 22  | a     | 746  | PSU  | C6-C5 | 9.64  | 1.46        | 1.35     |
| 22  | a     | 955  | PSU  | C6-C5 | 9.63  | 1.46        | 1.35     |
| 22  | a     | 2604 | PSU  | C6-C5 | 9.63  | 1.46        | 1.35     |
| 22  | a     | 1917 | PSU  | C6-C5 | 9.59  | 1.46        | 1.35     |
| 22  | a     | 1911 | PSU  | C6-C5 | 9.57  | 1.46        | 1.35     |
| 22  | a     | 1962 | 5MC  | C6-C5 | 9.56  | 1.50        | 1.34     |
| 22  | a     | 2580 | PSU  | C6-C5 | 9.56  | 1.46        | 1.35     |
| 1   | A     | 967  | 5MC  | C6-C5 | 9.56  | 1.50        | 1.34     |
| 22  | a     | 2457 | PSU  | C6-C5 | 9.55  | 1.46        | 1.35     |
| 1   | A     | 1407 | 5MC  | C6-C5 | 9.53  | 1.50        | 1.34     |
| 55  | X     | 54   | 5MU  | C4-C5 | 9.53  | 1.60        | 1.44     |
| 55  | X     | 55   | PSU  | C2-N1 | 9.52  | 1.49        | 1.36     |
| 53  | V     | 13   | PSU  | C2-N1 | 9.52  | 1.49        | 1.36     |
| 22  | a     | 2605 | PSU  | C2-N1 | 9.36  | 1.49        | 1.36     |
| 22  | a     | 746  | PSU  | C2-N1 | 9.35  | 1.49        | 1.36     |
| 22  | a     | 1911 | PSU  | C2-N1 | 9.34  | 1.49        | 1.36     |
| 22  | a     | 1917 | PSU  | C2-N1 | 9.34  | 1.49        | 1.36     |
| 55  | X     | 39   | PSU  | C2-N1 | 9.33  | 1.49        | 1.36     |
| 22  | a     | 955  | PSU  | C2-N1 | 9.32  | 1.49        | 1.36     |
| 22  | a     | 747  | 5MU  | C4-C5 | 9.32  | 1.60        | 1.44     |
| 53  | V     | 55   | PSU  | C2-N1 | 9.32  | 1.49        | 1.36     |
| 22  | a     | 2604 | PSU  | C2-N1 | 9.31  | 1.49        | 1.36     |
| 22  | a     | 2504 | PSU  | C2-N1 | 9.30  | 1.49        | 1.36     |
| 53  | V     | 54   | 5MU  | C4-C5 | 9.29  | 1.60        | 1.44     |
| 22  | a     | 2605 | PSU  | C6-C5 | 9.25  | 1.46        | 1.35     |
| 1   | A     | 516  | PSU  | C2-N1 | 9.23  | 1.49        | 1.36     |
| 22  | a     | 1939 | 5MU  | C4-C5 | 9.19  | 1.60        | 1.44     |
| 22  | a     | 2457 | PSU  | C2-N1 | 9.18  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | a     | 2580 | PSU  | C2-N1 | 9.14  | 1.49        | 1.36     |
| 22  | a     | 1915 | 3TD  | C2-N1 | 8.88  | 1.48        | 1.37     |
| 55  | X     | 8    | 4SU  | C4-N3 | 8.31  | 1.46        | 1.37     |
| 55  | X     | 34   | M3X  | C2-N2 | 8.25  | 1.45        | 1.33     |
| 22  | a     | 1835 | 2MG  | C2-N3 | 7.74  | 1.46        | 1.31     |
| 1   | A     | 1207 | 2MG  | C2-N3 | 7.73  | 1.46        | 1.31     |
| 1   | A     | 966  | 2MG  | C2-N3 | 7.73  | 1.46        | 1.31     |
| 22  | a     | 2445 | 2MG  | C2-N3 | 7.66  | 1.46        | 1.31     |
| 1   | A     | 1516 | 2MG  | C2-N3 | 7.51  | 1.46        | 1.31     |
| 22  | a     | 1939 | 5MU  | C4-N3 | -7.41 | 1.25        | 1.38     |
| 1   | A     | 967  | 5MC  | C4-N3 | 7.38  | 1.46        | 1.34     |
| 22  | a     | 1962 | 5MC  | C4-N3 | 7.35  | 1.46        | 1.34     |
| 55  | X     | 18   | OMG  | C4-N3 | 7.35  | 1.51        | 1.34     |
| 53  | V     | 38   | 2MA  | C2-N3 | 7.32  | 1.47        | 1.34     |
| 22  | a     | 2251 | OMG  | C4-N3 | 7.32  | 1.51        | 1.34     |
| 22  | a     | 747  | 5MU  | C4-N3 | -7.28 | 1.25        | 1.38     |
| 22  | a     | 2503 | 2MA  | C2-N3 | 7.25  | 1.46        | 1.34     |
| 1   | A     | 1407 | 5MC  | C4-N3 | 7.24  | 1.46        | 1.34     |
| 55  | X     | 54   | 5MU  | C4-N3 | -7.19 | 1.25        | 1.38     |
| 1   | A     | 1498 | UR3  | C2-N1 | 7.19  | 1.48        | 1.38     |
| 53  | V     | 54   | 5MU  | C4-N3 | -7.18 | 1.25        | 1.38     |
| 53  | V     | 55   | PSU  | C2-N3 | 7.03  | 1.49        | 1.37     |
| 22  | a     | 2552 | OMU  | C2-N1 | 7.00  | 1.49        | 1.38     |
| 1   | A     | 516  | PSU  | C2-N3 | 6.94  | 1.49        | 1.37     |
| 1   | A     | 1402 | 4OC  | C4-N3 | 6.93  | 1.44        | 1.32     |
| 22  | a     | 2504 | PSU  | C2-N3 | 6.92  | 1.49        | 1.37     |
| 53  | V     | 13   | PSU  | C2-N3 | 6.91  | 1.49        | 1.37     |
| 22  | a     | 1911 | PSU  | C2-N3 | 6.89  | 1.49        | 1.37     |
| 22  | a     | 955  | PSU  | C2-N3 | 6.87  | 1.49        | 1.37     |
| 22  | a     | 2580 | PSU  | C2-N3 | 6.87  | 1.49        | 1.37     |
| 22  | a     | 1917 | PSU  | C2-N3 | 6.86  | 1.49        | 1.37     |
| 22  | a     | 2457 | PSU  | C2-N3 | 6.86  | 1.49        | 1.37     |
| 55  | X     | 39   | PSU  | C2-N3 | 6.85  | 1.49        | 1.37     |
| 55  | X     | 55   | PSU  | C2-N3 | 6.79  | 1.49        | 1.37     |
| 55  | X     | 8    | 4SU  | C2-N3 | 6.79  | 1.50        | 1.38     |
| 22  | a     | 746  | PSU  | C2-N3 | 6.73  | 1.49        | 1.37     |
| 22  | a     | 2604 | PSU  | C2-N3 | 6.70  | 1.49        | 1.37     |
| 22  | a     | 2605 | PSU  | C2-N3 | 6.69  | 1.49        | 1.37     |
| 22  | a     | 1939 | 5MU  | C6-C5 | 6.69  | 1.45        | 1.34     |
| 53  | V     | 54   | 5MU  | C6-C5 | 6.68  | 1.45        | 1.34     |
| 22  | a     | 747  | 5MU  | C6-C5 | 6.63  | 1.45        | 1.34     |
| 1   | A     | 1207 | 2MG  | C4-N3 | 6.63  | 1.50        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | A     | 966  | 2MG  | C4-N3 | 6.62 | 1.50        | 1.34     |
| 1   | A     | 967  | 5MC  | C2-N3 | 6.61 | 1.49        | 1.36     |
| 53  | V     | 38   | 2MA  | C2-N1 | 6.59 | 1.45        | 1.34     |
| 22  | a     | 1835 | 2MG  | C4-N3 | 6.55 | 1.49        | 1.34     |
| 55  | X     | 46   | G7M  | C4-N3 | 6.55 | 1.49        | 1.34     |
| 55  | X     | 46   | G7M  | C2-N2 | 6.55 | 1.49        | 1.34     |
| 1   | A     | 527  | G7M  | C2-N2 | 6.54 | 1.49        | 1.34     |
| 22  | a     | 1962 | 5MC  | C2-N3 | 6.51 | 1.49        | 1.36     |
| 1   | A     | 527  | G7M  | C4-N3 | 6.51 | 1.49        | 1.34     |
| 22  | a     | 2445 | 2MG  | C4-N3 | 6.50 | 1.49        | 1.34     |
| 1   | A     | 1516 | 2MG  | C4-N3 | 6.49 | 1.49        | 1.34     |
| 22  | a     | 2069 | G7M  | C4-N3 | 6.49 | 1.49        | 1.34     |
| 22  | a     | 2069 | G7M  | C2-N2 | 6.49 | 1.49        | 1.34     |
| 1   | A     | 1407 | 5MC  | C2-N3 | 6.49 | 1.49        | 1.36     |
| 55  | X     | 8    | 4SU  | C2-N1 | 6.48 | 1.48        | 1.38     |
| 22  | a     | 2552 | OMU  | C2-N3 | 6.46 | 1.49        | 1.38     |
| 22  | a     | 2503 | 2MA  | C2-N1 | 6.43 | 1.45        | 1.34     |
| 22  | a     | 745  | 1MG  | C2-N3 | 6.31 | 1.45        | 1.34     |
| 22  | a     | 745  | 1MG  | C4-N3 | 6.27 | 1.49        | 1.34     |
| 1   | A     | 1402 | 4OC  | C6-C5 | 6.25 | 1.49        | 1.35     |
| 22  | a     | 2498 | OMC  | C2-N3 | 6.21 | 1.48        | 1.36     |
| 1   | A     | 1498 | UR3  | C6-C5 | 6.17 | 1.49        | 1.35     |
| 22  | a     | 745  | 1MG  | C2-N2 | 6.14 | 1.45        | 1.34     |
| 55  | X     | 47   | 3AU  | C2-N1 | 6.12 | 1.47        | 1.38     |
| 55  | X     | 47   | 3AU  | C2-N3 | 6.07 | 1.49        | 1.38     |
| 55  | X     | 47   | 3AU  | C6-C5 | 6.07 | 1.49        | 1.35     |
| 55  | X     | 54   | 5MU  | C6-C5 | 6.04 | 1.44        | 1.34     |
| 53  | V     | 35   | U8U  | C2-N3 | 5.98 | 1.51        | 1.37     |
| 22  | a     | 2498 | OMC  | C6-C5 | 5.97 | 1.48        | 1.35     |
| 22  | a     | 1915 | 3TD  | C6-N1 | 5.96 | 1.46        | 1.36     |
| 1   | A     | 1402 | 4OC  | C2-N3 | 5.95 | 1.48        | 1.36     |
| 55  | X     | 46   | G7M  | C2-N3 | 5.84 | 1.47        | 1.33     |
| 55  | X     | 8    | 4SU  | C6-C5 | 5.81 | 1.48        | 1.35     |
| 22  | a     | 2552 | OMU  | C6-C5 | 5.80 | 1.48        | 1.35     |
| 1   | A     | 527  | G7M  | C2-N3 | 5.74 | 1.47        | 1.33     |
| 22  | a     | 2069 | G7M  | C2-N3 | 5.65 | 1.46        | 1.33     |
| 55  | X     | 18   | OMG  | C2-N3 | 5.55 | 1.46        | 1.33     |
| 22  | a     | 2251 | OMG  | C2-N3 | 5.53 | 1.46        | 1.33     |
| 53  | V     | 35   | U8U  | C6-C5 | 5.43 | 1.50        | 1.34     |
| 22  | a     | 2503 | 2MA  | C5-C6 | 5.41 | 1.56        | 1.41     |
| 53  | V     | 38   | 2MA  | C5-C6 | 5.40 | 1.56        | 1.41     |
| 1   | A     | 967  | 5MC  | C6-N1 | 5.35 | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1407 | 5MC  | C6-N1 | 5.26  | 1.47        | 1.38     |
| 22  | a     | 1962 | 5MC  | C6-N1 | 5.24  | 1.47        | 1.38     |
| 55  | X     | 55   | PSU  | C6-N1 | 5.21  | 1.44        | 1.36     |
| 22  | a     | 1911 | PSU  | C6-N1 | 5.19  | 1.44        | 1.36     |
| 22  | a     | 955  | PSU  | C6-N1 | 5.18  | 1.44        | 1.36     |
| 53  | V     | 13   | PSU  | C6-N1 | 5.18  | 1.44        | 1.36     |
| 1   | A     | 966  | 2MG  | C2-N1 | 5.16  | 1.45        | 1.36     |
| 1   | A     | 1498 | UR3  | C2-N3 | 5.16  | 1.49        | 1.39     |
| 1   | A     | 1207 | 2MG  | C2-N1 | 5.15  | 1.45        | 1.36     |
| 55  | X     | 18   | OMG  | C2-N2 | 5.15  | 1.46        | 1.34     |
| 22  | a     | 2251 | OMG  | C2-N2 | 5.15  | 1.46        | 1.34     |
| 22  | a     | 746  | PSU  | C6-N1 | 5.15  | 1.44        | 1.36     |
| 1   | A     | 1516 | 2MG  | C2-N1 | 5.14  | 1.44        | 1.36     |
| 22  | a     | 2445 | 2MG  | C2-N1 | 5.12  | 1.44        | 1.36     |
| 53  | V     | 55   | PSU  | C6-N1 | 5.12  | 1.44        | 1.36     |
| 55  | X     | 39   | PSU  | C6-N1 | 5.08  | 1.44        | 1.36     |
| 22  | a     | 2605 | PSU  | C6-N1 | 5.07  | 1.44        | 1.36     |
| 1   | A     | 516  | PSU  | C6-N1 | 5.06  | 1.44        | 1.36     |
| 22  | a     | 2504 | PSU  | C6-N1 | 5.04  | 1.44        | 1.36     |
| 22  | a     | 1835 | 2MG  | C2-N1 | 5.02  | 1.44        | 1.36     |
| 22  | a     | 2604 | PSU  | C6-N1 | 5.02  | 1.44        | 1.36     |
| 22  | a     | 2498 | OMC  | C4-N3 | 5.01  | 1.44        | 1.34     |
| 22  | a     | 1917 | PSU  | C6-N1 | 5.00  | 1.44        | 1.36     |
| 22  | a     | 2580 | PSU  | C6-N1 | 4.91  | 1.44        | 1.36     |
| 22  | a     | 2457 | PSU  | C6-N1 | 4.91  | 1.44        | 1.36     |
| 22  | a     | 2498 | OMC  | C4-N4 | 4.89  | 1.45        | 1.33     |
| 22  | a     | 2503 | 2MA  | C6-N6 | -4.87 | 1.21        | 1.34     |
| 53  | V     | 38   | 2MA  | C6-N6 | -4.85 | 1.22        | 1.34     |
| 55  | X     | 8    | 4SU  | C4-S4 | -4.79 | 1.59        | 1.68     |
| 53  | V     | 35   | U8U  | C6-N1 | 4.72  | 1.46        | 1.38     |
| 55  | X     | 8    | 4SU  | C5-C4 | 4.72  | 1.48        | 1.42     |
| 1   | A     | 1402 | 4OC  | C4-N4 | 4.58  | 1.45        | 1.35     |
| 22  | a     | 2498 | OMC  | C2-N1 | 4.46  | 1.49        | 1.40     |
| 22  | a     | 1915 | 3TD  | C2-N3 | 4.38  | 1.48        | 1.38     |
| 53  | V     | 35   | U8U  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 1   | A     | 967  | 5MC  | C2-N1 | 4.35  | 1.49        | 1.40     |
| 1   | A     | 1407 | 5MC  | C2-N1 | 4.32  | 1.49        | 1.40     |
| 22  | a     | 1962 | 5MC  | C2-N1 | 4.19  | 1.49        | 1.40     |
| 1   | A     | 967  | 5MC  | C4-N4 | 4.18  | 1.45        | 1.34     |
| 1   | A     | 527  | G7M  | C5-N7 | -4.14 | 1.34        | 1.39     |
| 33  | l     | 82   | MS6  | CB-CA | 4.14  | 1.59        | 1.53     |
| 1   | A     | 1407 | 5MC  | C4-N4 | 4.11  | 1.44        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | a     | 1962 | 5MC  | C4-N4 | 4.11  | 1.44        | 1.34     |
| 1   | A     | 1402 | 4OC  | C2-N1 | 4.11  | 1.48        | 1.40     |
| 55  | X     | 46   | G7M  | C5-N7 | -4.07 | 1.34        | 1.39     |
| 22  | a     | 2069 | G7M  | C5-N7 | -4.02 | 1.34        | 1.39     |
| 53  | V     | 38   | 2MA  | C6-N1 | 4.00  | 1.40        | 1.35     |
| 1   | A     | 1402 | 4OC  | C5-C4 | 3.95  | 1.49        | 1.40     |
| 1   | A     | 527  | G7M  | C5-C6 | 3.89  | 1.54        | 1.43     |
| 55  | X     | 46   | G7M  | C5-C6 | 3.89  | 1.54        | 1.43     |
| 22  | a     | 2069 | G7M  | C5-C6 | 3.87  | 1.54        | 1.43     |
| 22  | a     | 2503 | 2MA  | C6-N1 | 3.86  | 1.40        | 1.35     |
| 55  | X     | 47   | 3AU  | O2-C2 | -3.69 | 1.15        | 1.22     |
| 55  | X     | 47   | 3AU  | C4-N3 | 3.58  | 1.46        | 1.40     |
| 55  | X     | 47   | 3AU  | C6-N1 | 3.58  | 1.46        | 1.38     |
| 33  | l     | 81   | 4D4  | CZ-NE | 3.53  | 1.40        | 1.33     |
| 55  | X     | 34   | M3X  | C4-N4 | 3.47  | 1.45        | 1.35     |
| 53  | V     | 55   | PSU  | C4-N3 | 3.42  | 1.45        | 1.38     |
| 1   | A     | 516  | PSU  | C4-N3 | 3.41  | 1.45        | 1.38     |
| 22  | a     | 2504 | PSU  | C4-N3 | 3.39  | 1.45        | 1.38     |
| 53  | V     | 13   | PSU  | C4-N3 | 3.39  | 1.45        | 1.38     |
| 22  | a     | 1911 | PSU  | C4-N3 | 3.38  | 1.45        | 1.38     |
| 53  | V     | 35   | U8U  | C2-S2 | -3.38 | 1.62        | 1.67     |
| 22  | a     | 2552 | OMU  | C4-N3 | 3.37  | 1.44        | 1.38     |
| 55  | X     | 39   | PSU  | C4-N3 | 3.37  | 1.45        | 1.38     |
| 22  | a     | 955  | PSU  | C4-N3 | 3.37  | 1.45        | 1.38     |
| 22  | a     | 1917 | PSU  | C4-N3 | 3.36  | 1.45        | 1.38     |
| 22  | a     | 2457 | PSU  | C4-N3 | 3.32  | 1.45        | 1.38     |
| 22  | a     | 2605 | PSU  | C4-N3 | 3.28  | 1.44        | 1.38     |
| 55  | X     | 55   | PSU  | C4-N3 | 3.28  | 1.44        | 1.38     |
| 22  | a     | 2580 | PSU  | C4-N3 | 3.26  | 1.44        | 1.38     |
| 22  | a     | 2604 | PSU  | C4-N3 | 3.25  | 1.44        | 1.38     |
| 55  | X     | 8    | 4SU  | C6-N1 | 3.19  | 1.45        | 1.38     |
| 22  | a     | 745  | 1MG  | C5-C6 | 3.18  | 1.53        | 1.45     |
| 22  | a     | 746  | PSU  | C4-N3 | 3.18  | 1.44        | 1.38     |
| 1   | A     | 1402 | 4OC  | C6-N1 | 3.17  | 1.45        | 1.38     |
| 22  | a     | 2498 | OMC  | C6-N1 | 3.14  | 1.45        | 1.38     |
| 55  | X     | 46   | G7M  | C2-N1 | 3.08  | 1.45        | 1.37     |
| 53  | V     | 35   | U8U  | C4-C5 | 3.07  | 1.51        | 1.45     |
| 1   | A     | 527  | G7M  | C2-N1 | 3.07  | 1.45        | 1.37     |
| 1   | A     | 1518 | MA6  | C6-N6 | 3.06  | 1.45        | 1.36     |
| 55  | X     | 46   | G7M  | C6-N1 | 3.06  | 1.44        | 1.38     |
| 1   | A     | 527  | G7M  | C6-N1 | 3.05  | 1.44        | 1.38     |
| 1   | A     | 1519 | MA6  | C6-N6 | 3.04  | 1.45        | 1.36     |

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| Mol | Chain | Res   | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 22  | a     | 2069  | G7M  | C6-N1   | 3.03  | 1.44        | 1.38     |
| 1   | A     | 1498  | UR3  | C6-N1   | 3.03  | 1.45        | 1.38     |
| 22  | a     | 2069  | G7M  | C2-N1   | 3.01  | 1.45        | 1.37     |
| 55  | X     | 47    | 3AU  | C11-C10 | 3.01  | 1.59        | 1.52     |
| 22  | a     | 745   | 1MG  | C5-N7   | -2.99 | 1.33        | 1.39     |
| 1   | A     | 1207  | 2MG  | C5-N7   | -2.98 | 1.33        | 1.39     |
| 22  | a     | 2503  | 2MA  | C5-N7   | -2.95 | 1.33        | 1.39     |
| 22  | a     | 2251  | OMG  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 55  | X     | 18    | OMG  | C5-C6   | 2.94  | 1.55        | 1.44     |
| 53  | V     | 38    | 2MA  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 22  | a     | 1835  | 2MG  | C5-N7   | -2.92 | 1.33        | 1.39     |
| 1   | A     | 966   | 2MG  | C5-N7   | -2.89 | 1.33        | 1.39     |
| 22  | a     | 2251  | OMG  | C5-C6   | 2.88  | 1.55        | 1.44     |
| 55  | X     | 20    | H2U  | C2-N3   | -2.86 | 1.32        | 1.38     |
| 22  | a     | 2445  | 2MG  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 1   | A     | 1516  | 2MG  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 1   | A     | 1402  | 4OC  | O2-C2   | -2.82 | 1.18        | 1.23     |
| 22  | a     | 2449  | H2U  | C2-N3   | -2.80 | 1.33        | 1.38     |
| 55  | X     | 18    | OMG  | C6-N1   | 2.76  | 1.44        | 1.38     |
| 22  | a     | 1915  | 3TD  | C4-N3   | 2.74  | 1.46        | 1.40     |
| 22  | a     | 2449  | H2U  | C4-N3   | -2.74 | 1.32        | 1.37     |
| 1   | A     | 1519  | MA6  | C5-C4   | -2.74 | 1.33        | 1.39     |
| 22  | a     | 2251  | OMG  | O6-C6   | -2.73 | 1.18        | 1.23     |
| 55  | X     | 20(A) | H2U  | C2-N3   | -2.72 | 1.33        | 1.38     |
| 22  | a     | 2552  | OMU  | O2-C2   | -2.71 | 1.18        | 1.23     |
| 22  | a     | 2498  | OMC  | O2-C2   | -2.70 | 1.18        | 1.23     |
| 22  | a     | 2445  | 2MG  | C5-C6   | 2.69  | 1.54        | 1.44     |
| 22  | a     | 2552  | OMU  | O4-C4   | -2.68 | 1.19        | 1.24     |
| 1   | A     | 1207  | 2MG  | C5-C6   | 2.68  | 1.54        | 1.44     |
| 55  | X     | 18    | OMG  | C5-N7   | -2.68 | 1.33        | 1.39     |
| 1   | A     | 1516  | 2MG  | C5-C6   | 2.67  | 1.54        | 1.44     |
| 1   | A     | 966   | 2MG  | C5-C6   | 2.66  | 1.54        | 1.44     |
| 55  | X     | 20    | H2U  | C4-N3   | -2.65 | 1.33        | 1.37     |
| 22  | a     | 1835  | 2MG  | C5-C6   | 2.63  | 1.54        | 1.44     |
| 1   | A     | 1518  | MA6  | C5-C4   | -2.62 | 1.34        | 1.39     |
| 55  | X     | 18    | OMG  | O6-C6   | -2.62 | 1.18        | 1.23     |
| 55  | X     | 18    | OMG  | C2-N1   | 2.61  | 1.44        | 1.37     |
| 22  | a     | 2251  | OMG  | C6-N1   | 2.61  | 1.43        | 1.38     |
| 55  | X     | 20(A) | H2U  | C4-N3   | -2.60 | 1.33        | 1.37     |
| 22  | a     | 2251  | OMG  | C2-N1   | 2.54  | 1.43        | 1.37     |
| 1   | A     | 527   | G7M  | O6-C6   | -2.53 | 1.18        | 1.23     |
| 55  | X     | 34    | M3X  | C6-N1   | -2.53 | 1.32        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 966  | 2MG  | C6-N1   | 2.49  | 1.43        | 1.38     |
| 22  | a     | 1618 | 6MZ  | C5-C4   | -2.47 | 1.34        | 1.39     |
| 22  | a     | 2030 | 6MZ  | C5-C4   | -2.46 | 1.34        | 1.39     |
| 55  | X     | 46   | G7M  | O6-C6   | -2.45 | 1.18        | 1.23     |
| 22  | a     | 2069 | G7M  | O6-C6   | -2.45 | 1.18        | 1.23     |
| 55  | X     | 8    | 4SU  | O2-C2   | -2.45 | 1.18        | 1.23     |
| 1   | A     | 1207 | 2MG  | C6-N1   | 2.45  | 1.43        | 1.38     |
| 22  | a     | 2498 | OMC  | C5-C4   | 2.44  | 1.48        | 1.42     |
| 1   | A     | 1518 | MA6  | C5-N7   | -2.44 | 1.34        | 1.39     |
| 1   | A     | 1519 | MA6  | C5-N7   | -2.42 | 1.34        | 1.39     |
| 55  | X     | 47   | 3AU  | O4-C4   | -2.41 | 1.18        | 1.23     |
| 22  | a     | 2445 | 2MG  | C6-N1   | 2.41  | 1.43        | 1.38     |
| 12  | L     | 89   | D2T  | CB-SB   | 2.39  | 1.84        | 1.82     |
| 1   | A     | 1516 | 2MG  | C6-N1   | 2.39  | 1.43        | 1.38     |
| 53  | V     | 38   | 2MA  | CM2-C2  | 2.35  | 1.56        | 1.49     |
| 1   | A     | 1407 | 5MC  | O2-C2   | -2.34 | 1.19        | 1.23     |
| 22  | a     | 2503 | 2MA  | CM2-C2  | 2.33  | 1.56        | 1.49     |
| 22  | a     | 1962 | 5MC  | O2-C2   | -2.32 | 1.19        | 1.23     |
| 22  | a     | 2580 | PSU  | O4'-C1' | -2.31 | 1.40        | 1.43     |
| 22  | a     | 1835 | 2MG  | C6-N1   | 2.31  | 1.43        | 1.38     |
| 1   | A     | 1498 | UR3  | O4-C4   | -2.27 | 1.18        | 1.23     |
| 1   | A     | 1407 | 5MC  | CM5-C5  | 2.27  | 1.56        | 1.50     |
| 1   | A     | 1518 | MA6  | C8-N9   | -2.26 | 1.33        | 1.37     |
| 22  | a     | 1962 | 5MC  | CM5-C5  | 2.26  | 1.56        | 1.50     |
| 1   | A     | 1516 | 2MG  | O6-C6   | -2.25 | 1.19        | 1.23     |
| 1   | A     | 1498 | UR3  | C5-C4   | 2.25  | 1.49        | 1.43     |
| 55  | X     | 47   | 3AU  | O30-C13 | 2.25  | 1.29        | 1.22     |
| 1   | A     | 967  | 5MC  | CM5-C5  | 2.25  | 1.56        | 1.50     |
| 22  | a     | 1835 | 2MG  | O6-C6   | -2.24 | 1.19        | 1.23     |
| 1   | A     | 1498 | UR3  | C4-N3   | 2.24  | 1.45        | 1.40     |
| 1   | A     | 1519 | MA6  | C8-N9   | -2.24 | 1.33        | 1.37     |
| 1   | A     | 967  | 5MC  | O2-C2   | -2.23 | 1.19        | 1.23     |
| 22  | a     | 2445 | 2MG  | O6-C6   | -2.23 | 1.19        | 1.23     |
| 22  | a     | 2030 | 6MZ  | C8-N7   | 2.20  | 1.35        | 1.31     |
| 22  | a     | 2069 | G7M  | C8-N7   | 2.19  | 1.37        | 1.33     |
| 1   | A     | 1207 | 2MG  | O6-C6   | -2.18 | 1.19        | 1.23     |
| 22  | a     | 955  | PSU  | O4-C4   | -2.18 | 1.19        | 1.23     |
| 1   | A     | 1498 | UR3  | O2-C2   | -2.18 | 1.18        | 1.22     |
| 55  | X     | 54   | 5MU  | O2-C2   | -2.17 | 1.19        | 1.23     |
| 22  | a     | 746  | PSU  | O4-C4   | -2.16 | 1.19        | 1.23     |
| 22  | a     | 2457 | PSU  | O4-C4   | -2.15 | 1.19        | 1.23     |
| 55  | X     | 55   | PSU  | O4-C4   | -2.15 | 1.19        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | X     | 46   | G7M  | C8-N7   | 2.14  | 1.36        | 1.33     |
| 1   | A     | 966  | 2MG  | O6-C6   | -2.14 | 1.19        | 1.23     |
| 1   | A     | 527  | G7M  | C8-N7   | 2.14  | 1.36        | 1.33     |
| 22  | a     | 1939 | 5MU  | O2-C2   | -2.13 | 1.19        | 1.23     |
| 22  | a     | 1915 | 3TD  | O4-C4   | -2.12 | 1.18        | 1.23     |
| 22  | a     | 1911 | PSU  | O4-C4   | -2.12 | 1.19        | 1.23     |
| 22  | a     | 2580 | PSU  | O4-C4   | -2.12 | 1.19        | 1.23     |
| 22  | a     | 745  | 1MG  | O6-C6   | -2.11 | 1.18        | 1.23     |
| 22  | a     | 745  | 1MG  | C4-N9   | -2.10 | 1.32        | 1.38     |
| 22  | a     | 2552 | OMU  | C6-N1   | 2.09  | 1.43        | 1.38     |
| 1   | A     | 516  | PSU  | O4'-C1' | -2.08 | 1.41        | 1.43     |
| 22  | a     | 1618 | 6MZ  | C8-N7   | 2.07  | 1.35        | 1.31     |
| 22  | a     | 1917 | PSU  | O4-C4   | -2.06 | 1.19        | 1.23     |
| 53  | V     | 13   | PSU  | O4-C4   | -2.06 | 1.19        | 1.23     |
| 53  | V     | 13   | PSU  | C4-C5   | 2.05  | 1.50        | 1.44     |
| 22  | a     | 2605 | PSU  | O4-C4   | -2.05 | 1.19        | 1.23     |
| 22  | a     | 2552 | OMU  | C5-C4   | 2.05  | 1.48        | 1.43     |
| 22  | a     | 747  | 5MU  | O2-C2   | -2.04 | 1.19        | 1.23     |
| 55  | X     | 39   | PSU  | O4-C4   | -2.04 | 1.19        | 1.23     |
| 22  | a     | 1618 | 6MZ  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 1   | A     | 1516 | 2MG  | C4-N9   | -2.04 | 1.32        | 1.38     |
| 22  | a     | 2604 | PSU  | O4-C4   | -2.02 | 1.19        | 1.23     |
| 1   | A     | 516  | PSU  | O4-C4   | -2.01 | 1.19        | 1.23     |
| 22  | a     | 2030 | 6MZ  | C5-N7   | -2.01 | 1.35        | 1.39     |

All (310) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 22  | a     | 1939 | 5MU  | C5-C4-N3  | 12.10  | 125.64      | 115.31   |
| 53  | V     | 54   | 5MU  | C5-C4-N3  | 12.03  | 125.58      | 115.31   |
| 22  | a     | 747  | 5MU  | C5-C4-N3  | 11.94  | 125.50      | 115.31   |
| 55  | X     | 54   | 5MU  | C5-C4-N3  | 10.90  | 124.61      | 115.31   |
| 22  | a     | 1939 | 5MU  | C5-C6-N1  | -10.36 | 112.68      | 123.34   |
| 22  | a     | 747  | 5MU  | C5-C6-N1  | -10.06 | 112.99      | 123.34   |
| 53  | V     | 54   | 5MU  | C5-C6-N1  | -9.63  | 113.43      | 123.34   |
| 55  | X     | 54   | 5MU  | C5-C6-N1  | -9.52  | 113.55      | 123.34   |
| 22  | a     | 2503 | 2MA  | C5-C4-N3  | -8.31  | 117.84      | 127.19   |
| 55  | X     | 8    | 4SU  | C4-N3-C2  | -7.94  | 119.63      | 127.34   |
| 53  | V     | 38   | 2MA  | C4-N9-C1' | -7.68  | 108.29      | 126.59   |
| 53  | V     | 38   | 2MA  | C5-C4-N3  | -7.62  | 118.62      | 127.19   |
| 53  | V     | 38   | 2MA  | C1'-N9-C8 | 7.60   | 144.31      | 127.14   |
| 55  | X     | 54   | 5MU  | C5M-C5-C6 | -7.21  | 113.22      | 122.85   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 55  | X     | 54   | 5MU  | C5M-C5-C4 | 7.05  | 126.53      | 118.77   |
| 22  | a     | 2503 | 2MA  | C1'-N9-C8 | 7.03  | 143.00      | 127.14   |
| 22  | a     | 2503 | 2MA  | C4-N9-C1' | -7.02 | 109.86      | 126.59   |
| 22  | a     | 1835 | 2MG  | C2-N3-C4  | 6.70  | 120.35      | 112.04   |
| 1   | A     | 966  | 2MG  | C2-N3-C4  | 6.67  | 120.31      | 112.04   |
| 22  | a     | 2445 | 2MG  | C2-N3-C4  | 6.54  | 120.15      | 112.04   |
| 1   | A     | 1207 | 2MG  | C2-N3-C4  | 6.48  | 120.08      | 112.04   |
| 1   | A     | 1516 | 2MG  | C2-N3-C4  | 6.23  | 119.77      | 112.04   |
| 55  | X     | 20   | H2U  | C4-N3-C2  | -6.13 | 120.70      | 125.79   |
| 1   | A     | 1518 | MA6  | N1-C2-N3  | -5.71 | 119.66      | 128.60   |
| 1   | A     | 1519 | MA6  | N1-C2-N3  | -5.68 | 119.72      | 128.60   |
| 55  | X     | 8    | 4SU  | C5-C4-N3  | 5.63  | 119.91      | 114.69   |
| 22  | a     | 2030 | 6MZ  | N1-C2-N3  | -5.54 | 119.94      | 128.60   |
| 22  | a     | 1618 | 6MZ  | N1-C2-N3  | -5.53 | 119.96      | 128.60   |
| 22  | a     | 1915 | 3TD  | N1-C2-N3  | 5.52  | 120.50      | 116.14   |
| 22  | a     | 2503 | 2MA  | N3-C4-N9  | 5.40  | 134.48      | 126.99   |
| 22  | a     | 2552 | OMU  | C4-N3-C2  | -5.39 | 119.47      | 126.58   |
| 22  | a     | 1835 | 2MG  | C5-C4-N3  | -5.39 | 119.72      | 128.46   |
| 22  | a     | 1618 | 6MZ  | C5-C4-N3  | -5.32 | 119.81      | 126.75   |
| 22  | a     | 2251 | OMG  | C5-C4-N3  | -5.30 | 119.86      | 128.46   |
| 1   | A     | 966  | 2MG  | C5-C4-N3  | -5.26 | 119.93      | 128.46   |
| 1   | A     | 1207 | 2MG  | C5-C4-N3  | -5.19 | 120.04      | 128.46   |
| 22  | a     | 2445 | 2MG  | C5-C4-N3  | -5.11 | 120.17      | 128.46   |
| 53  | V     | 54   | 5MU  | O4-C4-C5  | -5.06 | 119.03      | 124.90   |
| 22  | a     | 2030 | 6MZ  | C5-C4-N3  | -4.97 | 120.27      | 126.75   |
| 55  | X     | 18   | OMG  | C5-C4-N3  | -4.95 | 120.43      | 128.46   |
| 1   | A     | 1498 | UR3  | C4-N3-C2  | -4.95 | 119.91      | 124.56   |
| 22  | a     | 747  | 5MU  | O4-C4-C5  | -4.93 | 119.19      | 124.90   |
| 55  | X     | 55   | PSU  | C4-N3-C2  | -4.92 | 119.25      | 126.34   |
| 22  | a     | 1939 | 5MU  | C4-N3-C2  | -4.85 | 121.08      | 127.35   |
| 53  | V     | 38   | 2MA  | N3-C4-N9  | 4.84  | 133.71      | 126.99   |
| 1   | A     | 1519 | MA6  | C5-C4-N3  | -4.84 | 120.44      | 126.75   |
| 22  | a     | 1939 | 5MU  | O4-C4-C5  | -4.81 | 119.33      | 124.90   |
| 22  | a     | 955  | PSU  | C4-N3-C2  | -4.80 | 119.42      | 126.34   |
| 1   | A     | 1518 | MA6  | C5-C4-N3  | -4.80 | 120.49      | 126.75   |
| 22  | a     | 2605 | PSU  | C4-N3-C2  | -4.77 | 119.46      | 126.34   |
| 22  | a     | 745  | 1MG  | C5-C4-N3  | -4.75 | 120.75      | 128.46   |
| 55  | X     | 54   | 5MU  | N3-C2-N1  | 4.75  | 121.20      | 114.89   |
| 1   | A     | 1516 | 2MG  | C5-C4-N3  | -4.73 | 120.79      | 128.46   |
| 55  | X     | 54   | 5MU  | C4-N3-C2  | -4.72 | 121.24      | 127.35   |
| 22  | a     | 746  | PSU  | C4-N3-C2  | -4.72 | 119.54      | 126.34   |
| 53  | V     | 54   | 5MU  | C4-N3-C2  | -4.71 | 121.25      | 127.35   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22  | a     | 747  | 5MU  | C4-N3-C2 | -4.66 | 121.32      | 127.35   |
| 22  | a     | 2457 | PSU  | C4-N3-C2 | -4.58 | 119.75      | 126.34   |
| 22  | a     | 2030 | 6MZ  | N9-C8-N7 | -4.57 | 107.66      | 113.91   |
| 22  | a     | 2604 | PSU  | C4-N3-C2 | -4.57 | 119.76      | 126.34   |
| 22  | a     | 1911 | PSU  | C4-N3-C2 | -4.56 | 119.76      | 126.34   |
| 22  | a     | 1917 | PSU  | C4-N3-C2 | -4.56 | 119.77      | 126.34   |
| 53  | V     | 54   | 5MU  | N3-C2-N1 | 4.53  | 120.90      | 114.89   |
| 53  | V     | 13   | PSU  | C4-N3-C2 | -4.53 | 119.82      | 126.34   |
| 22  | a     | 1939 | 5MU  | N3-C2-N1 | 4.50  | 120.87      | 114.89   |
| 1   | A     | 1518 | MA6  | C2-N1-C6 | 4.49  | 122.37      | 111.75   |
| 22  | a     | 2504 | PSU  | C4-N3-C2 | -4.49 | 119.87      | 126.34   |
| 1   | A     | 1519 | MA6  | N9-C8-N7 | -4.48 | 107.79      | 113.91   |
| 22  | a     | 2030 | 6MZ  | C9-N6-C6 | -4.46 | 119.03      | 122.87   |
| 53  | V     | 55   | PSU  | C4-N3-C2 | -4.46 | 119.91      | 126.34   |
| 55  | X     | 39   | PSU  | C4-N3-C2 | -4.45 | 119.93      | 126.34   |
| 1   | A     | 516  | PSU  | C4-N3-C2 | -4.42 | 119.97      | 126.34   |
| 55  | X     | 55   | PSU  | N1-C2-N3 | 4.40  | 120.11      | 115.13   |
| 22  | a     | 1618 | 6MZ  | N9-C8-N7 | -4.39 | 107.90      | 113.91   |
| 22  | a     | 1835 | 2MG  | C2-N1-C6 | -4.39 | 119.43      | 124.48   |
| 22  | a     | 2580 | PSU  | C4-N3-C2 | -4.38 | 120.03      | 126.34   |
| 1   | A     | 1518 | MA6  | N9-C8-N7 | -4.38 | 107.93      | 113.91   |
| 1   | A     | 1519 | MA6  | C2-N1-C6 | 4.37  | 122.08      | 111.75   |
| 22  | a     | 2251 | OMG  | C2-N3-C4 | 4.35  | 120.05      | 112.30   |
| 22  | a     | 747  | 5MU  | N3-C2-N1 | 4.35  | 120.66      | 114.89   |
| 55  | X     | 46   | G7M  | C2-N3-C4 | 4.34  | 120.03      | 112.30   |
| 22  | a     | 2457 | PSU  | N1-C2-N3 | 4.34  | 120.05      | 115.13   |
| 22  | a     | 2069 | G7M  | C2-N3-C4 | 4.33  | 120.02      | 112.30   |
| 1   | A     | 527  | G7M  | C2-N3-C4 | 4.30  | 119.97      | 112.30   |
| 55  | X     | 18   | OMG  | C2-N3-C4 | 4.26  | 119.88      | 112.30   |
| 1   | A     | 966  | 2MG  | C2-N1-C6 | -4.25 | 119.58      | 124.48   |
| 22  | a     | 2445 | 2MG  | C2-N1-C6 | -4.25 | 119.59      | 124.48   |
| 1   | A     | 1518 | MA6  | C4-C5-C6 | 4.24  | 120.62      | 115.88   |
| 1   | A     | 1207 | 2MG  | C2-N1-C6 | -4.23 | 119.61      | 124.48   |
| 22  | a     | 2580 | PSU  | N1-C2-N3 | 4.21  | 119.90      | 115.13   |
| 1   | A     | 1519 | MA6  | C4-C5-C6 | 4.20  | 120.58      | 115.88   |
| 22  | a     | 746  | PSU  | N1-C2-N3 | 4.20  | 119.89      | 115.13   |
| 22  | a     | 955  | PSU  | N1-C2-N3 | 4.19  | 119.88      | 115.13   |
| 22  | a     | 1917 | PSU  | N1-C2-N3 | 4.10  | 119.78      | 115.13   |
| 22  | a     | 1915 | 3TD  | C4-N3-C2 | -4.10 | 120.16      | 124.61   |
| 53  | V     | 55   | PSU  | N1-C2-N3 | 4.09  | 119.77      | 115.13   |
| 22  | a     | 2605 | PSU  | N1-C2-N3 | 4.09  | 119.76      | 115.13   |
| 55  | X     | 39   | PSU  | N1-C2-N3 | 4.09  | 119.76      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 53  | V     | 13   | PSU  | N1-C2-N3  | 4.08  | 119.75      | 115.13   |
| 22  | a     | 747  | 5MU  | C5M-C5-C6 | -4.08 | 117.40      | 122.85   |
| 1   | A     | 516  | PSU  | N1-C2-N3  | 4.07  | 119.74      | 115.13   |
| 22  | a     | 2604 | PSU  | N1-C2-N3  | 4.05  | 119.72      | 115.13   |
| 55  | X     | 54   | 5MU  | O4-C4-C5  | -4.04 | 120.21      | 124.90   |
| 22  | a     | 1911 | PSU  | N1-C2-N3  | 4.02  | 119.68      | 115.13   |
| 22  | a     | 2552 | OMU  | N3-C2-N1  | 4.00  | 120.20      | 114.89   |
| 55  | X     | 46   | G7M  | C5-C6-N1  | 3.97  | 120.09      | 111.79   |
| 22  | a     | 2069 | G7M  | C5-C6-N1  | 3.93  | 119.99      | 111.79   |
| 22  | a     | 2504 | PSU  | N1-C2-N3  | 3.92  | 119.57      | 115.13   |
| 22  | a     | 747  | 5MU  | C5M-C5-C4 | 3.91  | 123.08      | 118.77   |
| 1   | A     | 527  | G7M  | C5-C6-N1  | 3.91  | 119.96      | 111.79   |
| 1   | A     | 1516 | 2MG  | C2-N1-C6  | -3.91 | 119.98      | 124.48   |
| 55  | X     | 46   | G7M  | C5-C4-N3  | -3.87 | 120.73      | 128.15   |
| 55  | X     | 34   | M3X  | C2-N3-C4  | 3.87  | 121.41      | 117.84   |
| 22  | a     | 1939 | 5MU  | C5M-C5-C6 | -3.86 | 117.69      | 122.85   |
| 53  | V     | 54   | 5MU  | C5M-C5-C6 | -3.81 | 117.76      | 122.85   |
| 55  | X     | 8    | 4SU  | N3-C2-N1  | 3.81  | 119.94      | 114.89   |
| 22  | a     | 1618 | 6MZ  | C9-N6-C6  | -3.80 | 119.60      | 122.87   |
| 53  | V     | 54   | 5MU  | C5M-C5-C4 | 3.77  | 122.91      | 118.77   |
| 1   | A     | 527  | G7M  | C5-C4-N3  | -3.76 | 120.95      | 128.15   |
| 33  | l     | 81   | 4D4  | NE-CZ-NH2 | 3.73  | 127.25      | 120.70   |
| 22  | a     | 2069 | G7M  | C5-C4-N3  | -3.72 | 121.02      | 128.15   |
| 1   | A     | 1518 | MA6  | C5-N7-C8  | 3.71  | 108.78      | 103.51   |
| 22  | a     | 1618 | 6MZ  | C2-N3-C4  | 3.70  | 120.49      | 111.75   |
| 1   | A     | 1519 | MA6  | C5-N7-C8  | 3.70  | 108.76      | 103.51   |
| 55  | X     | 47   | 3AU  | C4-N3-C2  | -3.68 | 120.02      | 124.63   |
| 53  | V     | 38   | 2MA  | N9-C8-N7  | -3.61 | 108.98      | 113.91   |
| 22  | a     | 1835 | 2MG  | N9-C4-N3  | 3.61  | 133.18      | 125.94   |
| 22  | a     | 2251 | OMG  | N9-C4-N3  | 3.60  | 133.18      | 125.94   |
| 22  | a     | 745  | 1MG  | C2-N3-C4  | 3.59  | 120.05      | 111.98   |
| 22  | a     | 2030 | 6MZ  | C2-N3-C4  | 3.57  | 120.19      | 111.75   |
| 22  | a     | 1939 | 5MU  | C5M-C5-C4 | 3.55  | 122.67      | 118.77   |
| 22  | a     | 1618 | 6MZ  | C4-C5-C6  | 3.52  | 119.53      | 116.81   |
| 55  | X     | 18   | OMG  | N9-C8-N7  | -3.51 | 106.78      | 113.39   |
| 1   | A     | 527  | G7M  | O6-C6-C5  | -3.50 | 120.17      | 128.06   |
| 22  | a     | 2503 | 2MA  | N9-C8-N7  | -3.49 | 109.14      | 113.91   |
| 22  | a     | 2069 | G7M  | O6-C6-C5  | -3.46 | 120.25      | 128.06   |
| 1   | A     | 966  | 2MG  | N9-C4-N3  | 3.44  | 132.85      | 125.94   |
| 1   | A     | 1207 | 2MG  | N9-C4-N3  | 3.43  | 132.82      | 125.94   |
| 55  | X     | 46   | G7M  | O6-C6-C5  | -3.42 | 120.34      | 128.06   |
| 1   | A     | 1516 | 2MG  | N9-C8-N7  | -3.39 | 107.02      | 113.39   |

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| Mol | Chain | Res   | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 55  | X     | 8     | 4SU  | C5-C4-S4  | -3.38 | 120.11      | 124.47   |
| 1   | A     | 1519  | MA6  | C2-N3-C4  | 3.38  | 119.73      | 111.75   |
| 22  | a     | 2445  | 2MG  | N9-C8-N7  | -3.37 | 107.04      | 113.39   |
| 55  | X     | 47    | 3AU  | C5-C4-N3  | 3.36  | 119.94      | 115.50   |
| 22  | a     | 2552  | OMU  | C5-C4-N3  | 3.35  | 119.86      | 114.84   |
| 12  | L     | 89    | D2T  | OD2-CG-CB | 3.32  | 120.33      | 113.15   |
| 22  | a     | 2445  | 2MG  | N9-C4-N3  | 3.32  | 132.60      | 125.94   |
| 53  | V     | 35    | U8U  | C5-C4-N3  | 3.32  | 119.63      | 114.97   |
| 1   | A     | 1518  | MA6  | C2-N3-C4  | 3.31  | 119.57      | 111.75   |
| 22  | a     | 2030  | 6MZ  | C5-N7-C8  | 3.31  | 108.21      | 103.51   |
| 55  | X     | 18    | OMG  | N9-C4-N3  | 3.29  | 132.54      | 125.94   |
| 22  | a     | 1962  | 5MC  | C5-C6-N1  | -3.26 | 119.98      | 123.34   |
| 22  | a     | 746   | PSU  | C6-C5-C4  | 3.26  | 120.48      | 118.20   |
| 22  | a     | 2580  | PSU  | C6-N1-C2  | -3.25 | 119.36      | 122.68   |
| 1   | A     | 966   | 2MG  | N9-C8-N7  | -3.19 | 107.37      | 113.39   |
| 22  | a     | 2251  | OMG  | N9-C8-N7  | -3.19 | 107.38      | 113.39   |
| 22  | a     | 1618  | 6MZ  | C5-N7-C8  | 3.19  | 108.03      | 103.51   |
| 22  | a     | 2457  | PSU  | C6-C5-C4  | 3.16  | 120.41      | 118.20   |
| 12  | L     | 89    | D2T  | OD1-CG-CB | -3.16 | 115.82      | 122.44   |
| 1   | A     | 1407  | 5MC  | C5-C6-N1  | -3.15 | 120.10      | 123.34   |
| 53  | V     | 35    | U8U  | C1'-N1-C6 | -3.14 | 115.90      | 121.12   |
| 1   | A     | 1518  | MA6  | C4-C5-N7  | -3.13 | 106.81      | 110.62   |
| 22  | a     | 1835  | 2MG  | N9-C8-N7  | -3.12 | 107.51      | 113.39   |
| 22  | a     | 2030  | 6MZ  | C4-C5-C6  | 3.12  | 119.22      | 116.81   |
| 1   | A     | 967   | 5MC  | C5-C6-N1  | -3.12 | 120.13      | 123.34   |
| 22  | a     | 2503  | 2MA  | N3-C2-N1  | -3.11 | 120.00      | 125.72   |
| 1   | A     | 1207  | 2MG  | N9-C8-N7  | -3.11 | 107.54      | 113.39   |
| 22  | a     | 745   | 1MG  | N9-C8-N7  | -3.11 | 107.54      | 113.39   |
| 22  | a     | 1618  | 6MZ  | N3-C4-N9  | 3.10  | 132.19      | 127.08   |
| 22  | a     | 2251  | OMG  | C2-N1-C6  | -3.08 | 119.49      | 125.10   |
| 1   | A     | 1519  | MA6  | C4-C5-N7  | -3.08 | 106.87      | 110.62   |
| 22  | a     | 2457  | PSU  | C6-N1-C2  | -3.06 | 119.55      | 122.68   |
| 22  | a     | 2580  | PSU  | C6-C5-C4  | 3.05  | 120.33      | 118.20   |
| 1   | A     | 516   | PSU  | C6-C5-C4  | 3.05  | 120.33      | 118.20   |
| 53  | V     | 38    | 2MA  | N3-C2-N1  | -3.05 | 120.12      | 125.72   |
| 55  | X     | 46    | G7M  | N9-C4-N3  | 3.00  | 131.97      | 125.94   |
| 55  | X     | 20(A) | H2U  | C4-N3-C2  | -3.00 | 123.30      | 125.79   |
| 22  | a     | 1917  | PSU  | C6-C5-C4  | 3.00  | 120.29      | 118.20   |
| 53  | V     | 55    | PSU  | C6-N1-C2  | -3.00 | 119.62      | 122.68   |
| 33  | l     | 82    | MS6  | CE-SD-CG  | 3.00  | 110.69      | 100.40   |
| 55  | X     | 46    | G7M  | C2-N1-C6  | -2.98 | 119.67      | 125.10   |
| 55  | X     | 39    | PSU  | C6-N1-C2  | -2.98 | 119.64      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22  | a     | 2503 | 2MA  | C5-N7-C8  | 2.97  | 107.73      | 103.51   |
| 55  | X     | 18   | OMG  | C1'-N9-C4 | -2.97 | 117.69      | 126.50   |
| 22  | a     | 2605 | PSU  | C6-C5-C4  | 2.96  | 120.27      | 118.20   |
| 1   | A     | 516  | PSU  | C6-N1-C2  | -2.95 | 119.66      | 122.68   |
| 55  | X     | 55   | PSU  | C6-C5-C4  | 2.92  | 120.24      | 118.20   |
| 22  | a     | 955  | PSU  | C6-C5-C4  | 2.92  | 120.24      | 118.20   |
| 53  | V     | 38   | 2MA  | C5-N7-C8  | 2.92  | 107.66      | 103.51   |
| 1   | A     | 1516 | 2MG  | N9-C4-N3  | 2.91  | 131.77      | 125.94   |
| 1   | A     | 527  | G7M  | N9-C4-N3  | 2.90  | 131.76      | 125.94   |
| 55  | X     | 18   | OMG  | C2-N1-C6  | -2.90 | 119.82      | 125.10   |
| 53  | V     | 35   | U8U  | O4-C4-C5  | -2.90 | 120.65      | 124.96   |
| 1   | A     | 527  | G7M  | C2-N1-C6  | -2.89 | 119.84      | 125.10   |
| 22  | a     | 2069 | G7M  | C2-N1-C6  | -2.86 | 119.88      | 125.10   |
| 53  | V     | 55   | PSU  | C6-C5-C4  | 2.82  | 120.17      | 118.20   |
| 53  | V     | 38   | 2MA  | C6-C5-C4  | 2.82  | 120.97      | 117.18   |
| 22  | a     | 2503 | 2MA  | C6-C5-C4  | 2.82  | 120.97      | 117.18   |
| 22  | a     | 1911 | PSU  | C6-N1-C2  | -2.81 | 119.81      | 122.68   |
| 22  | a     | 746  | PSU  | C6-N1-C2  | -2.80 | 119.83      | 122.68   |
| 22  | a     | 2457 | PSU  | O2-C2-N1  | -2.79 | 119.72      | 122.79   |
| 22  | a     | 2552 | OMU  | O4-C4-C5  | -2.79 | 120.26      | 125.16   |
| 53  | V     | 13   | PSU  | C6-N1-C2  | -2.78 | 119.84      | 122.68   |
| 55  | X     | 55   | PSU  | C6-N1-C2  | -2.78 | 119.84      | 122.68   |
| 22  | a     | 1917 | PSU  | C6-N1-C2  | -2.77 | 119.85      | 122.68   |
| 22  | a     | 1835 | 2MG  | C5-C6-N1  | 2.77  | 120.22      | 113.19   |
| 22  | a     | 2069 | G7M  | N9-C4-N3  | 2.76  | 131.48      | 125.94   |
| 55  | X     | 54   | 5MU  | O2-C2-N1  | -2.76 | 119.12      | 122.79   |
| 22  | a     | 1911 | PSU  | C6-C5-C4  | 2.73  | 120.11      | 118.20   |
| 22  | a     | 2251 | OMG  | C5-C6-N1  | 2.73  | 120.11      | 113.19   |
| 1   | A     | 966  | 2MG  | C5-C6-N1  | 2.72  | 120.10      | 113.19   |
| 53  | V     | 13   | PSU  | C6-C5-C4  | 2.72  | 120.10      | 118.20   |
| 22  | a     | 955  | PSU  | C6-N1-C2  | -2.71 | 119.91      | 122.68   |
| 22  | a     | 2604 | PSU  | C6-N1-C2  | -2.70 | 119.92      | 122.68   |
| 55  | X     | 54   | 5MU  | C1'-N1-C2 | 2.70  | 122.46      | 117.57   |
| 55  | X     | 39   | PSU  | C6-C5-C4  | 2.70  | 120.08      | 118.20   |
| 22  | a     | 745  | 1MG  | C1'-N9-C8 | -2.70 | 119.02      | 126.70   |
| 22  | a     | 2504 | PSU  | C6-N1-C2  | -2.70 | 119.93      | 122.68   |
| 22  | a     | 2445 | 2MG  | C5-C6-N1  | 2.69  | 120.02      | 113.19   |
| 22  | a     | 745  | 1MG  | N9-C4-N3  | 2.68  | 131.33      | 125.94   |
| 1   | A     | 1207 | 2MG  | C5-C6-N1  | 2.68  | 120.00      | 113.19   |
| 33  | l     | 81   | 4D4  | CB-CA-C   | -2.67 | 107.50      | 111.77   |
| 22  | a     | 2504 | PSU  | C6-C5-C4  | 2.67  | 120.06      | 118.20   |
| 55  | X     | 18   | OMG  | C5-C6-N1  | 2.66  | 119.94      | 113.19   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | X     | 54   | 5MU  | C6-C5-C4    | 2.66  | 120.25      | 118.03   |
| 22  | a     | 1939 | 5MU  | O4-C4-N3    | -2.66 | 115.03      | 120.12   |
| 22  | a     | 2605 | PSU  | C6-N1-C2    | -2.65 | 119.97      | 122.68   |
| 22  | a     | 745  | 1MG  | C5-C6-N1    | 2.64  | 120.01      | 114.91   |
| 1   | A     | 527  | G7M  | CN7-N7-C5   | 2.63  | 130.04      | 126.77   |
| 53  | V     | 55   | PSU  | O2-C2-N1    | -2.61 | 119.92      | 122.79   |
| 22  | a     | 2069 | G7M  | CN7-N7-C5   | 2.61  | 130.01      | 126.77   |
| 22  | a     | 2030 | 6MZ  | N3-C4-N9    | 2.60  | 131.36      | 127.08   |
| 1   | A     | 1516 | 2MG  | C5-C6-N1    | 2.60  | 119.78      | 113.19   |
| 55  | X     | 54   | 5MU  | O4-C4-N3    | -2.58 | 115.17      | 120.12   |
| 55  | X     | 46   | G7M  | CN7-N7-C5   | 2.56  | 129.95      | 126.77   |
| 55  | X     | 39   | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 1   | A     | 966  | 2MG  | N1-C2-N3    | -2.55 | 120.01      | 123.95   |
| 1   | A     | 516  | PSU  | O2-C2-N1    | -2.55 | 119.99      | 122.79   |
| 1   | A     | 1207 | 2MG  | O6-C6-C5    | -2.55 | 119.84      | 126.60   |
| 1   | A     | 1516 | 2MG  | N1-C2-N3    | -2.54 | 120.02      | 123.95   |
| 22  | a     | 2580 | PSU  | O2-C2-N1    | -2.54 | 119.99      | 122.79   |
| 22  | a     | 1917 | PSU  | O2-C2-N1    | -2.54 | 120.00      | 122.79   |
| 22  | a     | 2604 | PSU  | C6-C5-C4    | 2.54  | 119.97      | 118.20   |
| 22  | a     | 1835 | 2MG  | O6-C6-C5    | -2.52 | 119.92      | 126.60   |
| 1   | A     | 1519 | MA6  | C5-C4-N9    | 2.52  | 108.71      | 105.78   |
| 33  | l     | 81   | 4D4  | O-C-CA      | -2.52 | 118.18      | 124.78   |
| 22  | a     | 2030 | 6MZ  | C4-C5-N7    | -2.52 | 107.56      | 110.62   |
| 22  | a     | 747  | 5MU  | O4-C4-N3    | -2.51 | 115.31      | 120.12   |
| 1   | A     | 966  | 2MG  | O6-C6-C5    | -2.51 | 119.95      | 126.60   |
| 25  | d     | 150  | MEQ  | OE1-CD-CG   | 2.50  | 126.59      | 122.02   |
| 1   | A     | 1518 | MA6  | C5-C4-N9    | 2.49  | 108.68      | 105.78   |
| 22  | a     | 2445 | 2MG  | N1-C2-N3    | -2.49 | 120.10      | 123.95   |
| 22  | a     | 1835 | 2MG  | N1-C2-N3    | -2.49 | 120.10      | 123.95   |
| 1   | A     | 1516 | 2MG  | O6-C6-C5    | -2.47 | 120.05      | 126.60   |
| 53  | V     | 54   | 5MU  | O4-C4-N3    | -2.46 | 115.39      | 120.12   |
| 22  | a     | 2445 | 2MG  | O6-C6-C5    | -2.44 | 120.12      | 126.60   |
| 55  | X     | 18   | OMG  | O6-C6-C5    | -2.44 | 120.13      | 126.60   |
| 55  | X     | 34   | M3X  | N4-C4-N3    | 2.44  | 120.34      | 116.49   |
| 1   | A     | 1207 | 2MG  | N1-C2-N3    | -2.44 | 120.18      | 123.95   |
| 22  | a     | 2251 | OMG  | O6-C6-C5    | -2.44 | 120.14      | 126.60   |
| 22  | a     | 2251 | OMG  | C1'-N9-C4   | -2.40 | 119.37      | 126.50   |
| 22  | a     | 955  | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 22  | a     | 2445 | 2MG  | C8-N7-C5    | 2.37  | 108.53      | 104.24   |
| 22  | a     | 2580 | PSU  | O4'-C1'-C2' | 2.37  | 108.48      | 105.14   |
| 1   | A     | 1519 | MA6  | N1-C6-N6    | -2.36 | 114.50      | 117.08   |
| 22  | a     | 1939 | 5MU  | O2-C2-N1    | -2.35 | 119.66      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1518 | MA6  | N1-C6-N6    | -2.35 | 114.52      | 117.08   |
| 12  | L     | 89   | D2T  | O-C-CA      | -2.34 | 118.65      | 124.78   |
| 55  | X     | 18   | OMG  | C8-N7-C5    | 2.32  | 108.43      | 104.24   |
| 53  | V     | 54   | 5MU  | O2-C2-N1    | -2.30 | 119.73      | 122.79   |
| 22  | a     | 1911 | PSU  | O2-C2-N1    | -2.30 | 120.26      | 122.79   |
| 22  | a     | 2604 | PSU  | O2-C2-N1    | -2.30 | 120.26      | 122.79   |
| 22  | a     | 2504 | PSU  | O2-C2-N1    | -2.29 | 120.27      | 122.79   |
| 1   | A     | 1516 | 2MG  | C8-N7-C5    | 2.29  | 108.39      | 104.24   |
| 1   | A     | 1519 | MA6  | N3-C4-N9    | 2.29  | 130.85      | 127.08   |
| 55  | X     | 55   | PSU  | O2-C2-N1    | -2.28 | 120.28      | 122.79   |
| 25  | d     | 150  | MEQ  | CG-CD-NE2   | -2.28 | 113.12      | 116.29   |
| 22  | a     | 2030 | 6MZ  | C4-N9-C8    | 2.28  | 108.20      | 105.73   |
| 1   | A     | 1518 | MA6  | N3-C4-N9    | 2.27  | 130.83      | 127.08   |
| 1   | A     | 966  | 2MG  | C8-N7-C5    | 2.26  | 108.34      | 104.24   |
| 1   | A     | 1402 | 4OC  | C6-C5-C4    | 2.26  | 119.73      | 116.96   |
| 55  | X     | 20   | H2U  | O4-C4-N3    | 2.26  | 123.86      | 120.28   |
| 53  | V     | 13   | PSU  | O2-C2-N1    | -2.24 | 120.33      | 122.79   |
| 1   | A     | 516  | PSU  | O4'-C1'-C2' | 2.23  | 108.29      | 105.14   |
| 22  | a     | 1835 | 2MG  | C8-N7-C5    | 2.23  | 108.28      | 104.24   |
| 22  | a     | 2030 | 6MZ  | C5-C4-N9    | 2.23  | 108.37      | 105.78   |
| 22  | a     | 2251 | OMG  | C8-N7-C5    | 2.22  | 108.25      | 104.24   |
| 22  | a     | 1618 | 6MZ  | C4-N9-C8    | 2.21  | 108.13      | 105.73   |
| 22  | a     | 1618 | 6MZ  | C4-C5-N7    | -2.20 | 107.93      | 110.62   |
| 1   | A     | 1207 | 2MG  | C8-N7-C5    | 2.19  | 108.19      | 104.24   |
| 22  | a     | 747  | 5MU  | C1'-N1-C2   | 2.18  | 121.51      | 117.57   |
| 22  | a     | 746  | PSU  | O2-C2-N1    | -2.16 | 120.41      | 122.79   |
| 22  | a     | 2457 | PSU  | O4'-C1'-C2' | 2.15  | 108.18      | 105.14   |
| 22  | a     | 2552 | OMU  | O2-C2-N1    | -2.15 | 119.93      | 122.79   |
| 22  | a     | 2445 | 2MG  | CM2-N2-C2   | -2.13 | 119.15      | 123.86   |
| 22  | a     | 745  | 1MG  | C8-N7-C5    | 2.13  | 108.10      | 104.24   |
| 22  | a     | 2605 | PSU  | O2-C2-N1    | -2.13 | 120.45      | 122.79   |
| 55  | X     | 54   | 5MU  | C6-N1-C2    | -2.12 | 119.15      | 121.30   |
| 22  | a     | 1915 | 3TD  | C6-C5-C4    | 2.10  | 119.67      | 118.22   |
| 1   | A     | 1516 | 2MG  | C1'-N9-C4   | -2.08 | 120.31      | 126.50   |
| 22  | a     | 2069 | G7M  | N9-C8-N7    | -2.08 | 107.06      | 112.21   |
| 55  | X     | 18   | OMG  | C1'-N9-C8   | 2.08  | 132.61      | 126.70   |
| 1   | A     | 1407 | 5MC  | CM5-C5-C6   | -2.05 | 120.10      | 122.85   |
| 22  | a     | 1962 | 5MC  | CM5-C5-C6   | -2.05 | 120.11      | 122.85   |
| 1   | A     | 1498 | UR3  | C6-N1-C2    | -2.04 | 119.96      | 121.79   |
| 55  | X     | 34   | M3X  | C5-C4-N3    | -2.03 | 119.38      | 121.72   |
| 22  | a     | 2069 | G7M  | CN7-N7-C8   | -2.02 | 121.72      | 124.84   |
| 55  | X     | 46   | G7M  | CN7-N7-C8   | -2.02 | 121.72      | 124.84   |

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| Mol | Chain | Res   | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|----------|-------|-------------|----------|
| 55  | X     | 46    | G7M  | N9-C8-N7 | -2.02 | 107.22      | 112.21   |
| 55  | X     | 20(A) | H2U  | O4-C4-N3 | 2.00  | 123.46      | 120.28   |

There are no chirality outliers.

All (65) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | K     | 119  | IAS  | N-CA-CB-CG      |
| 22  | a     | 1618 | 6MZ  | N1-C6-N6-C9     |
| 22  | a     | 1915 | 3TD  | C3'-C4'-C5'-O5' |
| 22  | a     | 2251 | OMG  | C1'-C2'-O2'-CM2 |
| 53  | V     | 55   | PSU  | C3'-C4'-C5'-O5' |
| 53  | V     | 55   | PSU  | O4'-C4'-C5'-O5' |
| 55  | X     | 20   | H2U  | O4'-C4'-C5'-O5' |
| 55  | X     | 55   | PSU  | C3'-C4'-C5'-O5' |
| 55  | X     | 55   | PSU  | O4'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 22  | a     | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 22  | a     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 22  | a     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 22  | a     | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 22  | a     | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 53  | V     | 13   | PSU  | C3'-C4'-C5'-O5' |
| 53  | V     | 54   | 5MU  | O4'-C4'-C5'-O5' |
| 55  | X     | 18   | OMG  | O4'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 22  | a     | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 53  | V     | 54   | 5MU  | C3'-C4'-C5'-O5' |
| 55  | X     | 18   | OMG  | C3'-C4'-C5'-O5' |
| 55  | X     | 47   | 3AU  | C3'-C4'-C5'-O5' |
| 25  | d     | 150  | MEQ  | OE1-CD-CG-CB    |
| 25  | d     | 150  | MEQ  | NE2-CD-CG-CB    |
| 55  | X     | 34   | M3X  | CG-CD-CE-N2     |
| 55  | X     | 46   | G7M  | C3'-C4'-C5'-O5' |
| 55  | X     | 47   | 3AU  | O4'-C4'-C5'-O5' |
| 55  | X     | 34   | M3X  | CE-CD-CG-CB     |
| 55  | X     | 46   | G7M  | C4'-C5'-O5'-P   |
| 1   | A     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 53  | V     | 13   | PSU  | O4'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 1   | A     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 55  | X     | 34   | M3X  | O-C-CZ-N        |

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| Mol | Chain | Res   | Type | Atoms           |
|-----|-------|-------|------|-----------------|
| 55  | X     | 34    | M3X  | OXT-C-CZ-N      |
| 55  | X     | 47    | 3AU  | C10-C11-C12-N40 |
| 22  | a     | 2503  | 2MA  | C3'-C4'-C5'-O5' |
| 55  | X     | 20(A) | H2U  | O4'-C4'-C5'-O5' |
| 33  | l     | 82    | MS6  | CB-CG-SD-CE     |
| 55  | X     | 34    | M3X  | CG-CB-CZ-N      |
| 55  | X     | 20(A) | H2U  | C2'-C1'-N1-C6   |
| 55  | X     | 34    | M3X  | N1-C2-N2-CE     |
| 55  | X     | 47    | 3AU  | N3-C10-C11-C12  |
| 33  | l     | 81    | 4D4  | OB-CB-CG-CD     |
| 55  | X     | 34    | M3X  | N3-C2-N2-CE     |
| 55  | X     | 34    | M3X  | CD-CE-N2-C2     |
| 55  | X     | 18    | OMG  | C3'-C2'-O2'-CM2 |
| 55  | X     | 47    | 3AU  | C4'-C5'-O5'-P   |
| 1   | A     | 966   | 2MG  | C3'-C4'-C5'-O5' |
| 1   | A     | 1402  | 4OC  | C3'-C4'-C5'-O5' |
| 55  | X     | 46    | G7M  | O4'-C4'-C5'-O5' |
| 22  | a     | 2069  | G7M  | O4'-C4'-C5'-O5' |
| 55  | X     | 34    | M3X  | OXT-C-CZ-CB     |
| 55  | X     | 20(A) | H2U  | O4'-C1'-N1-C2   |
| 53  | V     | 35    | U8U  | C2'-C1'-N1-C2   |
| 55  | X     | 34    | M3X  | O-C-CZ-CB       |
| 55  | X     | 20(A) | H2U  | C2'-C1'-N1-C2   |
| 55  | X     | 34    | M3X  | C3'-C4'-C5'-O5' |
| 55  | X     | 34    | M3X  | CG-CB-CZ-C      |
| 12  | L     | 89    | D2T  | CG-CB-SB-CB1    |
| 22  | a     | 746   | PSU  | O4'-C1'-C5-C6   |
| 33  | l     | 81    | 4D4  | CA-CB-CG-CD     |
| 53  | V     | 13    | PSU  | C4'-C5'-O5'-P   |
| 1   | A     | 527   | G7M  | C4'-C5'-O5'-P   |

There are no ring outliers.

17 monomers are involved in 20 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | a     | 2503 | 2MA  | 1       | 0            |
| 22  | a     | 2605 | PSU  | 2       | 0            |
| 22  | a     | 2030 | 6MZ  | 2       | 0            |
| 53  | V     | 35   | U8U  | 2       | 0            |
| 1   | A     | 967  | 5MC  | 1       | 0            |
| 55  | X     | 54   | 5MU  | 1       | 0            |
| 55  | X     | 20   | H2U  | 2       | 0            |

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| Mol | Chain | Res   | Type | Clashes | Symm-Clashes |
|-----|-------|-------|------|---------|--------------|
| 12  | L     | 89    | D2T  | 1       | 0            |
| 55  | X     | 8     | 4SU  | 1       | 0            |
| 22  | a     | 2251  | OMG  | 1       | 0            |
| 22  | a     | 2552  | OMU  | 1       | 0            |
| 22  | a     | 2604  | PSU  | 1       | 0            |
| 55  | X     | 20(A) | H2U  | 2       | 0            |
| 22  | a     | 745   | 1MG  | 1       | 0            |
| 11  | K     | 119   | IAS  | 1       | 0            |
| 1   | A     | 966   | 2MG  | 1       | 0            |
| 22  | a     | 1939  | 5MU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 315 ligands modelled in this entry, 315 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

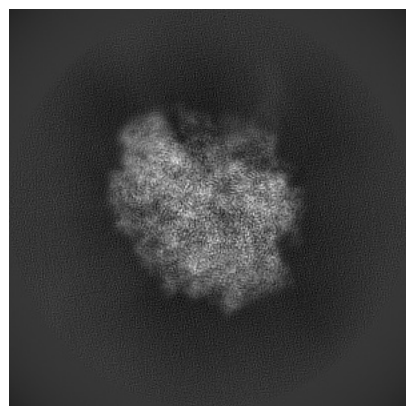
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35022. These allow visual inspection of the internal detail of the map and identification of artifacts.

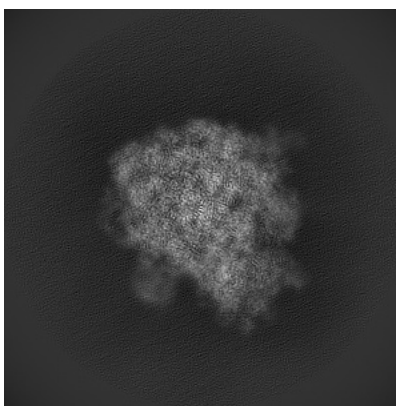
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

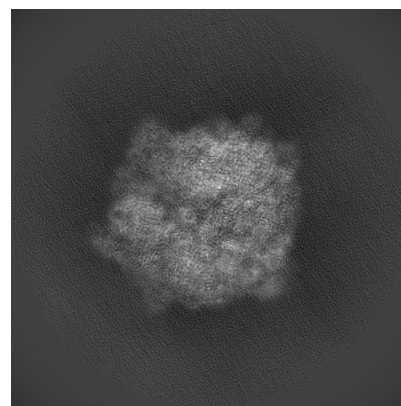
#### 6.1.1 Primary map



X

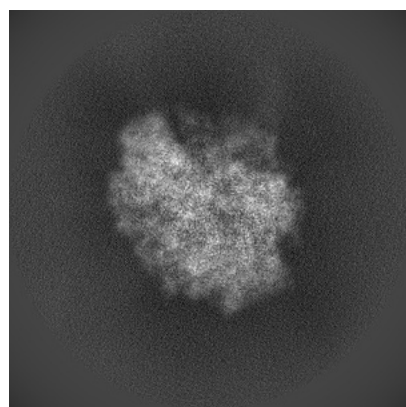


Y

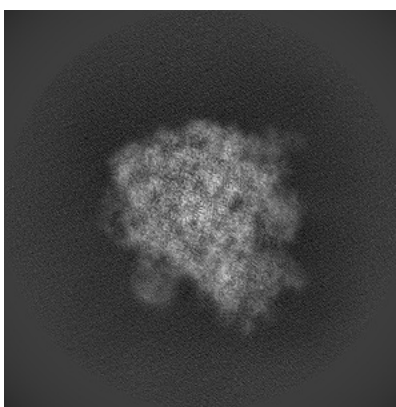


Z

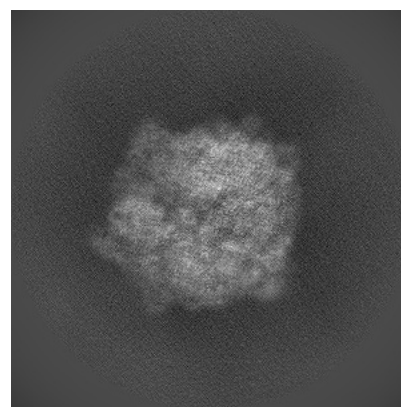
#### 6.1.2 Raw map



X



Y

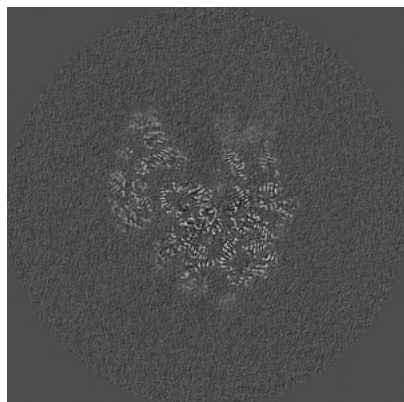


Z

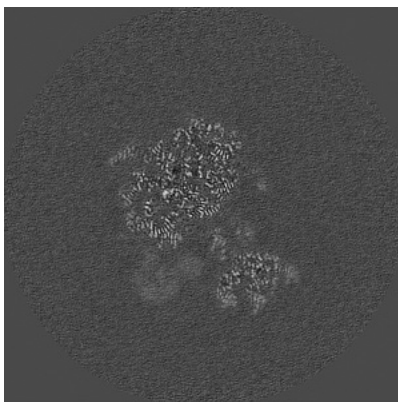
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

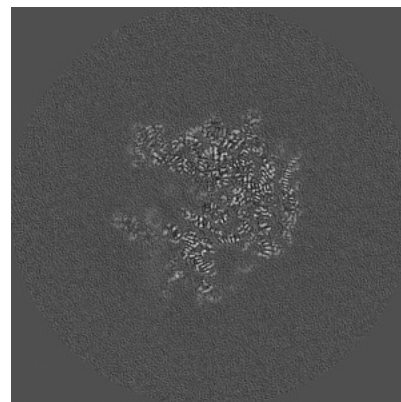
### 6.2.1 Primary map



X Index: 265

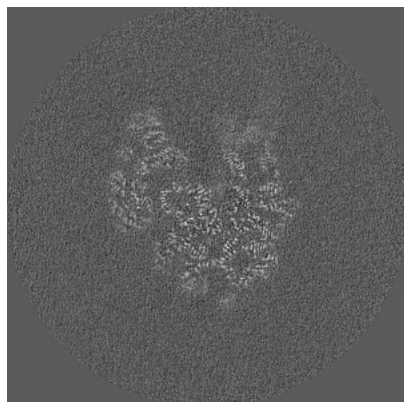


Y Index: 265

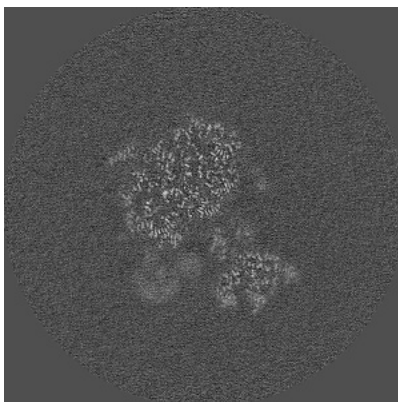


Z Index: 265

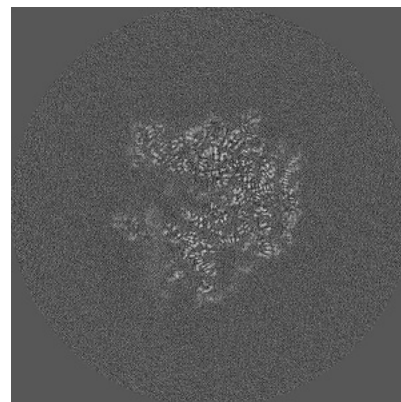
### 6.2.2 Raw map



X Index: 265



Y Index: 265

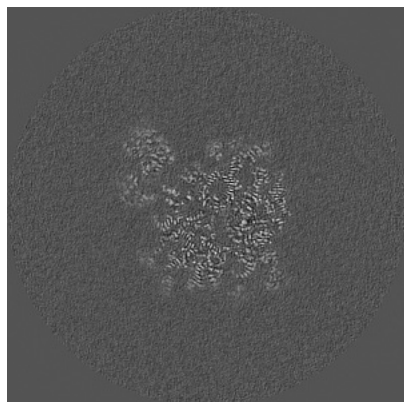


Z Index: 265

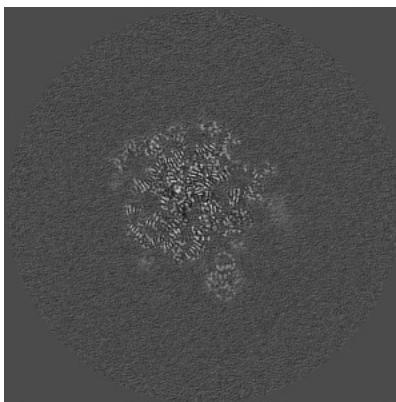
The images above show central slices of the map in three orthogonal directions.

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

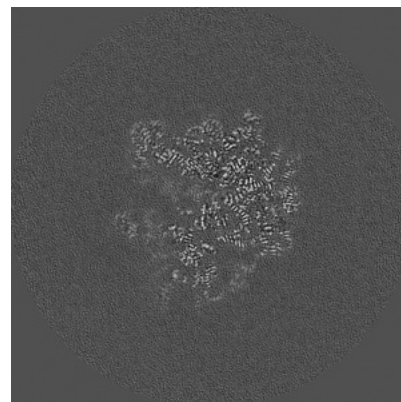
### 6.3.1 Primary map



X Index: 297

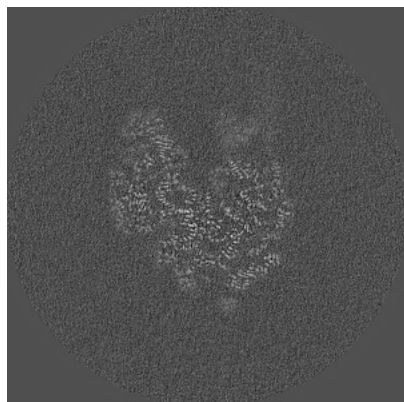


Y Index: 317

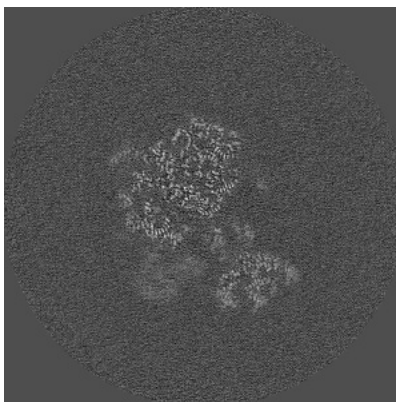


Z Index: 269

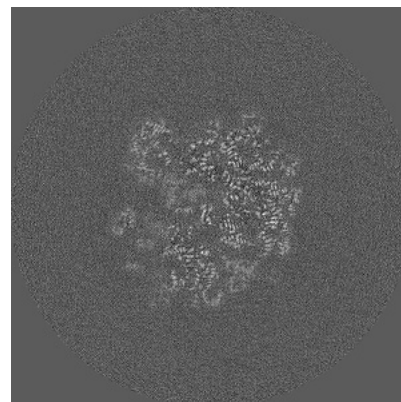
### 6.3.2 Raw map



X Index: 259



Y Index: 264

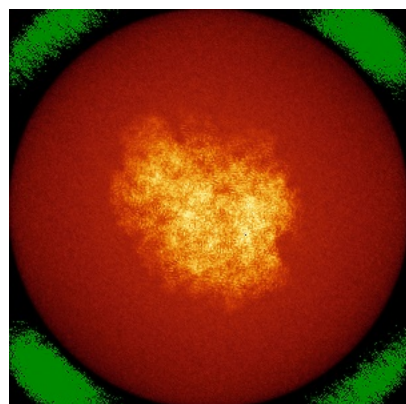


Z Index: 274

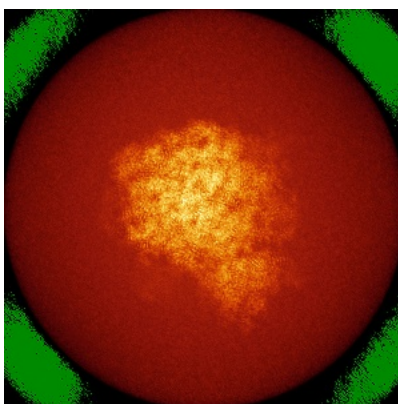
The images above show the largest variance slices of the map in three orthogonal directions.

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

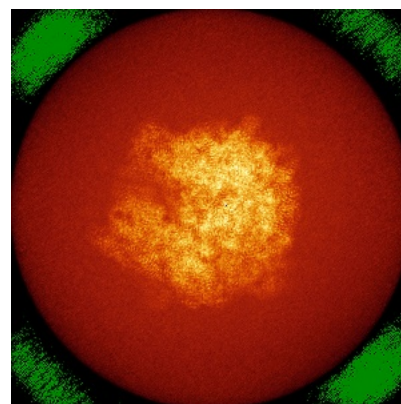
### 6.4.1 Primary map



X

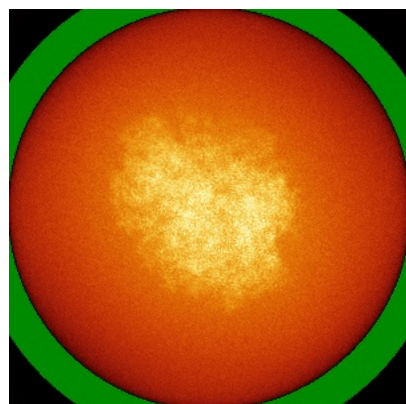


Y

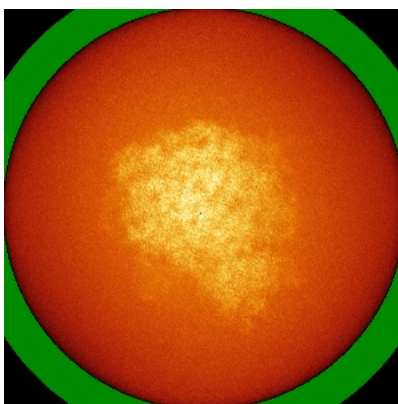


Z

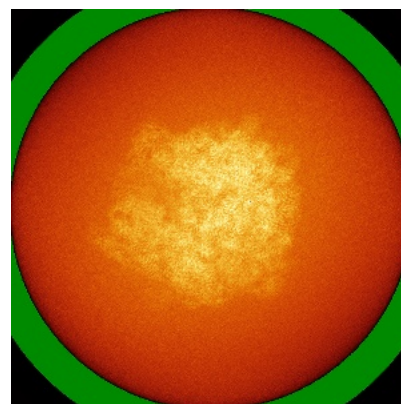
### 6.4.2 Raw map



X



Y

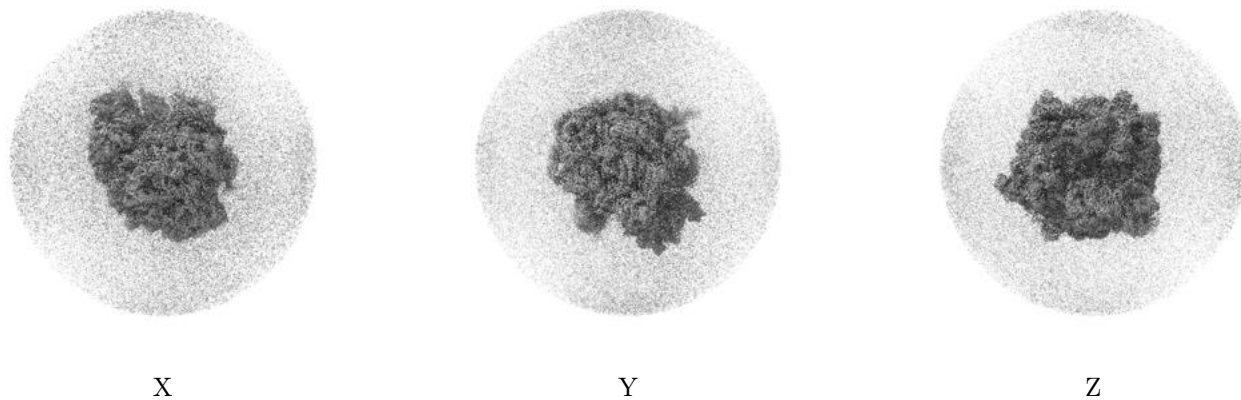


Z

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

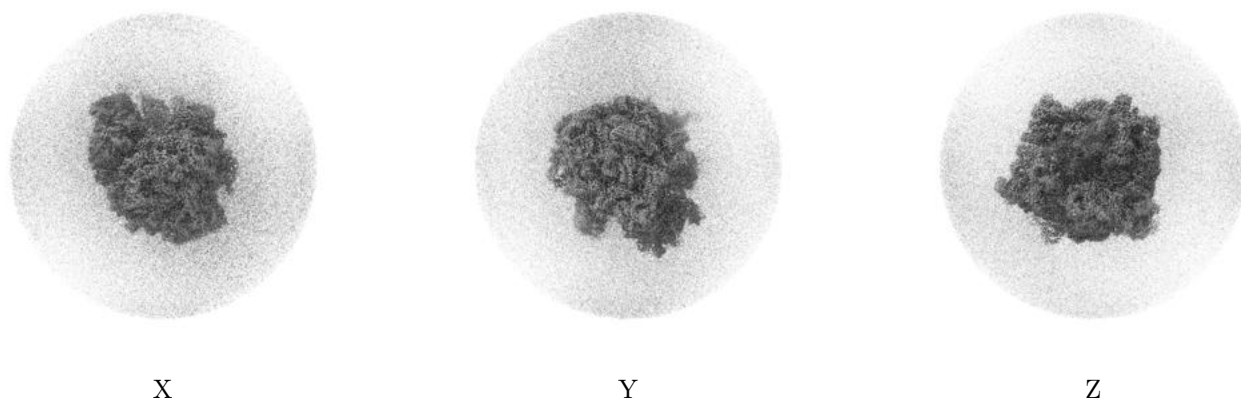
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

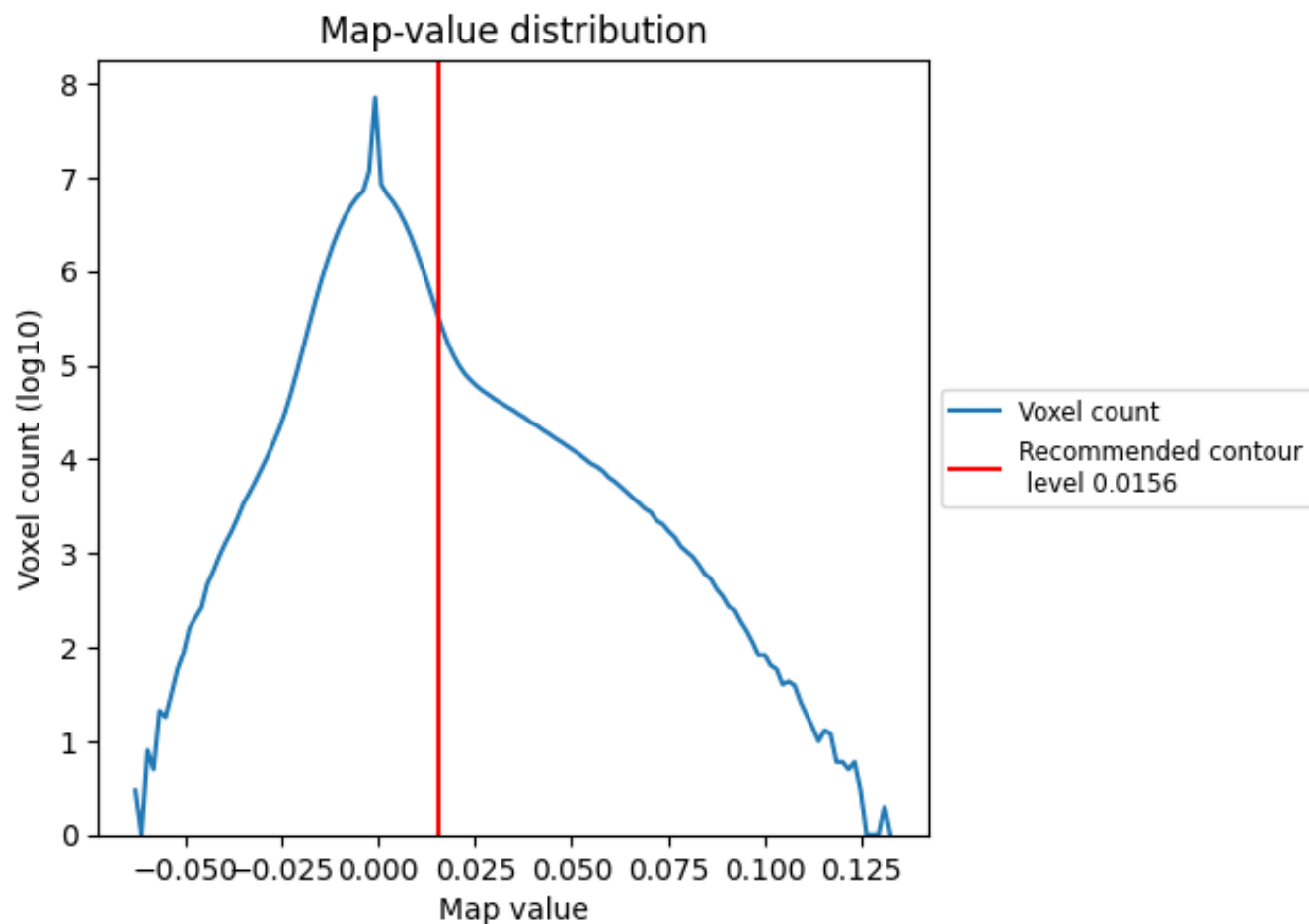
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

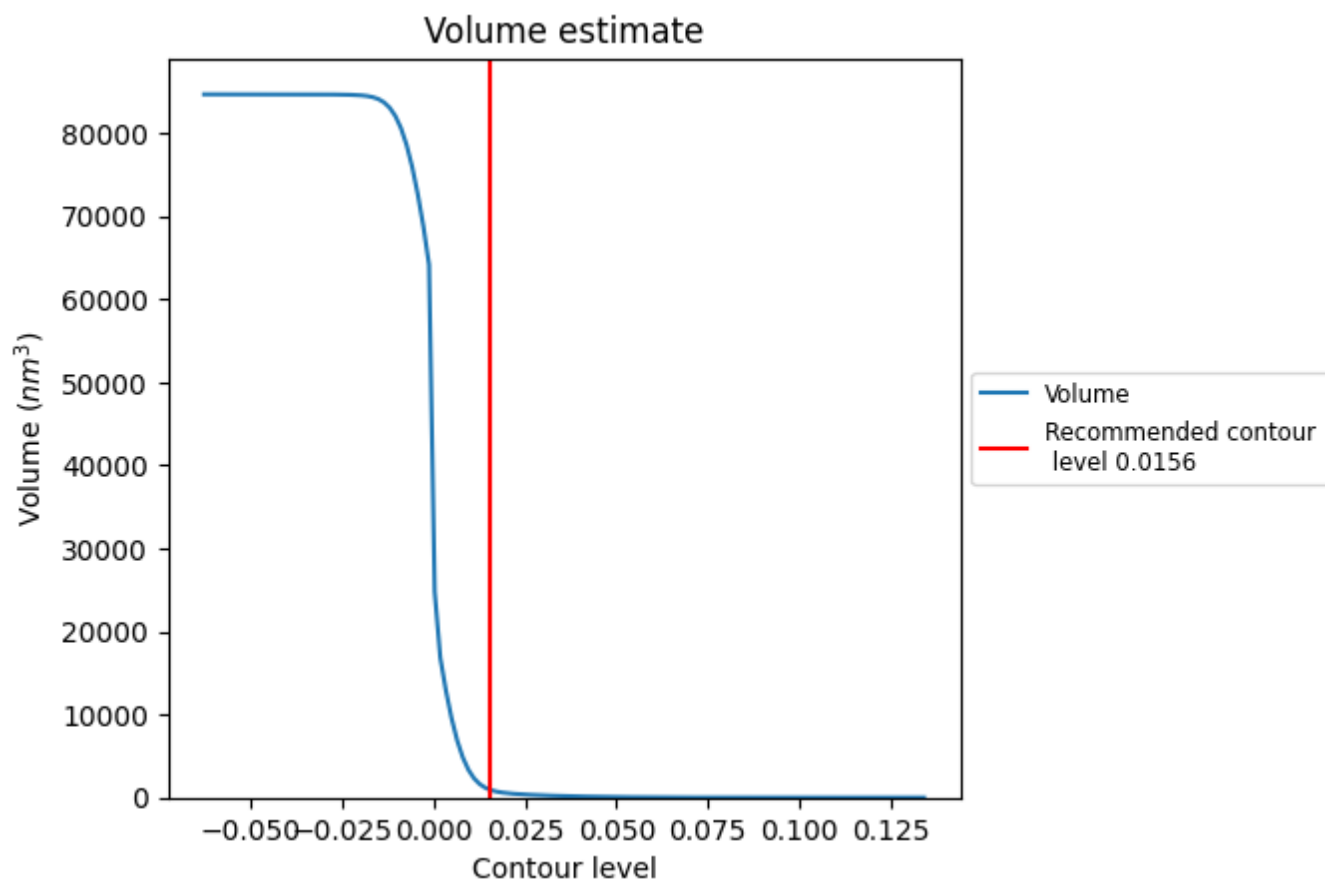
This section contains the results of statistical analysis of the map.

### 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.

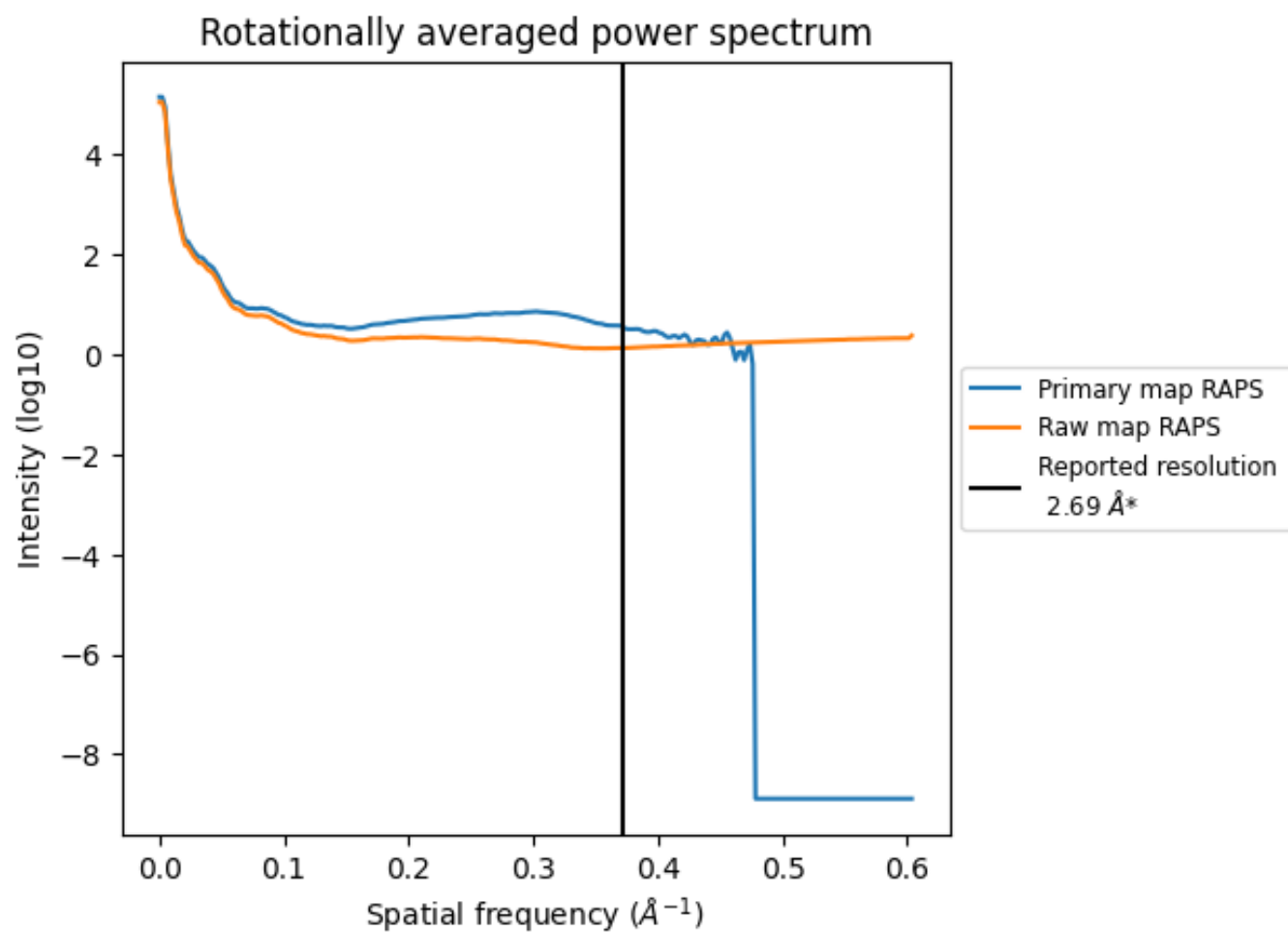
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 908  $\text{nm}^3$ ; this corresponds to an approximate mass of 821 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 ⓘ

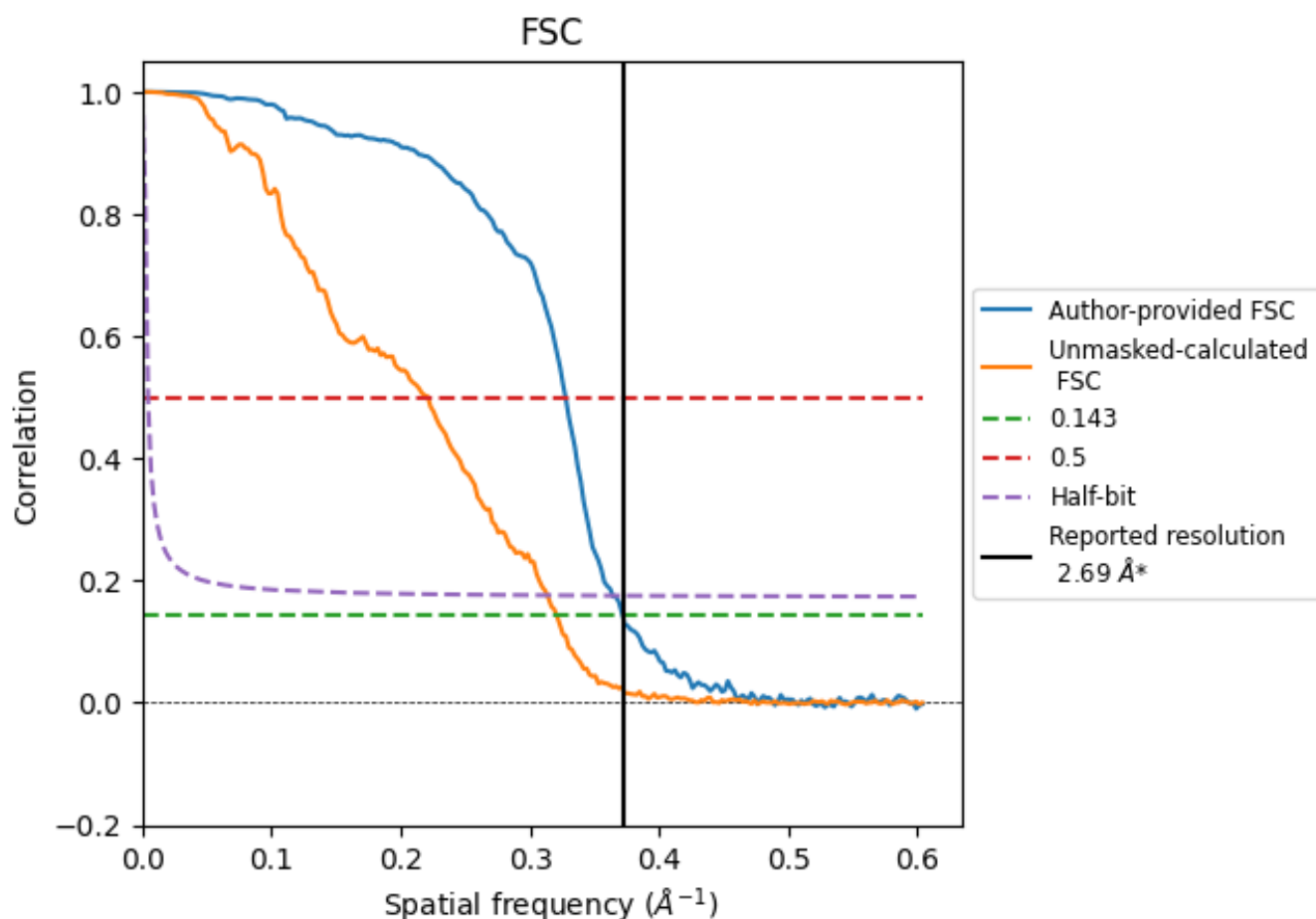


\*Reported resolution corresponds to spatial frequency of 0.372  $\text{\AA}^{-1}$

## 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 0.372  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

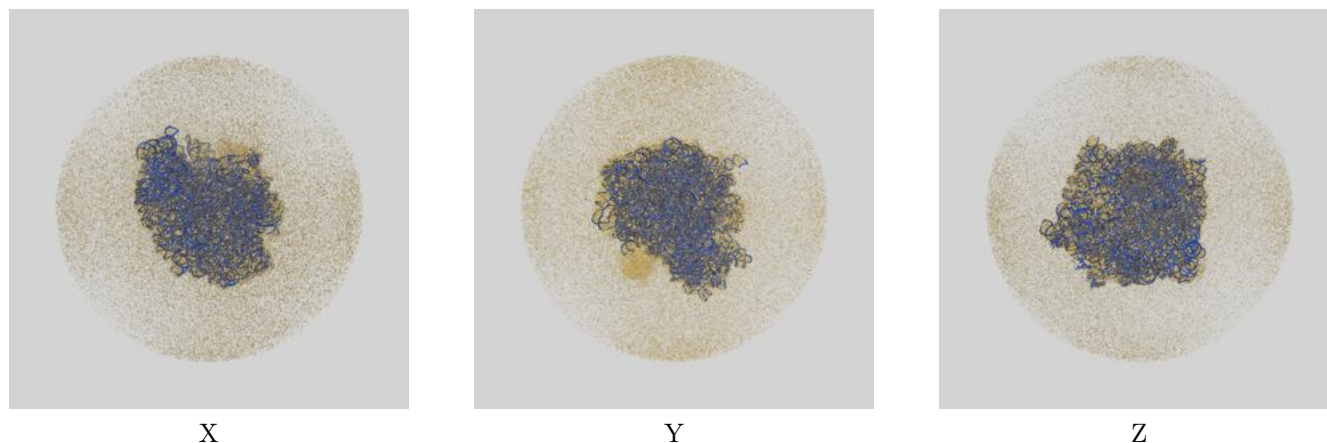
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.69                               | -    | -        |
| Author-provided FSC curve | 2.69                               | 3.05 | 2.75     |
| Unmasked-calculated*      | 3.12                               | 4.52 | 3.19     |

\*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 3.12 differs from the reported value 2.69 by more than 10 %

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

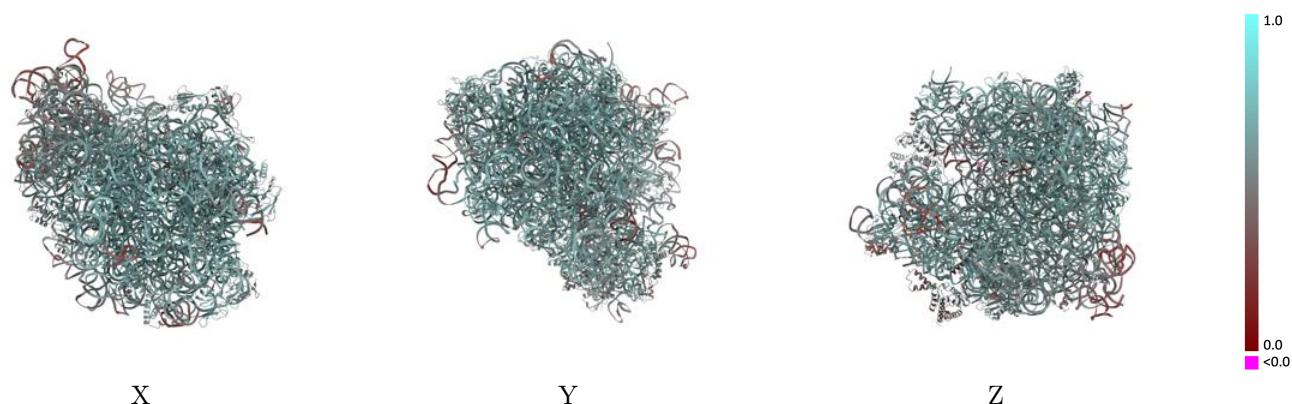
This section contains information regarding the fit between EMDB map EMD-35022 and PDB model 8HU1. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



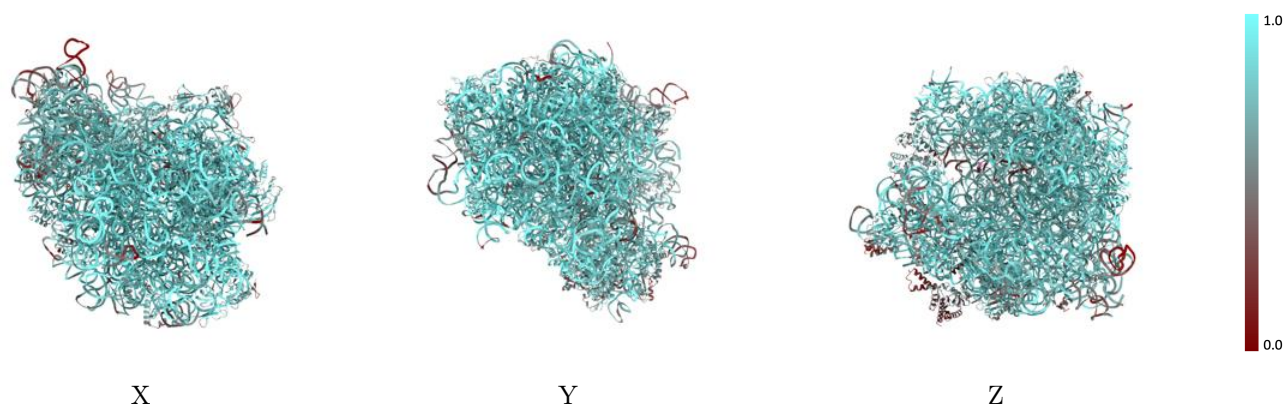
The images above show the 3D surface view of the map at the recommended contour level 0.0156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



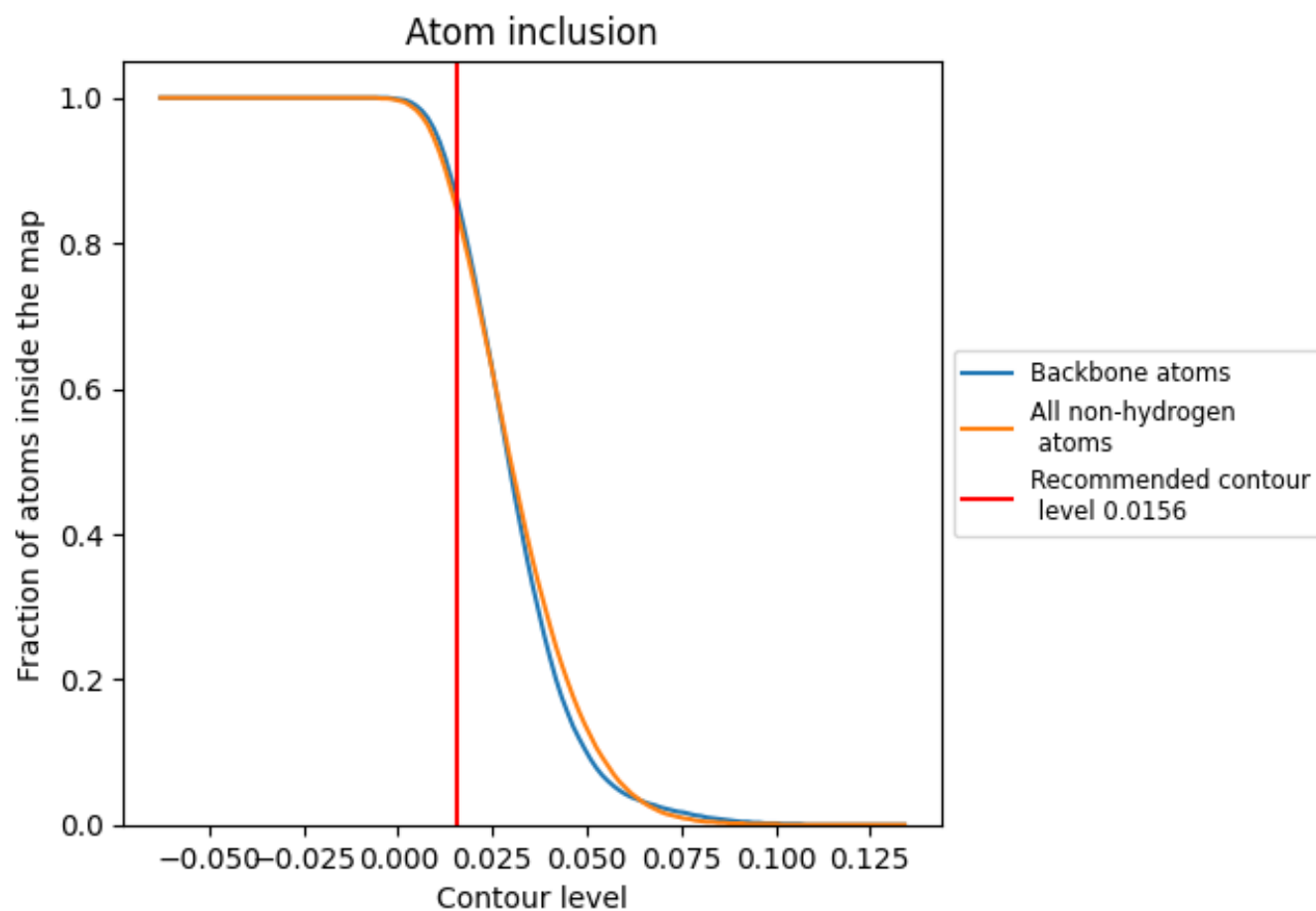
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0156).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.0156) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8460   |  0.5990   |
| 0     |  0.8310   |  0.6250   |
| 1     |  0.9410   |  0.6760   |
| 2     |  0.9350   |  0.6670   |
| 3     |  0.8660   |  0.6300   |
| 4     |  0.5670   |  0.5040   |
| A     |  0.8470   |  0.5800   |
| B     |  0.3820   |  0.4680   |
| C     |  0.7730   |  0.5930   |
| D     |  0.5780   |  0.5150   |
| E     |  0.8050   |  0.6010   |
| F     |  0.6710   |  0.5200   |
| G     |  0.6450   |  0.5360   |
| H     |  0.7970   |  0.5950   |
| I     |  0.7340  |  0.5760  |
| J     |  0.5940 |  0.5100 |
| K     |  0.7440 |  0.5690 |
| L     |  0.8130 |  0.6150 |
| M     |  0.7140 |  0.5580 |
| N     |  0.7680 |  0.5870 |
| O     |  0.7750 |  0.5810 |
| P     |  0.6230 |  0.5100 |
| Q     |  0.6830 |  0.5480 |
| R     |  0.7270 |  0.5700 |
| S     |  0.7550 |  0.5780 |
| T     |  0.5950 |  0.5100 |
| U     |  0.3900 |  0.4400 |
| V     |  0.6710 |  0.5030 |
| W     |  0.8390 |  0.5980 |
| X     |  0.6540 |  0.5020 |
| a     |  0.9190 |  0.6250 |
| b     |  0.8900 |  0.5950 |
| c     |  0.9220 |  0.6620 |
| d     |  0.8830 |  0.6420 |
| e     |  0.7800 |  0.5990 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| f     |  0.6880   |  0.5410   |
| g     |  0.6490   |  0.5300   |
| h     |  0.4170   |  0.4850   |
| i     |  0.8820   |  0.6370   |
| j     |  0.8520   |  0.6380   |
| k     |  0.8660   |  0.6360   |
| l     |  0.8660   |  0.6350   |
| m     |  0.9280   |  0.6540   |
| n     |  0.7990   |  0.5860   |
| o     |  0.8480   |  0.6320   |
| p     |  0.9110   |  0.6450   |
| q     |  0.8120   |  0.6050   |
| r     |  0.8590   |  0.6250   |
| s     |  0.7630   |  0.5890   |
| t     |  0.7310   |  0.5610   |
| u     |  0.7750   |  0.6000   |
| v     |  0.8930   |  0.6590   |
| w     |  0.8500  |  0.6250  |
| x     |  0.6730 |  0.5330 |
| y     |  0.8420 |  0.6140 |
| z     |  0.8720 |  0.6440 |