



## Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 04:34 PM EDT

PDB ID : 11DG / pdb\_000011dg  
EMDB ID : EMD-75634  
Title : Chimeric Escherichia coli 70S ribosome containing an evolved Vibrio cholerae 16S rRNA (VC-S4.4)  
Authors : Raskar, T.; Badran, A.; Fraser, J.; Costello, A.  
Deposited on : 2026-02-18  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.50

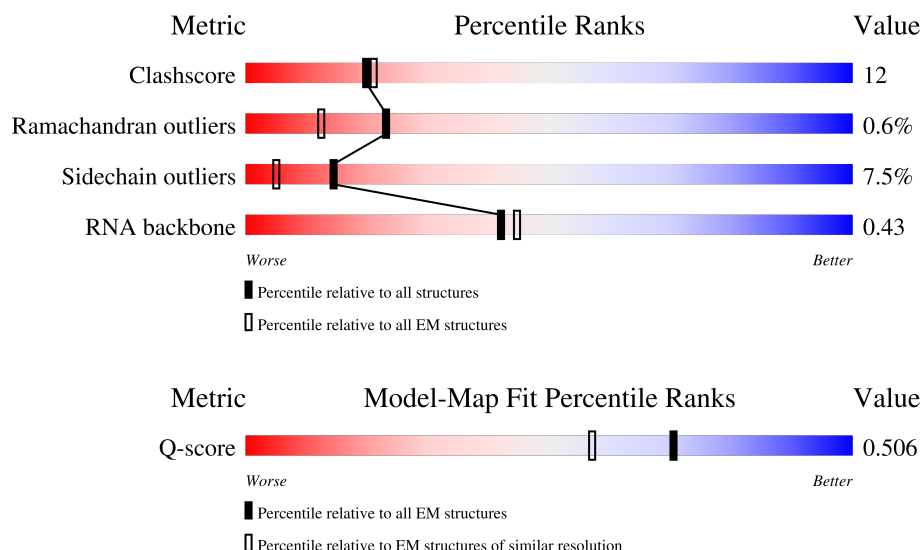
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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                       | 14081 ( 2.50 - 3.50 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 55     |                  |
| 2   | 1     | 46     |                  |
| 3   | 2     | 65     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 3     | 38     |                  |
| 5   | 4     | 70     |                  |
| 6   | 5     | 2      |                  |
| 7   | A     | 1517   |                  |
| 8   | B     | 241    |                  |
| 9   | C     | 233    |                  |
| 10  | D     | 206    |                  |
| 11  | E     | 167    |                  |
| 12  | F     | 135    |                  |
| 13  | G     | 179    |                  |
| 14  | H     | 130    |                  |
| 15  | I     | 130    |                  |
| 16  | J     | 103    |                  |
| 17  | K     | 129    |                  |
| 18  | L     | 124    |                  |
| 19  | M     | 118    |                  |
| 20  | N     | 101    |                  |
| 21  | O     | 89     |                  |
| 22  | P     | 82     |                  |
| 23  | Q     | 84     |                  |
| 24  | R     | 75     |                  |
| 25  | S     | 92     |                  |
| 26  | T     | 87     |                  |
| 27  | U     | 71     |                  |
| 28  | a     | 2904   |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | b     | 120    |                  |
| 30  | c     | 273    |                  |
| 31  | d     | 209    |                  |
| 32  | e     | 201    |                  |
| 33  | f     | 179    |                  |
| 34  | g     | 177    |                  |
| 35  | h     | 149    |                  |
| 36  | i     | 142    |                  |
| 37  | j     | 123    |                  |
| 38  | k     | 144    |                  |
| 39  | l     | 136    |                  |
| 40  | m     | 127    |                  |
| 41  | n     | 117    |                  |
| 42  | o     | 115    |                  |
| 43  | p     | 118    |                  |
| 44  | q     | 103    |                  |
| 45  | r     | 110    |                  |
| 46  | s     | 100    |                  |
| 47  | t     | 104    |                  |
| 48  | u     | 94     |                  |
| 49  | v     | 85     |                  |
| 50  | w     | 78     |                  |
| 51  | x     | 63     |                  |
| 52  | y     | 59     |                  |
| 53  | z     | 57     |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17  | BH2  | K     | 119 | X         | -        | -       | -                |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 138477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | 0     | 51       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 417   | 269 | 76 | 72 |         |       |

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 3   | 2     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 480   | 299 | 90 | 85 | 6 |         |       |

- Molecule 6 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|-------|
| 6   | 5     | 2        | Total | C  | N | O  | P | 0       | 0     |
|     |       |          | 42    | 19 | 8 | 13 | 2 |         |       |

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 7   | A     | 1517     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32564 | 14534 | 5976 | 10537 | 1517 |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 9 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | C     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | D     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 1026 | 315 | 297 | 4 |         |       |

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | E     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 717 | 217 | 212 | 6 |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein bS6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | F     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 530 | 151 | 151 | 7 |         |       |

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | G     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 750 | 231 | 218 | 4 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 978   | 616 | 173 | 183 | 6 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | I     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | J     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | K     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 540 | 173 | 160 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| K     | 119     | BH2      | ASN    | conflict | UNP A7ZSI6 |

- Molecule 18 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | L     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | M     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 552 | 179 | 157 | 3 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | N     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | O     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 22 is a protein called Small ribosomal subunit protein bS16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | P     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 403 | 127 | 112 | 1 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Q     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 641   | 406 | 120 | 112 | 3 |         |       |

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 24  | R     | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 345 | 102 | 96 | 1 |         |       |

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | S     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 427 | 127 | 112 | 2 |         |       |

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | T     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 669   | 412 | 138 | 115 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| T     | 58      | CYS      | VAL    | conflict | UNP A7ZHB2 |

- Molecule 27 is a protein called Small ribosomal subunit protein bS21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | U     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 589   | 366 | 125 | 97 | 1 |         |       |

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 28  | a     | 2753     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 59130 | 26384 | 10897 | 19096 | 2753 |         |       |

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 29  | b     | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2549  | 1135 | 466 | 829 | 119 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | c     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | d     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 980 | 288 | 294 | 4 |         |       |

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | e     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | f     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | g     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | h     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 303   | 194 | 54 | 54 | 1 |         |       |

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | i     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | j     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | k     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | l     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 686 | 205 | 177 | 7 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | m     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 585 | 194 | 161 | 5 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 41  | n     | 116      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |       |

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | o     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 43  | p     | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | q     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | r     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | s     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 47  | t     | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |         |       |

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 48  | u     | 94       | Total | C   | N   | O   | S       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3       | 0     |

- Molecule 49 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 49  | v     | 78       | Total | C   | N   | O   | S       | 0     |
|     |       |          | 586   | 362 | 116 | 107 | 1       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 50  | w     | 77       | Total | C   | N   | O   | S       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2       | 0     |

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 51  | x     | 62       | Total | C   | N  | O  | S       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1       | 0     |

- Molecule 52 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52  | y     | 58       | Total | C   | N  | O  | S       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2       | 0     |

- Molecule 53 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 53  | z     | 56       | Total | C   | N  | O  | S       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1       | 0     |

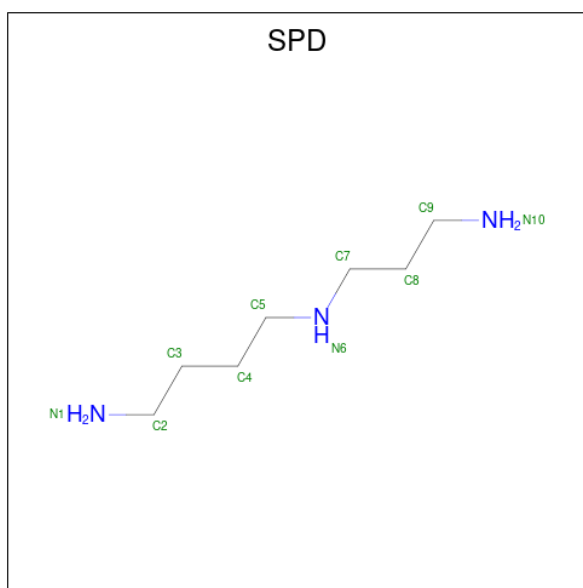
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 54  | 3     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 54  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

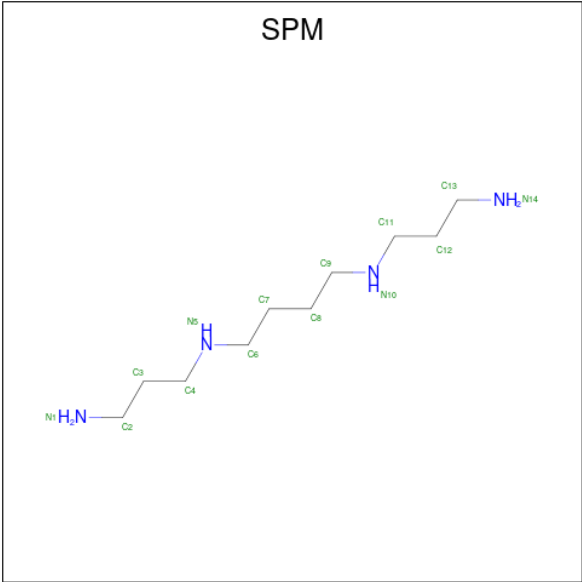
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 55  | A     | 55       | Total | Mg  | 0       |
|     |       |          | 55    | 55  |         |
| 55  | Q     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 55  | a     | 207      | Total | Mg  | 0       |
|     |       |          | 207   | 207 |         |
| 55  | b     | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 55  | c     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 55  | m     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 55  | n     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 55  | z     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 56 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 56  | a     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 57 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).

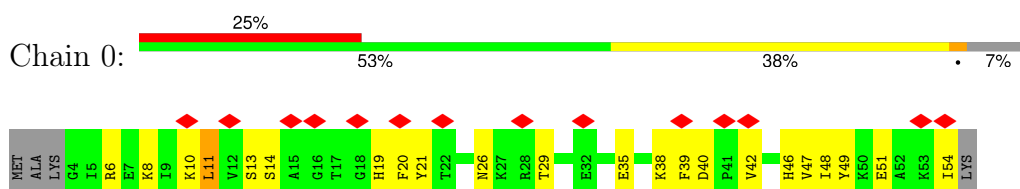


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 57  | a     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

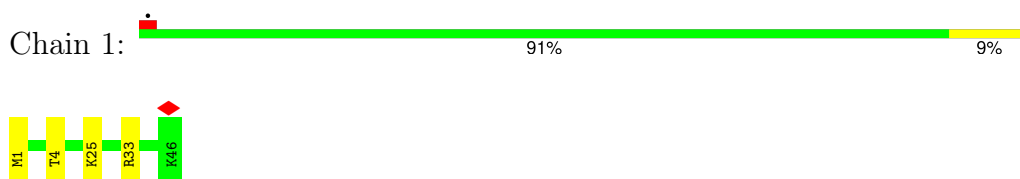
### 3 Residue-property plots [i](#)

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

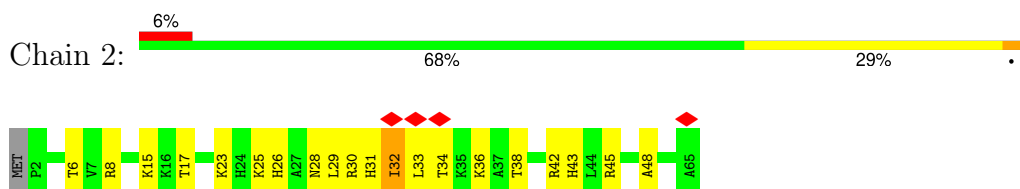
- Molecule 1: 50S ribosomal protein L33



- Molecule 2: Large ribosomal subunit protein bL34

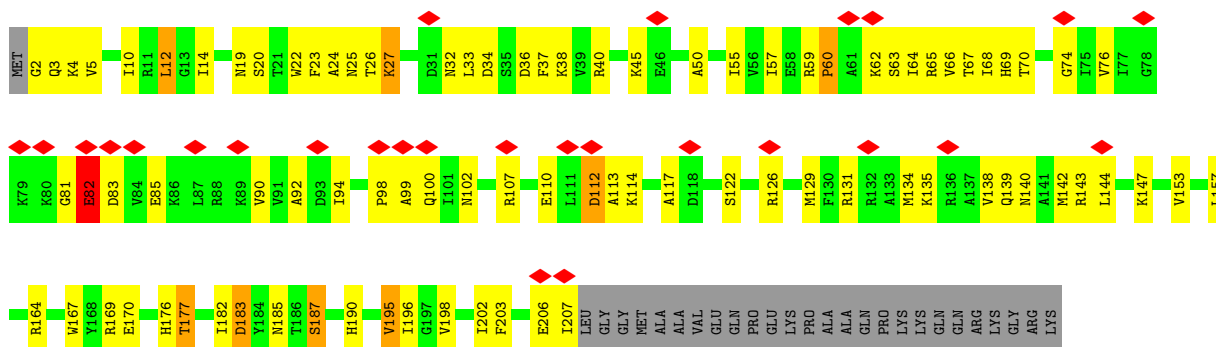


- Molecule 3: 50S ribosomal protein L35

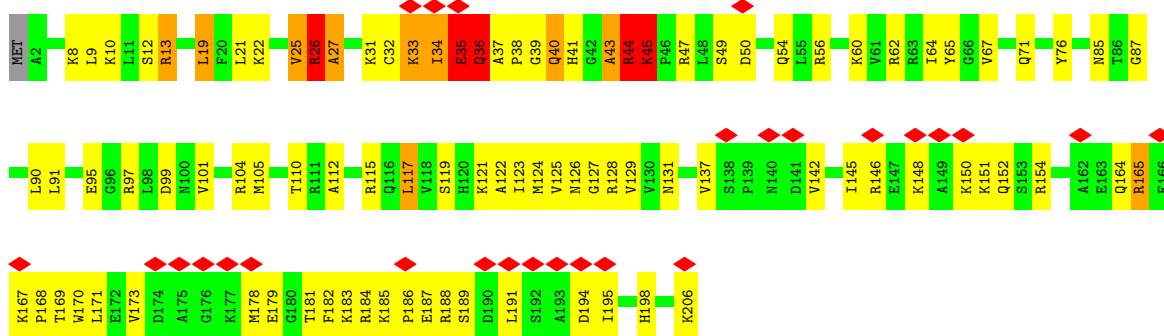




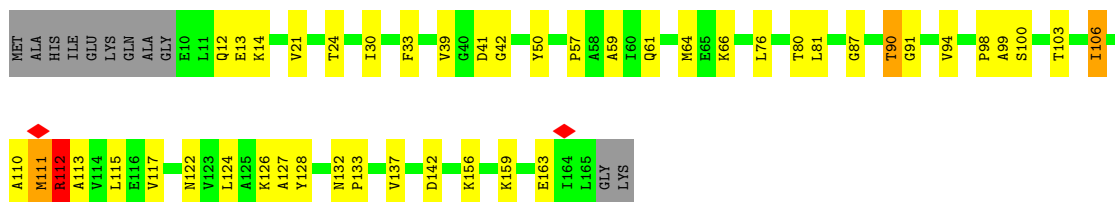




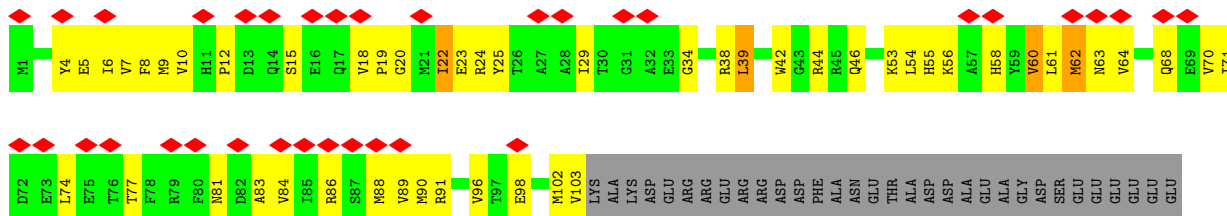
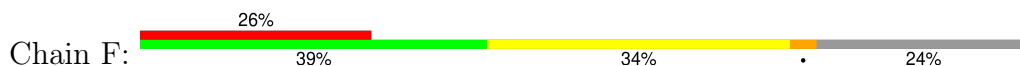
- Molecule 10: Small ribosomal subunit protein uS4



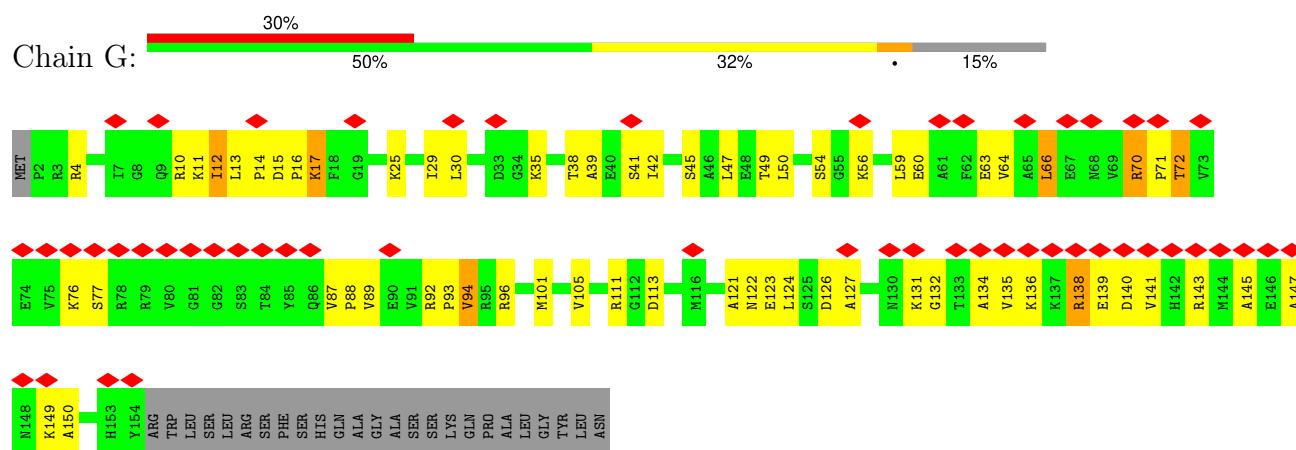
- Molecule 11: Small ribosomal subunit protein uS5



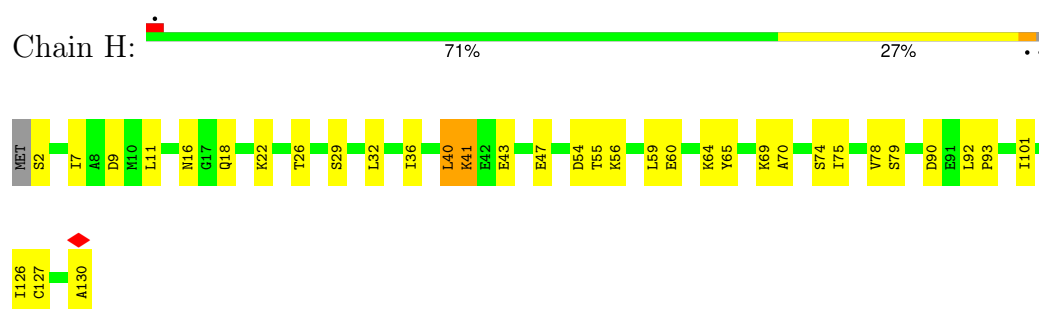
- Molecule 12: Small ribosomal subunit protein bS6



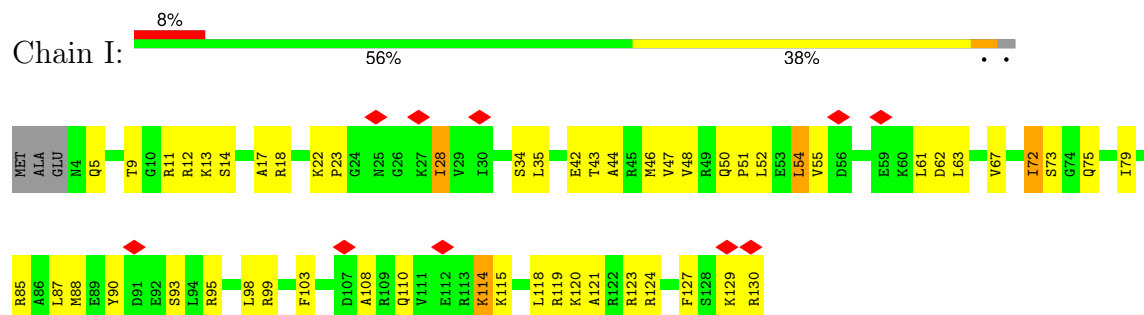
- Molecule 13: Small ribosomal subunit protein uS7



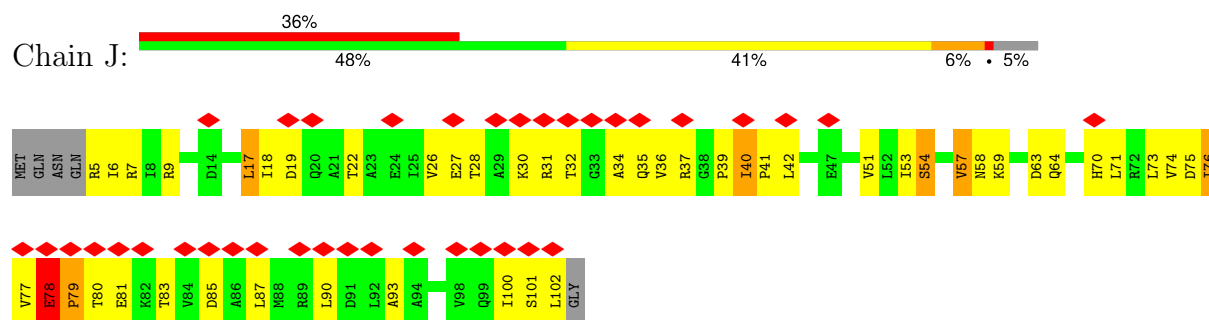
- Molecule 14: Small ribosomal subunit protein uS8



- Molecule 15: Small ribosomal subunit protein uS9

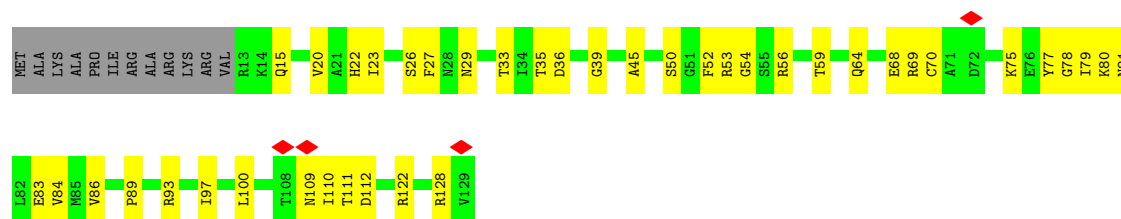


- Molecule 16: Small ribosomal subunit protein uS10



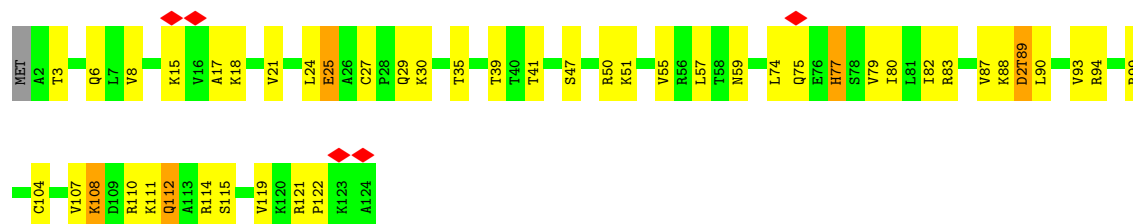
- Molecule 17: Small ribosomal subunit protein uS11





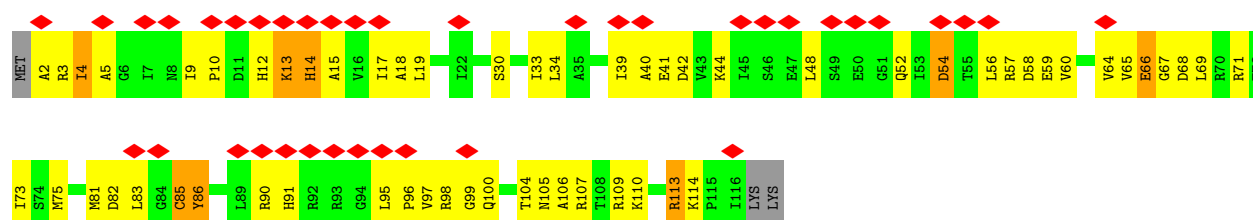
- Molecule 18: 30S ribosomal protein S12

Chain L: 62% 33%



- Molecule 19: Small ribosomal subunit protein uS13

Chain M: 32% 47% 43% 7%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N: 5% 69% 27%



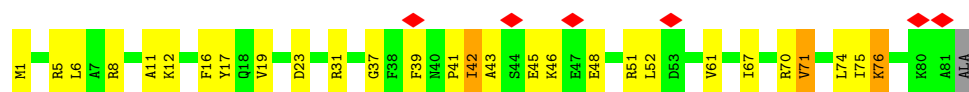
- Molecule 21: Small ribosomal subunit protein uS15

Chain O: 71% 25%

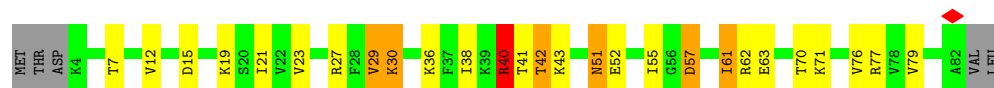


- Molecule 22: Small ribosomal subunit protein bS16

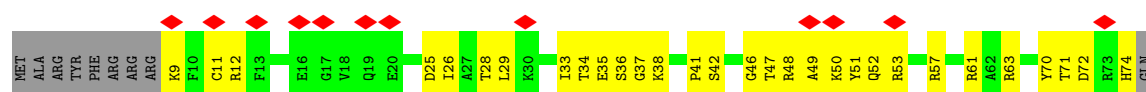
Chain P: 7% 65% 30%



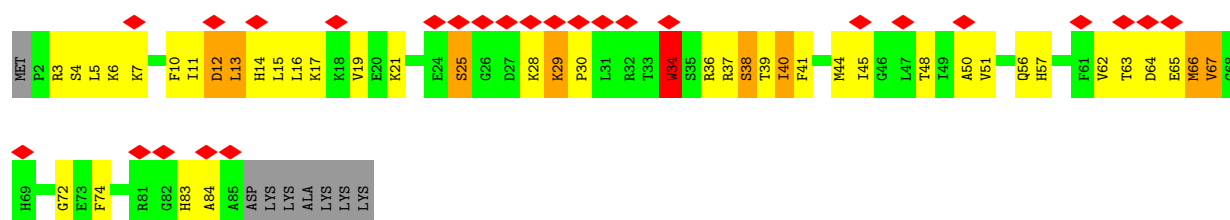
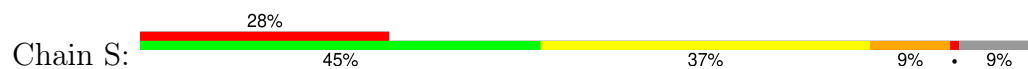
- Molecule 23: Small ribosomal subunit protein uS17



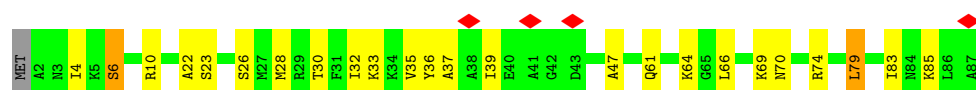
- Molecule 24: Small ribosomal subunit protein bS18



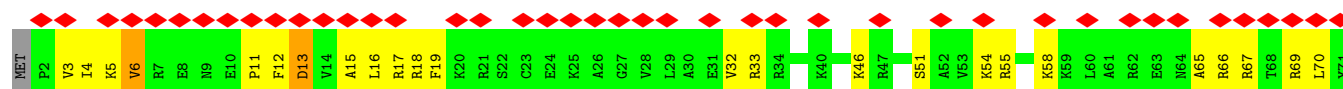
- Molecule 25: Small ribosomal subunit protein uS19



- Molecule 26: Small ribosomal subunit protein bS20



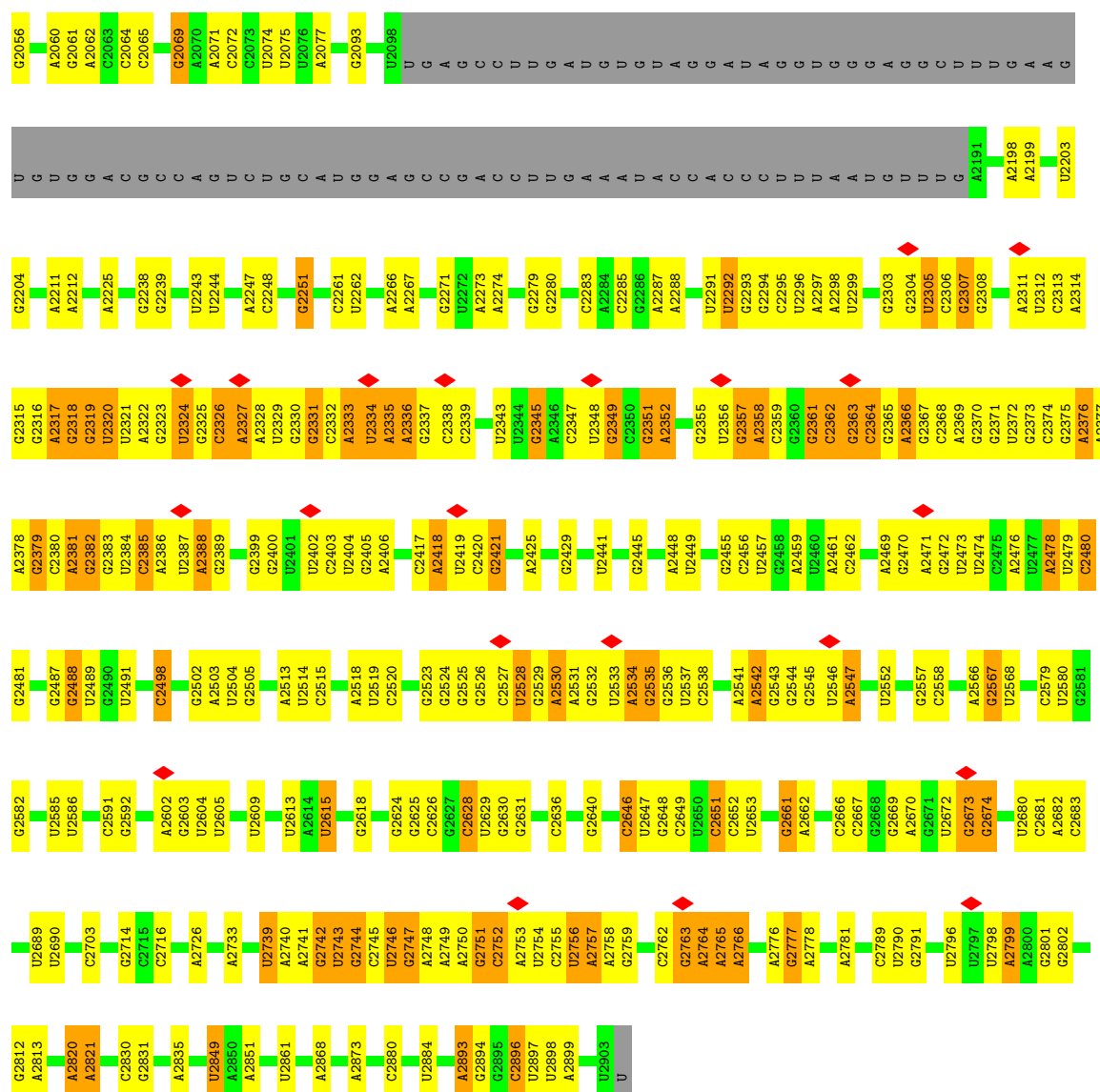
- Molecule 27: Small ribosomal subunit protein bS21



- Molecule 28: 23S ribosomal RNA



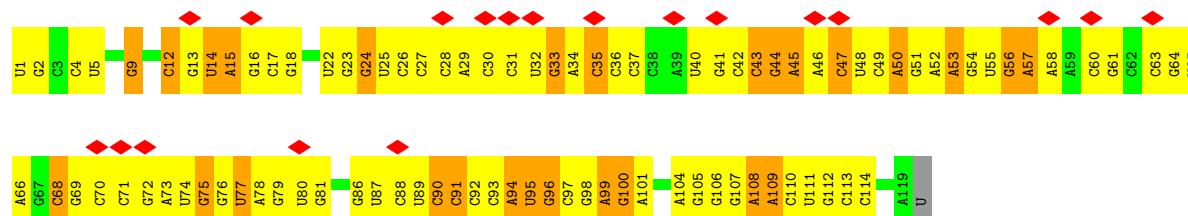




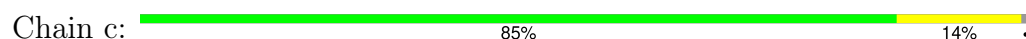
• Molecule 29: 5S ribosomal RNA



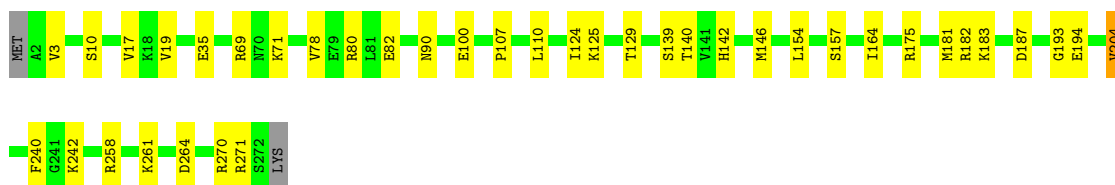
Chain b:



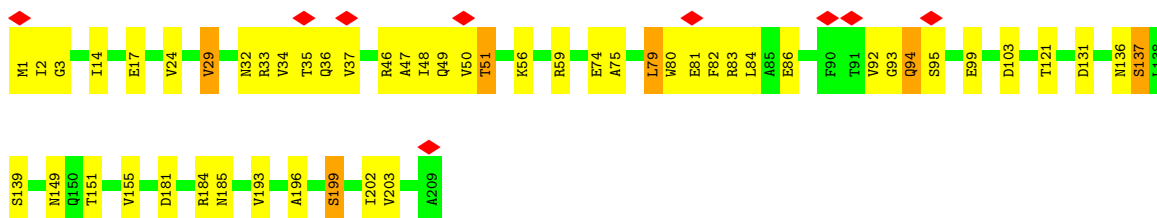
• Molecule 30: 50S ribosomal protein L2



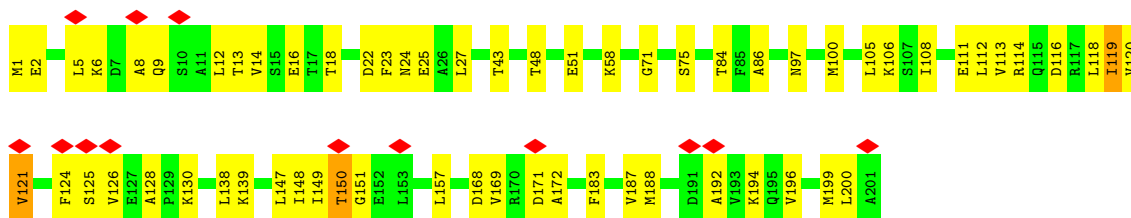
Chain c:



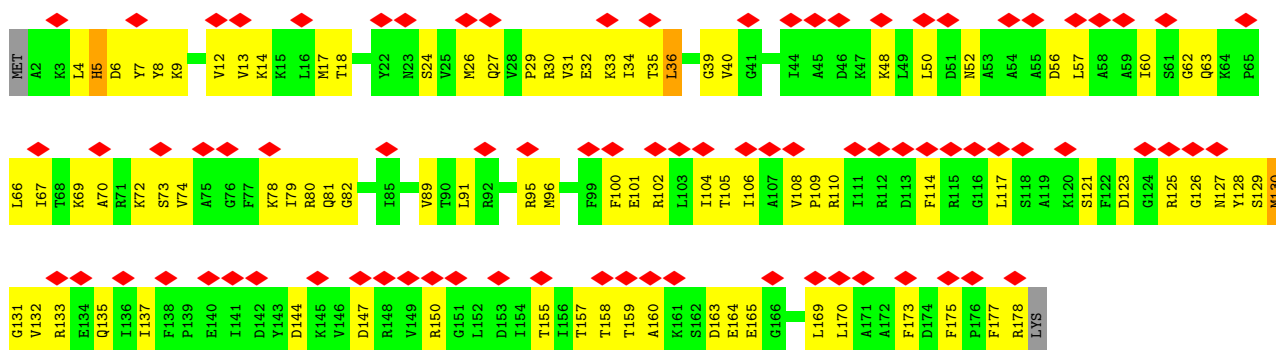
- Molecule 31: 50S ribosomal protein L3



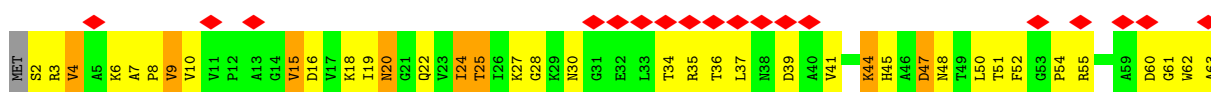
- Molecule 32: Large ribosomal subunit protein uL4



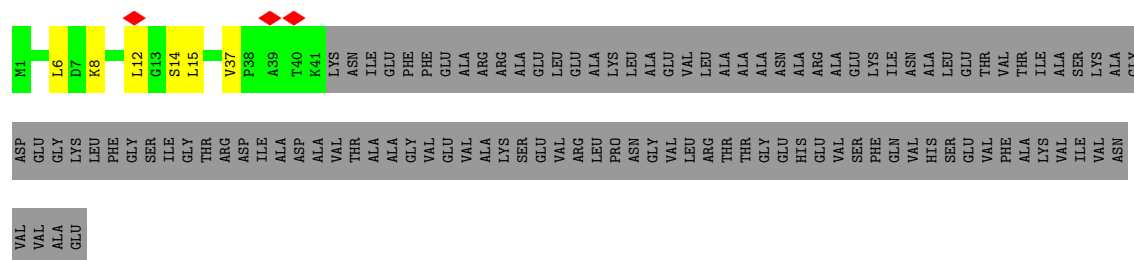
- Molecule 33: Large ribosomal subunit protein uL5



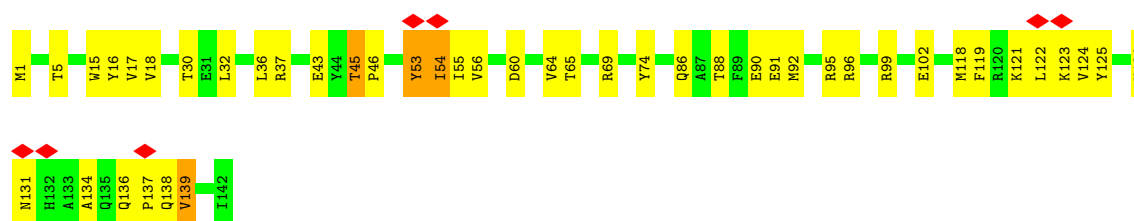
- Molecule 34: Large ribosomal subunit protein uL6



- Molecule 35: Large ribosomal subunit protein bL9



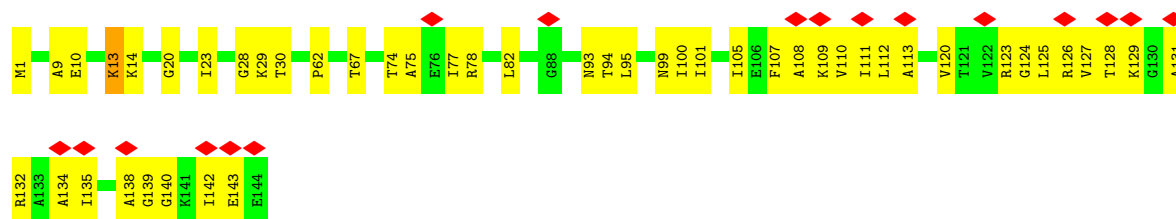
- Molecule 36: Large ribosomal subunit protein uL13



- Molecule 37: Large ribosomal subunit protein uL14

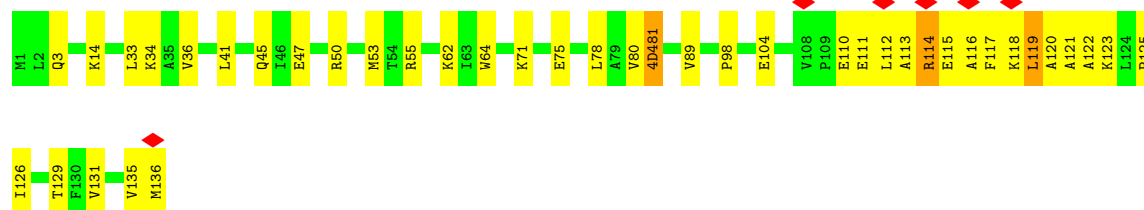


- Molecule 38: Large ribosomal subunit protein uL15



- Molecule 39: Large ribosomal subunit protein uL16

Chain l: 



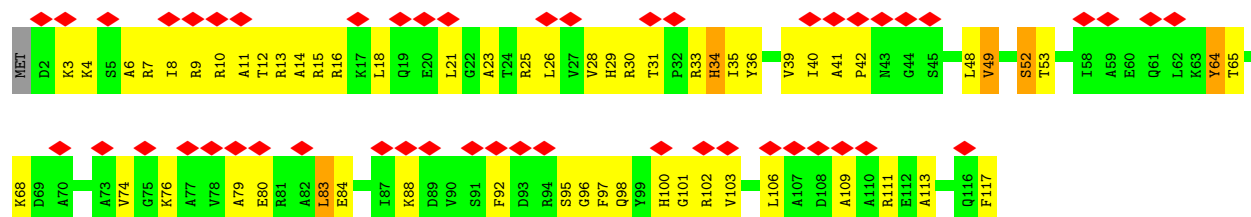
- Molecule 40: Large ribosomal subunit protein bL17

Chain m: 



- Molecule 41: Large ribosomal subunit protein uL18

Chain n: 



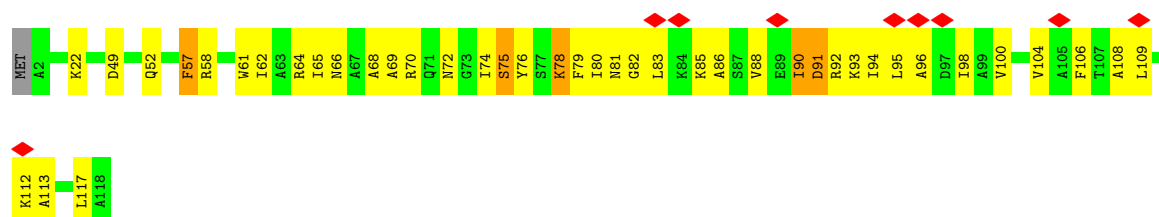
- Molecule 42: Large ribosomal subunit protein bL19

Chain o: 



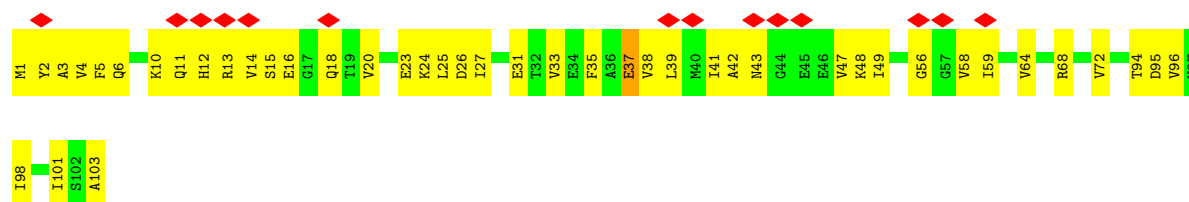
- Molecule 43: 50S ribosomal protein L20

Chain p: 

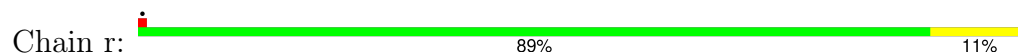


- Molecule 44: Large ribosomal subunit protein bL21

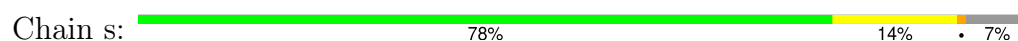
Chain q: 



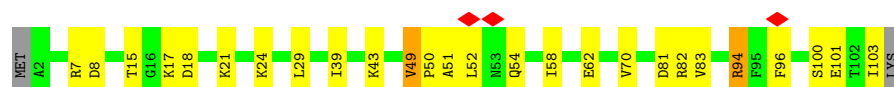
- Molecule 45: Large ribosomal subunit protein uL22



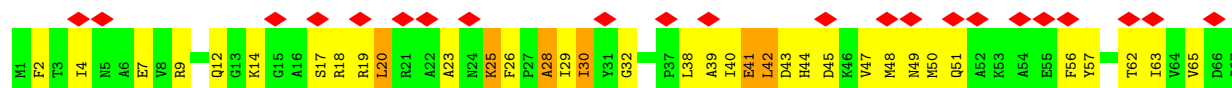
- Molecule 46: 50S ribosomal protein L23



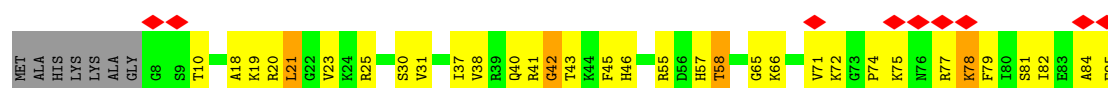
- Molecule 47: 50S ribosomal protein L24



- Molecule 48: Large ribosomal subunit protein bL25



- Molecule 49: 50S ribosomal protein L27



- Molecule 50: 50S ribosomal protein L28

Chain w:  78% 19% ..



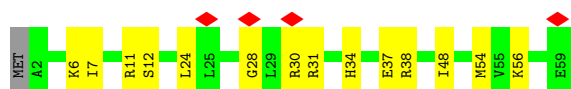
- Molecule 51: Large ribosomal subunit protein uL29

Chain x:  78% 21% .



- Molecule 52: 50S ribosomal protein L30

Chain y:  7% 75% 24% .



- Molecule 53: 50S ribosomal protein L32

Chain z:  79% 19% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 450287                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS GLACIOS                             | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 43.573                                  | Depositor |
| Minimum map value                    | -23.645                                 | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 2.8                                     | Depositor |
| Map size (Å)                         | 579.36, 579.36, 579.36                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.207, 1.207, 1.207                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, UR3, MA6, 1MG, OMU, MG, BH2, H2U, SPM, OMC, 6MZ, 5MU, MS6, PSU, OMG, G7M, 2MA, SPD, 2MG, D2T, 3TD, ZN, 4OC, MEQ, 4D4

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

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 1   | 0     | 0.25         | 0/424         | 0.58        | 1/565 (0.2%)    |
| 2   | 1     | 0.24         | 0/380         | 0.38        | 0/498           |
| 3   | 2     | 0.27         | 0/513         | 0.45        | 0/676           |
| 4   | 3     | 0.33         | 0/303         | 0.76        | 0/397           |
| 5   | 4     | 0.23         | 0/488         | 0.49        | 0/649           |
| 6   | 5     | 0.10         | 0/46          | 0.09        | 0/69            |
| 7   | A     | 0.25         | 0/36183       | 0.45        | 10/56432 (0.0%) |
| 8   | B     | 0.26         | 0/1784        | 0.64        | 2/2403 (0.1%)   |
| 9   | C     | 0.24         | 0/1651        | 0.63        | 1/2225 (0.0%)   |
| 10  | D     | 0.41         | 0/1664        | 0.80        | 2/2226 (0.1%)   |
| 11  | E     | 0.25         | 0/1165        | 0.65        | 1/1568 (0.1%)   |
| 12  | F     | 0.25         | 0/858         | 0.60        | 0/1160          |
| 13  | G     | 0.55         | 2/1219 (0.2%) | 0.92        | 4/1635 (0.2%)   |
| 14  | H     | 0.22         | 0/988         | 0.59        | 1/1326 (0.1%)   |
| 15  | I     | 0.22         | 0/1034        | 0.61        | 0/1375          |
| 16  | J     | 0.55         | 1/796 (0.1%)  | 0.99        | 3/1077 (0.3%)   |
| 17  | K     | 0.20         | 0/884         | 0.54        | 0/1191          |
| 18  | L     | 0.21         | 0/960         | 0.52        | 1/1286 (0.1%)   |
| 19  | M     | 0.24         | 0/900         | 0.78        | 2/1204 (0.2%)   |
| 20  | N     | 0.21         | 0/817         | 0.59        | 0/1088          |
| 21  | O     | 0.37         | 0/722         | 0.55        | 1/964 (0.1%)    |
| 22  | P     | 0.24         | 0/653         | 0.65        | 0/877           |
| 23  | Q     | 0.30         | 0/650         | 0.71        | 0/871           |
| 24  | R     | 0.19         | 0/553         | 0.55        | 0/742           |
| 25  | S     | 0.26         | 0/685         | 0.75        | 1/922 (0.1%)    |
| 26  | T     | 0.20         | 0/675         | 0.58        | 1/893 (0.1%)    |
| 27  | U     | 0.24         | 0/597         | 0.55        | 0/792           |
| 28  | a     | 0.26         | 0/65651       | 0.36        | 0/102413        |
| 29  | b     | 0.26         | 0/2850        | 0.43        | 0/4444          |
| 30  | c     | 0.22         | 0/2121        | 0.36        | 0/2852          |
| 31  | d     | 0.26         | 0/1576        | 0.47        | 0/2119          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 32  | e     | 0.24         | 0/1571          | 0.48        | 0/2113           |
| 33  | f     | 0.21         | 0/1434          | 0.41        | 0/1926           |
| 34  | g     | 0.22         | 0/1343          | 0.53        | 0/1816           |
| 35  | h     | 0.20         | 0/306           | 0.54        | 0/413            |
| 36  | i     | 0.29         | 0/1152          | 0.54        | 0/1551           |
| 37  | j     | 0.22         | 0/955           | 0.37        | 0/1279           |
| 38  | k     | 0.23         | 0/1062          | 0.46        | 0/1413           |
| 39  | l     | 0.26         | 0/1073          | 0.54        | 0/1433           |
| 40  | m     | 0.23         | 0/958           | 0.39        | 0/1281           |
| 41  | n     | 0.53         | 1/902 (0.1%)    | 0.47        | 0/1209           |
| 42  | o     | 0.21         | 0/929           | 0.35        | 0/1242           |
| 43  | p     | 0.36         | 0/960           | 0.66        | 0/1278           |
| 44  | q     | 0.27         | 0/829           | 0.56        | 0/1107           |
| 45  | r     | 0.20         | 0/864           | 0.29        | 0/1156           |
| 46  | s     | 0.21         | 0/744           | 0.42        | 0/994            |
| 47  | t     | 0.21         | 0/787           | 0.49        | 0/1051           |
| 48  | u     | 0.33         | 1/766 (0.1%)    | 0.63        | 0/1025           |
| 49  | v     | 0.29         | 0/593           | 0.67        | 1/785 (0.1%)     |
| 50  | w     | 0.20         | 0/635           | 0.35        | 0/848            |
| 51  | x     | 0.22         | 0/502           | 0.52        | 0/667            |
| 52  | y     | 0.25         | 0/453           | 0.54        | 0/605            |
| 53  | z     | 0.21         | 0/450           | 0.37        | 0/599            |
| All | All   | 0.27         | 5/149058 (0.0%) | 0.45        | 32/222730 (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 |
|-----|-------|---------------------|---------------------|
| 10  | D     | 0                   | 3                   |
| 11  | E     | 0                   | 1                   |
| 16  | J     | 0                   | 1                   |
| 17  | K     | 1                   | 0                   |
| 20  | N     | 0                   | 1                   |
| 21  | O     | 0                   | 1                   |
| 23  | Q     | 0                   | 1                   |
| 34  | g     | 0                   | 1                   |
| 39  | l     | 0                   | 3                   |
| All | All   | 1                   | 12                  |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 13  | G     | 14  | PRO  | CG-CD | -15.01 | 0.99        | 1.50     |
| 41  | n     | 34  | HIS  | C-N   | -13.82 | 1.25        | 1.33     |
| 16  | J     | 79  | PRO  | CG-CD | -12.36 | 1.08        | 1.50     |
| 13  | G     | 14  | PRO  | N-CD  | 6.37   | 1.56        | 1.47     |
| 48  | u     | 28  | ALA  | C-N   | -5.12  | 1.30        | 1.33     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 13  | G     | 14   | PRO  | N-CD-CG     | -18.57 | 75.34       | 103.20   |
| 16  | J     | 79   | PRO  | N-CD-CG     | -16.56 | 78.36       | 103.20   |
| 16  | J     | 79   | PRO  | CA-CB-CG    | -12.96 | 79.88       | 104.50   |
| 13  | G     | 14   | PRO  | CA-CB-CG    | -11.90 | 81.90       | 104.50   |
| 13  | G     | 14   | PRO  | CA-N-CD     | -9.30  | 98.98       | 112.00   |
| 13  | G     | 14   | PRO  | CB-CG-CD    | 8.77   | 134.16      | 106.10   |
| 7   | A     | 413  | A    | P-O3'-C3'   | -8.73  | 107.11      | 120.20   |
| 7   | A     | 422  | C    | P-O3'-C3'   | -8.48  | 107.48      | 120.20   |
| 7   | A     | 425  | G    | P-O3'-C3'   | -8.29  | 107.77      | 120.20   |
| 7   | A     | 415  | A    | P-O3'-C3'   | -8.05  | 108.13      | 120.20   |
| 11  | E     | 106  | ILE  | N-CA-C      | -7.83  | 104.94      | 111.91   |
| 7   | A     | 1004 | A    | C2'-C3'-O3' | 7.23   | 120.34      | 109.50   |
| 10  | D     | 39   | GLY  | CA-C-O      | -6.84  | 117.52      | 122.45   |
| 16  | J     | 19   | ASP  | N-CA-C      | -6.80  | 104.13      | 113.18   |
| 7   | A     | 420  | U    | P-O3'-C3'   | -6.77  | 110.04      | 120.20   |
| 26  | T     | 66   | LEU  | N-CA-C      | -6.54  | 106.51      | 114.75   |
| 1   | 0     | 11   | LEU  | CA-CB-CG    | 6.41   | 138.72      | 116.30   |
| 9   | C     | 82   | GLU  | CA-CB-CG    | 6.33   | 126.75      | 114.10   |
| 7   | A     | 424  | G    | P-O3'-C3'   | -6.15  | 110.97      | 120.20   |
| 18  | L     | 25   | GLU  | CA-CB-CG    | 5.70   | 125.50      | 114.10   |
| 25  | S     | 34   | TRP  | N-CA-C      | -5.62  | 107.67      | 114.75   |
| 19  | M     | 86   | TYR  | N-CA-C      | -5.55  | 105.49      | 114.09   |
| 14  | H     | 93   | PRO  | CA-N-CD     | -5.53  | 104.26      | 112.00   |
| 7   | A     | 412  | C    | P-O3'-C3'   | -5.51  | 111.93      | 120.20   |
| 21  | O     | 22   | THR  | N-CA-C      | -5.35  | 106.92      | 113.50   |
| 10  | D     | 19   | LEU  | N-CA-C      | -5.32  | 106.57      | 113.16   |
| 8   | B     | 207  | ILE  | N-CA-C      | -5.27  | 108.70      | 113.71   |
| 8   | B     | 107  | VAL  | N-CA-C      | -5.26  | 108.37      | 113.53   |
| 49  | v     | 42   | GLY  | N-CA-C      | -5.26  | 106.11      | 112.48   |
| 19  | M     | 66   | GLU  | CB-CA-C     | -5.23  | 110.56      | 116.63   |
| 7   | A     | 423  | G    | C2'-C3'-O3' | 5.22   | 117.33      | 109.50   |
| 7   | A     | 421  | U    | P-O3'-C3'   | -5.13  | 112.50      | 120.20   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 17  | K     | 119 | BH2  | CB   |

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 10  | D     | 13  | ARG  | Sidechain |
| 10  | D     | 26  | ARG  | Sidechain |
| 10  | D     | 44  | ARG  | Sidechain |
| 11  | E     | 112 | ARG  | Sidechain |
| 16  | J     | 78  | GLU  | Peptide   |
| 20  | N     | 85  | ARG  | Sidechain |
| 21  | O     | 17  | ARG  | Sidechain |
| 23  | Q     | 40  | ARG  | Sidechain |
| 34  | g     | 47  | ASP  | Peptide   |
| 39  | l     | 119 | LEU  | Peptide   |
| 39  | l     | 80  | VAL  | Mainchain |
| 39  | l     | 81  | 4D4  | Mainchain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 417   | 0        | 451      | 21      | 0            |
| 2   | 1     | 377   | 0        | 418      | 5       | 0            |
| 3   | 2     | 504   | 0        | 572      | 18      | 0            |
| 4   | 3     | 302   | 0        | 340      | 31      | 0            |
| 5   | 4     | 480   | 0        | 478      | 22      | 0            |
| 6   | 5     | 42    | 0        | 23       | 0       | 0            |
| 7   | A     | 32564 | 0        | 16407    | 523     | 0            |
| 8   | B     | 1753  | 0        | 1780     | 58      | 0            |
| 9   | C     | 1624  | 0        | 1696     | 63      | 0            |
| 10  | D     | 1642  | 0        | 1704     | 73      | 0            |
| 11  | E     | 1152  | 0        | 1196     | 29      | 0            |
| 12  | F     | 839   | 0        | 833      | 42      | 0            |
| 13  | G     | 1203  | 0        | 1254     | 49      | 0            |
| 14  | H     | 978   | 0        | 1031     | 24      | 0            |
| 15  | I     | 1022  | 0        | 1070     | 46      | 0            |
| 16  | J     | 786   | 0        | 828      | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17  | K     | 876   | 0        | 882      | 35      | 0            |
| 18  | L     | 957   | 0        | 1016     | 27      | 0            |
| 19  | M     | 891   | 0        | 952      | 60      | 0            |
| 20  | N     | 805   | 0        | 844      | 28      | 0            |
| 21  | O     | 714   | 0        | 734      | 12      | 0            |
| 22  | P     | 643   | 0        | 661      | 23      | 0            |
| 23  | Q     | 641   | 0        | 682      | 16      | 0            |
| 24  | R     | 544   | 0        | 565      | 28      | 0            |
| 25  | S     | 668   | 0        | 693      | 43      | 0            |
| 26  | T     | 669   | 0        | 715      | 17      | 0            |
| 27  | U     | 589   | 0        | 629      | 27      | 0            |
| 28  | a     | 59130 | 0        | 29768    | 760     | 0            |
| 29  | b     | 2549  | 0        | 1291     | 121     | 0            |
| 30  | c     | 2082  | 0        | 2154     | 19      | 0            |
| 31  | d     | 1566  | 0        | 1617     | 46      | 0            |
| 32  | e     | 1552  | 0        | 1619     | 56      | 0            |
| 33  | f     | 1410  | 0        | 1444     | 79      | 0            |
| 34  | g     | 1323  | 0        | 1371     | 106     | 0            |
| 35  | h     | 303   | 0        | 327      | 4       | 0            |
| 36  | i     | 1129  | 0        | 1162     | 66      | 0            |
| 37  | j     | 946   | 0        | 1023     | 20      | 0            |
| 38  | k     | 1053  | 0        | 1129     | 49      | 0            |
| 39  | l     | 1075  | 0        | 1145     | 33      | 0            |
| 40  | m     | 945   | 0        | 989      | 11      | 0            |
| 41  | n     | 892   | 0        | 923      | 55      | 0            |
| 42  | o     | 917   | 0        | 962      | 9       | 0            |
| 43  | p     | 947   | 0        | 1019     | 67      | 0            |
| 44  | q     | 816   | 0        | 839      | 45      | 0            |
| 45  | r     | 857   | 0        | 922      | 6       | 0            |
| 46  | s     | 738   | 0        | 807      | 8       | 0            |
| 47  | t     | 779   | 0        | 831      | 22      | 0            |
| 48  | u     | 753   | 0        | 780      | 77      | 0            |
| 49  | v     | 586   | 0        | 596      | 48      | 0            |
| 50  | w     | 625   | 0        | 652      | 5       | 0            |
| 51  | x     | 501   | 0        | 531      | 7       | 0            |
| 52  | y     | 449   | 0        | 488      | 11      | 0            |
| 53  | z     | 444   | 0        | 458      | 7       | 0            |
| 54  | 3     | 1     | 0        | 0        | 0       | 0            |
| 54  | 4     | 1     | 0        | 0        | 0       | 0            |
| 55  | A     | 55    | 0        | 0        | 0       | 0            |
| 55  | Q     | 1     | 0        | 0        | 0       | 0            |
| 55  | a     | 207   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55  | b     | 5      | 0        | 0        | 0       | 0            |
| 55  | c     | 1      | 0        | 0        | 0       | 0            |
| 55  | m     | 1      | 0        | 0        | 0       | 0            |
| 55  | n     | 1      | 0        | 0        | 0       | 0            |
| 55  | z     | 1      | 0        | 0        | 0       | 0            |
| 56  | a     | 140    | 0        | 266      | 12      | 0            |
| 57  | a     | 14     | 0        | 26       | 1       | 0            |
| All | All   | 138477 | 0        | 93593    | 2821    | 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 12.

All (2821) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 29:b:78:A:H62   | 29:b:98:G:N2    | 1.20                     | 1.38              |
| 7:A:998:C:C6    | 7:A:1044:A:C5'  | 2.07                     | 1.37              |
| 28:a:1418:G:H21 | 28:a:1580:A:N6  | 1.23                     | 1.37              |
| 28:a:1020:A:N6  | 28:a:1141:U:C2  | 2.00                     | 1.29              |
| 7:A:73:C:N4     | 7:A:96:U:H3     | 1.30                     | 1.29              |
| 28:a:2739:U:H3  | 28:a:2764:A:N6  | 1.28                     | 1.28              |
| 29:b:77:U:H3    | 29:b:99:A:N6    | 1.31                     | 1.28              |
| 29:b:78:A:N6    | 29:b:98:G:H21   | 1.30                     | 1.28              |
| 28:a:1418:G:N2  | 28:a:1580:A:H62 | 1.31                     | 1.25              |
| 7:A:998:C:C2'   | 7:A:999:C:O2    | 1.90                     | 1.19              |
| 28:a:2352:A:N6  | 28:a:2365:G:H21 | 1.42                     | 1.18              |
| 7:A:998:C:H2'   | 7:A:999:C:O2    | 1.41                     | 1.17              |
| 28:a:2352:A:H62 | 28:a:2365:G:N2  | 1.39                     | 1.17              |
| 7:A:998:C:C6    | 7:A:1044:A:H5'  | 1.81                     | 1.13              |
| 28:a:2472:G:H21 | 28:a:2478:A:N6  | 1.46                     | 1.12              |
| 3:2:33:LEU:HB2  | 3:2:36:LYS:HG3  | 1.41                     | 1.02              |
| 7:A:998:C:C6    | 7:A:1044:A:H5'' | 1.89                     | 1.02              |
| 7:A:998:C:O2'   | 7:A:999:C:O2    | 1.77                     | 1.02              |
| 28:a:2472:G:N2  | 28:a:2478:A:H62 | 1.59                     | 1.01              |
| 29:b:76:G:N1    | 29:b:100:G:O6   | 1.92                     | 1.01              |
| 29:b:77:U:O4    | 29:b:99:A:N7    | 1.94                     | 1.01              |
| 7:A:836:G:H1    | 7:A:850:U:H3    | 1.06                     | 1.01              |
| 28:a:996:A:H4'  | 44:q:11:GLN:HG3 | 1.42                     | 0.99              |
| 28:a:600:G:H1   | 28:a:657:U:H3   | 1.04                     | 0.99              |
| 28:a:2739:U:O4  | 28:a:2764:A:N7  | 1.97                     | 0.97              |
| 28:a:1039:A:H2  | 28:a:1116:G:H1  | 0.99                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:i:53:TYR:HA    | 36:i:121:LYS:HB3  | 1.47                     | 0.96              |
| 28:a:2345:G:O6    | 28:a:2371:G:N1    | 1.98                     | 0.95              |
| 3:2:31:HIS:HD2    | 3:2:32:ILE:HG13   | 1.31                     | 0.95              |
| 28:a:2648:G:O6    | 28:a:2672:U:O4    | 1.85                     | 0.94              |
| 7:A:998:C:C5      | 7:A:1044:A:H5''   | 2.02                     | 0.94              |
| 28:a:600:G:O6     | 28:a:657:U:O4     | 1.85                     | 0.94              |
| 10:D:8:LYS:HE3    | 10:D:21:LEU:HB3   | 1.47                     | 0.93              |
| 7:A:1151:C:H1'    | 16:J:41:PRO:HB3   | 1.47                     | 0.93              |
| 29:b:77:U:N3      | 29:b:99:A:N6      | 1.97                     | 0.93              |
| 7:A:1023:A:H1'    | 7:A:1024:G:H5'    | 1.49                     | 0.91              |
| 28:a:2331:G:N2    | 28:a:2336:A:O2'   | 2.03                     | 0.91              |
| 7:A:998:C:C5      | 7:A:1044:A:C5'    | 2.54                     | 0.91              |
| 43:p:81:ASN:O     | 43:p:85:LYS:HB3   | 1.70                     | 0.91              |
| 28:a:2356:U:H4'   | 49:v:20:ARG:HE    | 1.35                     | 0.90              |
| 28:a:2519:U:O4    | 28:a:2542:A:N6    | 2.04                     | 0.90              |
| 28:a:2351:G:H21   | 28:a:2366:A:H8    | 1.17                     | 0.90              |
| 7:A:73:C:N4       | 7:A:96:U:N3       | 2.11                     | 0.90              |
| 28:a:2523:G:H21   | 28:a:2764:A:H1'   | 1.37                     | 0.90              |
| 32:e:121:VAL:HG21 | 32:e:187:VAL:HG23 | 1.53                     | 0.89              |
| 4:3:2:LYS:O       | 4:3:36:ARG:N      | 2.04                     | 0.89              |
| 28:a:2472:G:H21   | 28:a:2478:A:H62   | 0.92                     | 0.89              |
| 28:a:1020:A:C6    | 28:a:1141:U:N3    | 2.41                     | 0.89              |
| 28:a:284:U:H3     | 28:a:356:G:H1     | 0.90                     | 0.89              |
| 28:a:1027:A:H2'   | 28:a:1028:A:H8    | 1.36                     | 0.89              |
| 29:b:77:U:C2      | 29:b:99:A:N6      | 2.40                     | 0.88              |
| 7:A:736:C:O2'     | 12:F:89:VAL:O     | 1.92                     | 0.88              |
| 28:a:2305:U:H5''  | 33:f:131:GLY:HA3  | 1.55                     | 0.88              |
| 7:A:998:C:H2'     | 7:A:999:C:C2      | 2.08                     | 0.88              |
| 5:4:64:PHE:O      | 25:S:7:LYS:NZ     | 2.07                     | 0.87              |
| 39:l:113:ALA:O    | 39:l:117:PHE:N    | 2.08                     | 0.87              |
| 28:a:2262:U:O2'   | 28:a:2329:U:O2'   | 1.93                     | 0.87              |
| 7:A:765:G:N1      | 7:A:812:G:N3      | 2.23                     | 0.86              |
| 31:d:37:VAL:H     | 31:d:92:VAL:HG22  | 1.40                     | 0.86              |
| 28:a:424:G:N1     | 28:a:425:G:N3     | 2.24                     | 0.86              |
| 28:a:1027:A:H2'   | 28:a:1028:A:C8    | 2.12                     | 0.85              |
| 28:a:1183:U:OP1   | 52:y:31:ARG:NH2   | 2.10                     | 0.85              |
| 10:D:146:ARG:HE   | 10:D:178:MET:HG3  | 1.41                     | 0.85              |
| 28:a:1418:G:N2    | 28:a:1580:A:N6    | 2.02                     | 0.85              |
| 28:a:2757:A:N1    | 34:g:67:THR:OG1   | 2.09                     | 0.84              |
| 7:A:1130:A:O2'    | 15:I:18:ARG:NH2   | 2.11                     | 0.84              |
| 36:i:16:TYR:N     | 36:i:53:TYR:O     | 2.11                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 32:e:97:ASN:HB2  | 32:e:100:MET:HG3 | 1.60                     | 0.84              |
| 29:b:9:G:O6      | 29:b:111:U:O2    | 1.95                     | 0.84              |
| 7:A:484:G:H4'    | 7:A:485:U:H5'    | 1.59                     | 0.83              |
| 28:a:85:G:H2'    | 28:a:86:G:H4'    | 1.59                     | 0.83              |
| 7:A:1125:U:H5'   | 16:J:37:ARG:HH11 | 1.42                     | 0.83              |
| 10:D:178:MET:HG2 | 10:D:179:GLU:HG2 | 1.59                     | 0.83              |
| 28:a:1583:A:O2'  | 28:a:1585:C:N4   | 2.12                     | 0.83              |
| 28:a:2336:A:N6   | 49:v:57:HIS:HD2  | 1.77                     | 0.83              |
| 7:A:1280:A:H8    | 7:A:1283:C:H42   | 1.24                     | 0.82              |
| 4:3:4:ARG:N      | 4:3:36:ARG:O     | 2.12                     | 0.82              |
| 7:A:778:G:H21    | 17:K:122:ARG:HD3 | 1.42                     | 0.82              |
| 28:a:2261:C:H4'  | 28:a:2387:U:H2'  | 1.61                     | 0.82              |
| 28:a:646:U:O4    | 28:a:2368:C:O2'  | 1.96                     | 0.82              |
| 7:A:35:G:H1      | 7:A:549:C:H5     | 1.27                     | 0.82              |
| 7:A:1001:G:O2'   | 7:A:1041:G:O6    | 1.97                     | 0.82              |
| 29:b:78:A:N6     | 29:b:98:G:N2     | 2.05                     | 0.82              |
| 18:L:121:ARG:HD2 | 18:L:122:PRO:HD2 | 1.62                     | 0.82              |
| 7:A:609:A:O2'    | 7:A:610:G:O5'    | 1.98                     | 0.81              |
| 48:u:78:GLN:HB2  | 48:u:88:HIS:HB3  | 1.60                     | 0.81              |
| 11:E:13:GLU:HG2  | 11:E:64:MET:HE1  | 1.62                     | 0.81              |
| 19:M:54:ASP:HA   | 19:M:57:ARG:HE   | 1.45                     | 0.81              |
| 43:p:95:LEU:HA   | 43:p:98:ILE:HD12 | 1.63                     | 0.81              |
| 49:v:72:LYS:HD2  | 49:v:79:PHE:HB2  | 1.61                     | 0.81              |
| 28:a:1020:A:N6   | 28:a:1141:U:N3   | 2.28                     | 0.81              |
| 43:p:68:ALA:O    | 43:p:72:ASN:ND2  | 2.14                     | 0.81              |
| 28:a:643:A:H61   | 28:a:2370:G:H4'  | 1.45                     | 0.80              |
| 29:b:40:U:H1'    | 29:b:45:A:H61    | 1.47                     | 0.80              |
| 28:a:97:C:N4     | 28:a:98:G:O6     | 2.13                     | 0.80              |
| 28:a:2519:U:N3   | 28:a:2541:A:N1   | 2.28                     | 0.80              |
| 28:a:2525:G:H2'  | 28:a:2526:G:C8   | 2.15                     | 0.80              |
| 39:l:47:GLU:OE1  | 39:l:50:ARG:NH1  | 2.15                     | 0.80              |
| 7:A:1158:A:H61   | 7:A:1182:G:H5'   | 1.47                     | 0.80              |
| 28:a:2796:U:H3   | 28:a:2799:A:H61  | 1.28                     | 0.79              |
| 7:A:1252:G:H3'   | 7:A:1253:A:H5'   | 1.63                     | 0.79              |
| 28:a:2262:U:HO2' | 28:a:2329:U:HO2' | 1.28                     | 0.79              |
| 49:v:66:LYS:NZ   | 49:v:85:GLU:OE1  | 2.15                     | 0.79              |
| 27:U:6:VAL:HG12  | 27:U:18:ARG:HH22 | 1.47                     | 0.79              |
| 29:b:31:C:H1'    | 29:b:53:A:H61    | 1.46                     | 0.79              |
| 7:A:998:C:H6     | 7:A:1044:A:C5'   | 1.94                     | 0.79              |
| 39:l:114:ARG:O   | 39:l:118:LYS:N   | 2.16                     | 0.79              |
| 12:F:38:ARG:HD3  | 12:F:98:GLU:H    | 1.46                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:a:2297:A:H62   | 28:a:2319:G:H21   | 1.28                     | 0.79              |
| 34:g:126:PRO:HG3  | 34:g:132:VAL:HG23 | 1.64                     | 0.79              |
| 38:k:82:LEU:HD21  | 38:k:120:VAL:HG21 | 1.64                     | 0.79              |
| 28:a:1028:A:C2    | 28:a:2487:G:H4'   | 2.17                     | 0.79              |
| 28:a:1036:G:O6    | 28:a:1119:U:O2    | 2.00                     | 0.79              |
| 28:a:643:A:N6     | 28:a:2370:G:O2'   | 2.16                     | 0.79              |
| 31:d:50:VAL:N     | 31:d:80:TRP:O     | 2.16                     | 0.78              |
| 28:a:636:G:H5''   | 38:k:128:THR:HB   | 1.63                     | 0.78              |
| 48:u:9:ARG:NH1    | 48:u:17:SER:OG    | 2.17                     | 0.78              |
| 1:0:19:HIS:ND1    | 1:0:49:TYR:OH     | 2.16                     | 0.78              |
| 7:A:683:G:N2      | 17:K:39:GLY:O     | 2.17                     | 0.78              |
| 28:a:660:C:H2'    | 28:a:661:A:C8     | 2.19                     | 0.78              |
| 39:l:119:LEU:HD22 | 39:l:123:LYS:HE2  | 1.63                     | 0.78              |
| 7:A:61:G:N2       | 7:A:105:G:H22     | 1.82                     | 0.78              |
| 47:t:96:PHE:HB2   | 47:t:101:GLU:HG3  | 1.64                     | 0.78              |
| 4:3:1:MET:HB3     | 4:3:35:GLN:HA     | 1.66                     | 0.77              |
| 28:a:1880:U:C4    | 28:a:1881:C:N4    | 2.52                     | 0.77              |
| 28:a:277:G:N2     | 28:a:361:G:OP2    | 2.18                     | 0.77              |
| 32:e:196:VAL:HA   | 32:e:199:MET:HE2  | 1.65                     | 0.77              |
| 36:i:15:TRP:HA    | 36:i:53:TYR:H     | 1.48                     | 0.77              |
| 48:u:32:GLY:O     | 48:u:93:ARG:NH1   | 2.16                     | 0.77              |
| 9:C:65:ARG:HG3    | 9:C:100:GLN:HG2   | 1.65                     | 0.77              |
| 28:a:877:A:O2'    | 28:a:900:A:N6     | 2.16                     | 0.77              |
| 29:b:66:A:OP2     | 29:b:108:A:N6     | 2.17                     | 0.77              |
| 41:n:18:LEU:HD22  | 41:n:25:ARG:HG3   | 1.67                     | 0.77              |
| 29:b:76:G:OP1     | 48:u:17:SER:OG    | 2.03                     | 0.77              |
| 18:L:30:LYS:HE3   | 18:L:59:ASN:HD22  | 1.48                     | 0.77              |
| 19:M:30:SER:O     | 19:M:34:LEU:HB2   | 1.84                     | 0.77              |
| 38:k:110:VAL:O    | 38:k:128:THR:OG1  | 2.03                     | 0.76              |
| 39:l:116:ALA:HA   | 39:l:119:LEU:HB2  | 1.65                     | 0.76              |
| 7:A:599:C:H2'     | 7:A:600:A:H8      | 1.49                     | 0.76              |
| 40:m:103:ARG:HD3  | 40:m:110:MET:HE2  | 1.64                     | 0.76              |
| 7:A:143:A:H2      | 7:A:220:G:H1      | 1.30                     | 0.76              |
| 7:A:1321:C:O2'    | 7:A:1322:U:O5'    | 2.03                     | 0.76              |
| 48:u:78:GLN:N     | 48:u:88:HIS:O     | 2.18                     | 0.76              |
| 36:i:69:ARG:NH1   | 36:i:90:GLU:OE2   | 2.19                     | 0.76              |
| 28:a:1020:A:N1    | 28:a:1141:U:C4    | 2.53                     | 0.76              |
| 28:a:1035:U:O2    | 28:a:1120:G:O6    | 2.03                     | 0.76              |
| 39:l:118:LYS:O    | 39:l:122:ALA:N    | 2.12                     | 0.76              |
| 1:0:21:TYR:OH     | 1:0:39:PHE:O      | 2.04                     | 0.76              |
| 28:a:2306:C:H42   | 33:f:39:GLY:HA3   | 1.51                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:a:2345:G:O6    | 28:a:2371:G:C6    | 2.39                     | 0.76              |
| 53:z:54:VAL:HG12  | 53:z:55:ILE:HG23  | 1.67                     | 0.76              |
| 28:a:1168:G:N2    | 28:a:1181:U:O2    | 2.14                     | 0.76              |
| 4:3:5:ALA:HA      | 4:3:37:GLN:HG2    | 1.68                     | 0.76              |
| 4:3:19:ARG:NH1    | 28:a:2754:U:O2'   | 2.19                     | 0.76              |
| 7:A:82:A:H3'      | 7:A:83:C:H4'      | 1.68                     | 0.76              |
| 7:A:448:A:H2'     | 7:A:449:G:H4'     | 1.68                     | 0.75              |
| 36:i:54:ILE:N     | 36:i:121:LYS:O    | 2.16                     | 0.75              |
| 43:p:93:LYS:NZ    | 44:q:11:GLN:O     | 2.19                     | 0.75              |
| 4:3:32:LYS:O      | 4:3:35:GLN:NE2    | 2.18                     | 0.75              |
| 28:a:2630:G:H2'   | 28:a:2631:G:H8    | 1.49                     | 0.75              |
| 7:A:66:G:O6       | 7:A:102:G:N2      | 2.19                     | 0.75              |
| 10:D:142:VAL:HG22 | 10:D:181:THR:HG22 | 1.67                     | 0.75              |
| 28:a:2336:A:N6    | 49:v:57:HIS:CD2   | 2.53                     | 0.75              |
| 23:Q:57:ASP:N     | 23:Q:57:ASP:OD1   | 2.20                     | 0.75              |
| 28:a:1235:G:OP1   | 56:a:6211:SPD:N1  | 2.20                     | 0.75              |
| 28:a:2333:A:OP2   | 49:v:77:ARG:NH2   | 2.20                     | 0.75              |
| 34:g:39:ASP:O     | 34:g:55:ARG:NH1   | 2.20                     | 0.75              |
| 39:l:115:GLU:O    | 39:l:119:LEU:N    | 2.17                     | 0.75              |
| 34:g:87:LEU:HD22  | 34:g:148:LEU:HB2  | 1.67                     | 0.74              |
| 38:k:78:ARG:HB2   | 38:k:78:ARG:HH11  | 1.52                     | 0.74              |
| 28:a:1023:U:H2'   | 28:a:1024:G:H5'   | 1.69                     | 0.74              |
| 41:n:33:ARG:NH2   | 41:n:65:THR:OG1   | 2.19                     | 0.74              |
| 43:p:61:TRP:CE2   | 43:p:93:LYS:HB2   | 2.23                     | 0.74              |
| 7:A:981:U:H3'     | 7:A:982:U:H5''    | 1.70                     | 0.74              |
| 28:a:2648:G:H1    | 28:a:2672:U:H3    | 0.82                     | 0.74              |
| 7:A:67:C:H42      | 7:A:101:A:H61     | 1.33                     | 0.74              |
| 28:a:1029:A:H61   | 28:a:1125:G:H1'   | 1.52                     | 0.74              |
| 28:a:2750:A:H5''  | 34:g:3:ARG:HH12   | 1.51                     | 0.74              |
| 7:A:1186:G:N2     | 20:N:101:TRP:O    | 2.20                     | 0.74              |
| 32:e:6:LYS:HD3    | 32:e:119:ILE:HD12 | 1.69                     | 0.74              |
| 50:w:43:GLU:OE1   | 50:w:45:ARG:NH1   | 2.20                     | 0.74              |
| 7:A:129:A:H2      | 7:A:232:G:H22     | 1.36                     | 0.73              |
| 39:l:36:VAL:HA    | 48:u:82:TYR:HB2   | 1.70                     | 0.73              |
| 32:e:112:LEU:HG   | 32:e:118:LEU:HB2  | 1.70                     | 0.73              |
| 36:i:36:LEU:O     | 36:i:121:LYS:NZ   | 2.22                     | 0.73              |
| 28:a:285:G:O6     | 28:a:355:U:O2     | 2.07                     | 0.73              |
| 28:a:631:A:O2'    | 28:a:632:A:OP1    | 2.06                     | 0.73              |
| 28:a:2334:U:H1'   | 41:n:13:ARG:HD3   | 1.70                     | 0.73              |
| 38:k:10:GLU:N     | 38:k:10:GLU:OE2   | 2.20                     | 0.73              |
| 8:B:13:GLY:O      | 8:B:17:GLY:N      | 2.17                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:L:114:ARG:HB3  | 18:L:119:VAL:HB   | 1.70                     | 0.73              |
| 28:a:84:A:H3'     | 47:t:7:ARG:HH22   | 1.50                     | 0.73              |
| 29:b:66:A:N6      | 29:b:108:A:OP2    | 2.21                     | 0.73              |
| 7:A:61:G:H22      | 7:A:105:G:H1      | 1.36                     | 0.73              |
| 28:a:2525:G:H2'   | 28:a:2526:G:H8    | 1.51                     | 0.73              |
| 28:a:2741:A:H2'   | 28:a:2742:G:H8    | 1.53                     | 0.73              |
| 36:i:55:ILE:HG23  | 36:i:124:VAL:HA   | 1.69                     | 0.73              |
| 13:G:92:ARG:HE    | 13:G:94:VAL:HG12  | 1.53                     | 0.73              |
| 39:l:64:TRP:HB2   | 39:l:104:GLU:HB2  | 1.70                     | 0.73              |
| 3:2:31:HIS:CD2    | 3:2:32:ILE:HG13   | 2.20                     | 0.73              |
| 10:D:33:LYS:O     | 10:D:35:GLU:N     | 2.21                     | 0.73              |
| 28:a:2741:A:H2'   | 28:a:2742:G:C8    | 2.24                     | 0.73              |
| 41:n:31:THR:O     | 41:n:102:ARG:NH1  | 2.18                     | 0.73              |
| 8:B:114:LEU:HD12  | 8:B:144:LEU:HB3   | 1.70                     | 0.72              |
| 38:k:134:ALA:O    | 38:k:138:ALA:N    | 2.20                     | 0.72              |
| 36:i:17:VAL:HA    | 36:i:55:ILE:O     | 1.89                     | 0.72              |
| 28:a:1417:C:H2'   | 28:a:1418:G:C8    | 2.24                     | 0.72              |
| 29:b:27:C:H2'     | 29:b:28:C:C5      | 2.23                     | 0.72              |
| 49:v:65:GLY:HA3   | 49:v:84:ALA:HA    | 1.71                     | 0.72              |
| 28:a:2329:U:H2'   | 28:a:2330:G:C8    | 2.24                     | 0.72              |
| 38:k:78:ARG:HE    | 38:k:113:ALA:HB3  | 1.54                     | 0.72              |
| 32:e:112:LEU:HD23 | 32:e:118:LEU:HD12 | 1.71                     | 0.72              |
| 33:f:30:ARG:NH1   | 33:f:31:VAL:O     | 2.23                     | 0.72              |
| 7:A:393:A:O2'     | 7:A:483:C:OP1     | 2.06                     | 0.72              |
| 7:A:1059:C:H4'    | 20:N:85:ARG:NH2   | 2.04                     | 0.72              |
| 10:D:148:LYS:HG3  | 10:D:150:LYS:HG2  | 1.72                     | 0.72              |
| 28:a:505:A:OP2    | 56:a:6211:SPD:N1  | 2.23                     | 0.72              |
| 7:A:176:C:H3'     | 7:A:177:G:H21     | 1.55                     | 0.71              |
| 28:a:550:C:H2'    | 28:a:551:G:H8     | 1.54                     | 0.71              |
| 49:v:25:ARG:HD2   | 49:v:31:VAL:HG12  | 1.72                     | 0.71              |
| 15:I:129:LYS:HD2  | 15:I:130:ARG:HH21 | 1.55                     | 0.71              |
| 28:a:2525:G:O2'   | 28:a:2742:G:O2'   | 2.04                     | 0.71              |
| 28:a:2750:A:O2'   | 28:a:2752:C:N4    | 2.23                     | 0.71              |
| 48:u:7:GLU:HA     | 48:u:65:VAL:HG21  | 1.71                     | 0.71              |
| 7:A:1506:G:O2'    | 7:A:1507:U:OP2    | 2.09                     | 0.71              |
| 28:a:1880:U:H2'   | 28:a:1881:C:C6    | 2.26                     | 0.71              |
| 28:a:2740:A:N7    | 28:a:2764:A:N6    | 2.39                     | 0.71              |
| 8:B:66:LYS:HB2    | 8:B:158:PRO:HA    | 1.73                     | 0.71              |
| 9:C:34:ASP:OD2    | 9:C:38:LYS:NZ     | 2.24                     | 0.71              |
| 28:a:2297:A:H62   | 28:a:2319:G:N2    | 1.88                     | 0.71              |
| 28:a:2744:G:H21   | 34:g:143:GLN:HE22 | 1.35                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:A:383:A:H5'    | 7:A:384:G:H5'    | 1.71                     | 0.71              |
| 28:a:630:G:N1    | 28:a:632:A:OP2   | 2.23                     | 0.71              |
| 7:A:998:C:C6     | 7:A:1044:A:O5'   | 2.43                     | 0.71              |
| 22:P:48:GLU:OE1  | 22:P:51:ARG:NH1  | 2.23                     | 0.71              |
| 36:i:96:ARG:HD3  | 36:i:99:ARG:HD3  | 1.71                     | 0.71              |
| 43:p:58:ARG:HA   | 43:p:61:TRP:CE3  | 2.25                     | 0.71              |
| 28:a:1039:A:N1   | 28:a:1116:G:O6   | 2.24                     | 0.71              |
| 7:A:959:A:HO2'   | 7:A:984:C:HO2'   | 1.37                     | 0.71              |
| 7:A:1158:A:N7    | 7:A:1178:G:N2    | 2.39                     | 0.71              |
| 29:b:74:U:H2'    | 48:u:29:ILE:HD13 | 1.71                     | 0.71              |
| 33:f:117:LEU:H   | 33:f:177:PHE:HA  | 1.55                     | 0.71              |
| 7:A:440:C:OP1    | 10:D:121:LYS:NZ  | 2.23                     | 0.71              |
| 28:a:2386:A:OP1  | 49:v:55:ARG:NH2  | 2.23                     | 0.71              |
| 28:a:2530:A:OP1  | 28:a:2535:G:N2   | 2.24                     | 0.71              |
| 39:l:114:ARG:HA  | 39:l:117:PHE:HB2 | 1.73                     | 0.71              |
| 43:p:61:TRP:HA   | 43:p:96:ALA:HB2  | 1.71                     | 0.71              |
| 28:a:2317:A:H3'  | 28:a:2318:G:C8   | 2.25                     | 0.70              |
| 28:a:2329:U:H2'  | 28:a:2330:G:H8   | 1.55                     | 0.70              |
| 13:G:145:ALA:O   | 13:G:149:LYS:NZ  | 2.25                     | 0.70              |
| 26:T:69:LYS:H    | 26:T:69:LYS:HD2  | 1.55                     | 0.70              |
| 36:i:118:MET:HA  | 36:i:121:LYS:HG3 | 1.73                     | 0.70              |
| 7:A:459:A:H61    | 7:A:473:A:H61    | 1.39                     | 0.70              |
| 43:p:66:ASN:HD21 | 43:p:70:ARG:HH21 | 1.39                     | 0.70              |
| 25:S:29:LYS:HB3  | 25:S:30:PRO:HD2  | 1.74                     | 0.70              |
| 36:i:15:TRP:CG   | 36:i:53:TYR:HB2  | 2.26                     | 0.70              |
| 48:u:76:ASP:O    | 48:u:90:ASP:N    | 2.18                     | 0.70              |
| 7:A:415:A:H2'    | 7:A:416:G:C8     | 2.26                     | 0.70              |
| 7:A:836:G:O6     | 7:A:850:U:O4     | 2.09                     | 0.70              |
| 12:F:9:MET:N     | 12:F:9:MET:SD    | 2.65                     | 0.70              |
| 24:R:50:LYS:HD3  | 24:R:53:ARG:HH22 | 1.56                     | 0.70              |
| 28:a:1040:A:N1   | 28:a:1115:G:O6   | 2.25                     | 0.70              |
| 28:a:2683:C:O2   | 37:j:70:ARG:NH2  | 2.22                     | 0.70              |
| 47:t:96:PHE:N    | 47:t:101:GLU:O   | 2.22                     | 0.70              |
| 1:O:39:PHE:HA    | 1:O:46:HIS:HA    | 1.73                     | 0.70              |
| 28:a:1050:A:H2'  | 28:a:1051:G:H8   | 1.56                     | 0.70              |
| 7:A:74:A:N6      | 7:A:95:G:OP1     | 2.25                     | 0.70              |
| 28:a:1418:G:H21  | 28:a:1580:A:H62  | 0.72                     | 0.70              |
| 29:b:29:A:H2     | 29:b:57:A:H61    | 1.38                     | 0.70              |
| 41:n:41:ALA:HB2  | 41:n:48:LEU:HD11 | 1.72                     | 0.70              |
| 19:M:69:LEU:O    | 19:M:73:ILE:HG13 | 1.92                     | 0.70              |
| 28:a:1028:A:H62  | 28:a:1126:A:N6   | 1.90                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:g:74:SER:OG    | 34:g:138:LYS:NZ   | 2.22                     | 0.70              |
| 3:2:45:ARG:NH1    | 28:a:2349:G:OP1   | 2.24                     | 0.69              |
| 25:S:3:ARG:HE     | 25:S:10:PHE:HB2   | 1.57                     | 0.69              |
| 28:a:1023:U:OP2   | 28:a:1025:G:O2'   | 2.10                     | 0.69              |
| 39:l:110:GLU:O    | 39:l:114:ARG:N    | 2.25                     | 0.69              |
| 20:N:27:LEU:HA    | 20:N:30:ILE:HD12  | 1.74                     | 0.69              |
| 28:a:1880:U:N3    | 28:a:1881:C:C4    | 2.61                     | 0.69              |
| 31:d:51:THR:HB    | 31:d:79:LEU:HD13  | 1.75                     | 0.69              |
| 32:e:168:ASP:HB2  | 32:e:183:PHE:HE2  | 1.57                     | 0.69              |
| 7:A:120:A:H2'     | 7:A:122:G:H8      | 1.56                     | 0.69              |
| 7:A:673:A:H2'     | 7:A:674:G:C8      | 2.28                     | 0.69              |
| 7:A:933:G:OP1     | 13:G:4:ARG:NH1    | 2.25                     | 0.69              |
| 28:a:2292:U:OP1   | 28:a:2378:A:N6    | 2.26                     | 0.69              |
| 39:l:135:VAL:HG23 | 39:l:136:MET:HG2  | 1.74                     | 0.69              |
| 7:A:484:G:H4'     | 7:A:485:U:C5'     | 2.22                     | 0.69              |
| 28:a:634:C:H2'    | 28:a:635:C:C6     | 2.27                     | 0.69              |
| 28:a:2739:U:N3    | 28:a:2764:A:N6    | 2.09                     | 0.69              |
| 46:s:69:ARG:NH1   | 46:s:69:ARG:HB2   | 2.07                     | 0.69              |
| 7:A:37:U:H3       | 7:A:397:A:H61     | 1.39                     | 0.69              |
| 10:D:105:MET:HG3  | 10:D:171:LEU:HD13 | 1.75                     | 0.69              |
| 49:v:43:THR:HG22  | 49:v:57:HIS:HB3   | 1.75                     | 0.69              |
| 7:A:449:G:OP1     | 7:A:450:G:N2      | 2.25                     | 0.69              |
| 13:G:150:ALA:HB1  | 17:K:59:THR:HG21  | 1.75                     | 0.69              |
| 29:b:80:U:O2      | 29:b:96:G:O6      | 2.09                     | 0.69              |
| 34:g:127:THR:OG1  | 34:g:128:GLN:N    | 2.25                     | 0.69              |
| 29:b:14:U:H4'     | 29:b:69:G:H22     | 1.57                     | 0.69              |
| 9:C:65:ARG:NH1    | 9:C:100:GLN:OE1   | 2.26                     | 0.68              |
| 48:u:75:GLN:HB2   | 48:u:92:VAL:HG23  | 1.75                     | 0.68              |
| 48:u:80:HIS:HB3   | 48:u:83:LYS:HZ3   | 1.58                     | 0.68              |
| 19:M:13:LYS:O     | 19:M:13:LYS:HD2   | 1.93                     | 0.68              |
| 28:a:1417:C:H2'   | 28:a:1418:G:H8    | 1.58                     | 0.68              |
| 28:a:1039:A:C2    | 28:a:1116:G:N1    | 2.53                     | 0.68              |
| 28:a:1042:G:O6    | 28:a:1113:U:O4    | 2.10                     | 0.68              |
| 28:a:2747:G:N1    | 28:a:2756:U:OP1   | 2.27                     | 0.68              |
| 34:g:103:ILE:HD12 | 34:g:115:HIS:HB3  | 1.76                     | 0.68              |
| 27:U:66:ARG:HH11  | 27:U:67:ARG:HH12  | 1.42                     | 0.68              |
| 39:l:75:GLU:N     | 39:l:75:GLU:OE2   | 2.26                     | 0.68              |
| 7:A:1159:C:OP1    | 7:A:1182:G:N1     | 2.26                     | 0.68              |
| 8:B:9:MET:HE3     | 8:B:14:VAL:HG21   | 1.73                     | 0.68              |
| 29:b:77:U:H3      | 29:b:99:A:H62     | 0.76                     | 0.68              |
| 33:f:32:GLU:N     | 33:f:157:THR:O    | 2.25                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:1067:A:N6     | 7:A:1110:A:OP2    | 2.26                     | 0.68              |
| 28:a:325:G:O6     | 56:a:6214:SPD:N1  | 2.26                     | 0.68              |
| 28:a:661:A:H2'    | 28:a:662:G:H5'    | 1.74                     | 0.68              |
| 29:b:63:C:H2'     | 29:b:64:G:H8      | 1.59                     | 0.68              |
| 7:A:100:G:N2      | 7:A:152:A:O2'     | 2.25                     | 0.68              |
| 28:a:1125:G:H3'   | 28:a:1126:A:H2'   | 1.76                     | 0.68              |
| 48:u:42:LEU:HD13  | 48:u:43:ASP:H     | 1.57                     | 0.68              |
| 7:A:1442:A:H2'    | 7:A:1443:G:H5'    | 1.76                     | 0.68              |
| 7:A:484:G:H5'     | 7:A:486:U:H5''    | 1.75                     | 0.67              |
| 7:A:921:U:O2      | 11:E:24:THR:OG1   | 2.12                     | 0.67              |
| 7:A:1531:G:N7     | 27:U:46:LYS:NZ    | 2.41                     | 0.67              |
| 28:a:636:G:OP1    | 38:k:129:LYS:N    | 2.26                     | 0.67              |
| 32:e:150:THR:O    | 32:e:172:ALA:N    | 2.23                     | 0.67              |
| 33:f:31:VAL:HA    | 33:f:158:THR:HA   | 1.77                     | 0.67              |
| 7:A:239:U:O3'     | 7:A:240:G:H8      | 1.78                     | 0.67              |
| 36:i:1:MET:HE2    | 44:q:13:ARG:H     | 1.59                     | 0.67              |
| 51:x:11:VAL:O     | 51:x:15:ASN:ND2   | 2.24                     | 0.67              |
| 48:u:9:ARG:O      | 48:u:12:GLN:NE2   | 2.23                     | 0.67              |
| 28:a:268:C:N3     | 28:a:269:C:H5     | 1.92                     | 0.67              |
| 41:n:34:HIS:O     | 41:n:102:ARG:NH2  | 2.27                     | 0.67              |
| 28:a:1583:A:HO2'  | 28:a:1585:C:H41   | 1.41                     | 0.67              |
| 32:e:113:VAL:HG23 | 32:e:118:LEU:HD13 | 1.77                     | 0.67              |
| 7:A:413:A:H5'     | 7:A:414:A:H8      | 1.59                     | 0.67              |
| 7:A:1223:G:OP2    | 7:A:1323:C:N4     | 2.21                     | 0.67              |
| 19:M:95:LEU:HA    | 19:M:110:LYS:HB2  | 1.77                     | 0.67              |
| 28:a:629:G:H2'    | 28:a:630:G:O4'    | 1.95                     | 0.67              |
| 28:a:2351:G:N2    | 28:a:2366:A:H8    | 1.91                     | 0.67              |
| 15:I:28:ILE:HG23  | 15:I:63:LEU:HD12  | 1.76                     | 0.66              |
| 20:N:47:LYS:O     | 20:N:50:THR:OG1   | 2.13                     | 0.66              |
| 27:U:13:ASP:OD1   | 27:U:13:ASP:N     | 2.28                     | 0.66              |
| 29:b:92:C:OP1     | 48:u:18:ARG:NH2   | 2.15                     | 0.66              |
| 7:A:714:G:H2'     | 7:A:715:A:C8      | 2.30                     | 0.66              |
| 28:a:1043:C:O2    | 28:a:1112:G:N2    | 2.16                     | 0.66              |
| 34:g:126:PRO:HB2  | 34:g:127:THR:HG22 | 1.78                     | 0.66              |
| 36:i:17:VAL:HG12  | 36:i:137:PRO:HB2  | 1.77                     | 0.66              |
| 28:a:327:G:N7     | 56:a:6214:SPD:N10 | 2.42                     | 0.66              |
| 28:a:1168:G:O6    | 28:a:1181:U:O4    | 2.13                     | 0.66              |
| 32:e:2:GLU:OE2    | 32:e:12:LEU:N     | 2.27                     | 0.66              |
| 38:k:110:VAL:HB   | 38:k:127:VAL:HG13 | 1.77                     | 0.66              |
| 41:n:30:ARG:NH1   | 41:n:100:HIS:O    | 2.24                     | 0.66              |
| 5:4:37:CYS:O      | 5:4:41:HIS:HB2    | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 28:a:1027:A:C2'  | 28:a:1028:A:H8   | 2.07                     | 0.66              |
| 41:n:29:HIS:HD1  | 41:n:97:PHE:HZ   | 1.44                     | 0.66              |
| 48:u:83:LYS:HB3  | 48:u:85:LYS:HG3  | 1.76                     | 0.66              |
| 13:G:140:ASP:HA  | 13:G:143:ARG:HE  | 1.61                     | 0.66              |
| 28:a:2751:G:OP1  | 28:a:2751:G:N2   | 2.29                     | 0.66              |
| 45:r:48:LYS:O    | 45:r:52:GLU:HG3  | 1.95                     | 0.66              |
| 7:A:501:C:H2'    | 7:A:502:A:C8     | 2.30                     | 0.66              |
| 9:C:36:ASP:HB3   | 9:C:40:ARG:HH11  | 1.61                     | 0.66              |
| 18:L:57:LEU:HD21 | 18:L:82:ILE:HD11 | 1.78                     | 0.66              |
| 41:n:25:ARG:HB2  | 41:n:40:ILE:HB   | 1.78                     | 0.66              |
| 43:p:83:LEU:HA   | 43:p:112:LYS:NZ  | 2.10                     | 0.66              |
| 53:z:34:SER:OG   | 53:z:36:GLU:OE1  | 2.14                     | 0.66              |
| 14:H:32:LEU:O    | 14:H:36:ILE:HD12 | 1.95                     | 0.66              |
| 49:v:75:LYS:HD3  | 49:v:77:ARG:HB2  | 1.78                     | 0.66              |
| 7:A:194:C:H2'    | 7:A:195:A:H4'    | 1.78                     | 0.66              |
| 48:u:79:ARG:HA   | 48:u:86:LEU:HA   | 1.77                     | 0.66              |
| 7:A:998:C:H6     | 7:A:1044:A:H5'   | 1.54                     | 0.66              |
| 8:B:188:ASP:HB2  | 8:B:204:ASP:HB3  | 1.77                     | 0.66              |
| 28:a:1881:C:H2'  | 28:a:1882:U:C6   | 2.30                     | 0.66              |
| 28:a:1881:C:H2'  | 28:a:1882:U:H6   | 1.59                     | 0.66              |
| 28:a:2333:A:H1'  | 41:n:9:ARG:NH2   | 2.10                     | 0.66              |
| 38:k:108:ALA:O   | 38:k:125:LEU:HB3 | 1.96                     | 0.66              |
| 43:p:69:ALA:HB2  | 43:p:106:PHE:HZ  | 1.61                     | 0.66              |
| 15:I:23:PRO:HA   | 15:I:61:LEU:HD12 | 1.77                     | 0.65              |
| 28:a:2324:U:C2   | 28:a:2331:G:O6   | 2.48                     | 0.65              |
| 36:i:15:TRP:CD2  | 36:i:53:TYR:HB2  | 2.31                     | 0.65              |
| 47:t:50:PRO:O    | 47:t:54:GLN:NE2  | 2.29                     | 0.65              |
| 34:g:39:ASP:OD1  | 34:g:55:ARG:NH1  | 2.30                     | 0.65              |
| 14:H:29:SER:HB2  | 14:H:59:LEU:HB2  | 1.78                     | 0.65              |
| 28:a:1020:A:C6   | 28:a:1141:U:C2   | 2.80                     | 0.65              |
| 28:a:1392:A:N6   | 46:s:18:GLU:OE1  | 2.29                     | 0.65              |
| 29:b:50:A:N6     | 29:b:51:G:O6     | 2.29                     | 0.65              |
| 40:m:114:GLU:OE1 | 40:m:118:ARG:NH1 | 2.30                     | 0.65              |
| 28:a:2261:C:O2'  | 28:a:2387:U:O2   | 2.12                     | 0.65              |
| 30:c:71:LYS:NZ   | 30:c:100:GLU:OE2 | 2.26                     | 0.65              |
| 7:A:376:G:H2'    | 7:A:377:G:H8     | 1.61                     | 0.65              |
| 28:a:2303:G:O2'  | 33:f:121:SER:O   | 2.15                     | 0.65              |
| 28:a:2319:G:H1'  | 28:a:2320:U:C5   | 2.32                     | 0.65              |
| 44:q:14:VAL:HG11 | 44:q:20:VAL:HG13 | 1.79                     | 0.65              |
| 1:0:8:LYS:NZ     | 28:a:2420:C:OP1  | 2.22                     | 0.65              |
| 28:a:2748:A:H4'  | 34:g:4:VAL:HG11  | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:i:15:TRP:HA    | 36:i:53:TYR:N     | 2.10                     | 0.65              |
| 8:B:9:MET:HG3     | 8:B:209:ALA:HB2   | 1.79                     | 0.65              |
| 9:C:113:ALA:HB3   | 9:C:185:ASN:HB2   | 1.79                     | 0.65              |
| 30:c:124:ILE:HD12 | 30:c:124:ILE:O    | 1.97                     | 0.65              |
| 7:A:891:U:HO2'    | 7:A:892:A:H8      | 1.45                     | 0.65              |
| 28:a:549:G:H2'    | 28:a:550:C:C6     | 2.32                     | 0.65              |
| 28:a:2293:G:H4'   | 41:n:98:GLN:CD    | 2.21                     | 0.65              |
| 15:I:72:ILE:HD12  | 15:I:73:SER:H     | 1.62                     | 0.64              |
| 28:a:2528:U:N3    | 28:a:2536:G:N1    | 2.44                     | 0.64              |
| 29:b:78:A:N6      | 29:b:98:G:C2      | 2.61                     | 0.64              |
| 32:e:121:VAL:HG23 | 32:e:188:MET:H    | 1.61                     | 0.64              |
| 44:q:10:LYS:C     | 44:q:11:GLN:HG2   | 2.22                     | 0.64              |
| 31:d:149:ASN:O    | 31:d:151:THR:N    | 2.29                     | 0.64              |
| 43:p:61:TRP:CG    | 43:p:93:LYS:HA    | 2.31                     | 0.64              |
| 48:u:77:VAL:HA    | 48:u:89:ILE:HA    | 1.80                     | 0.64              |
| 7:A:136:C:H41     | 7:A:227:G:H22     | 1.44                     | 0.64              |
| 7:A:157:U:H3      | 7:A:164:G:H1      | 1.45                     | 0.64              |
| 29:b:29:A:O2'     | 29:b:58:A:N6      | 2.23                     | 0.64              |
| 7:A:1267:G:N2     | 7:A:1327:U:O2'    | 2.29                     | 0.64              |
| 11:E:12:GLN:OE1   | 11:E:14:LYS:NZ    | 2.26                     | 0.64              |
| 28:a:1021:A:OP1   | 28:a:1122:G:O2'   | 2.16                     | 0.64              |
| 28:a:84:A:N1      | 28:a:98:G:O2'     | 2.30                     | 0.64              |
| 28:a:1418:G:N2    | 28:a:1580:A:C6    | 2.65                     | 0.64              |
| 28:a:2318:G:H2'   | 28:a:2319:G:C2    | 2.33                     | 0.64              |
| 5:4:56:ARG:HE     | 25:S:65:GLU:H     | 1.45                     | 0.64              |
| 11:E:13:GLU:N     | 11:E:13:GLU:OE1   | 2.30                     | 0.64              |
| 28:a:1021:A:H5'   | 28:a:1022:G:OP2   | 1.98                     | 0.64              |
| 28:a:2355:G:H2'   | 28:a:2356:U:C6    | 2.33                     | 0.64              |
| 28:a:996:A:C4'    | 44:q:11:GLN:HG3   | 2.24                     | 0.64              |
| 33:f:48:LYS:NZ    | 33:f:48:LYS:O     | 2.28                     | 0.64              |
| 38:k:108:ALA:N    | 38:k:125:LEU:HD22 | 2.12                     | 0.64              |
| 32:e:196:VAL:O    | 32:e:200:LEU:HG   | 1.98                     | 0.64              |
| 47:t:62:GLU:N     | 47:t:62:GLU:OE2   | 2.31                     | 0.64              |
| 19:M:113:ARG:H    | 19:M:113:ARG:HD3  | 1.63                     | 0.64              |
| 12:F:70:VAL:O     | 12:F:74:LEU:HD12  | 1.97                     | 0.63              |
| 19:M:41:GLU:HG2   | 19:M:41:GLU:O     | 1.98                     | 0.63              |
| 29:b:28:C:H2'     | 29:b:29:A:O4'     | 1.98                     | 0.63              |
| 7:A:1533:U:H4'    | 7:A:1534:C:H5'    | 1.79                     | 0.63              |
| 2:1:33:ARG:NH1    | 28:a:467:G:OP1    | 2.31                     | 0.63              |
| 10:D:87:GLY:HA3   | 10:D:198:HIS:CD2  | 2.34                     | 0.63              |
| 13:G:56:LYS:HB3   | 13:G:60:GLU:HG2   | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 42:o:33:VAL:HG22 | 42:o:38:LYS:HZ3  | 1.63                     | 0.63              |
| 28:a:840:C:H2'   | 28:a:841:G:H8    | 1.64                     | 0.63              |
| 28:a:2630:G:H2'  | 28:a:2631:G:C8   | 2.34                     | 0.63              |
| 43:p:65:ILE:HG12 | 43:p:95:LEU:HD22 | 1.81                     | 0.63              |
| 7:A:437:U:O5'    | 10:D:154:ARG:NH1 | 2.23                     | 0.63              |
| 28:a:544:C:N4    | 28:a:548:G:O6    | 2.31                     | 0.63              |
| 28:a:1048:A:N1   | 28:a:1112:G:O2'  | 2.24                     | 0.63              |
| 29:b:27:C:N3     | 29:b:28:C:N4     | 2.46                     | 0.63              |
| 29:b:79:G:N7     | 48:u:14:LYS:NZ   | 2.44                     | 0.63              |
| 29:b:94:A:OP1    | 48:u:19:ARG:NE   | 2.31                     | 0.63              |
| 7:A:410:G:H21    | 7:A:432:A:H62    | 1.46                     | 0.63              |
| 8:B:73:LYS:HB3   | 8:B:76:ALA:HB3   | 1.81                     | 0.63              |
| 28:a:2523:G:N2   | 28:a:2764:A:H1'  | 2.12                     | 0.63              |
| 34:g:164:TYR:HB2 | 34:g:167:GLU:HB2 | 1.81                     | 0.63              |
| 47:t:50:PRO:HA   | 47:t:54:GLN:HG3  | 1.81                     | 0.63              |
| 7:A:642:A:HO2'   | 7:A:643:C:H6     | 1.45                     | 0.63              |
| 7:A:778:G:N2     | 17:K:122:ARG:HD3 | 2.12                     | 0.63              |
| 8:B:143:LYS:O    | 8:B:147:SER:OG   | 2.14                     | 0.63              |
| 8:B:162:PHE:HD1  | 8:B:184:PHE:HE2  | 1.46                     | 0.63              |
| 9:C:5:VAL:HG21   | 9:C:10:ILE:HD11  | 1.80                     | 0.63              |
| 19:M:67:GLY:O    | 19:M:71:ARG:HG3  | 1.99                     | 0.63              |
| 8:B:13:GLY:HA2   | 8:B:16:PHE:HB2   | 1.80                     | 0.63              |
| 10:D:184:ARG:HG2 | 10:D:186:PRO:HD3 | 1.81                     | 0.63              |
| 28:a:600:G:C6    | 28:a:657:U:O4    | 2.52                     | 0.63              |
| 28:a:848:C:H2'   | 28:a:849:A:H8    | 1.63                     | 0.63              |
| 28:a:2356:U:N3   | 28:a:2357:G:N7   | 2.46                     | 0.63              |
| 28:a:2893:A:H1'  | 28:a:2894:G:C6   | 2.34                     | 0.63              |
| 29:b:34:A:C6     | 29:b:44:G:H1'    | 2.34                     | 0.63              |
| 33:f:30:ARG:O    | 33:f:159:THR:N   | 2.31                     | 0.63              |
| 36:i:96:ARG:HG2  | 36:i:96:ARG:HH11 | 1.64                     | 0.63              |
| 38:k:74:THR:HG22 | 38:k:107:PHE:HB2 | 1.81                     | 0.63              |
| 41:n:3:LYS:O     | 41:n:7:ARG:HB2   | 1.98                     | 0.63              |
| 41:n:76:LYS:HD3  | 41:n:109:ALA:HB1 | 1.80                     | 0.63              |
| 7:A:123:C:H42    | 7:A:238:G:H1     | 1.47                     | 0.62              |
| 11:E:111:MET:HG2 | 11:E:133:PRO:HA  | 1.81                     | 0.62              |
| 17:K:20:VAL:HG13 | 17:K:83:GLU:HG2  | 1.81                     | 0.62              |
| 27:U:5:LYS:O     | 27:U:18:ARG:NH1  | 2.32                     | 0.62              |
| 34:g:105:LEU:HB2 | 34:g:113:VAL:HB  | 1.81                     | 0.62              |
| 7:A:1253:A:H2    | 7:A:1370:C:H1'   | 1.64                     | 0.62              |
| 9:C:182:ILE:HD13 | 9:C:203:PHE:HB2  | 1.80                     | 0.62              |
| 19:M:12:HIS:O    | 19:M:15:ALA:N    | 2.29                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 36:i:18:VAL:HA   | 36:i:139:VAL:HG13 | 1.80                     | 0.62              |
| 40:m:22:ARG:HD2  | 40:m:70:THR:H     | 1.63                     | 0.62              |
| 42:o:27:GLU:HB2  | 42:o:44:GLU:HG3   | 1.80                     | 0.62              |
| 1:0:11:LEU:HD23  | 1:0:49:TYR:CD2    | 2.34                     | 0.62              |
| 3:2:42:ARG:HG3   | 28:a:2349:G:OP2   | 1.99                     | 0.62              |
| 7:A:41:G:H1      | 7:A:401:C:H5      | 1.47                     | 0.62              |
| 9:C:153:VAL:HG22 | 9:C:198:VAL:HG22  | 1.81                     | 0.62              |
| 28:a:284:U:O2    | 28:a:356:G:N2     | 2.25                     | 0.62              |
| 28:a:597:G:H2'   | 28:a:598:U:O4'    | 1.99                     | 0.62              |
| 28:a:1036:G:C6   | 28:a:1119:U:O2    | 2.52                     | 0.62              |
| 29:b:14:U:OP2    | 29:b:70:C:O2'     | 2.17                     | 0.62              |
| 49:v:18:ALA:O    | 49:v:20:ARG:NH1   | 2.32                     | 0.62              |
| 7:A:472:U:H2'    | 7:A:473:A:H8      | 1.64                     | 0.62              |
| 19:M:75:MET:O    | 19:M:75:MET:HE3   | 1.99                     | 0.62              |
| 24:R:34:THR:HG22 | 24:R:36:SER:H     | 1.64                     | 0.62              |
| 28:a:938:G:C2    | 28:a:939:G:N7     | 2.67                     | 0.62              |
| 29:b:17:C:H2'    | 29:b:18:G:C8      | 2.35                     | 0.62              |
| 41:n:111:ARG:NH2 | 41:n:117:PHE:O    | 2.32                     | 0.62              |
| 7:A:619:U:H5     | 10:D:131:ASN:HB3  | 1.64                     | 0.62              |
| 11:E:41:ASP:OD1  | 11:E:42:GLY:N     | 2.33                     | 0.62              |
| 28:a:1581:G:H2'  | 28:a:1582:C:C6    | 2.35                     | 0.62              |
| 28:a:2307:G:N2   | 28:a:2311:A:O2'   | 2.32                     | 0.62              |
| 29:b:80:U:O2     | 29:b:96:G:C6      | 2.52                     | 0.62              |
| 7:A:1121:U:H2'   | 7:A:1122:U:C6     | 2.35                     | 0.62              |
| 10:D:35:GLU:O    | 10:D:36:GLN:C     | 2.42                     | 0.62              |
| 13:G:111:ARG:NH1 | 13:G:113:ASP:OD2  | 2.32                     | 0.62              |
| 28:a:1416:G:O2'  | 28:a:1417:C:OP2   | 2.13                     | 0.62              |
| 28:a:2043:C:N4   | 28:a:2625:G:N2    | 2.47                     | 0.62              |
| 29:b:86:G:N1     | 29:b:88:C:O4'     | 2.33                     | 0.62              |
| 5:4:24:ILE:HD11  | 33:f:102:ARG:HG2  | 1.82                     | 0.62              |
| 28:a:534:U:O2'   | 43:p:49:ASP:OD2   | 2.12                     | 0.62              |
| 30:c:142:HIS:ND1 | 30:c:193:GLY:O    | 2.28                     | 0.62              |
| 7:A:404:G:OP2    | 10:D:115:ARG:NH2  | 2.33                     | 0.62              |
| 12:F:6:ILE:HG12  | 12:F:89:VAL:HG22  | 1.82                     | 0.62              |
| 28:a:816:C:H5'   | 28:a:1166:G:H1'   | 1.81                     | 0.62              |
| 28:a:1039:A:H2   | 28:a:1116:G:N1    | 1.83                     | 0.62              |
| 28:a:1125:G:H2'  | 28:a:1126:A:C8    | 2.34                     | 0.62              |
| 28:a:1315:C:O2'  | 28:a:1392:A:N3    | 2.32                     | 0.62              |
| 28:a:2334:U:H5'  | 41:n:12:THR:HB    | 1.82                     | 0.62              |
| 28:a:2336:A:H61  | 49:v:57:HIS:CD2   | 2.16                     | 0.62              |
| 4:3:24:ARG:HA    | 4:3:36:ARG:HA     | 1.80                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:1228:A:H8    | 25:S:84:ALA:HB2   | 1.65                     | 0.62              |
| 28:a:1166:G:O6   | 28:a:1184:U:C4    | 2.52                     | 0.62              |
| 28:a:2334:U:H5'' | 41:n:9:ARG:HH22   | 1.64                     | 0.62              |
| 28:a:2545:G:H2'  | 28:a:2546:U:O4'   | 2.00                     | 0.62              |
| 36:i:122:LEU:O   | 36:i:123:LYS:HD3  | 2.00                     | 0.62              |
| 45:r:31:GLN:O    | 45:r:35:ILE:HG13  | 2.00                     | 0.62              |
| 7:A:713:G:H2'    | 7:A:714:G:C8      | 2.35                     | 0.62              |
| 28:a:1028:A:N1   | 28:a:2487:G:O2'   | 2.32                     | 0.62              |
| 36:i:54:ILE:HG23 | 36:i:122:LEU:HA   | 1.81                     | 0.62              |
| 37:j:112:PHE:HB3 | 37:j:115:ILE:HD12 | 1.82                     | 0.62              |
| 41:n:36:TYR:HA   | 41:n:52:SER:HB2   | 1.81                     | 0.62              |
| 7:A:998:C:C5     | 7:A:1044:A:O5'    | 2.53                     | 0.61              |
| 28:a:1802:A:H2'  | 28:a:1803:A:C8    | 2.35                     | 0.61              |
| 28:a:2666:C:N4   | 34:g:108:GLY:O    | 2.33                     | 0.61              |
| 33:f:128:TYR:OH  | 33:f:130:MET:SD   | 2.57                     | 0.61              |
| 7:A:1039:C:H1'   | 7:A:1040:U:H2'    | 1.82                     | 0.61              |
| 19:M:95:LEU:HD12 | 19:M:96:PRO:HD2   | 1.81                     | 0.61              |
| 23:Q:76:VAL:HG12 | 23:Q:77:ARG:HG2   | 1.81                     | 0.61              |
| 28:a:1880:U:H2'  | 28:a:1881:C:H6    | 1.65                     | 0.61              |
| 31:d:34:VAL:HG22 | 31:d:50:VAL:HB    | 1.83                     | 0.61              |
| 7:A:346:G:OP1    | 42:o:39:ARG:NH2   | 2.32                     | 0.61              |
| 7:A:642:A:O2'    | 7:A:643:C:O5'     | 2.17                     | 0.61              |
| 7:A:653:A:H3'    | 7:A:654:G:H21     | 1.63                     | 0.61              |
| 8:B:184:PHE:HB2  | 8:B:198:PHE:HB2   | 1.81                     | 0.61              |
| 28:a:1021:A:C6   | 28:a:1023:U:C4    | 2.88                     | 0.61              |
| 34:g:98:VAL:HG21 | 34:g:131:ILE:HG21 | 1.81                     | 0.61              |
| 36:i:53:TYR:CD1  | 36:i:121:LYS:HD2  | 2.35                     | 0.61              |
| 7:A:548:G:O2'    | 7:A:549:C:OP2     | 2.14                     | 0.61              |
| 28:a:2758:A:N1   | 34:g:139:GLN:NE2  | 2.48                     | 0.61              |
| 34:g:101:ASN:HA  | 34:g:117:LEU:HB2  | 1.82                     | 0.61              |
| 43:p:64:ARG:CZ   | 43:p:100:VAL:HG21 | 2.30                     | 0.61              |
| 43:p:61:TRP:CD2  | 43:p:93:LYS:HB2   | 2.35                     | 0.61              |
| 4:3:25:VAL:CG1   | 4:3:35:GLN:H      | 2.12                     | 0.61              |
| 4:3:25:VAL:HG13  | 4:3:35:GLN:H      | 1.65                     | 0.61              |
| 7:A:1012:G:H21   | 7:A:1013:G:H8     | 1.48                     | 0.61              |
| 7:A:1108:G:H22   | 7:A:1111:A:H62    | 1.48                     | 0.61              |
| 7:A:1302:U:O2'   | 7:A:1303:C:OP1    | 2.18                     | 0.61              |
| 15:I:127:PHE:HE2 | 15:I:129:LYS:HE2  | 1.65                     | 0.61              |
| 16:J:79:PRO:HG2  | 16:J:79:PRO:O     | 1.97                     | 0.61              |
| 28:a:2524:G:C5   | 28:a:2525:G:C8    | 2.88                     | 0.61              |
| 28:a:2740:A:C5   | 28:a:2741:A:C5    | 2.89                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:d:33:ARG:HA   | 31:d:94:GLN:O     | 2.01                     | 0.61              |
| 38:k:78:ARG:HB2  | 38:k:78:ARG:NH1   | 2.14                     | 0.61              |
| 13:G:127:ALA:HA  | 13:G:131:LYS:HB2  | 1.82                     | 0.61              |
| 28:a:1024:G:OP2  | 28:a:1025:G:H5''  | 2.01                     | 0.61              |
| 28:a:2519:U:C4   | 28:a:2542:A:N6    | 2.68                     | 0.61              |
| 38:k:74:THR:HG21 | 38:k:126:ARG:HH12 | 1.65                     | 0.61              |
| 7:A:202:G:O2'    | 7:A:468:A:O2'     | 2.18                     | 0.61              |
| 8:B:153:ASP:O    | 8:B:155:GLY:N     | 2.34                     | 0.61              |
| 19:M:64:VAL:HB   | 19:M:68:ASP:HB3   | 1.83                     | 0.61              |
| 7:A:28:A:O2'     | 7:A:296:U:OP1     | 2.15                     | 0.61              |
| 15:I:5:GLN:HB2   | 15:I:22:LYS:HZ2   | 1.66                     | 0.61              |
| 31:d:50:VAL:HG11 | 31:d:82:PHE:CZ    | 2.35                     | 0.61              |
| 7:A:507:C:H3'    | 7:A:508:U:H5'     | 1.83                     | 0.60              |
| 7:A:1315:C:OP2   | 25:S:4:SER:OG     | 2.12                     | 0.60              |
| 28:a:917:A:HO2'  | 29:b:99:A:HO2'    | 1.23                     | 0.60              |
| 7:A:1356:A:H2'   | 7:A:1357:A:H8     | 1.64                     | 0.60              |
| 9:C:92:ALA:HB2   | 9:C:98:PRO:HG3    | 1.82                     | 0.60              |
| 28:a:476:G:N1    | 28:a:479:A:OP2    | 2.32                     | 0.60              |
| 7:A:492:C:H2'    | 7:A:493:A:C8      | 2.37                     | 0.60              |
| 7:A:1312:A:H61   | 7:A:1327:U:H3     | 1.49                     | 0.60              |
| 7:A:1318:C:C4    | 20:N:53:ARG:HD3   | 2.36                     | 0.60              |
| 10:D:19:LEU:HG   | 10:D:64:ILE:HD12  | 1.83                     | 0.60              |
| 28:a:2336:A:H61  | 49:v:57:HIS:HD2   | 1.48                     | 0.60              |
| 28:a:2472:G:N2   | 28:a:2478:A:N6    | 2.28                     | 0.60              |
| 31:d:74:GLU:N    | 31:d:74:GLU:OE2   | 2.34                     | 0.60              |
| 36:i:53:TYR:CA   | 36:i:121:LYS:HB3  | 2.28                     | 0.60              |
| 43:p:88:VAL:HG13 | 43:p:90:ILE:HG13  | 1.83                     | 0.60              |
| 7:A:885:G:N7     | 7:A:912:C:N4      | 2.49                     | 0.60              |
| 7:A:994:A:H61    | 7:A:1044:A:H2     | 1.49                     | 0.60              |
| 46:s:6:ARG:NH2   | 46:s:37:ASP:OD1   | 2.33                     | 0.60              |
| 12:F:20:GLY:O    | 12:F:24:ARG:HD3   | 2.02                     | 0.60              |
| 28:a:2741:A:H62  | 28:a:2763:G:H21   | 1.49                     | 0.60              |
| 26:T:35:VAL:HG22 | 26:T:39:ILE:HD11  | 1.84                     | 0.60              |
| 28:a:603:A:H4'   | 28:a:604:G:H4'    | 1.83                     | 0.60              |
| 28:a:1028:A:H62  | 28:a:1126:A:H62   | 1.47                     | 0.60              |
| 28:a:2315:G:O4'  | 33:f:127:ASN:ND2  | 2.35                     | 0.60              |
| 43:p:91:ASP:OD1  | 43:p:91:ASP:N     | 2.31                     | 0.60              |
| 7:A:994:A:N6     | 7:A:1044:A:H2     | 2.00                     | 0.60              |
| 15:I:44:ALA:O    | 15:I:48:VAL:HG12  | 2.02                     | 0.60              |
| 28:a:634:C:C4    | 28:a:635:C:N4     | 2.69                     | 0.60              |
| 33:f:35:THR:HB   | 33:f:155:THR:HB   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:A:1264:A:H61    | 7:A:1274:G:H1'   | 1.66                     | 0.60              |
| 8:B:35:ARG:HB3    | 8:B:38:VAL:HG12  | 1.83                     | 0.60              |
| 10:D:110:THR:HG22 | 10:D:112:ALA:H   | 1.67                     | 0.60              |
| 22:P:17:TYR:HD2   | 22:P:42:ILE:HD11 | 1.66                     | 0.60              |
| 33:f:8:TYR:HA     | 33:f:12:VAL:HB   | 1.82                     | 0.60              |
| 43:p:91:ASP:O     | 43:p:95:LEU:N    | 2.35                     | 0.60              |
| 49:v:46:HIS:N     | 49:v:78:LYS:O    | 2.29                     | 0.60              |
| 23:Q:62:ARG:NH1   | 23:Q:63:GLU:O    | 2.35                     | 0.60              |
| 29:b:70:C:H2'     | 29:b:71:C:C6     | 2.36                     | 0.60              |
| 48:u:75:GLN:HB3   | 48:u:90:ASP:HB3  | 1.84                     | 0.60              |
| 1:0:13:SER:OG     | 1:0:14:SER:N     | 2.32                     | 0.60              |
| 7:A:72:G:H1       | 7:A:97:G:H21     | 1.50                     | 0.60              |
| 28:a:2355:G:O2'   | 28:a:2356:U:O4'  | 2.13                     | 0.60              |
| 29:b:92:C:O5'     | 48:u:18:ARG:NH1  | 2.34                     | 0.60              |
| 7:A:362:G:N2      | 7:A:365:U:OP2    | 2.32                     | 0.59              |
| 28:a:2313:C:H2'   | 28:a:2314:A:H8   | 1.66                     | 0.59              |
| 28:a:2541:A:OP2   | 56:a:6210:SPD:N1 | 2.35                     | 0.59              |
| 32:e:5:LEU:HB2    | 32:e:9:GLN:N     | 2.17                     | 0.59              |
| 39:l:113:ALA:HA   | 39:l:116:ALA:HB3 | 1.84                     | 0.59              |
| 20:N:47:LYS:HZ2   | 20:N:48:LEU:HD13 | 1.67                     | 0.59              |
| 28:a:2298:A:H61   | 28:a:2318:G:H1'  | 1.67                     | 0.59              |
| 28:a:2333:A:O5'   | 28:a:2335:A:H1'  | 2.01                     | 0.59              |
| 30:c:3:VAL:HG12   | 30:c:19:VAL:HG22 | 1.83                     | 0.59              |
| 34:g:44:LYS:HG2   | 34:g:45:HIS:H    | 1.67                     | 0.59              |
| 44:q:15:SER:HB2   | 44:q:18:GLN:HB2  | 1.83                     | 0.59              |
| 48:u:57:TYR:OH    | 48:u:79:ARG:NH1  | 2.21                     | 0.59              |
| 7:A:363:A:N6      | 18:L:27:CYS:SG   | 2.75                     | 0.59              |
| 28:a:1589:U:H2'   | 28:a:1590:A:C8   | 2.36                     | 0.59              |
| 39:l:45:GLN:NE2   | 39:l:125:PRO:HD3 | 2.18                     | 0.59              |
| 41:n:29:HIS:HA    | 41:n:97:PHE:CE2  | 2.37                     | 0.59              |
| 48:u:4:ILE:N      | 48:u:62:THR:O    | 2.35                     | 0.59              |
| 5:4:37:CYS:HB2    | 5:4:40:CYS:SG    | 2.42                     | 0.59              |
| 7:A:1108:G:N2     | 7:A:1111:A:H62   | 2.00                     | 0.59              |
| 28:a:2640:G:OP1   | 36:i:96:ARG:NH2  | 2.26                     | 0.59              |
| 39:l:116:ALA:O    | 39:l:120:ALA:N   | 2.35                     | 0.59              |
| 12:F:4:TYR:O      | 12:F:63:ASN:ND2  | 2.36                     | 0.59              |
| 32:e:148:ILE:HG23 | 32:e:169:VAL:HA  | 1.84                     | 0.59              |
| 33:f:69:LYS:HB3   | 33:f:82:GLY:HA2  | 1.83                     | 0.59              |
| 34:g:155:GLU:N    | 34:g:160:LYS:O   | 2.32                     | 0.59              |
| 7:A:195:A:H2'     | 7:A:196:A:C5     | 2.37                     | 0.59              |
| 23:Q:19:LYS:H     | 23:Q:51:ASN:ND2  | 2.01                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:a:628:G:H2'    | 28:a:629:G:O4'    | 2.03                     | 0.59              |
| 28:a:2746:U:H4'   | 34:g:138:LYS:HG2  | 1.84                     | 0.59              |
| 34:g:44:LYS:HD2   | 34:g:51:THR:H     | 1.67                     | 0.59              |
| 7:A:615:G:H2'     | 7:A:616:G:H5'     | 1.84                     | 0.59              |
| 26:T:26:SER:O     | 26:T:30:THR:HG23  | 2.03                     | 0.59              |
| 28:a:2324:U:O3'   | 28:a:2337:G:H5''  | 2.03                     | 0.59              |
| 15:I:17:ALA:HB2   | 15:I:67:VAL:HG23  | 1.85                     | 0.59              |
| 19:M:10:PRO:HB3   | 19:M:13:LYS:HG2   | 1.85                     | 0.59              |
| 28:a:2352:A:H62   | 28:a:2365:G:H21   | 0.70                     | 0.59              |
| 28:a:2630:G:C4    | 28:a:2894:G:C6    | 2.90                     | 0.59              |
| 33:f:91:LEU:HD12  | 33:f:95:ARG:HB3   | 1.83                     | 0.59              |
| 7:A:473:A:OP1     | 22:P:76:LYS:NZ    | 2.30                     | 0.59              |
| 7:A:1445:U:H2'    | 7:A:1446:U:O4'    | 2.02                     | 0.59              |
| 12:F:77:THR:O     | 12:F:81:ASN:HB2   | 2.03                     | 0.59              |
| 28:a:602:A:N6     | 28:a:655:A:O2'    | 2.36                     | 0.59              |
| 28:a:2324:U:O2    | 28:a:2331:G:O6    | 2.21                     | 0.59              |
| 48:u:48:MET:HA    | 48:u:51:GLN:OE1   | 2.03                     | 0.59              |
| 48:u:79:ARG:HA    | 48:u:87:GLN:H     | 1.68                     | 0.59              |
| 16:J:27:GLU:O     | 16:J:31:ARG:HB3   | 2.03                     | 0.59              |
| 28:a:2469:A:N6    | 28:a:2481:G:O2'   | 2.35                     | 0.59              |
| 7:A:143:A:C2      | 7:A:220:G:N1      | 2.59                     | 0.58              |
| 25:S:62:VAL:HG12  | 25:S:64:ASP:H     | 1.68                     | 0.58              |
| 29:b:9:G:O6       | 29:b:111:U:C2     | 2.56                     | 0.58              |
| 29:b:70:C:H2'     | 29:b:71:C:H6      | 1.68                     | 0.58              |
| 44:q:3:ALA:O      | 44:q:14:VAL:N     | 2.28                     | 0.58              |
| 48:u:63:ILE:O     | 48:u:69:GLU:HA    | 2.03                     | 0.58              |
| 7:A:657:U:H2'     | 7:A:658:A:H8      | 1.69                     | 0.58              |
| 7:A:1312:A:H3'    | 7:A:1313:G:H5''   | 1.85                     | 0.58              |
| 28:a:1021:A:H3'   | 28:a:1022:G:H4'   | 1.85                     | 0.58              |
| 34:g:98:VAL:HG22  | 34:g:103:ILE:HG23 | 1.85                     | 0.58              |
| 34:g:111:HIS:NE2  | 34:g:113:VAL:HG22 | 2.17                     | 0.58              |
| 7:A:91:U:H2'      | 7:A:92:U:C6       | 2.38                     | 0.58              |
| 7:A:1321:C:OP2    | 25:S:37:ARG:NH1   | 2.36                     | 0.58              |
| 22:P:1:MET:HE2    | 22:P:1:MET:HA     | 1.85                     | 0.58              |
| 7:A:1240:A:H4'    | 7:A:1242:G:H1'    | 1.86                     | 0.58              |
| 12:F:5:GLU:OE2    | 12:F:63:ASN:ND2   | 2.33                     | 0.58              |
| 15:I:118:LEU:HD22 | 15:I:124:ARG:HG2  | 1.85                     | 0.58              |
| 28:a:602:A:O2'    | 28:a:604:G:O2'    | 2.16                     | 0.58              |
| 31:d:48:ILE:HD11  | 31:d:82:PHE:CE1   | 2.38                     | 0.58              |
| 32:e:5:LEU:HB2    | 32:e:9:GLN:H      | 1.67                     | 0.58              |
| 34:g:94:TYR:HB3   | 34:g:107:LEU:HD22 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 43:p:58:ARG:HA    | 43:p:61:TRP:CD2  | 2.38                     | 0.58              |
| 8:B:10:LEU:HD12   | 8:B:43:LEU:HD23  | 1.85                     | 0.58              |
| 16:J:22:THR:O     | 16:J:26:VAL:HG23 | 2.04                     | 0.58              |
| 24:R:48:ARG:HB2   | 24:R:51:TYR:HD2  | 1.68                     | 0.58              |
| 28:a:1880:U:C2    | 28:a:1881:C:C5   | 2.91                     | 0.58              |
| 28:a:2745:C:H5'   | 34:g:146:ALA:HB2 | 1.84                     | 0.58              |
| 38:k:123:ARG:HB2  | 38:k:143:GLU:OE1 | 2.03                     | 0.58              |
| 46:s:17:SER:OG    | 46:s:18:GLU:N    | 2.37                     | 0.58              |
| 7:A:1163:C:H2'    | 7:A:1164:G:C8    | 2.39                     | 0.58              |
| 15:I:55:VAL:HG11  | 15:I:87:LEU:HD11 | 1.86                     | 0.58              |
| 24:R:42:SER:HB3   | 24:R:52:GLN:HG3  | 1.86                     | 0.58              |
| 41:n:35:ILE:HB    | 41:n:102:ARG:NH2 | 2.18                     | 0.58              |
| 44:q:31:GLU:N     | 44:q:31:GLU:OE2  | 2.37                     | 0.58              |
| 8:B:21:ARG:NH2    | 8:B:22:TYR:OH    | 2.36                     | 0.58              |
| 17:K:78:GLY:O     | 17:K:79:ILE:HD13 | 2.03                     | 0.58              |
| 34:g:2:SER:OG     | 34:g:3:ARG:N     | 2.34                     | 0.58              |
| 12:F:5:GLU:O      | 12:F:90:MET:N    | 2.25                     | 0.58              |
| 28:a:636:G:OP2    | 38:k:128:THR:HA  | 2.03                     | 0.58              |
| 7:A:199:C:H2'     | 7:A:200:A:H8     | 1.68                     | 0.58              |
| 7:A:952:U:H5'     | 7:A:972:C:H41    | 1.68                     | 0.58              |
| 7:A:1028:C:H1'    | 7:A:1035:A:N6    | 2.18                     | 0.58              |
| 7:A:1219:U:H2'    | 7:A:1220:A:C8    | 2.38                     | 0.58              |
| 10:D:125:VAL:HG12 | 10:D:126:ASN:OD1 | 2.04                     | 0.58              |
| 22:P:17:TYR:CD2   | 22:P:42:ILE:HD11 | 2.38                     | 0.58              |
| 26:T:35:VAL:O     | 26:T:39:ILE:HG13 | 2.04                     | 0.58              |
| 43:p:79:PHE:CZ    | 43:p:109:LEU:HB3 | 2.39                     | 0.58              |
| 1:0:8:LYS:NZ      | 28:a:2421:G:OP2  | 2.29                     | 0.58              |
| 3:2:28:ASN:O      | 3:2:36:LYS:NZ    | 2.37                     | 0.58              |
| 28:a:638:G:H2'    | 28:a:639:U:C6    | 2.39                     | 0.58              |
| 28:a:2319:G:H1'   | 28:a:2320:U:H5   | 1.68                     | 0.58              |
| 42:o:16:ASP:N     | 42:o:16:ASP:OD1  | 2.36                     | 0.58              |
| 7:A:1057:G:H8     | 7:A:1057:G:OP1   | 1.87                     | 0.57              |
| 24:R:35:GLU:OE2   | 24:R:35:GLU:N    | 2.25                     | 0.57              |
| 28:a:424:G:C6     | 28:a:425:G:C4    | 2.92                     | 0.57              |
| 41:n:4:LYS:O      | 41:n:8:ILE:HG12  | 2.03                     | 0.57              |
| 3:2:15:LYS:HE3    | 28:a:630:G:N7    | 2.18                     | 0.57              |
| 3:2:34:THR:OG1    | 28:a:2420:C:OP1  | 2.22                     | 0.57              |
| 22:P:41:PRO:C     | 22:P:42:ILE:HD12 | 2.28                     | 0.57              |
| 11:E:159:LYS:HD3  | 11:E:163:GLU:HG3 | 1.86                     | 0.57              |
| 12:F:81:ASN:HB3   | 12:F:84:VAL:HG12 | 1.86                     | 0.57              |
| 28:a:856:G:H2'    | 28:a:857:G:C8    | 2.39                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:a:2893:A:H1'  | 28:a:2894:G:C5    | 2.39                     | 0.57              |
| 48:u:30:ILE:HD11 | 48:u:93:ARG:HE    | 1.68                     | 0.57              |
| 7:A:1140:G:H1'   | 7:A:1141:G:N7     | 2.20                     | 0.57              |
| 12:F:29:ILE:HD12 | 12:F:64:VAL:HG22  | 1.86                     | 0.57              |
| 17:K:23:ILE:HB   | 17:K:86:VAL:HG12  | 1.85                     | 0.57              |
| 28:a:275:C:O2    | 28:a:362:A:N6     | 2.38                     | 0.57              |
| 7:A:8:A:C6       | 10:D:206:LYS:HG3  | 2.39                     | 0.57              |
| 15:I:62:ASP:O    | 15:I:63:LEU:HD23  | 2.04                     | 0.57              |
| 28:a:2541:A:H2'  | 28:a:2542:A:C8    | 2.39                     | 0.57              |
| 28:a:2762:C:H2'  | 28:a:2763:G:O4'   | 2.03                     | 0.57              |
| 49:v:72:LYS:CD   | 49:v:79:PHE:HB2   | 2.33                     | 0.57              |
| 7:A:1190:C:H4'   | 7:A:1191:G:O5'    | 2.05                     | 0.57              |
| 7:A:1319:A:H4'   | 25:S:10:PHE:CE1   | 2.40                     | 0.57              |
| 19:M:114:LYS:HD2 | 19:M:114:LYS:O    | 2.05                     | 0.57              |
| 26:T:22:ALA:O    | 26:T:26:SER:OG    | 2.19                     | 0.57              |
| 28:a:631:A:HO2'  | 28:a:632:A:P      | 2.26                     | 0.57              |
| 28:a:2356:U:H2'  | 28:a:2357:G:O4'   | 2.04                     | 0.57              |
| 29:b:40:U:H1'    | 29:b:45:A:N6      | 2.16                     | 0.57              |
| 33:f:144:ASP:OD1 | 33:f:144:ASP:N    | 2.35                     | 0.57              |
| 7:A:7:A:H2'      | 11:E:124:LEU:HD23 | 1.85                     | 0.57              |
| 7:A:96:U:H2'     | 7:A:97:G:O4'      | 2.05                     | 0.57              |
| 7:A:272:C:H2'    | 7:A:273:A:H8      | 1.69                     | 0.57              |
| 14:H:90:ASP:OD1  | 14:H:90:ASP:N     | 2.36                     | 0.57              |
| 15:I:115:LYS:HB3 | 15:I:118:LEU:HD12 | 1.87                     | 0.57              |
| 28:a:2305:U:H1'  | 33:f:133:ARG:HE   | 1.70                     | 0.57              |
| 30:c:146:MET:HE3 | 30:c:146:MET:HA   | 1.87                     | 0.57              |
| 31:d:2:ILE:HD11  | 31:d:48:ILE:HD13  | 1.85                     | 0.57              |
| 4:3:15:LYS:HD3   | 4:3:16:ILE:N      | 2.19                     | 0.57              |
| 7:A:413:A:H5'    | 7:A:414:A:C8      | 2.40                     | 0.57              |
| 7:A:521:G:O2'    | 7:A:537:G:OP1     | 2.23                     | 0.57              |
| 7:A:1012:G:N2    | 7:A:1017:C:OP2    | 2.36                     | 0.57              |
| 7:A:1234:G:OP1   | 15:I:119:ARG:NH2  | 2.37                     | 0.57              |
| 19:M:30:SER:O    | 19:M:34:LEU:CB    | 2.53                     | 0.57              |
| 28:a:86:G:C2     | 28:a:87:U:C4      | 2.93                     | 0.57              |
| 28:a:2479:U:C2   | 28:a:2480:C:H1'   | 2.39                     | 0.57              |
| 33:f:110:ARG:NE  | 33:f:137:ILE:O    | 2.31                     | 0.57              |
| 49:v:40:GLN:NE2  | 49:v:45:PHE:O     | 2.25                     | 0.57              |
| 10:D:44:ARG:O    | 10:D:45:LYS:HB2   | 2.03                     | 0.57              |
| 28:a:841:G:C6    | 28:a:842:U:C4     | 2.93                     | 0.57              |
| 28:a:2316:G:H4'  | 33:f:125:ARG:NH1  | 2.19                     | 0.57              |
| 28:a:2544:G:H2'  | 28:a:2545:G:O4'   | 2.05                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:A:1159:C:O2'    | 7:A:1160:U:OP1   | 2.22                     | 0.56              |
| 13:G:50:LEU:HG    | 13:G:121:ALA:HB1 | 1.87                     | 0.56              |
| 19:M:30:SER:HA    | 19:M:33:ILE:HG22 | 1.87                     | 0.56              |
| 28:a:636:G:P      | 38:k:128:THR:HA  | 2.45                     | 0.56              |
| 38:k:127:VAL:HG11 | 38:k:132:ARG:HB3 | 1.87                     | 0.56              |
| 48:u:44:HIS:CE1   | 48:u:85:LYS:HB3  | 2.39                     | 0.56              |
| 28:a:1040:A:H2    | 28:a:1115:G:H1   | 1.50                     | 0.56              |
| 34:g:20:ASN:OD1   | 34:g:20:ASN:N    | 2.38                     | 0.56              |
| 1:0:39:PHE:HD1    | 1:0:46:HIS:CG    | 2.23                     | 0.56              |
| 5:4:9:TYR:CE2     | 33:f:62:GLY:HA3  | 2.40                     | 0.56              |
| 7:A:522:C:H5      | 18:L:50:ARG:HH12 | 1.53                     | 0.56              |
| 7:A:642:A:O2'     | 7:A:643:C:H6     | 1.87                     | 0.56              |
| 23:Q:51:ASN:OD1   | 23:Q:51:ASN:N    | 2.35                     | 0.56              |
| 24:R:11:CYS:HB2   | 24:R:47:THR:HA   | 1.88                     | 0.56              |
| 28:a:84:A:C3'     | 47:t:7:ARG:HH22  | 2.19                     | 0.56              |
| 28:a:634:C:C4     | 28:a:635:C:C4    | 2.93                     | 0.56              |
| 28:a:2327:A:N6    | 28:a:2388:A:H61  | 2.03                     | 0.56              |
| 29:b:12:C:O2'     | 49:v:74:PRO:O    | 2.22                     | 0.56              |
| 29:b:52:A:H2      | 29:b:53:A:H62    | 1.52                     | 0.56              |
| 32:e:2:GLU:OE1    | 32:e:13:THR:OG1  | 2.16                     | 0.56              |
| 41:n:8:ILE:O      | 41:n:12:THR:OG1  | 2.23                     | 0.56              |
| 41:n:79:ALA:HB3   | 41:n:113:ALA:HB3 | 1.88                     | 0.56              |
| 44:q:1:MET:HA     | 44:q:42:ALA:O    | 2.04                     | 0.56              |
| 48:u:4:ILE:HB     | 48:u:63:ILE:HA   | 1.87                     | 0.56              |
| 7:A:1015:G:N2     | 7:A:1220:A:N3    | 2.54                     | 0.56              |
| 7:A:1442:A:N6     | 7:A:1461:C:O2    | 2.39                     | 0.56              |
| 9:C:82:GLU:HG3    | 9:C:83:ASP:H     | 1.69                     | 0.56              |
| 13:G:93:PRO:HA    | 13:G:96:ARG:HD2  | 1.87                     | 0.56              |
| 32:e:147:LEU:HB2  | 32:e:183:PHE:CD2 | 2.40                     | 0.56              |
| 49:v:71:VAL:HA    | 49:v:78:LYS:HA   | 1.87                     | 0.56              |
| 9:C:65:ARG:HA     | 9:C:100:GLN:HB2  | 1.88                     | 0.56              |
| 19:M:57:ARG:HD2   | 19:M:57:ARG:C    | 2.31                     | 0.56              |
| 19:M:91:HIS:HB2   | 19:M:97:VAL:HG21 | 1.86                     | 0.56              |
| 28:a:1418:G:N1    | 28:a:1579:A:N7   | 2.53                     | 0.56              |
| 7:A:198:G:H4'     | 7:A:199:C:OP1    | 2.05                     | 0.56              |
| 7:A:1133:A:N3     | 7:A:1143:G:N2    | 2.53                     | 0.56              |
| 10:D:13:ARG:HB3   | 10:D:38:PRO:HD3  | 1.87                     | 0.56              |
| 10:D:32:CYS:O     | 10:D:33:LYS:C    | 2.49                     | 0.56              |
| 18:L:99:ARG:HD3   | 18:L:104:CYS:SG  | 2.45                     | 0.56              |
| 28:a:596:U:H2'    | 28:a:597:G:H8    | 1.71                     | 0.56              |
| 28:a:2376:A:H61   | 41:n:92:PHE:HB3  | 1.71                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:b:65:U:H3'    | 29:b:108:A:H61    | 1.70                     | 0.56              |
| 33:f:4:LEU:HD21  | 33:f:104:ILE:HD11 | 1.87                     | 0.56              |
| 5:4:42:PRO:HB3   | 5:4:47:LYS:HB2    | 1.88                     | 0.56              |
| 7:A:608:A:H2'    | 7:A:609:A:H5'     | 1.88                     | 0.56              |
| 7:A:1163:C:H2'   | 7:A:1164:G:H8     | 1.69                     | 0.56              |
| 28:a:660:C:H2'   | 28:a:661:A:N9     | 2.20                     | 0.56              |
| 28:a:1166:G:H2'  | 28:a:1167:C:H6    | 1.70                     | 0.56              |
| 31:d:3:GLY:HA3   | 31:d:203:VAL:O    | 2.05                     | 0.56              |
| 34:g:88:GLN:NE2  | 34:g:165:ALA:O    | 2.39                     | 0.56              |
| 34:g:111:HIS:CE1 | 34:g:113:VAL:HG22 | 2.41                     | 0.56              |
| 7:A:482:A:H2'    | 7:A:484:G:H2'     | 1.88                     | 0.56              |
| 7:A:998:C:O4'    | 7:A:1044:A:H5'    | 2.05                     | 0.56              |
| 16:J:42:LEU:HD13 | 16:J:71:LEU:N     | 2.21                     | 0.56              |
| 22:P:8:ARG:NH2   | 22:P:11:ALA:O     | 2.31                     | 0.56              |
| 28:a:1168:G:H2'  | 28:a:1169:A:C8    | 2.41                     | 0.56              |
| 28:a:2740:A:C4   | 28:a:2741:A:C8    | 2.94                     | 0.56              |
| 29:b:90:C:H2'    | 29:b:91:C:H6      | 1.70                     | 0.56              |
| 32:e:171:ASP:OD1 | 32:e:171:ASP:N    | 2.37                     | 0.56              |
| 33:f:13:VAL:O    | 33:f:17:MET:HG2   | 2.06                     | 0.56              |
| 36:i:36:LEU:HD21 | 36:i:54:ILE:HB    | 1.88                     | 0.56              |
| 7:A:652:U:O4     | 7:A:752:G:O2'     | 2.19                     | 0.56              |
| 7:A:1229:C:H2'   | 7:A:1230:A:H8     | 1.71                     | 0.56              |
| 16:J:57:VAL:HG22 | 16:J:58:ASN:H     | 1.70                     | 0.56              |
| 19:M:4:ILE:HG23  | 19:M:5:ALA:H      | 1.70                     | 0.56              |
| 31:d:33:ARG:NH2  | 31:d:75:ALA:O     | 2.38                     | 0.56              |
| 33:f:6:ASP:HA    | 33:f:9:LYS:HE3    | 1.88                     | 0.56              |
| 9:C:134:MET:O    | 9:C:138:VAL:HG23  | 2.06                     | 0.56              |
| 28:a:279:A:N6    | 28:a:361:G:H21    | 2.04                     | 0.56              |
| 28:a:938:G:C2'   | 28:a:939:G:H5'    | 2.36                     | 0.56              |
| 28:a:1527:G:N1   | 28:a:1544:A:OP2   | 2.33                     | 0.56              |
| 44:q:35:PHE:HD1  | 44:q:59:ILE:HB    | 1.70                     | 0.56              |
| 7:A:1118:U:O2'   | 15:I:108:ALA:HB2  | 2.07                     | 0.55              |
| 28:a:544:C:O3'   | 28:a:545:U:H2'    | 2.05                     | 0.55              |
| 28:a:1026:G:H2'  | 28:a:1027:A:C8    | 2.41                     | 0.55              |
| 34:g:22:GLN:HA   | 34:g:37:LEU:HD12  | 1.89                     | 0.55              |
| 5:4:56:ARG:HE    | 25:S:65:GLU:N     | 2.04                     | 0.55              |
| 7:A:501:C:H2'    | 7:A:502:A:H8      | 1.69                     | 0.55              |
| 8:B:67:ILE:HG13  | 8:B:160:ALA:HB3   | 1.88                     | 0.55              |
| 10:D:169:THR:O   | 10:D:184:ARG:NH1  | 2.39                     | 0.55              |
| 19:M:12:HIS:O    | 19:M:14:HIS:N     | 2.39                     | 0.55              |
| 20:N:45:VAL:O    | 20:N:49:GLN:NE2   | 2.39                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:a:879:G:H2'   | 28:a:880:G:H8     | 1.70                     | 0.55              |
| 28:a:1050:A:H2'  | 28:a:1051:G:C8    | 2.39                     | 0.55              |
| 28:a:1863:G:C5   | 28:a:1864:U:C4    | 2.94                     | 0.55              |
| 28:a:1864:U:H2'  | 28:a:1865:U:C2    | 2.41                     | 0.55              |
| 28:a:1880:U:O4   | 28:a:1881:C:N4    | 2.39                     | 0.55              |
| 28:a:2327:A:H61  | 28:a:2388:A:N6    | 2.04                     | 0.55              |
| 31:d:136:ASN:OD1 | 31:d:137:SER:N    | 2.39                     | 0.55              |
| 32:e:188:MET:N   | 32:e:188:MET:HE3  | 2.21                     | 0.55              |
| 38:k:112:LEU:HB2 | 38:k:131:ALA:HA   | 1.88                     | 0.55              |
| 46:s:69:ARG:HB2  | 46:s:69:ARG:HH11  | 1.71                     | 0.55              |
| 7:A:143:A:H2     | 7:A:220:G:N1      | 2.01                     | 0.55              |
| 19:M:97:VAL:HG12 | 19:M:109:ARG:HD3  | 1.88                     | 0.55              |
| 29:b:95:U:O2'    | 29:b:96:G:H5'     | 2.06                     | 0.55              |
| 53:z:53:LYS:HE2  | 53:z:53:LYS:HA    | 1.88                     | 0.55              |
| 12:F:62:MET:HE2  | 12:F:62:MET:HA    | 1.89                     | 0.55              |
| 13:G:138:ARG:HA  | 13:G:141:VAL:HB   | 1.87                     | 0.55              |
| 16:J:26:VAL:HG12 | 16:J:30:LYS:HD3   | 1.88                     | 0.55              |
| 28:a:1166:G:H2'  | 28:a:1167:C:O4'   | 2.06                     | 0.55              |
| 28:a:2318:G:O2'  | 28:a:2321:U:O4    | 2.24                     | 0.55              |
| 28:a:2382:G:H2'  | 28:a:2382:G:OP2   | 2.07                     | 0.55              |
| 28:a:2739:U:H3   | 28:a:2764:A:H62   | 0.63                     | 0.55              |
| 34:g:152:ARG:O   | 34:g:162:VAL:HG22 | 2.07                     | 0.55              |
| 4:3:30:GLU:HG3   | 4:3:32:LYS:H      | 1.70                     | 0.55              |
| 7:A:194:C:C2'    | 7:A:195:A:H4'     | 2.36                     | 0.55              |
| 7:A:1125:U:H5'   | 16:J:37:ARG:NH1   | 2.19                     | 0.55              |
| 7:A:1372:G:OP1   | 15:I:14:SER:HB3   | 2.07                     | 0.55              |
| 16:J:27:GLU:HA   | 16:J:30:LYS:HE2   | 1.88                     | 0.55              |
| 16:J:39:PRO:HB3  | 16:J:74:VAL:HG22  | 1.89                     | 0.55              |
| 19:M:81:MET:HG3  | 19:M:81:MET:O     | 2.07                     | 0.55              |
| 7:A:448:A:O2'    | 7:A:450:G:OP2     | 2.16                     | 0.55              |
| 8:B:32:PHE:HB2   | 8:B:42:ASN:HB3    | 1.89                     | 0.55              |
| 16:J:7:ARG:HB2   | 16:J:73:LEU:HD11  | 1.88                     | 0.55              |
| 28:a:2373:G:H2'  | 28:a:2374:C:C6    | 2.42                     | 0.55              |
| 29:b:68:C:H3'    | 29:b:69:G:H8      | 1.72                     | 0.55              |
| 32:e:48:THR:OG1  | 32:e:51:GLU:OE1   | 2.25                     | 0.55              |
| 34:g:144:VAL:O   | 34:g:148:LEU:HG   | 2.07                     | 0.55              |
| 36:i:95:ARG:HE   | 36:i:96:ARG:HH12  | 1.55                     | 0.55              |
| 7:A:83:C:H2'     | 7:A:88:U:H3       | 1.71                     | 0.55              |
| 7:A:451:A:N6     | 7:A:480:U:O2      | 2.40                     | 0.55              |
| 7:A:1143:G:H3'   | 7:A:1144:G:H8     | 1.72                     | 0.55              |
| 10:D:124:MET:SD  | 10:D:127:GLY:HA2  | 2.47                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:E:115:LEU:HD21 | 11:E:137:VAL:HG12 | 1.88                     | 0.55              |
| 13:G:138:ARG:HD3  | 13:G:139:GLU:N    | 2.22                     | 0.55              |
| 28:a:1733:G:H2'   | 28:a:1734:G:H8    | 1.71                     | 0.55              |
| 28:a:1853:A:H2'   | 28:a:1854:A:C8    | 2.42                     | 0.55              |
| 28:a:2043:C:N4    | 28:a:2044:C:C2    | 2.75                     | 0.55              |
| 28:a:2741:A:C5    | 28:a:2742:G:C5    | 2.95                     | 0.55              |
| 29:b:86:G:H21     | 29:b:87:U:HO2'    | 1.54                     | 0.55              |
| 7:A:201:G:H22     | 7:A:216:U:H3      | 1.54                     | 0.55              |
| 7:A:602:A:H2'     | 7:A:603:U:H6      | 1.71                     | 0.55              |
| 7:A:613:C:H2'     | 7:A:614:U:C6      | 2.42                     | 0.55              |
| 7:A:1518:G:O2'    | 7:A:1519:MA6:OP1  | 2.24                     | 0.55              |
| 22:P:67:ILE:HG23  | 22:P:71:VAL:HB    | 1.89                     | 0.55              |
| 28:a:1026:G:O2'   | 28:a:1027:A:O4'   | 2.14                     | 0.55              |
| 28:a:2297:A:P     | 28:a:2297:A:H8    | 2.29                     | 0.55              |
| 29:b:76:G:H22     | 29:b:100:G:H1     | 1.55                     | 0.55              |
| 31:d:32:ASN:O     | 31:d:95:SER:HA    | 2.07                     | 0.55              |
| 34:g:44:LYS:HB3   | 34:g:50:LEU:HD22  | 1.89                     | 0.55              |
| 7:A:344:A:H5''    | 7:A:345:C:H5      | 1.72                     | 0.55              |
| 7:A:1253:A:H3'    | 7:A:1254:G:C8     | 2.42                     | 0.55              |
| 24:R:48:ARG:HB2   | 24:R:51:TYR:CD2   | 2.42                     | 0.55              |
| 28:a:282:A:N6     | 28:a:359:G:O6     | 2.40                     | 0.55              |
| 28:a:596:U:C2     | 28:a:597:G:N7     | 2.75                     | 0.55              |
| 43:p:65:ILE:HD11  | 43:p:106:PHE:CE1  | 2.41                     | 0.55              |
| 7:A:1228:A:OP2    | 19:M:95:LEU:HD11  | 2.06                     | 0.55              |
| 7:A:1331:U:O2'    | 7:A:1332:G:O4'    | 2.20                     | 0.55              |
| 24:R:71:THR:OG1   | 24:R:72:ASP:N     | 2.39                     | 0.55              |
| 28:a:2745:C:H2'   | 28:a:2746:U:C6    | 2.41                     | 0.55              |
| 31:d:37:VAL:H     | 31:d:92:VAL:CG2   | 2.18                     | 0.55              |
| 34:g:152:ARG:HD3  | 34:g:161:GLY:HA2  | 1.89                     | 0.55              |
| 2:1:1:MET:N       | 2:1:1:MET:HE3     | 2.22                     | 0.54              |
| 7:A:9:G:OP2       | 11:E:126:LYS:NZ   | 2.40                     | 0.54              |
| 7:A:69:G:H22      | 7:A:98:G:N2       | 2.05                     | 0.54              |
| 7:A:260:G:H2'     | 7:A:261:U:C4      | 2.41                     | 0.54              |
| 27:U:16:LEU:HG    | 27:U:17:ARG:HH12  | 1.71                     | 0.54              |
| 28:a:841:G:C5     | 28:a:842:U:C5     | 2.94                     | 0.54              |
| 28:a:1434:A:H2'   | 28:a:1435:G:H8    | 1.71                     | 0.54              |
| 28:a:2357:G:H2'   | 28:a:2359:C:H5    | 1.72                     | 0.54              |
| 29:b:1:U:H2'      | 29:b:2:G:H8       | 1.71                     | 0.54              |
| 29:b:15:A:H5''    | 29:b:16:G:N7      | 2.22                     | 0.54              |
| 32:e:168:ASP:HB2  | 32:e:183:PHE:CE2  | 2.39                     | 0.54              |
| 7:A:10:A:O2'      | 7:A:507:C:O2'     | 2.25                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:720:C:H5'    | 24:R:41:PRO:HA    | 1.89                     | 0.54              |
| 15:I:129:LYS:HD2 | 15:I:130:ARG:NH2  | 2.22                     | 0.54              |
| 28:a:2332:C:H5'  | 49:v:43:THR:OG1   | 2.07                     | 0.54              |
| 29:b:27:C:H2'    | 29:b:28:C:C6      | 2.42                     | 0.54              |
| 29:b:99:A:H2'    | 29:b:100:G:C8     | 2.42                     | 0.54              |
| 43:p:81:ASN:HB3  | 43:p:117:LEU:HD21 | 1.90                     | 0.54              |
| 44:q:10:LYS:NZ   | 44:q:23:GLU:OE1   | 2.40                     | 0.54              |
| 28:a:1126:A:H4'  | 28:a:1127:A:H5''  | 1.88                     | 0.54              |
| 34:g:93:GLY:HA2  | 34:g:95:ARG:NH2   | 2.23                     | 0.54              |
| 43:p:76:TYR:CZ   | 43:p:80:ILE:HG13  | 2.42                     | 0.54              |
| 44:q:24:LYS:HA   | 44:q:94:THR:HG23  | 1.88                     | 0.54              |
| 4:3:30:GLU:HG2   | 4:3:33:HIS:H      | 1.72                     | 0.54              |
| 7:A:194:C:C3'    | 7:A:195:A:H4'     | 2.36                     | 0.54              |
| 7:A:660:U:H3     | 7:A:745:G:H1      | 1.55                     | 0.54              |
| 7:A:1106:G:O2'   | 9:C:169:ARG:NH2   | 2.38                     | 0.54              |
| 28:a:2741:A:C4   | 28:a:2742:G:C8    | 2.96                     | 0.54              |
| 29:b:29:A:HO2'   | 29:b:58:A:H61     | 1.51                     | 0.54              |
| 33:f:33:LYS:HA   | 33:f:96:MET:HE2   | 1.89                     | 0.54              |
| 41:n:35:ILE:HB   | 41:n:102:ARG:HH21 | 1.73                     | 0.54              |
| 45:r:73:LYS:HB2  | 45:r:106:VAL:HB   | 1.89                     | 0.54              |
| 48:u:68:LYS:HE3  | 48:u:70:ILE:HG12  | 1.89                     | 0.54              |
| 7:A:69:G:H1      | 7:A:98:G:H22      | 1.56                     | 0.54              |
| 16:J:5:ARG:HH21  | 16:J:7:ARG:HB3    | 1.73                     | 0.54              |
| 28:a:2334:U:C4   | 41:n:16:ARG:HG2   | 2.42                     | 0.54              |
| 38:k:123:ARG:HG3 | 38:k:143:GLU:HB2  | 1.88                     | 0.54              |
| 44:q:6:GLN:HB3   | 44:q:37:GLU:CD    | 2.32                     | 0.54              |
| 48:u:76:ASP:O    | 48:u:89:ILE:HD12  | 2.06                     | 0.54              |
| 8:B:9:MET:O      | 8:B:14:VAL:HB     | 2.08                     | 0.54              |
| 9:C:23:PHE:O     | 9:C:23:PHE:HD2    | 1.90                     | 0.54              |
| 28:a:2377:A:H3'  | 28:a:2378:A:H8    | 1.72                     | 0.54              |
| 28:a:2759:G:N2   | 34:g:139:GLN:OE1  | 2.41                     | 0.54              |
| 44:q:5:PHE:HE1   | 44:q:12:HIS:HB2   | 1.71                     | 0.54              |
| 44:q:6:GLN:HB3   | 44:q:37:GLU:OE1   | 2.08                     | 0.54              |
| 52:y:31:ARG:HG2  | 52:y:34:HIS:HB2   | 1.89                     | 0.54              |
| 28:a:2538:C:O2   | 28:a:2538:C:H2'   | 2.06                     | 0.54              |
| 43:p:58:ARG:HG3  | 43:p:92:ARG:HD3   | 1.90                     | 0.54              |
| 7:A:105:G:H21    | 7:A:379:C:H5''    | 1.73                     | 0.54              |
| 8:B:16:PHE:HD1   | 8:B:38:VAL:HG11   | 1.73                     | 0.54              |
| 28:a:2291:U:H2'  | 28:a:2292:U:C6    | 2.42                     | 0.54              |
| 29:b:54:G:H2'    | 29:b:55:U:C6      | 2.43                     | 0.54              |
| 38:k:135:ILE:O   | 38:k:139:GLY:N    | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 41:n:6:ALA:O     | 41:n:10:ARG:HB2  | 2.08                     | 0.54              |
| 7:A:778:G:O2'    | 7:A:779:C:OP1    | 2.25                     | 0.54              |
| 9:C:24:ALA:HB2   | 9:C:32:ASN:HD22  | 1.72                     | 0.54              |
| 14:H:11:LEU:HD11 | 14:H:127:CYS:SG  | 2.48                     | 0.54              |
| 24:R:48:ARG:O    | 24:R:52:GLN:N    | 2.32                     | 0.54              |
| 27:U:65:ALA:HA   | 27:U:69:ARG:HG2  | 1.90                     | 0.54              |
| 28:a:2748:A:H1'  | 28:a:2757:A:N6   | 2.23                     | 0.54              |
| 36:i:55:ILE:HG21 | 36:i:130:HIS:CE1 | 2.43                     | 0.54              |
| 36:i:55:ILE:HG22 | 36:i:56:VAL:H    | 1.71                     | 0.54              |
| 7:A:195:A:H2'    | 7:A:196:A:N7     | 2.23                     | 0.54              |
| 8:B:88:ASP:O     | 8:B:89:GLN:NE2   | 2.41                     | 0.54              |
| 12:F:64:VAL:HB   | 12:F:71:ILE:HD11 | 1.90                     | 0.54              |
| 15:I:72:ILE:HD12 | 15:I:73:SER:N    | 2.23                     | 0.54              |
| 28:a:2636:C:OP1  | 31:d:81:GLU:HB2  | 2.07                     | 0.54              |
| 37:j:88:ASN:ND2  | 37:j:91:SER:OG   | 2.35                     | 0.54              |
| 7:A:1115:U:N3    | 7:A:1186:G:O6    | 2.19                     | 0.53              |
| 7:A:1228:A:C8    | 25:S:84:ALA:HB2  | 2.43                     | 0.53              |
| 22:P:5:ARG:NH2   | 22:P:23:ASP:O    | 2.41                     | 0.53              |
| 28:a:1023:U:H2'  | 28:a:1024:G:C5'  | 2.38                     | 0.53              |
| 28:a:2044:C:C2   | 28:a:2045:C:C6   | 2.96                     | 0.53              |
| 28:a:2324:U:O2   | 28:a:2331:G:C6   | 2.61                     | 0.53              |
| 29:b:17:C:H2'    | 29:b:18:G:H8     | 1.72                     | 0.53              |
| 43:p:76:TYR:CE2  | 43:p:80:ILE:HG13 | 2.42                     | 0.53              |
| 4:3:17:VAL:O     | 4:3:18:LYS:HD3   | 2.08                     | 0.53              |
| 7:A:166:U:H2'    | 7:A:167:G:H8     | 1.72                     | 0.53              |
| 9:C:167:TRP:HZ3  | 9:C:169:ARG:HG3  | 1.73                     | 0.53              |
| 19:M:98:ARG:HD3  | 19:M:99:GLY:H    | 1.74                     | 0.53              |
| 21:O:72:ARG:NH2  | 21:O:73:LYS:HA   | 2.23                     | 0.53              |
| 28:a:2529:G:H5'  | 34:g:175:LYS:HG3 | 1.90                     | 0.53              |
| 31:d:34:VAL:HG13 | 31:d:50:VAL:HG12 | 1.89                     | 0.53              |
| 31:d:99:GLU:OE1  | 31:d:99:GLU:N    | 2.22                     | 0.53              |
| 47:t:17:LYS:HG3  | 47:t:18:ASP:OD2  | 2.09                     | 0.53              |
| 4:3:30:GLU:OE1   | 4:3:32:LYS:HB2   | 2.09                     | 0.53              |
| 5:4:37:CYS:HB2   | 5:4:40:CYS:H     | 1.73                     | 0.53              |
| 21:O:24:SER:O    | 21:O:28:GLN:HG3  | 2.08                     | 0.53              |
| 28:a:1020:A:N6   | 28:a:1141:U:N1   | 2.51                     | 0.53              |
| 28:a:2331:G:O2'  | 49:v:42:GLY:HA2  | 2.08                     | 0.53              |
| 29:b:23:G:N7     | 29:b:56:G:O2'    | 2.42                     | 0.53              |
| 29:b:86:G:N2     | 29:b:87:U:O2'    | 2.39                     | 0.53              |
| 29:b:94:A:P      | 48:u:19:ARG:HE   | 2.30                     | 0.53              |
| 33:f:50:LEU:HD21 | 33:f:67:ILE:HG21 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:k:108:ALA:HB3  | 38:k:125:LEU:HD13 | 1.90                     | 0.53              |
| 3:2:42:ARG:HH12   | 28:a:2382:G:N2    | 2.07                     | 0.53              |
| 7:A:73:C:H42      | 7:A:96:U:H3       | 0.62                     | 0.53              |
| 7:A:196:A:H1'     | 7:A:221:C:O2'     | 2.08                     | 0.53              |
| 10:D:145:ILE:HG22 | 10:D:146:ARG:N    | 2.23                     | 0.53              |
| 17:K:89:PRO:HG3   | 27:U:32:VAL:HG11  | 1.89                     | 0.53              |
| 23:Q:42:THR:OG1   | 23:Q:43:LYS:N     | 2.41                     | 0.53              |
| 28:a:85:G:C6      | 28:a:86:G:C2      | 2.95                     | 0.53              |
| 7:A:601:G:H1'     | 7:A:602:A:H5'     | 1.89                     | 0.53              |
| 7:A:1133:A:HO2'   | 7:A:1143:G:H1     | 1.56                     | 0.53              |
| 9:C:131:ARG:NH1   | 9:C:131:ARG:HB3   | 2.24                     | 0.53              |
| 10:D:148:LYS:HG3  | 10:D:150:LYS:CG   | 2.39                     | 0.53              |
| 12:F:9:MET:HE1    | 12:F:86:ARG:HD2   | 1.89                     | 0.53              |
| 16:J:35:GLN:NE2   | 16:J:78:GLU:HB3   | 2.23                     | 0.53              |
| 28:a:2303:G:H1'   | 33:f:123:ASP:OD1  | 2.08                     | 0.53              |
| 45:r:4:ILE:HG12   | 45:r:106:VAL:HG22 | 1.89                     | 0.53              |
| 52:y:7:ILE:HD11   | 52:y:48:ILE:HD11  | 1.91                     | 0.53              |
| 7:A:6:G:H4'       | 7:A:298:A:H4'     | 1.90                     | 0.53              |
| 7:A:61:G:H22      | 7:A:105:G:H22     | 1.57                     | 0.53              |
| 7:A:973:G:H3'     | 7:A:974:A:H5''    | 1.90                     | 0.53              |
| 17:K:53:ARG:HD3   | 17:K:54:GLY:H     | 1.73                     | 0.53              |
| 19:M:98:ARG:HD2   | 19:M:100:GLN:CD   | 2.33                     | 0.53              |
| 20:N:36:ALA:HB3   | 20:N:41:ARG:HH12  | 1.72                     | 0.53              |
| 24:R:53:ARG:O     | 24:R:57:ARG:HG2   | 2.08                     | 0.53              |
| 28:a:638:G:H2'    | 28:a:639:U:H6     | 1.73                     | 0.53              |
| 28:a:643:A:H61    | 28:a:2370:G:C4'   | 2.20                     | 0.53              |
| 28:a:1033:U:O2'   | 28:a:1034:G:H5''  | 2.08                     | 0.53              |
| 30:c:17:VAL:HB    | 30:c:204:VAL:HG13 | 1.90                     | 0.53              |
| 41:n:30:ARG:HA    | 41:n:35:ILE:HG13  | 1.91                     | 0.53              |
| 7:A:472:U:H2'     | 7:A:473:A:C8      | 2.44                     | 0.53              |
| 7:A:1086:U:H3     | 7:A:1099:G:H22    | 1.54                     | 0.53              |
| 7:A:1180:A:O2'    | 7:A:1181:A:OP1    | 2.26                     | 0.53              |
| 13:G:72:THR:O     | 13:G:72:THR:OG1   | 2.25                     | 0.53              |
| 15:I:42:GLU:O     | 15:I:46:MET:HG2   | 2.08                     | 0.53              |
| 28:a:358:U:H2'    | 28:a:359:G:H8     | 1.73                     | 0.53              |
| 28:a:919:U:OP1    | 29:b:97:C:O2'     | 2.25                     | 0.53              |
| 28:a:2523:G:O2'   | 28:a:2764:A:H5''  | 2.09                     | 0.53              |
| 39:l:110:GLU:OE1  | 39:l:114:ARG:HG3  | 2.09                     | 0.53              |
| 41:n:25:ARG:O     | 41:n:40:ILE:N     | 2.28                     | 0.53              |
| 7:A:326:G:O2'     | 7:A:327:A:OP1     | 2.19                     | 0.53              |
| 7:A:1086:U:H3     | 7:A:1099:G:H1     | 1.55                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:F:5:GLU:HA    | 12:F:62:MET:O     | 2.08                     | 0.53              |
| 28:a:2330:G:C2   | 28:a:2331:G:H1'   | 2.44                     | 0.53              |
| 28:a:2526:G:O6   | 28:a:2538:C:N4    | 2.42                     | 0.53              |
| 39:l:118:LYS:HA  | 39:l:121:ALA:HB3  | 1.91                     | 0.53              |
| 41:n:11:ALA:O    | 41:n:14:ALA:N     | 2.42                     | 0.53              |
| 4:3:26:ILE:HA    | 4:3:34:LYS:HG2    | 1.91                     | 0.53              |
| 7:A:437:U:P      | 10:D:154:ARG:HH12 | 2.32                     | 0.53              |
| 7:A:674:G:H2'    | 7:A:675:A:H8      | 1.74                     | 0.53              |
| 7:A:1149:U:O2'   | 7:A:1150:C:H6     | 1.92                     | 0.53              |
| 8:B:16:PHE:O     | 8:B:38:VAL:HG13   | 2.09                     | 0.53              |
| 15:I:12:ARG:HG3  | 15:I:13:LYS:H     | 1.74                     | 0.53              |
| 28:a:1223:G:OP1  | 44:q:68:ARG:NH1   | 2.41                     | 0.53              |
| 28:a:1746:A:H2'  | 28:a:1747:U:C6    | 2.44                     | 0.53              |
| 28:a:1029:A:N6   | 28:a:1125:G:H1'   | 2.22                     | 0.53              |
| 32:e:139:LYS:HD2 | 32:e:139:LYS:C    | 2.34                     | 0.53              |
| 34:g:71:LEU:O    | 34:g:75:MET:HG3   | 2.09                     | 0.53              |
| 49:v:43:THR:HB   | 49:v:46:HIS:CE1   | 2.44                     | 0.53              |
| 49:v:71:VAL:HG12 | 49:v:78:LYS:HG2   | 1.89                     | 0.53              |
| 4:3:1:MET:O      | 28:a:2538:C:O2'   | 2.19                     | 0.52              |
| 7:A:597:G:H2'    | 7:A:598:U:H5'     | 1.90                     | 0.52              |
| 7:A:944:G:N1     | 7:A:1339:G:OP2    | 2.36                     | 0.52              |
| 7:A:1127:G:N7    | 16:J:7:ARG:NH2    | 2.56                     | 0.52              |
| 14:H:65:TYR:HB3  | 14:H:69:LYS:HA    | 1.91                     | 0.52              |
| 28:a:997:G:OP1   | 43:p:91:ASP:HB2   | 2.09                     | 0.52              |
| 28:a:1007:C:OP1  | 36:i:37:ARG:NH1   | 2.42                     | 0.52              |
| 28:a:2315:G:O2'  | 33:f:125:ARG:HD3  | 2.10                     | 0.52              |
| 28:a:2471:A:N6   | 28:a:2480:C:C2    | 2.78                     | 0.52              |
| 32:e:120:VAL:HA  | 32:e:188:MET:SD   | 2.49                     | 0.52              |
| 37:j:4:GLU:HG2   | 37:j:23:LYS:HA    | 1.91                     | 0.52              |
| 7:A:105:G:H21    | 7:A:379:C:C5'     | 2.21                     | 0.52              |
| 8:B:151:ILE:HG23 | 8:B:154:MET:SD    | 2.48                     | 0.52              |
| 8:B:191:SER:OG   | 8:B:192:ASP:N     | 2.40                     | 0.52              |
| 11:E:80:THR:HG22 | 11:E:122:ASN:HB2  | 1.91                     | 0.52              |
| 11:E:90:THR:HG22 | 11:E:91:GLY:N     | 2.25                     | 0.52              |
| 14:H:74:SER:H    | 14:H:130:ALA:HB2  | 1.74                     | 0.52              |
| 19:M:5:ALA:HB1   | 19:M:9:ILE:HB     | 1.91                     | 0.52              |
| 28:a:2377:A:H3'  | 28:a:2378:A:C8    | 2.44                     | 0.52              |
| 29:b:90:C:C2     | 29:b:91:C:C5      | 2.97                     | 0.52              |
| 48:u:30:ILE:HG23 | 48:u:38:LEU:O     | 2.09                     | 0.52              |
| 7:A:259:G:H2'    | 7:A:260:G:H4'     | 1.90                     | 0.52              |
| 22:P:41:PRO:HG2  | 22:P:45:GLU:OE1   | 2.10                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:a:599:A:H5''  | 38:k:9:ALA:HB3    | 1.91                     | 0.52              |
| 28:a:1469:A:H2'  | 28:a:1470:A:C8    | 2.45                     | 0.52              |
| 28:a:2043:C:C4   | 28:a:2044:C:C2    | 2.98                     | 0.52              |
| 28:a:2741:A:H62  | 28:a:2763:G:N2    | 2.07                     | 0.52              |
| 34:g:156:PRO:HB2 | 34:g:172:LYS:HE2  | 1.89                     | 0.52              |
| 34:g:174:ALA:O   | 34:g:176:LYS:NZ   | 2.42                     | 0.52              |
| 13:G:143:ARG:O   | 13:G:147:ALA:HB3  | 2.10                     | 0.52              |
| 28:a:840:C:H2'   | 28:a:841:G:C8     | 2.45                     | 0.52              |
| 28:a:2071:A:H2'  | 28:a:2072:C:C6    | 2.45                     | 0.52              |
| 31:d:80:TRP:HB3  | 31:d:202:ILE:HD11 | 1.91                     | 0.52              |
| 33:f:35:THR:O    | 33:f:155:THR:N    | 2.42                     | 0.52              |
| 40:m:22:ARG:HG3  | 40:m:70:THR:HA    | 1.90                     | 0.52              |
| 7:A:402:G:OP1    | 10:D:71:GLN:NE2   | 2.32                     | 0.52              |
| 7:A:608:A:C2'    | 7:A:609:A:H5'     | 2.40                     | 0.52              |
| 7:A:718:A:H2     | 24:R:38:LYS:HZ3   | 1.58                     | 0.52              |
| 22:P:71:VAL:O    | 22:P:75:ILE:HG13  | 2.09                     | 0.52              |
| 25:S:12:ASP:HB3  | 25:S:16:LEU:HG    | 1.90                     | 0.52              |
| 32:e:16:GLU:HA   | 32:e:16:GLU:OE2   | 2.10                     | 0.52              |
| 36:i:16:TYR:O    | 36:i:54:ILE:HA    | 2.09                     | 0.52              |
| 40:m:106:ASP:OD1 | 40:m:106:ASP:N    | 2.42                     | 0.52              |
| 7:A:1311:G:H3'   | 7:A:1312:A:H5''   | 1.92                     | 0.52              |
| 12:F:19:PRO:O    | 12:F:22:ILE:HG23  | 2.10                     | 0.52              |
| 14:H:41:LYS:NZ   | 14:H:47:GLU:O     | 2.42                     | 0.52              |
| 19:M:13:LYS:HE3  | 19:M:15:ALA:HB2   | 1.91                     | 0.52              |
| 28:a:1020:A:C6   | 28:a:1141:U:C4    | 2.96                     | 0.52              |
| 28:a:1040:A:H4'  | 48:u:49:ASN:ND2   | 2.24                     | 0.52              |
| 28:a:2356:U:C2   | 28:a:2357:G:C8    | 2.97                     | 0.52              |
| 28:a:2471:A:N6   | 28:a:2480:C:O2    | 2.43                     | 0.52              |
| 28:a:2526:G:H2'  | 28:a:2526:G:N3    | 2.24                     | 0.52              |
| 36:i:54:ILE:O    | 36:i:122:LEU:HA   | 2.09                     | 0.52              |
| 44:q:2:TYR:CD1   | 44:q:13:ARG:HD2   | 2.44                     | 0.52              |
| 7:A:501:C:OP1    | 18:L:114:ARG:NH2  | 2.35                     | 0.52              |
| 7:A:1156:A:O3'   | 7:A:1157:G:H4'    | 2.09                     | 0.52              |
| 7:A:1440:G:H3'   | 7:A:1441:U:C6     | 2.44                     | 0.52              |
| 8:B:197:ASP:OD1  | 8:B:197:ASP:N     | 2.42                     | 0.52              |
| 9:C:55:ILE:HD12  | 9:C:55:ILE:O      | 2.10                     | 0.52              |
| 28:a:1021:A:C3'  | 28:a:1022:G:H4'   | 2.39                     | 0.52              |
| 28:a:2479:U:C5   | 28:a:2480:C:C6    | 2.97                     | 0.52              |
| 32:e:124:PHE:CD2 | 32:e:187:VAL:HG11 | 2.45                     | 0.52              |
| 43:p:91:ASP:OD2  | 44:q:11:GLN:NE2   | 2.42                     | 0.52              |
| 51:x:34:SER:O    | 51:x:34:SER:OG    | 2.24                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:42:ARG:HD3    | 28:a:2349:G:N7    | 2.25                     | 0.52              |
| 7:A:458:U:N3      | 7:A:475:U:O2      | 2.42                     | 0.52              |
| 7:A:983:A:O2'     | 7:A:1049:U:OP2    | 2.26                     | 0.52              |
| 7:A:1525:G:H2'    | 7:A:1526:A:C8     | 2.43                     | 0.52              |
| 12:F:12:PRO:O     | 12:F:44:ARG:NH2   | 2.43                     | 0.52              |
| 17:K:15:GLN:NE2   | 17:K:77:TYR:O     | 2.43                     | 0.52              |
| 26:T:33:LYS:HZ2   | 26:T:37:ALA:HB2   | 1.74                     | 0.52              |
| 26:T:33:LYS:NZ    | 26:T:37:ALA:HB2   | 2.25                     | 0.52              |
| 28:a:282:A:H2'    | 28:a:283:G:H8     | 1.74                     | 0.52              |
| 28:a:627:A:H62    | 38:k:112:LEU:HB3  | 1.74                     | 0.52              |
| 7:A:108:G:H22     | 7:A:332:G:H5''    | 1.74                     | 0.52              |
| 7:A:1002:A:H2'    | 7:A:1041:G:C6     | 2.45                     | 0.52              |
| 7:A:1320:A:H4'    | 7:A:1321:C:OP2    | 2.09                     | 0.52              |
| 20:N:31:ILE:HA    | 20:N:41:ARG:HH21  | 1.75                     | 0.52              |
| 29:b:64:G:H2'     | 29:b:65:U:O4'     | 2.10                     | 0.52              |
| 31:d:196:ALA:O    | 31:d:199:SER:OG   | 2.27                     | 0.52              |
| 34:g:54:PRO:HB3   | 34:g:61:GLY:C     | 2.35                     | 0.52              |
| 38:k:109:LYS:HG2  | 38:k:128:THR:HG23 | 1.91                     | 0.52              |
| 49:v:66:LYS:NZ    | 49:v:66:LYS:HB3   | 2.24                     | 0.52              |
| 7:A:674:G:H2'     | 7:A:675:A:C8      | 2.45                     | 0.52              |
| 7:A:891:U:O2'     | 7:A:892:A:H8      | 1.92                     | 0.52              |
| 7:A:1181:A:OP2    | 15:I:99:ARG:NH2   | 2.39                     | 0.52              |
| 9:C:40:ARG:HG2    | 9:C:55:ILE:HD11   | 1.92                     | 0.52              |
| 9:C:117:ALA:HB1   | 9:C:187:SER:HB2   | 1.92                     | 0.52              |
| 10:D:19:LEU:HG    | 10:D:64:ILE:CD1   | 2.40                     | 0.52              |
| 12:F:8:PHE:CE1    | 12:F:60:VAL:HG12  | 2.45                     | 0.52              |
| 15:I:22:LYS:HB2   | 15:I:62:ASP:OD2   | 2.10                     | 0.52              |
| 16:J:53:ILE:O     | 16:J:54:SER:HB3   | 2.10                     | 0.52              |
| 27:U:54:LYS:O     | 27:U:58:LYS:HG2   | 2.09                     | 0.52              |
| 28:a:290:U:H3     | 28:a:350:G:H1     | 1.58                     | 0.52              |
| 28:a:841:G:H2'    | 28:a:842:U:H6     | 1.73                     | 0.52              |
| 28:a:2528:U:C2    | 28:a:2536:G:C2    | 2.98                     | 0.52              |
| 28:a:2625:G:H1    | 28:a:2777:G:H1    | 1.57                     | 0.52              |
| 32:e:147:LEU:HB2  | 32:e:183:PHE:HD2  | 1.75                     | 0.52              |
| 38:k:127:VAL:HG21 | 38:k:142:ILE:HD13 | 1.92                     | 0.52              |
| 7:A:255:G:OP1     | 23:Q:71:LYS:NZ    | 2.42                     | 0.51              |
| 28:a:1028:A:H3'   | 28:a:1029:A:H8    | 1.75                     | 0.51              |
| 28:a:1434:A:H2'   | 28:a:1435:G:C8    | 2.44                     | 0.51              |
| 39:l:98:PRO:C     | 48:u:82:TYR:HB3   | 2.34                     | 0.51              |
| 48:u:57:TYR:HE2   | 48:u:77:VAL:HB    | 1.75                     | 0.51              |
| 7:A:299:G:H1      | 7:A:566:A:H61     | 1.56                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:1009:A:H61    | 7:A:1020:U:H3     | 1.57                     | 0.51              |
| 7:A:1066:C:O2'    | 7:A:1067:A:O5'    | 2.23                     | 0.51              |
| 8:B:43:LEU:HA     | 8:B:46:THR:HB     | 1.92                     | 0.51              |
| 18:L:110:ARG:NH1  | 18:L:112:GLN:O    | 2.43                     | 0.51              |
| 28:a:586:A:H5'    | 32:e:84:THR:HG21  | 1.91                     | 0.51              |
| 28:a:1873:G:H2'   | 28:a:1874:C:C6    | 2.45                     | 0.51              |
| 31:d:17:GLU:CD    | 31:d:17:GLU:H     | 2.17                     | 0.51              |
| 31:d:50:VAL:O     | 31:d:80:TRP:N     | 2.42                     | 0.51              |
| 32:e:119:ILE:O    | 32:e:188:MET:HE1  | 2.10                     | 0.51              |
| 34:g:63:ALA:O     | 34:g:67:THR:OG1   | 2.28                     | 0.51              |
| 34:g:101:ASN:OD1  | 34:g:116:GLN:NE2  | 2.43                     | 0.51              |
| 36:i:15:TRP:HZ3   | 36:i:55:ILE:HD11  | 1.74                     | 0.51              |
| 36:i:36:LEU:HD11  | 36:i:54:ILE:HG21  | 1.91                     | 0.51              |
| 7:A:131:A:H3'     | 7:A:132:U:H5''    | 1.92                     | 0.51              |
| 7:A:415:A:H2'     | 7:A:416:G:H8      | 1.75                     | 0.51              |
| 10:D:10:LYS:HD2   | 10:D:38:PRO:HB3   | 1.93                     | 0.51              |
| 22:P:19:VAL:HB    | 22:P:37:GLY:HA2   | 1.92                     | 0.51              |
| 28:a:1589:U:H2'   | 28:a:1590:A:H8    | 1.74                     | 0.51              |
| 28:a:2472:G:H5''  | 28:a:2473:U:H5''  | 1.92                     | 0.51              |
| 31:d:33:ARG:O     | 31:d:51:THR:HG22  | 2.11                     | 0.51              |
| 34:g:16:ASP:HB2   | 34:g:27:LYS:HB3   | 1.92                     | 0.51              |
| 34:g:105:LEU:O    | 34:g:112:PRO:HA   | 2.11                     | 0.51              |
| 43:p:76:TYR:O     | 43:p:80:ILE:HG12  | 2.11                     | 0.51              |
| 48:u:80:HIS:N     | 48:u:85:LYS:O     | 2.43                     | 0.51              |
| 7:A:1024:G:H2'    | 7:A:1025:U:H4'    | 1.93                     | 0.51              |
| 9:C:45:LYS:NZ     | 9:C:45:LYS:HB3    | 2.25                     | 0.51              |
| 28:a:1418:G:N2    | 28:a:1580:A:C5    | 2.78                     | 0.51              |
| 29:b:23:G:H2'     | 29:b:24:G:N7      | 2.25                     | 0.51              |
| 30:c:270:ARG:HG2  | 30:c:271:ARG:N    | 2.25                     | 0.51              |
| 32:e:151:GLY:N    | 32:e:192:ALA:HB2  | 2.25                     | 0.51              |
| 34:g:156:PRO:HB2  | 34:g:172:LYS:CE   | 2.40                     | 0.51              |
| 18:L:75:GLN:OE1   | 18:L:75:GLN:N     | 2.43                     | 0.51              |
| 23:Q:7:THR:OG1    | 23:Q:61:ILE:O     | 2.23                     | 0.51              |
| 33:f:147:ASP:OD1  | 33:f:147:ASP:N    | 2.43                     | 0.51              |
| 34:g:129:THR:HG23 | 34:g:130:GLU:HG3  | 1.92                     | 0.51              |
| 36:i:54:ILE:HD13  | 36:i:122:LEU:HD13 | 1.92                     | 0.51              |
| 44:q:25:LEU:H     | 44:q:94:THR:HG21  | 1.76                     | 0.51              |
| 7:A:458:U:H2'     | 7:A:459:A:H8      | 1.76                     | 0.51              |
| 7:A:500:G:H2'     | 7:A:501:C:C6      | 2.45                     | 0.51              |
| 7:A:1014:A:N1     | 25:S:34:TRP:HB3   | 2.26                     | 0.51              |
| 8:B:112:LYS:HA    | 8:B:115:LYS:HG2   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:C:25:ASN:O     | 9:C:27:LYS:N      | 2.44                     | 0.51              |
| 9:C:64:ILE:O     | 9:C:66:VAL:HG23   | 2.11                     | 0.51              |
| 9:C:135:LYS:O    | 9:C:139:GLN:HG3   | 2.10                     | 0.51              |
| 10:D:128:ARG:HB3 | 10:D:128:ARG:CZ   | 2.38                     | 0.51              |
| 19:M:85:CYS:SG   | 19:M:86:TYR:N     | 2.84                     | 0.51              |
| 25:S:5:LEU:HD23  | 25:S:5:LEU:O      | 2.11                     | 0.51              |
| 28:a:1028:A:N6   | 28:a:1126:A:H62   | 2.08                     | 0.51              |
| 28:a:1028:A:H2   | 28:a:2487:G:H4'   | 1.73                     | 0.51              |
| 33:f:14:LYS:O    | 33:f:18:THR:OG1   | 2.28                     | 0.51              |
| 34:g:101:ASN:O   | 34:g:117:LEU:N    | 2.43                     | 0.51              |
| 40:m:32:GLU:OE2  | 40:m:115:LEU:HD12 | 2.10                     | 0.51              |
| 41:n:83:LEU:HD12 | 41:n:88:LYS:HD2   | 1.92                     | 0.51              |
| 5:4:56:ARG:HD3   | 25:S:67:VAL:HB    | 1.93                     | 0.51              |
| 7:A:596:A:H62    | 7:A:644:U:H3      | 1.59                     | 0.51              |
| 7:A:1444:U:H2'   | 7:A:1445:U:O4'    | 2.11                     | 0.51              |
| 8:B:96:TRP:HA    | 8:B:100:MET:SD    | 2.51                     | 0.51              |
| 9:C:5:VAL:HG11   | 9:C:10:ILE:HG13   | 1.92                     | 0.51              |
| 29:b:48:U:H2'    | 29:b:49:C:C6      | 2.45                     | 0.51              |
| 33:f:24:SER:HB3  | 33:f:27:GLN:HG3   | 1.92                     | 0.51              |
| 33:f:126:GLY:O   | 33:f:158:THR:OG1  | 2.16                     | 0.51              |
| 34:g:48:ASN:OD1  | 34:g:48:ASN:N     | 2.43                     | 0.51              |
| 38:k:78:ARG:NE   | 38:k:113:ALA:HB3  | 2.24                     | 0.51              |
| 38:k:112:LEU:HB2 | 38:k:131:ALA:CA   | 2.41                     | 0.51              |
| 38:k:129:LYS:HA  | 38:k:132:ARG:CG   | 2.41                     | 0.51              |
| 48:u:20:LEU:HA   | 48:u:23:ALA:HB3   | 1.91                     | 0.51              |
| 48:u:49:ASN:C    | 48:u:50:MET:HE2   | 2.36                     | 0.51              |
| 7:A:413:A:H2'    | 7:A:413:A:N3      | 2.26                     | 0.51              |
| 9:C:40:ARG:CZ    | 20:N:92:GLU:HG3   | 2.41                     | 0.51              |
| 18:L:21:VAL:HB   | 18:L:24:LEU:HD23  | 1.93                     | 0.51              |
| 20:N:49:GLN:HE21 | 25:S:10:PHE:HE2   | 1.59                     | 0.51              |
| 27:U:11:PRO:HB2  | 27:U:13:ASP:OD1   | 2.11                     | 0.51              |
| 28:a:85:G:C2'    | 28:a:86:G:H4'     | 2.36                     | 0.51              |
| 28:a:548:G:C5    | 28:a:549:G:C6     | 2.99                     | 0.51              |
| 28:a:644:A:N1    | 28:a:2369:A:O2'   | 2.44                     | 0.51              |
| 29:b:92:C:H2'    | 29:b:93:C:C6      | 2.45                     | 0.51              |
| 30:c:107:PRO:HD2 | 30:c:110:LEU:HD22 | 1.93                     | 0.51              |
| 32:e:124:PHE:CE2 | 32:e:138:LEU:HD11 | 2.46                     | 0.51              |
| 36:i:45:THR:HG22 | 36:i:46:PRO:HD2   | 1.92                     | 0.51              |
| 1:0:13:SER:HA    | 1:0:49:TYR:HA     | 1.91                     | 0.51              |
| 7:A:73:C:N4      | 7:A:96:U:C4       | 2.78                     | 0.51              |
| 15:I:85:ARG:O    | 15:I:88:MET:HG3   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:b:78:A:H2'    | 29:b:79:G:O4'     | 2.10                     | 0.51              |
| 34:g:44:LYS:HD3  | 34:g:50:LEU:HA    | 1.93                     | 0.51              |
| 38:k:129:LYS:HA  | 38:k:132:ARG:HG2  | 1.93                     | 0.51              |
| 51:x:20:ASN:O    | 51:x:24:GLU:HG2   | 2.10                     | 0.51              |
| 3:2:25:LYS:HD3   | 38:k:62:PRO:HG2   | 1.92                     | 0.51              |
| 7:A:1049:U:H4'   | 7:A:1050:G:H4'    | 1.93                     | 0.51              |
| 8:B:83:ALA:HB3   | 8:B:214:LEU:HD12  | 1.92                     | 0.51              |
| 9:C:2:GLY:O      | 9:C:4:LYS:N       | 2.43                     | 0.51              |
| 22:P:6:LEU:HG    | 22:P:17:TYR:HB3   | 1.93                     | 0.51              |
| 25:S:66:MET:HG3  | 25:S:74:PHE:CZ    | 2.46                     | 0.51              |
| 28:a:279:A:H62   | 28:a:361:G:H21    | 1.58                     | 0.51              |
| 28:a:2043:C:C5   | 28:a:2044:C:C5    | 2.99                     | 0.51              |
| 5:4:18:CYS:HB3   | 5:4:40:CYS:HB3    | 1.93                     | 0.50              |
| 7:A:447:G:N1     | 7:A:486:U:OP2     | 2.44                     | 0.50              |
| 7:A:600:A:N6     | 7:A:639:G:O6      | 2.44                     | 0.50              |
| 7:A:1000:A:H2'   | 7:A:1001:G:C8     | 2.46                     | 0.50              |
| 10:D:168:PRO:O   | 10:D:170:TRP:N    | 2.36                     | 0.50              |
| 13:G:122:ASN:OD1 | 13:G:123:GLU:N    | 2.44                     | 0.50              |
| 25:S:21:LYS:O    | 25:S:21:LYS:HD3   | 2.11                     | 0.50              |
| 28:a:2789:C:N4   | 28:a:2893:A:C5    | 2.79                     | 0.50              |
| 29:b:63:C:H2'    | 29:b:64:G:C8      | 2.42                     | 0.50              |
| 29:b:65:U:H3'    | 29:b:108:A:N6     | 2.26                     | 0.50              |
| 31:d:1:MET:SD    | 31:d:2:ILE:HG22   | 2.51                     | 0.50              |
| 33:f:70:ALA:O    | 33:f:82:GLY:N     | 2.37                     | 0.50              |
| 34:g:41:VAL:O    | 34:g:55:ARG:NH2   | 2.44                     | 0.50              |
| 36:i:138:GLN:N   | 36:i:138:GLN:OE1  | 2.44                     | 0.50              |
| 37:j:64:ARG:NH2  | 37:j:100:PHE:O    | 2.45                     | 0.50              |
| 43:p:98:ILE:HG21 | 43:p:109:LEU:HD12 | 1.93                     | 0.50              |
| 44:q:14:VAL:HB   | 44:q:20:VAL:HG22  | 1.93                     | 0.50              |
| 48:u:71:LYS:HB3  | 48:u:73:LYS:HZ1   | 1.76                     | 0.50              |
| 7:A:1285:C:H5''  | 7:A:1286:A:H2'    | 1.93                     | 0.50              |
| 7:A:1370:C:HO2'  | 7:A:1371:G:P      | 2.34                     | 0.50              |
| 8:B:19:GLN:OE1   | 8:B:19:GLN:N      | 2.33                     | 0.50              |
| 24:R:9:LYS:N     | 24:R:46:GLY:HA3   | 2.26                     | 0.50              |
| 28:a:85:G:C8     | 28:a:86:G:H1'     | 2.46                     | 0.50              |
| 28:a:661:A:C5    | 28:a:662:G:C8     | 3.00                     | 0.50              |
| 28:a:879:G:H2'   | 28:a:880:G:C8     | 2.46                     | 0.50              |
| 30:c:240:PHE:O   | 30:c:242:LYS:HD2  | 2.11                     | 0.50              |
| 1:0:6:ARG:NH1    | 28:a:2285:C:OP2   | 2.40                     | 0.50              |
| 7:A:376:G:H2'    | 7:A:377:G:C8      | 2.45                     | 0.50              |
| 7:A:458:U:H2'    | 7:A:459:A:C8      | 2.46                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:A:1321:C:H41   | 25:S:36:ARG:HH11  | 1.59                     | 0.50              |
| 10:D:189:SER:OG  | 10:D:194:ASP:O    | 2.29                     | 0.50              |
| 28:a:424:G:C6    | 28:a:425:G:N3     | 2.79                     | 0.50              |
| 29:b:77:U:C4     | 29:b:99:A:N7      | 2.76                     | 0.50              |
| 32:e:24:ASN:HB3  | 32:e:27:LEU:HB3   | 1.93                     | 0.50              |
| 43:p:64:ARG:NH1  | 43:p:100:VAL:HG21 | 2.27                     | 0.50              |
| 1:O:20:PHE:CZ    | 28:a:2419:U:H1'   | 2.47                     | 0.50              |
| 7:A:465:A:H2'    | 7:A:465:A:N3      | 2.26                     | 0.50              |
| 7:A:1122:U:H1'   | 7:A:1123:G:C8     | 2.47                     | 0.50              |
| 15:I:129:LYS:O   | 15:I:130:ARG:HG3  | 2.11                     | 0.50              |
| 25:S:41:PHE:O    | 25:S:44:MET:HG2   | 2.11                     | 0.50              |
| 28:a:1167:C:H3'  | 28:a:1168:G:H8    | 1.76                     | 0.50              |
| 28:a:1720:U:H2'  | 28:a:1721:G:O4'   | 2.12                     | 0.50              |
| 28:a:1733:G:H2'  | 28:a:1734:G:C8    | 2.47                     | 0.50              |
| 28:a:2351:G:H22  | 28:a:2366:A:H5''  | 1.76                     | 0.50              |
| 28:a:2744:G:H21  | 34:g:143:GLN:NE2  | 2.07                     | 0.50              |
| 36:i:15:TRP:HB3  | 36:i:137:PRO:HB3  | 1.93                     | 0.50              |
| 36:i:134:ALA:C   | 36:i:136:GLN:H    | 2.19                     | 0.50              |
| 43:p:61:TRP:HB3  | 43:p:92:ARG:O     | 2.11                     | 0.50              |
| 47:t:81:ASP:OD1  | 47:t:82:ARG:N     | 2.44                     | 0.50              |
| 7:A:411:A:H2'    | 7:A:412:C:C4'     | 2.41                     | 0.50              |
| 7:A:486:U:H2'    | 7:A:487:A:H8      | 1.76                     | 0.50              |
| 7:A:748:U:O4     | 7:A:749:A:N6      | 2.45                     | 0.50              |
| 13:G:30:LEU:HD12 | 13:G:39:ALA:HB1   | 1.94                     | 0.50              |
| 15:I:14:SER:O    | 15:I:14:SER:OG    | 2.27                     | 0.50              |
| 16:J:40:ILE:HD11 | 16:J:73:LEU:HB3   | 1.93                     | 0.50              |
| 19:M:34:LEU:HD11 | 19:M:39:ILE:HB    | 1.92                     | 0.50              |
| 28:a:840:C:C2    | 28:a:841:G:N7     | 2.79                     | 0.50              |
| 28:a:1020:A:H1'  | 28:a:1021:A:C2    | 2.47                     | 0.50              |
| 28:a:1433:A:H2'  | 28:a:1434:A:C8    | 2.46                     | 0.50              |
| 28:a:2304:G:OP1  | 33:f:121:SER:OG   | 2.30                     | 0.50              |
| 7:A:231:U:H1'    | 7:A:262:A:H61     | 1.76                     | 0.50              |
| 17:K:50:SER:OG   | 17:K:69:ARG:NH1   | 2.44                     | 0.50              |
| 20:N:47:LYS:HD2  | 20:N:47:LYS:C     | 2.37                     | 0.50              |
| 28:a:1042:G:H2'  | 28:a:1043:C:C6    | 2.47                     | 0.50              |
| 28:a:1183:U:P    | 52:y:31:ARG:NH2   | 2.83                     | 0.50              |
| 28:a:2335:A:H5'  | 41:n:13:ARG:NH2   | 2.27                     | 0.50              |
| 28:a:2546:U:H5'' | 28:a:2547:A:O5'   | 2.12                     | 0.50              |
| 29:b:96:G:H2'    | 29:b:97:C:O4'     | 2.11                     | 0.50              |
| 32:e:124:PHE:HB3 | 32:e:148:ILE:HD13 | 1.92                     | 0.50              |
| 43:p:79:PHE:HZ   | 43:p:109:LEU:HB3  | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:x:12:GLU:HG2   | 51:x:13:GLU:OE1   | 2.11                     | 0.50              |
| 10:D:60:LYS:O     | 10:D:64:ILE:HD13  | 2.11                     | 0.50              |
| 28:a:2461:A:H2'   | 28:a:2462:C:C6    | 2.46                     | 0.50              |
| 31:d:37:VAL:HG13  | 31:d:48:ILE:HG22  | 1.92                     | 0.50              |
| 46:s:3:ARG:HH12   | 46:s:5:GLU:HG2    | 1.77                     | 0.50              |
| 7:A:66:G:O6       | 7:A:102:G:C2      | 2.65                     | 0.50              |
| 7:A:618:C:N4      | 7:A:621:A:OP2     | 2.41                     | 0.50              |
| 7:A:1164:G:H2'    | 7:A:1165:G:H8     | 1.77                     | 0.50              |
| 12:F:46:GLN:OE1   | 12:F:46:GLN:N     | 2.28                     | 0.50              |
| 28:a:2324:U:H5''  | 28:a:2326:C:P     | 2.52                     | 0.50              |
| 28:a:2472:G:N2    | 28:a:2479:U:O4    | 2.44                     | 0.50              |
| 29:b:74:U:O2      | 48:u:29:ILE:HD13  | 2.12                     | 0.50              |
| 29:b:92:C:P       | 48:u:18:ARG:HH12  | 2.35                     | 0.50              |
| 41:n:15:ARG:HE    | 41:n:95:SER:HA    | 1.75                     | 0.50              |
| 4:3:2:LYS:HE3     | 28:a:2478:A:H5'   | 1.93                     | 0.50              |
| 7:A:967:5MC:H3'   | 7:A:968:A:H2'     | 1.94                     | 0.50              |
| 7:A:1130:A:H2'    | 7:A:1131:G:C8     | 2.47                     | 0.50              |
| 28:a:2741:A:C2'   | 28:a:2742:G:H8    | 2.24                     | 0.50              |
| 7:A:849:G:H3'     | 7:A:850:U:H5''    | 1.94                     | 0.49              |
| 8:B:32:PHE:HB3    | 8:B:40:ILE:HG12   | 1.94                     | 0.49              |
| 10:D:104:ARG:HH11 | 10:D:104:ARG:HG3  | 1.77                     | 0.49              |
| 28:a:640:C:H2'    | 28:a:641:U:C6     | 2.47                     | 0.49              |
| 28:a:1126:A:H5''  | 56:a:6210:SPD:H92 | 1.94                     | 0.49              |
| 28:a:1141:U:H4'   | 28:a:1142:A:O4'   | 2.12                     | 0.49              |
| 7:A:91:U:H2'      | 7:A:92:U:H6       | 1.77                     | 0.49              |
| 7:A:260:G:H2'     | 7:A:261:U:C5      | 2.47                     | 0.49              |
| 7:A:1229:C:H2'    | 7:A:1230:A:C8     | 2.45                     | 0.49              |
| 28:a:1026:G:C2    | 28:a:1027:A:C6    | 3.00                     | 0.49              |
| 36:i:55:ILE:HG12  | 36:i:123:LYS:O    | 2.12                     | 0.49              |
| 43:p:93:LYS:HD3   | 43:p:94:ILE:HG12  | 1.94                     | 0.49              |
| 7:A:176:C:OP2     | 26:T:64:LYS:NZ    | 2.45                     | 0.49              |
| 7:A:837:U:H3      | 7:A:849:G:H1      | 1.57                     | 0.49              |
| 7:A:902:G:H2'     | 7:A:903:A:H8      | 1.77                     | 0.49              |
| 7:A:1003:G:OP2    | 7:A:1039:C:N4     | 2.45                     | 0.49              |
| 7:A:1157:G:H5'    | 7:A:1158:A:O3'    | 2.11                     | 0.49              |
| 9:C:59:ARG:HE     | 9:C:64:ILE:HD13   | 1.76                     | 0.49              |
| 24:R:50:LYS:HA    | 24:R:53:ARG:NH1   | 2.27                     | 0.49              |
| 27:U:55:ARG:NH1   | 27:U:55:ARG:HB3   | 2.27                     | 0.49              |
| 28:a:360:U:H2'    | 28:a:361:G:C8     | 2.47                     | 0.49              |
| 28:a:424:G:C4     | 28:a:425:G:H1'    | 2.47                     | 0.49              |
| 28:a:841:G:C6     | 28:a:938:G:N2     | 2.80                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 28:a:2399:G:H2'  | 28:a:2400:G:C8   | 2.47                     | 0.49              |
| 29:b:106:G:H2'   | 29:b:107:G:O4'   | 2.12                     | 0.49              |
| 4:3:2:LYS:HB2    | 4:3:35:GLN:CG    | 2.42                     | 0.49              |
| 7:A:127:G:OP1    | 7:A:605:U:O2'    | 2.25                     | 0.49              |
| 7:A:254:G:O6     | 7:A:273:A:N6     | 2.45                     | 0.49              |
| 7:A:337:G:H2'    | 7:A:338:A:C8     | 2.47                     | 0.49              |
| 8:B:213:TYR:O    | 8:B:217:VAL:HG22 | 2.12                     | 0.49              |
| 9:C:60:PRO:HB3   | 16:J:93:ALA:HA   | 1.95                     | 0.49              |
| 12:F:8:PHE:HE2   | 12:F:10:VAL:HG23 | 1.77                     | 0.49              |
| 19:M:98:ARG:HH11 | 19:M:99:GLY:H    | 1.60                     | 0.49              |
| 25:S:11:ILE:CG2  | 25:S:38:SER:HA   | 2.42                     | 0.49              |
| 28:a:603:A:H4'   | 28:a:604:G:C4'   | 2.42                     | 0.49              |
| 28:a:1023:U:C4   | 28:a:1024:G:C4   | 3.01                     | 0.49              |
| 28:a:2323:G:N1   | 28:a:2331:G:O6   | 2.45                     | 0.49              |
| 28:a:2830:C:H5'' | 31:d:56:LYS:HE3  | 1.94                     | 0.49              |
| 36:i:53:TYR:CD2  | 36:i:121:LYS:HA  | 2.46                     | 0.49              |
| 4:3:4:ARG:HH22   | 4:3:10:LEU:HD11  | 1.77                     | 0.49              |
| 7:A:1100:C:H5'   | 8:B:95:ARG:NE    | 2.28                     | 0.49              |
| 8:B:128:LYS:HD2  | 8:B:128:LYS:N    | 2.27                     | 0.49              |
| 10:D:49:SER:OG   | 10:D:50:ASP:N    | 2.44                     | 0.49              |
| 19:M:13:LYS:HG3  | 19:M:15:ALA:HB2  | 1.94                     | 0.49              |
| 19:M:96:PRO:HA   | 19:M:109:ARG:HB2 | 1.94                     | 0.49              |
| 28:a:2305:U:H2'  | 28:a:2306:C:O4'  | 2.13                     | 0.49              |
| 28:a:2362:C:C2   | 28:a:2363:G:N7   | 2.80                     | 0.49              |
| 32:e:5:LEU:HD22  | 32:e:8:ALA:HB3   | 1.95                     | 0.49              |
| 48:u:44:HIS:O    | 48:u:48:MET:HB2  | 2.13                     | 0.49              |
| 7:A:502:A:OP1    | 18:L:115:SER:OG  | 2.18                     | 0.49              |
| 7:A:1017:C:N4    | 20:N:53:ARG:H    | 2.11                     | 0.49              |
| 7:A:1398:C:O2'   | 7:A:1403:4OC:OP1 | 2.31                     | 0.49              |
| 12:F:10:VAL:HG13 | 12:F:83:ALA:HB1  | 1.94                     | 0.49              |
| 17:K:45:ALA:HB3  | 17:K:70:CYS:HB2  | 1.94                     | 0.49              |
| 23:Q:15:ASP:CG   | 23:Q:21:ILE:HG22 | 2.38                     | 0.49              |
| 25:S:14:HIS:HD2  | 25:S:15:LEU:HD23 | 1.77                     | 0.49              |
| 26:T:4:ILE:HG22  | 26:T:6:SER:H     | 1.76                     | 0.49              |
| 28:a:2356:U:H2'  | 28:a:2357:G:H5'' | 1.95                     | 0.49              |
| 34:g:88:GLN:N    | 34:g:163:ARG:O   | 2.45                     | 0.49              |
| 36:i:43:GLU:OE1  | 36:i:43:GLU:N    | 2.45                     | 0.49              |
| 43:p:79:PHE:CZ   | 43:p:106:PHE:HE1 | 2.30                     | 0.49              |
| 48:u:47:VAL:HG13 | 48:u:56:PHE:CZ   | 2.48                     | 0.49              |
| 48:u:77:VAL:HG21 | 48:u:79:ARG:NH1  | 2.27                     | 0.49              |
| 7:A:194:C:O2'    | 7:A:196:A:OP1    | 2.24                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:G:131:LYS:HB3 | 13:G:135:VAL:HG21 | 1.94                     | 0.49              |
| 16:J:6:ILE:HG12  | 16:J:76:ILE:HG22  | 1.94                     | 0.49              |
| 28:a:2333:A:N3   | 41:n:9:ARG:NE     | 2.60                     | 0.49              |
| 28:a:2380:C:C2   | 28:a:2381:A:H1'   | 2.46                     | 0.49              |
| 28:a:2524:G:C6   | 28:a:2525:G:C8    | 3.01                     | 0.49              |
| 28:a:2896:C:H2'  | 28:a:2897:U:C6    | 2.48                     | 0.49              |
| 33:f:34:ILE:HD12 | 33:f:96:MET:HG2   | 1.93                     | 0.49              |
| 33:f:80:ARG:NE   | 33:f:80:ARG:HA    | 2.27                     | 0.49              |
| 36:i:119:PHE:HD1 | 36:i:122:LEU:HD23 | 1.78                     | 0.49              |
| 48:u:2:PHE:CE2   | 48:u:50:MET:HB3   | 2.47                     | 0.49              |
| 48:u:9:ARG:HH12  | 48:u:17:SER:HA    | 1.78                     | 0.49              |
| 50:w:20:HIS:O    | 50:w:20:HIS:ND1   | 2.41                     | 0.49              |
| 52:y:38:ARG:NE   | 52:y:38:ARG:HA    | 2.26                     | 0.49              |
| 7:A:22:G:HO2'    | 7:A:885:G:H8      | 1.60                     | 0.49              |
| 7:A:108:G:H5'    | 7:A:109:A:H3'     | 1.95                     | 0.49              |
| 7:A:373:A:H62    | 7:A:391:G:H1'     | 1.77                     | 0.49              |
| 7:A:1280:A:H5''  | 16:J:9:ARG:NH2    | 2.27                     | 0.49              |
| 8:B:15:HIS:HA    | 8:B:40:ILE:HA     | 1.95                     | 0.49              |
| 11:E:126:LYS:HG2 | 11:E:128:TYR:CZ   | 2.48                     | 0.49              |
| 13:G:59:LEU:HD12 | 13:G:59:LEU:O     | 2.13                     | 0.49              |
| 25:S:11:ILE:HD12 | 25:S:12:ASP:N     | 2.28                     | 0.49              |
| 28:a:749:A:N1    | 28:a:753:A:O2'    | 2.38                     | 0.49              |
| 28:a:2043:C:N4   | 28:a:2044:C:N3    | 2.61                     | 0.49              |
| 28:a:2591:C:H2'  | 28:a:2592:G:H8    | 1.78                     | 0.49              |
| 49:v:23:VAL:HA   | 49:v:38:VAL:HG12  | 1.95                     | 0.49              |
| 49:v:75:LYS:H    | 49:v:75:LYS:HD2   | 1.78                     | 0.49              |
| 7:A:456:G:H8     | 7:A:477:A:C2      | 2.30                     | 0.49              |
| 8:B:95:ARG:HG2   | 8:B:96:TRP:H      | 1.78                     | 0.49              |
| 10:D:25:VAL:HG23 | 10:D:26:ARG:HG2   | 1.95                     | 0.49              |
| 11:E:106:ILE:O   | 11:E:106:ILE:HG22 | 2.12                     | 0.49              |
| 13:G:92:ARG:NH2  | 13:G:93:PRO:HG2   | 2.28                     | 0.49              |
| 15:I:34:SER:OG   | 15:I:35:LEU:N     | 2.46                     | 0.49              |
| 18:L:55:VAL:HG21 | 18:L:80:ILE:HD11  | 1.94                     | 0.49              |
| 28:a:219:A:N3    | 28:a:234:U:O2'    | 2.43                     | 0.49              |
| 28:a:424:G:N1    | 28:a:425:G:C2     | 2.80                     | 0.49              |
| 28:a:629:G:N7    | 28:a:630:G:C4     | 2.80                     | 0.49              |
| 28:a:2471:A:N7   | 28:a:2472:G:C8    | 2.81                     | 0.49              |
| 28:a:2630:G:H1'  | 28:a:2894:G:C4    | 2.48                     | 0.49              |
| 28:a:2646:C:H2'  | 28:a:2647:U:O4'   | 2.13                     | 0.49              |
| 33:f:175:PHE:HB3 | 33:f:177:PHE:HD1  | 1.78                     | 0.49              |
| 43:p:85:LYS:HD3  | 43:p:86:ALA:N     | 2.28                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 48:u:80:HIS:HA   | 48:u:87:GLN:HG3  | 1.94                     | 0.49              |
| 49:v:46:HIS:HB2  | 49:v:79:PHE:CE1  | 2.48                     | 0.49              |
| 7:A:712:A:H2'    | 7:A:713:G:C8     | 2.48                     | 0.49              |
| 8:B:134:ALA:O    | 8:B:138:THR:HG22 | 2.13                     | 0.49              |
| 13:G:88:PRO:HG3  | 13:G:149:LYS:HD2 | 1.94                     | 0.49              |
| 28:a:424:G:C2    | 28:a:425:G:H1'   | 2.46                     | 0.49              |
| 28:a:628:G:O4'   | 28:a:636:G:N2    | 2.46                     | 0.49              |
| 28:a:1880:U:C4   | 28:a:1881:C:C4   | 3.01                     | 0.49              |
| 28:a:2557:G:H2'  | 28:a:2558:C:C6   | 2.48                     | 0.49              |
| 28:a:2651:C:O2   | 28:a:2651:C:H2'  | 2.13                     | 0.49              |
| 28:a:2673:G:N2   | 28:a:2674:G:O6   | 2.46                     | 0.49              |
| 43:p:85:LYS:HD3  | 43:p:85:LYS:C    | 2.38                     | 0.49              |
| 1:0:40:ASP:OD1   | 1:0:42:VAL:HG12  | 2.14                     | 0.48              |
| 7:A:410:G:OP1    | 10:D:26:ARG:HD3  | 2.13                     | 0.48              |
| 7:A:678:U:H2'    | 7:A:679:U:C6     | 2.48                     | 0.48              |
| 7:A:1002:A:O2'   | 7:A:1003:G:N3    | 2.46                     | 0.48              |
| 7:A:1231:C:H2'   | 7:A:1232:G:H8    | 1.77                     | 0.48              |
| 8:B:72:THR:HG22  | 8:B:93:ASN:HA    | 1.94                     | 0.48              |
| 9:C:142:MET:SD   | 9:C:170:GLU:HG2  | 2.53                     | 0.48              |
| 16:J:42:LEU:HD13 | 16:J:71:LEU:H    | 1.78                     | 0.48              |
| 27:U:69:ARG:O    | 27:U:70:LEU:HB3  | 2.13                     | 0.48              |
| 28:a:703:U:H2'   | 28:a:704:G:O4'   | 2.13                     | 0.48              |
| 28:a:1029:A:H2'  | 28:a:1030:C:C6   | 2.48                     | 0.48              |
| 28:a:2591:C:H2'  | 28:a:2592:G:C8   | 2.48                     | 0.48              |
| 31:d:181:ASP:OD1 | 31:d:184:ARG:HB2 | 2.13                     | 0.48              |
| 33:f:63:GLN:HB2  | 33:f:95:ARG:NH2  | 2.28                     | 0.48              |
| 37:j:34:GLY:N    | 37:j:37:ASP:OD2  | 2.46                     | 0.48              |
| 4:3:30:GLU:HG2   | 4:3:33:HIS:N     | 2.27                     | 0.48              |
| 7:A:765:G:H2'    | 7:A:765:G:N3     | 2.27                     | 0.48              |
| 7:A:1067:A:C5    | 7:A:1109:C:H5''  | 2.48                     | 0.48              |
| 7:A:1292:U:H2'   | 7:A:1293:A:H5''  | 1.95                     | 0.48              |
| 9:C:23:PHE:O     | 9:C:23:PHE:CD2   | 2.65                     | 0.48              |
| 9:C:206:GLU:O    | 9:C:207:ILE:HD13 | 2.14                     | 0.48              |
| 25:S:19:VAL:HG21 | 25:S:44:MET:HE1  | 1.94                     | 0.48              |
| 25:S:36:ARG:HB3  | 25:S:72:GLY:HA3  | 1.94                     | 0.48              |
| 28:a:1022:G:N2   | 28:a:1141:U:H3   | 2.11                     | 0.48              |
| 28:a:1548:A:H2'  | 28:a:1549:A:C8   | 2.48                     | 0.48              |
| 28:a:1809:A:H2'  | 28:a:1810:A:C8   | 2.47                     | 0.48              |
| 28:a:2336:A:H61  | 49:v:43:THR:HG21 | 1.78                     | 0.48              |
| 28:a:2625:G:C6   | 28:a:2626:C:C4   | 3.01                     | 0.48              |
| 29:b:50:A:C6     | 29:b:51:G:N7     | 2.81                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:b:75:G:H2'    | 29:b:76:G:C8      | 2.48                     | 0.48              |
| 32:e:5:LEU:HA    | 32:e:120:VAL:HG13 | 1.95                     | 0.48              |
| 34:g:97:ALA:HB3  | 34:g:104:ASN:HB2  | 1.95                     | 0.48              |
| 1:0:11:LEU:HA    | 1:0:51:GLU:HA     | 1.95                     | 0.48              |
| 7:A:95:G:H4'     | 7:A:96:U:C6       | 2.48                     | 0.48              |
| 7:A:721:G:H4'    | 7:A:722:G:O4'     | 2.14                     | 0.48              |
| 7:A:974:A:H8     | 7:A:974:A:OP1     | 1.96                     | 0.48              |
| 7:A:1321:C:H1'   | 7:A:1322:U:OP1    | 2.13                     | 0.48              |
| 8:B:76:ALA:HA    | 8:B:79:ALA:HB3    | 1.94                     | 0.48              |
| 8:B:94:HIS:C     | 8:B:94:HIS:CD2    | 2.92                     | 0.48              |
| 28:a:2386:A:H2'  | 28:a:2387:U:C6    | 2.48                     | 0.48              |
| 34:g:54:PRO:HB3  | 34:g:61:GLY:HA3   | 1.94                     | 0.48              |
| 8:B:73:LYS:O     | 8:B:76:ALA:N      | 2.45                     | 0.48              |
| 19:M:2:ALA:N     | 19:M:9:ILE:HG22   | 2.28                     | 0.48              |
| 28:a:2280:G:O2'  | 28:a:2327:A:C2    | 2.65                     | 0.48              |
| 28:a:2419:U:H2'  | 28:a:2420:C:H6    | 1.78                     | 0.48              |
| 29:b:17:C:N4     | 29:b:109:A:OP2    | 2.37                     | 0.48              |
| 34:g:9:VAL:HG12  | 34:g:10:VAL:H     | 1.79                     | 0.48              |
| 48:u:29:ILE:HA   | 48:u:40:ILE:HG12  | 1.94                     | 0.48              |
| 7:A:765:G:C2     | 7:A:812:G:N3      | 2.81                     | 0.48              |
| 7:A:1112:C:H42   | 9:C:177:THR:HB    | 1.78                     | 0.48              |
| 7:A:1286:A:H5'   | 7:A:1287:C:C5     | 2.49                     | 0.48              |
| 10:D:43:ALA:O    | 10:D:44:ARG:C     | 2.56                     | 0.48              |
| 10:D:97:ARG:O    | 10:D:101:VAL:HG23 | 2.14                     | 0.48              |
| 13:G:70:ARG:HG2  | 13:G:71:PRO:O     | 2.13                     | 0.48              |
| 14:H:78:VAL:HG12 | 14:H:79:SER:H     | 1.78                     | 0.48              |
| 28:a:1800:C:OP2  | 30:c:182:ARG:NH1  | 2.34                     | 0.48              |
| 28:a:2374:C:H2'  | 28:a:2375:G:C8    | 2.48                     | 0.48              |
| 29:b:113:C:H2'   | 29:b:114:C:C6     | 2.49                     | 0.48              |
| 34:g:103:ILE:O   | 34:g:114:ASP:HA   | 2.14                     | 0.48              |
| 7:A:219:C:H2'    | 7:A:220:G:H8      | 1.78                     | 0.48              |
| 7:A:1011:C:H42   | 7:A:1018:G:H1     | 1.62                     | 0.48              |
| 7:A:1336:U:H5'   | 7:A:1337:C:H5'    | 1.95                     | 0.48              |
| 12:F:9:MET:SD    | 12:F:86:ARG:HB3   | 2.54                     | 0.48              |
| 16:J:9:ARG:HG2   | 16:J:73:LEU:HD13  | 1.96                     | 0.48              |
| 28:a:282:A:H2'   | 28:a:283:G:C8     | 2.48                     | 0.48              |
| 28:a:849:A:H2'   | 28:a:850:U:C6     | 2.49                     | 0.48              |
| 28:a:1798:U:OP2  | 30:c:271:ARG:NH2  | 2.43                     | 0.48              |
| 29:b:43:C:N4     | 29:b:45:A:C6      | 2.82                     | 0.48              |
| 29:b:86:G:N2     | 29:b:87:U:HO2'    | 2.11                     | 0.48              |
| 39:l:110:GLU:HA  | 39:l:113:ALA:HB3  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 40:m:69:ARG:O    | 40:m:70:THR:OG1   | 2.27                     | 0.48              |
| 7:A:123:C:H2'    | 7:A:124:C:C6      | 2.49                     | 0.48              |
| 7:A:383:A:N6     | 7:A:455:U:OP2     | 2.39                     | 0.48              |
| 28:a:595:C:H2'   | 28:a:596:U:C6     | 2.48                     | 0.48              |
| 28:a:1043:C:H2'  | 28:a:1044:C:O4'   | 2.13                     | 0.48              |
| 28:a:2524:G:H2'  | 28:a:2525:G:O4'   | 2.14                     | 0.48              |
| 32:e:48:THR:HG23 | 32:e:86:ALA:HB3   | 1.95                     | 0.48              |
| 33:f:40:VAL:O    | 33:f:40:VAL:HG12  | 2.13                     | 0.48              |
| 41:n:23:ALA:C    | 41:n:42:PRO:HG3   | 2.38                     | 0.48              |
| 7:A:1339:G:H2'   | 7:A:1340:A:C8     | 2.49                     | 0.48              |
| 7:A:1457:A:H2'   | 7:A:1458:G:O4'    | 2.14                     | 0.48              |
| 16:J:76:ILE:HD13 | 16:J:76:ILE:HA    | 1.71                     | 0.48              |
| 28:a:2740:A:H3'  | 28:a:2741:A:H8    | 1.78                     | 0.48              |
| 41:n:68:LYS:NZ   | 41:n:101:GLY:HA2  | 2.29                     | 0.48              |
| 7:A:299:G:H2'    | 7:A:300:A:C8      | 2.49                     | 0.48              |
| 7:A:373:A:C8     | 7:A:374:A:C8      | 3.01                     | 0.48              |
| 7:A:615:G:C2'    | 7:A:616:G:H5'     | 2.43                     | 0.48              |
| 7:A:1157:G:O5'   | 7:A:1158:A:H4'    | 2.13                     | 0.48              |
| 7:A:1164:G:H2'   | 7:A:1165:G:C8     | 2.49                     | 0.48              |
| 7:A:1356:A:H2'   | 7:A:1357:A:C8     | 2.46                     | 0.48              |
| 9:C:131:ARG:HB3  | 9:C:131:ARG:HH11  | 1.79                     | 0.48              |
| 10:D:105:MET:HE3 | 10:D:105:MET:HB2  | 1.70                     | 0.48              |
| 26:T:47:ALA:HB1  | 26:T:83:ILE:HD11  | 1.95                     | 0.48              |
| 27:U:4:ILE:HD13  | 27:U:19:PHE:CE1   | 2.48                     | 0.48              |
| 28:a:2546:U:O2'  | 28:a:2567:G:OP2   | 2.27                     | 0.48              |
| 31:d:34:VAL:HA   | 31:d:50:VAL:HA    | 1.94                     | 0.48              |
| 31:d:37:VAL:HA   | 31:d:47:ALA:O     | 2.14                     | 0.48              |
| 42:o:52:ASN:O    | 42:o:53:ARG:HD3   | 2.13                     | 0.48              |
| 7:A:744:C:H2'    | 7:A:745:G:C8      | 2.49                     | 0.48              |
| 7:A:1003:G:H21   | 7:A:1039:C:H42    | 1.62                     | 0.48              |
| 7:A:1143:G:H3'   | 7:A:1144:G:C8     | 2.49                     | 0.48              |
| 13:G:140:ASP:HA  | 13:G:143:ARG:HH21 | 1.79                     | 0.48              |
| 19:M:64:VAL:O    | 19:M:64:VAL:HG23  | 2.13                     | 0.48              |
| 29:b:15:A:H3'    | 29:b:16:G:C8      | 2.49                     | 0.48              |
| 36:i:119:PHE:CD1 | 36:i:122:LEU:HD23 | 2.49                     | 0.48              |
| 48:u:30:ILE:HD11 | 48:u:93:ARG:NE    | 2.28                     | 0.48              |
| 7:A:157:U:O4     | 7:A:164:G:O6      | 2.31                     | 0.47              |
| 9:C:122:SER:O    | 9:C:126:ARG:HG3   | 2.13                     | 0.47              |
| 10:D:101:VAL:O   | 10:D:105:MET:HE2  | 2.14                     | 0.47              |
| 28:a:263:G:O2'   | 28:a:429:A:N3     | 2.44                     | 0.47              |
| 28:a:2323:G:O2'  | 28:a:2337:G:O2'   | 2.17                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:b:4:C:H2'     | 29:b:5:U:C6       | 2.49                     | 0.47              |
| 33:f:74:VAL:O    | 33:f:79:ILE:HG22  | 2.14                     | 0.47              |
| 36:i:92:MET:SD   | 36:i:96:ARG:HD2   | 2.54                     | 0.47              |
| 49:v:45:PHE:CE1  | 49:v:78:LYS:HB3   | 2.49                     | 0.47              |
| 7:A:1112:C:H3'   | 7:A:1113:C:H5''   | 1.96                     | 0.47              |
| 10:D:35:GLU:O    | 10:D:37:ALA:N     | 2.47                     | 0.47              |
| 18:L:77:HIS:ND1  | 18:L:77:HIS:N     | 2.62                     | 0.47              |
| 19:M:12:HIS:HD2  | 19:M:44:LYS:NZ    | 2.12                     | 0.47              |
| 24:R:25:ASP:OD1  | 24:R:26:ILE:N     | 2.47                     | 0.47              |
| 28:a:841:G:H2'   | 28:a:842:U:C6     | 2.47                     | 0.47              |
| 28:a:2480:C:H2'  | 28:a:2481:G:O4'   | 2.14                     | 0.47              |
| 28:a:2661:G:H2'  | 28:a:2662:A:C8    | 2.48                     | 0.47              |
| 38:k:111:ILE:C   | 38:k:131:ALA:HB2  | 2.39                     | 0.47              |
| 52:y:24:LEU:O    | 52:y:28:GLY:N     | 2.46                     | 0.47              |
| 1:0:19:HIS:O     | 1:0:49:TYR:OH     | 2.29                     | 0.47              |
| 5:4:1:MET:N      | 29:b:35:C:OP2     | 2.47                     | 0.47              |
| 7:A:123:C:H2'    | 7:A:124:C:H6      | 1.78                     | 0.47              |
| 11:E:14:LYS:HE2  | 11:E:117:VAL:HG13 | 1.96                     | 0.47              |
| 26:T:61:GLN:OE1  | 26:T:61:GLN:HA    | 2.15                     | 0.47              |
| 28:a:1027:A:C6   | 28:a:1126:A:C6    | 3.03                     | 0.47              |
| 44:q:5:PHE:CE1   | 44:q:12:HIS:HB2   | 2.48                     | 0.47              |
| 7:A:8:A:H4'      | 7:A:9:G:OP1       | 2.13                     | 0.47              |
| 7:A:384:G:O2'    | 7:A:385:C:O5'     | 2.31                     | 0.47              |
| 7:A:892:A:H2'    | 7:A:893:C:H6      | 1.78                     | 0.47              |
| 9:C:202:ILE:HD12 | 9:C:202:ILE:H     | 1.80                     | 0.47              |
| 10:D:169:THR:O   | 10:D:169:THR:HG22 | 2.14                     | 0.47              |
| 12:F:18:VAL:HG11 | 12:F:58:HIS:CE1   | 2.49                     | 0.47              |
| 12:F:20:GLY:HA2  | 12:F:23:GLU:OE2   | 2.14                     | 0.47              |
| 17:K:27:PHE:HZ   | 27:U:33:ARG:HH12  | 1.60                     | 0.47              |
| 23:Q:12:VAL:HG12 | 23:Q:23:VAL:HG12  | 1.95                     | 0.47              |
| 25:S:6:LYS:H     | 25:S:6:LYS:HD3    | 1.78                     | 0.47              |
| 28:a:1123:C:H2'  | 28:a:1124:G:C8    | 2.49                     | 0.47              |
| 28:a:2362:C:O2'  | 28:a:2363:G:H5'   | 2.14                     | 0.47              |
| 29:b:47:C:H2'    | 29:b:48:U:O4'     | 2.14                     | 0.47              |
| 29:b:97:C:H2'    | 29:b:98:G:O4'     | 2.14                     | 0.47              |
| 30:c:187:ASP:OD1 | 30:c:187:ASP:N    | 2.47                     | 0.47              |
| 31:d:34:VAL:HG13 | 31:d:50:VAL:HA    | 1.95                     | 0.47              |
| 34:g:22:GLN:HE21 | 34:g:55:ARG:HH22  | 1.61                     | 0.47              |
| 34:g:27:LYS:HD3  | 34:g:28:GLY:N     | 2.29                     | 0.47              |
| 39:l:111:GLU:CD  | 39:l:111:GLU:H    | 2.22                     | 0.47              |
| 43:p:92:ARG:O    | 43:p:95:LEU:HB2   | 2.13                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 45:r:38:TYR:HE2  | 53:z:28:LEU:HD21  | 1.79                     | 0.47              |
| 7:A:607:A:H2'    | 7:A:608:A:O4'     | 2.14                     | 0.47              |
| 7:A:720:C:O2'    | 24:R:52:GLN:OE1   | 2.32                     | 0.47              |
| 7:A:1253:A:H3'   | 7:A:1254:G:H8     | 1.79                     | 0.47              |
| 28:a:2373:G:H2'  | 28:a:2374:C:H6    | 1.79                     | 0.47              |
| 28:a:2378:A:H3'  | 28:a:2379:G:C8    | 2.49                     | 0.47              |
| 32:e:125:SER:HA  | 32:e:157:LEU:HD13 | 1.96                     | 0.47              |
| 33:f:135:GLN:N   | 33:f:150:ARG:O    | 2.47                     | 0.47              |
| 34:g:105:LEU:N   | 34:g:113:VAL:O    | 2.47                     | 0.47              |
| 37:j:93:GLN:HG3  | 37:j:94:PRO:HD2   | 1.97                     | 0.47              |
| 39:l:41:LEU:HD22 | 39:l:45:GLN:HE21  | 1.80                     | 0.47              |
| 49:v:21:LEU:HD21 | 49:v:41:ARG:HB2   | 1.97                     | 0.47              |
| 49:v:72:LYS:H    | 49:v:78:LYS:HA    | 1.80                     | 0.47              |
| 7:A:526:C:OP2    | 18:L:88:LYS:NZ    | 2.39                     | 0.47              |
| 7:A:601:G:C8     | 7:A:602:A:C8      | 3.03                     | 0.47              |
| 7:A:1159:C:HO2'  | 7:A:1160:U:P      | 2.38                     | 0.47              |
| 8:B:68:LEU:HD12  | 8:B:90:PHE:HB2    | 1.96                     | 0.47              |
| 13:G:76:LYS:HG2  | 13:G:89:VAL:HG21  | 1.97                     | 0.47              |
| 14:H:22:LYS:O    | 14:H:65:TYR:OH    | 2.32                     | 0.47              |
| 19:M:57:ARG:O    | 19:M:60:VAL:HG22  | 2.14                     | 0.47              |
| 22:P:41:PRO:O    | 22:P:43:ALA:N     | 2.46                     | 0.47              |
| 28:a:2326:C:OP2  | 28:a:2326:C:H6    | 1.97                     | 0.47              |
| 28:a:2418:A:C6   | 28:a:2419:U:C4    | 3.02                     | 0.47              |
| 28:a:2831:G:OP2  | 31:d:59:ARG:NH1   | 2.47                     | 0.47              |
| 34:g:22:GLN:NE2  | 34:g:41:VAL:O     | 2.46                     | 0.47              |
| 36:i:118:MET:O   | 36:i:121:LYS:HB2  | 2.14                     | 0.47              |
| 41:n:26:LEU:HG   | 41:n:92:PHE:CD1   | 2.50                     | 0.47              |
| 44:q:56:GLY:O    | 44:q:58:VAL:HG13  | 2.14                     | 0.47              |
| 5:4:7:PRO:HB2    | 33:f:62:GLY:HA2   | 1.95                     | 0.47              |
| 7:A:144:G:N2     | 7:A:144:G:OP2     | 2.47                     | 0.47              |
| 7:A:486:U:H2'    | 7:A:487:A:C8      | 2.48                     | 0.47              |
| 7:A:602:A:H2'    | 7:A:603:U:C6      | 2.50                     | 0.47              |
| 7:A:826:C:O2     | 14:H:16:ASN:ND2   | 2.48                     | 0.47              |
| 9:C:81:GLY:HA3   | 9:C:85:GLU:HB2    | 1.97                     | 0.47              |
| 12:F:8:PHE:HB2   | 12:F:84:VAL:HG21  | 1.96                     | 0.47              |
| 14:H:26:THR:OG1  | 14:H:60:GLU:OE2   | 2.33                     | 0.47              |
| 14:H:92:LEU:HD23 | 14:H:92:LEU:HA    | 1.71                     | 0.47              |
| 27:U:5:LYS:C     | 27:U:18:ARG:HH12  | 2.23                     | 0.47              |
| 27:U:54:LYS:HB3  | 27:U:54:LYS:HE3   | 1.80                     | 0.47              |
| 28:a:891:G:O6    | 28:a:892:A:N6     | 2.47                     | 0.47              |
| 28:a:1865:U:H3   | 28:a:1877:A:N6    | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:a:2615:U:C2    | 53:z:4:GLN:HA     | 2.50                     | 0.47              |
| 28:a:2740:A:H2'   | 28:a:2741:A:O4'   | 2.14                     | 0.47              |
| 31:d:37:VAL:HG22  | 31:d:48:ILE:HG22  | 1.97                     | 0.47              |
| 38:k:74:THR:HA    | 38:k:107:PHE:O    | 2.14                     | 0.47              |
| 38:k:93:ASN:OD1   | 38:k:94:THR:N     | 2.46                     | 0.47              |
| 38:k:95:LEU:HD22  | 38:k:100:ILE:HD11 | 1.97                     | 0.47              |
| 39:l:14:LYS:O     | 39:l:71:LYS:NZ    | 2.47                     | 0.47              |
| 43:p:61:TRP:HE3   | 43:p:92:ARG:HB3   | 1.80                     | 0.47              |
| 51:x:4:LYS:HZ2    | 51:x:7:ARG:HH11   | 1.63                     | 0.47              |
| 4:3:18:LYS:HD2    | 4:3:23:ILE:HG13   | 1.96                     | 0.47              |
| 7:A:563:A:HO2'    | 7:A:566:A:HO2'    | 1.53                     | 0.47              |
| 7:A:599:C:O2'     | 7:A:600:A:OP1     | 2.33                     | 0.47              |
| 7:A:654:G:H1      | 7:A:752:G:H21     | 1.63                     | 0.47              |
| 7:A:1071:C:H2'    | 7:A:1072:G:H8     | 1.80                     | 0.47              |
| 11:E:126:LYS:HG3  | 11:E:127:ALA:N    | 2.30                     | 0.47              |
| 18:L:87:VAL:HG21  | 18:L:90:LEU:HD23  | 1.97                     | 0.47              |
| 19:M:91:HIS:CG    | 19:M:97:VAL:HG11  | 2.49                     | 0.47              |
| 24:R:11:CYS:SG    | 24:R:47:THR:HG23  | 2.55                     | 0.47              |
| 28:a:1266:G:O2'   | 28:a:2012:G:O6    | 2.32                     | 0.47              |
| 29:b:24:G:H21     | 29:b:26:C:N4      | 2.13                     | 0.47              |
| 32:e:58:LYS:HG3   | 32:e:71:GLY:HA2   | 1.97                     | 0.47              |
| 37:j:113:MET:N    | 37:j:113:MET:SD   | 2.87                     | 0.47              |
| 47:t:49:VAL:HG13  | 47:t:52:LEU:O     | 2.15                     | 0.47              |
| 47:t:94:ARG:HE    | 47:t:103:ILE:HD11 | 1.79                     | 0.47              |
| 7:A:588:G:O2'     | 7:A:589:U:OP1     | 2.32                     | 0.47              |
| 15:I:54:LEU:HD11  | 15:I:103:PHE:HE2  | 1.80                     | 0.47              |
| 24:R:70:TYR:HB2   | 24:R:74:HIS:CE1   | 2.50                     | 0.47              |
| 28:a:886:A:H2'    | 28:a:887:U:O4'    | 2.15                     | 0.47              |
| 28:a:2314:A:H5'   | 33:f:33:LYS:NZ    | 2.30                     | 0.47              |
| 28:a:2386:A:H2'   | 28:a:2387:U:O4'   | 2.15                     | 0.47              |
| 28:a:2479:U:N3    | 28:a:2480:C:H1'   | 2.29                     | 0.47              |
| 28:a:2740:A:C6    | 28:a:2741:A:C4    | 3.03                     | 0.47              |
| 28:a:2758:A:C2'   | 34:g:35:ARG:HH22  | 2.27                     | 0.47              |
| 7:A:120:A:O2'     | 7:A:122:G:H5'     | 2.15                     | 0.47              |
| 7:A:751:U:H1'     | 21:O:23:GLY:O     | 2.15                     | 0.47              |
| 7:A:963:G:C6      | 7:A:964:A:N7      | 2.83                     | 0.47              |
| 19:M:12:HIS:O     | 19:M:44:LYS:NZ    | 2.47                     | 0.47              |
| 28:a:3:U:H2'      | 28:a:4:U:C6       | 2.50                     | 0.47              |
| 28:a:2479:U:H5'   | 28:a:2537:U:H4'   | 1.97                     | 0.47              |
| 31:d:47:ALA:HA    | 31:d:84:LEU:N     | 2.29                     | 0.47              |
| 32:e:149:ILE:HD11 | 32:e:188:MET:HB2  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:t:58:ILE:HD12  | 47:t:58:ILE:O     | 2.14                     | 0.47              |
| 7:A:77:G:O6       | 7:A:91:U:O2'      | 2.32                     | 0.46              |
| 7:A:757:U:O2'     | 7:A:879:C:H1'     | 2.15                     | 0.46              |
| 7:A:922:G:H2'     | 7:A:923:A:C8      | 2.50                     | 0.46              |
| 10:D:145:ILE:C    | 10:D:146:ARG:HG3  | 2.39                     | 0.46              |
| 17:K:97:ILE:HD11  | 27:U:16:LEU:HB3   | 1.97                     | 0.46              |
| 28:a:85:G:C6      | 28:a:86:G:N3      | 2.83                     | 0.46              |
| 28:a:2014:A:H2'   | 28:a:2015:A:C8    | 2.49                     | 0.46              |
| 28:a:2335:A:H5'   | 41:n:13:ARG:HH21  | 1.80                     | 0.46              |
| 30:c:182:ARG:HG3  | 30:c:183:LYS:N    | 2.30                     | 0.46              |
| 33:f:4:LEU:HD12   | 33:f:100:PHE:HB3  | 1.96                     | 0.46              |
| 43:p:90:ILE:HG12  | 44:q:39:LEU:O     | 2.15                     | 0.46              |
| 48:u:9:ARG:HH12   | 48:u:17:SER:CA    | 2.28                     | 0.46              |
| 7:A:135:C:H1'     | 7:A:325:A:C2      | 2.50                     | 0.46              |
| 7:A:192:A:C2'     | 7:A:193:C:H5'     | 2.45                     | 0.46              |
| 7:A:323:U:H2'     | 7:A:324:G:O4'     | 2.16                     | 0.46              |
| 9:C:129:MET:HE3   | 9:C:129:MET:HB3   | 1.83                     | 0.46              |
| 12:F:5:GLU:N      | 12:F:90:MET:O     | 2.48                     | 0.46              |
| 17:K:100:LEU:HD23 | 17:K:100:LEU:HA   | 1.79                     | 0.46              |
| 29:b:14:U:H3'     | 29:b:15:A:N7      | 2.29                     | 0.46              |
| 29:b:74:U:O2      | 48:u:29:ILE:HG21  | 2.15                     | 0.46              |
| 34:g:24:ILE:HD12  | 34:g:72:LEU:HD23  | 1.96                     | 0.46              |
| 37:j:113:MET:SD   | 37:j:114:LYS:N    | 2.88                     | 0.46              |
| 37:j:114:LYS:HE2  | 37:j:114:LYS:HB3  | 1.51                     | 0.46              |
| 38:k:29:LYS:HB3   | 38:k:30:THR:H     | 1.48                     | 0.46              |
| 44:q:35:PHE:CD1   | 44:q:59:ILE:HB    | 2.48                     | 0.46              |
| 48:u:9:ARG:HG3    | 48:u:39:ALA:HB1   | 1.96                     | 0.46              |
| 5:4:44:PHE:CZ     | 33:f:109:PRO:HG3  | 2.50                     | 0.46              |
| 7:A:609:A:O2'     | 7:A:610:G:H8      | 1.98                     | 0.46              |
| 7:A:673:A:H2'     | 7:A:674:G:H8      | 1.78                     | 0.46              |
| 7:A:1370:C:O2'    | 7:A:1371:G:OP1    | 2.26                     | 0.46              |
| 9:C:64:ILE:HG22   | 9:C:99:ALA:H      | 1.81                     | 0.46              |
| 10:D:105:MET:HB3  | 10:D:173:VAL:HG11 | 1.97                     | 0.46              |
| 12:F:8:PHE:CE2    | 12:F:10:VAL:HG23  | 2.51                     | 0.46              |
| 13:G:140:ASP:HA   | 13:G:143:ARG:NE   | 2.29                     | 0.46              |
| 21:O:88:ARG:HH12  | 28:a:715:A:H5''   | 1.80                     | 0.46              |
| 28:a:1039:A:N1    | 28:a:1116:G:C6    | 2.83                     | 0.46              |
| 28:a:1863:G:H2'   | 28:a:1864:U:C6    | 2.51                     | 0.46              |
| 28:a:2376:A:H61   | 41:n:92:PHE:CB    | 2.27                     | 0.46              |
| 43:p:62:ILE:HD11  | 43:p:92:ARG:HE    | 1.78                     | 0.46              |
| 43:p:74:ILE:HG12  | 43:p:75:SER:H     | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 43:p:81:ASN:O    | 43:p:85:LYS:CB   | 2.55                     | 0.46              |
| 4:3:2:LYS:H      | 4:3:35:GLN:HA    | 1.81                     | 0.46              |
| 7:A:33:A:H8      | 18:L:29:GLN:HE22 | 1.64                     | 0.46              |
| 7:A:79:G:H2'     | 7:A:80:G:O4'     | 2.16                     | 0.46              |
| 13:G:11:LYS:HG3  | 13:G:12:ILE:N    | 2.31                     | 0.46              |
| 15:I:75:GLN:O    | 15:I:79:ILE:HG12 | 2.16                     | 0.46              |
| 16:J:27:GLU:O    | 16:J:31:ARG:CB   | 2.64                     | 0.46              |
| 27:U:66:ARG:HH11 | 27:U:67:ARG:NH1  | 2.09                     | 0.46              |
| 28:a:938:G:H2'   | 28:a:939:G:H5'   | 1.97                     | 0.46              |
| 28:a:1028:A:C2   | 28:a:1029:A:C4   | 3.03                     | 0.46              |
| 31:d:37:VAL:N    | 31:d:92:VAL:HG22 | 2.20                     | 0.46              |
| 34:g:41:VAL:HG22 | 34:g:65:ALA:HA   | 1.98                     | 0.46              |
| 7:A:1324:G:H2'   | 7:A:1325:A:C8    | 2.51                     | 0.46              |
| 7:A:1449:C:H2'   | 7:A:1450:C:H6    | 1.81                     | 0.46              |
| 7:A:1478:U:H2'   | 7:A:1479:U:C6    | 2.50                     | 0.46              |
| 12:F:7:VAL:HB    | 12:F:88:MET:HG2  | 1.98                     | 0.46              |
| 13:G:136:LYS:HB3 | 13:G:136:LYS:HE2 | 1.67                     | 0.46              |
| 28:a:629:G:H21   | 28:a:640:C:H5'   | 1.79                     | 0.46              |
| 28:a:1049:C:H3'  | 28:a:1050:A:C8   | 2.51                     | 0.46              |
| 28:a:1930:G:O2'  | 28:a:1968:G:O6   | 2.30                     | 0.46              |
| 28:a:2298:A:N6   | 28:a:2318:G:H1'  | 2.31                     | 0.46              |
| 31:d:34:VAL:HA   | 31:d:51:THR:H    | 1.80                     | 0.46              |
| 34:g:66:GLY:O    | 34:g:69:ARG:HB3  | 2.15                     | 0.46              |
| 34:g:176:LYS:HA  | 34:g:176:LYS:HD3 | 1.76                     | 0.46              |
| 48:u:83:LYS:HE2  | 48:u:83:LYS:HB2  | 1.52                     | 0.46              |
| 51:x:13:GLU:OE1  | 51:x:13:GLU:N    | 2.40                     | 0.46              |
| 5:4:28:VAL:HG21  | 5:4:32:LEU:HD13  | 1.97                     | 0.46              |
| 7:A:951:G:HO2'   | 7:A:970:C:HO2'   | 1.60                     | 0.46              |
| 7:A:967:5MC:H2'  | 7:A:968:A:C8     | 2.50                     | 0.46              |
| 17:K:35:THR:OG1  | 17:K:36:ASP:N    | 2.49                     | 0.46              |
| 20:N:80:SER:O    | 20:N:84:VAL:HG13 | 2.15                     | 0.46              |
| 28:a:277:G:H4'   | 28:a:278:A:C4    | 2.50                     | 0.46              |
| 28:a:2293:G:N3   | 28:a:2293:G:H2'  | 2.29                     | 0.46              |
| 28:a:2532:G:C2   | 28:a:2533:U:C5   | 3.04                     | 0.46              |
| 28:a:2669:G:H2'  | 28:a:2669:G:N3   | 2.31                     | 0.46              |
| 35:h:6:LEU:HD21  | 35:h:37:VAL:HG13 | 1.96                     | 0.46              |
| 48:u:28:ALA:HB1  | 48:u:89:ILE:O    | 2.16                     | 0.46              |
| 10:D:104:ARG:HA  | 10:D:104:ARG:HD3 | 1.68                     | 0.46              |
| 13:G:12:ILE:H    | 13:G:12:ILE:HG12 | 1.67                     | 0.46              |
| 13:G:132:GLY:C   | 13:G:134:ALA:H   | 2.23                     | 0.46              |
| 19:M:96:PRO:HB3  | 19:M:106:ALA:O   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:P:19:VAL:H     | 22:P:37:GLY:HA3   | 1.80                     | 0.46              |
| 28:a:305:C:H2'    | 28:a:306:U:C6     | 2.51                     | 0.46              |
| 28:a:549:G:C5     | 28:a:550:C:C4     | 3.03                     | 0.46              |
| 29:b:24:G:C6      | 29:b:56:G:C6      | 3.03                     | 0.46              |
| 29:b:108:A:H3'    | 29:b:109:A:H4'    | 1.98                     | 0.46              |
| 32:e:125:SER:CB   | 32:e:157:LEU:HB2  | 2.45                     | 0.46              |
| 44:q:16:GLU:CD    | 44:q:16:GLU:N     | 2.74                     | 0.46              |
| 7:A:106:C:OP1     | 7:A:106:C:H4'     | 2.13                     | 0.46              |
| 7:A:272:C:H2'     | 7:A:273:A:C8      | 2.50                     | 0.46              |
| 7:A:549:C:O2'     | 7:A:550:G:O5'     | 2.28                     | 0.46              |
| 7:A:657:U:H2'     | 7:A:658:A:C8      | 2.48                     | 0.46              |
| 7:A:998:C:N1      | 7:A:1044:A:H5'    | 2.26                     | 0.46              |
| 7:A:1190:C:O4'    | 7:A:1191:G:N2     | 2.49                     | 0.46              |
| 10:D:76:TYR:HA    | 10:D:90:LEU:HD21  | 1.97                     | 0.46              |
| 17:K:53:ARG:HD3   | 17:K:54:GLY:N     | 2.30                     | 0.46              |
| 28:a:2527:C:O2    | 28:a:2527:C:H2'   | 2.15                     | 0.46              |
| 28:a:2533:U:H2'   | 28:a:2534:A:H5'   | 1.96                     | 0.46              |
| 41:n:100:HIS:O    | 41:n:103:VAL:HG12 | 2.16                     | 0.46              |
| 7:A:106:C:H5      | 26:T:10:ARG:HH12  | 1.64                     | 0.46              |
| 7:A:199:C:H2'     | 7:A:200:A:C8      | 2.49                     | 0.46              |
| 7:A:449:G:H1      | 22:P:70:ARG:HH22  | 1.63                     | 0.46              |
| 7:A:1030:U:C4     | 7:A:1032:G:H8     | 2.34                     | 0.46              |
| 23:Q:77:ARG:HH12  | 23:Q:79:VAL:HA    | 1.81                     | 0.46              |
| 24:R:72:ASP:HB3   | 27:U:3:VAL:HG23   | 1.97                     | 0.46              |
| 28:a:784:G:H5'    | 28:a:785:G:OP1    | 2.15                     | 0.46              |
| 28:a:849:A:H2'    | 28:a:850:U:H6     | 1.81                     | 0.46              |
| 28:a:1005:C:O2'   | 36:i:30:THR:HG21  | 2.16                     | 0.46              |
| 28:a:1028:A:C2    | 28:a:1029:A:C5    | 3.04                     | 0.46              |
| 28:a:2745:C:O2'   | 34:g:142:GLY:HA3  | 2.16                     | 0.46              |
| 28:a:2749:A:C8    | 28:a:2750:A:H2'   | 2.51                     | 0.46              |
| 28:a:2765:A:N3    | 28:a:2765:A:H2'   | 2.31                     | 0.46              |
| 28:a:2851:A:N7    | 56:a:6208:SPD:H92 | 2.30                     | 0.46              |
| 33:f:70:ALA:O     | 33:f:81:GLN:HG2   | 2.16                     | 0.46              |
| 34:g:24:ILE:O     | 34:g:35:ARG:N     | 2.39                     | 0.46              |
| 39:l:119:LEU:HA   | 39:l:119:LEU:HD23 | 1.69                     | 0.46              |
| 43:p:78:LYS:HG3   | 43:p:117:LEU:HD22 | 1.98                     | 0.46              |
| 7:A:999:C:H4'     | 7:A:1000:A:O4'    | 2.16                     | 0.46              |
| 7:A:1049:U:O2'    | 7:A:1215:C:O4'    | 2.33                     | 0.46              |
| 10:D:137:VAL:HG12 | 10:D:182:PHE:HD2  | 1.81                     | 0.46              |
| 13:G:12:ILE:O     | 13:G:13:LEU:HB2   | 2.16                     | 0.46              |
| 13:G:66:LEU:O     | 13:G:70:ARG:NH2   | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:16:LEU:HG    | 27:U:17:ARG:NH1   | 2.31                     | 0.46              |
| 28:a:720:U:H2'    | 28:a:721:A:C8     | 2.50                     | 0.46              |
| 28:a:1042:G:H2'   | 28:a:1043:C:H6    | 1.81                     | 0.46              |
| 28:a:1508:A:H2'   | 28:a:1509:A:C8    | 2.51                     | 0.46              |
| 28:a:2524:G:C6    | 28:a:2525:G:N7    | 2.84                     | 0.46              |
| 28:a:2526:G:N1    | 28:a:2538:C:C4    | 2.84                     | 0.46              |
| 29:b:32:U:H2'     | 29:b:33:G:C8      | 2.52                     | 0.46              |
| 32:e:172:ALA:HB2  | 32:e:192:ALA:HB1  | 1.98                     | 0.46              |
| 33:f:7:TYR:HE2    | 33:f:173:PHE:HA   | 1.80                     | 0.46              |
| 33:f:56:ASP:O     | 33:f:60:ILE:HG23  | 2.16                     | 0.46              |
| 34:g:171:THR:O    | 34:g:171:THR:OG1  | 2.29                     | 0.46              |
| 7:A:64:G:H4'      | 7:A:65:A:O5'      | 2.14                     | 0.45              |
| 19:M:66:GLU:HB3   | 19:M:67:GLY:H     | 1.56                     | 0.45              |
| 24:R:37:GLY:O     | 24:R:63:ARG:NH2   | 2.49                     | 0.45              |
| 28:a:596:U:O2     | 28:a:662:G:N2     | 2.48                     | 0.45              |
| 28:a:749:A:OP2    | 56:a:6217:SPD:N10 | 2.49                     | 0.45              |
| 28:a:1027:A:N7    | 28:a:1126:A:N1    | 2.63                     | 0.45              |
| 28:a:2266:A:H4'   | 28:a:2267:A:N3    | 2.32                     | 0.45              |
| 29:b:13:G:H5'     | 29:b:15:A:C2      | 2.50                     | 0.45              |
| 32:e:108:ILE:HA   | 38:k:1:MET:HE1    | 1.97                     | 0.45              |
| 43:p:66:ASN:HD21  | 43:p:70:ARG:NH2   | 2.10                     | 0.45              |
| 49:v:46:HIS:HB2   | 49:v:79:PHE:CZ    | 2.50                     | 0.45              |
| 7:A:782:A:H62     | 7:A:800:G:H21     | 1.62                     | 0.45              |
| 7:A:1280:A:H2'    | 7:A:1280:A:N3     | 2.32                     | 0.45              |
| 9:C:55:ILE:HG22   | 9:C:68:ILE:HG12   | 1.98                     | 0.45              |
| 14:H:126:ILE:HG22 | 14:H:127:CYS:SG   | 2.56                     | 0.45              |
| 18:L:30:LYS:HE3   | 18:L:59:ASN:ND2   | 2.23                     | 0.45              |
| 28:a:146:A:H2'    | 28:a:147:C:C6     | 2.51                     | 0.45              |
| 28:a:632:A:H2'    | 28:a:633:A:C8     | 2.51                     | 0.45              |
| 28:a:1049:C:H3'   | 28:a:1050:A:H8    | 1.80                     | 0.45              |
| 28:a:2388:A:OP1   | 28:a:2388:A:H4'   | 2.16                     | 0.45              |
| 28:a:2739:U:C5    | 28:a:2763:G:C6    | 3.04                     | 0.45              |
| 41:n:80:GLU:O     | 41:n:84:GLU:HG2   | 2.17                     | 0.45              |
| 43:p:78:LYS:HB2   | 43:p:78:LYS:HE3   | 1.70                     | 0.45              |
| 47:t:96:PHE:HD2   | 47:t:101:GLU:OE2  | 1.99                     | 0.45              |
| 49:v:43:THR:O     | 49:v:46:HIS:NE2   | 2.33                     | 0.45              |
| 7:A:485:U:H4'     | 7:A:485:U:OP2     | 2.15                     | 0.45              |
| 9:C:70:THR:HG21   | 9:C:76:VAL:HG21   | 1.98                     | 0.45              |
| 9:C:74:GLY:O      | 9:C:76:VAL:N      | 2.44                     | 0.45              |
| 10:D:13:ARG:HG3   | 10:D:32:CYS:HA    | 1.98                     | 0.45              |
| 25:S:40:ILE:H     | 25:S:40:ILE:HG12  | 1.48                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:a:145:C:H2'    | 28:a:146:A:C8     | 2.52                     | 0.45              |
| 28:a:1021:A:C5    | 28:a:1023:U:C5    | 3.04                     | 0.45              |
| 28:a:2064:C:H2'   | 28:a:2065:C:C6    | 2.52                     | 0.45              |
| 28:a:2683:C:OP1   | 42:o:51:ARG:NH2   | 2.49                     | 0.45              |
| 28:a:2751:G:OP1   | 34:g:3:ARG:HD2    | 2.16                     | 0.45              |
| 7:A:578:C:O2'     | 7:A:728:A:N3      | 2.48                     | 0.45              |
| 7:A:1012:G:N2     | 7:A:1013:G:H8     | 2.14                     | 0.45              |
| 28:a:413:C:O2'    | 28:a:1863:G:N2    | 2.49                     | 0.45              |
| 28:a:2628:C:O2'   | 28:a:2781:A:H2'   | 2.16                     | 0.45              |
| 28:a:2739:U:C6    | 28:a:2763:G:C6    | 3.05                     | 0.45              |
| 29:b:71:C:H2'     | 29:b:72:G:O4'     | 2.16                     | 0.45              |
| 34:g:126:PRO:HD3  | 34:g:132:VAL:H    | 1.82                     | 0.45              |
| 36:i:96:ARG:HG2   | 36:i:96:ARG:NH1   | 2.30                     | 0.45              |
| 37:j:53:LYS:HE2   | 37:j:53:LYS:HB2   | 1.78                     | 0.45              |
| 38:k:95:LEU:HB3   | 38:k:101:ILE:HG12 | 1.97                     | 0.45              |
| 46:s:14:PRO:HD3   | 51:x:30:MET:HE3   | 1.97                     | 0.45              |
| 7:A:457:G:H22     | 7:A:475:U:H2'     | 1.80                     | 0.45              |
| 7:A:539:A:O2'     | 7:A:540:G:O5'     | 2.31                     | 0.45              |
| 8:B:64:LYS:HD2    | 8:B:64:LYS:HA     | 1.68                     | 0.45              |
| 10:D:33:LYS:O     | 10:D:34:ILE:C     | 2.58                     | 0.45              |
| 17:K:97:ILE:HA    | 17:K:100:LEU:HB2  | 1.98                     | 0.45              |
| 18:L:108:LYS:HB2  | 18:L:108:LYS:HE3  | 1.80                     | 0.45              |
| 24:R:49:ALA:HB3   | 24:R:50:LYS:NZ    | 2.32                     | 0.45              |
| 28:a:172:A:H2'    | 28:a:173:A:C8     | 2.52                     | 0.45              |
| 28:a:841:G:C6     | 28:a:938:G:C2     | 3.03                     | 0.45              |
| 28:a:1021:A:C4    | 28:a:1023:U:C5    | 3.05                     | 0.45              |
| 28:a:1754:A:N1    | 28:a:2716:C:O2'   | 2.44                     | 0.45              |
| 28:a:2739:U:C6    | 28:a:2763:G:N1    | 2.84                     | 0.45              |
| 29:b:27:C:P       | 41:n:34:HIS:HE2   | 2.38                     | 0.45              |
| 29:b:68:C:H2'     | 29:b:69:G:O4'     | 2.17                     | 0.45              |
| 37:j:116:ILE:C    | 37:j:116:ILE:HD12 | 2.41                     | 0.45              |
| 3:2:26:HIS:CE1    | 3:2:48:ALA:HB2    | 2.52                     | 0.45              |
| 7:A:1125:U:O2'    | 7:A:1146:A:N6     | 2.50                     | 0.45              |
| 7:A:1319:A:O2'    | 25:S:37:ARG:HG2   | 2.16                     | 0.45              |
| 18:L:15:LYS:HE2   | 18:L:17:ALA:HA    | 1.99                     | 0.45              |
| 19:M:107:ARG:HH11 | 19:M:107:ARG:HG2  | 1.81                     | 0.45              |
| 23:Q:38:ILE:HD13  | 23:Q:40:ARG:HD3   | 1.99                     | 0.45              |
| 25:S:15:LEU:O     | 25:S:19:VAL:HG23  | 2.16                     | 0.45              |
| 28:a:938:G:C2     | 28:a:939:G:C5     | 3.04                     | 0.45              |
| 28:a:1245:G:OP1   | 38:k:13:LYS:NZ    | 2.48                     | 0.45              |
| 28:a:2303:G:C6    | 28:a:2314:A:N6    | 2.84                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:a:2327:A:N6   | 28:a:2388:A:N6    | 2.63                     | 0.45              |
| 28:a:2471:A:C8   | 28:a:2472:G:C8    | 3.05                     | 0.45              |
| 28:a:2820:A:O2'  | 28:a:2821:A:OP1   | 2.33                     | 0.45              |
| 29:b:45:A:C6     | 29:b:46:A:C8      | 3.04                     | 0.45              |
| 32:e:18:THR:HA   | 32:e:106:LYS:HG2  | 1.97                     | 0.45              |
| 35:h:8:LYS:HD3   | 35:h:8:LYS:HA     | 1.67                     | 0.45              |
| 36:i:17:VAL:O    | 36:i:139:VAL:HG22 | 2.17                     | 0.45              |
| 41:n:39:VAL:HB   | 41:n:49:VAL:HG13  | 1.98                     | 0.45              |
| 44:q:1:MET:HE1   | 44:q:41:ILE:HA    | 1.99                     | 0.45              |
| 7:A:1057:G:P     | 7:A:1057:G:O4'    | 2.75                     | 0.45              |
| 7:A:1377:U:O4    | 13:G:10:ARG:HD2   | 2.17                     | 0.45              |
| 8:B:79:ALA:HB1   | 8:B:210:VAL:HG21  | 1.99                     | 0.45              |
| 19:M:90:ARG:HD3  | 19:M:90:ARG:HA    | 1.71                     | 0.45              |
| 28:a:861:A:OP2   | 56:a:6218:SPD:N1  | 2.50                     | 0.45              |
| 28:a:1036:G:H3'  | 28:a:1037:G:C8    | 2.51                     | 0.45              |
| 28:a:2618:G:H21  | 31:d:155:VAL:HG21 | 1.81                     | 0.45              |
| 28:a:2739:U:C4   | 28:a:2766:A:N6    | 2.85                     | 0.45              |
| 29:b:86:G:O2'    | 29:b:87:U:H2'     | 2.16                     | 0.45              |
| 36:i:36:LEU:HD22 | 36:i:121:LYS:HE3  | 1.99                     | 0.45              |
| 36:i:56:VAL:HB   | 36:i:124:VAL:HG13 | 1.98                     | 0.45              |
| 46:s:79:ASP:OD1  | 46:s:79:ASP:N     | 2.49                     | 0.45              |
| 7:A:95:G:H4'     | 7:A:96:U:C5       | 2.51                     | 0.45              |
| 7:A:1446:U:H1'   | 7:A:1458:G:H22    | 1.82                     | 0.45              |
| 7:A:1493:A:H3'   | 7:A:1494:A:H8     | 1.82                     | 0.45              |
| 14:H:47:GLU:HA   | 14:H:47:GLU:OE1   | 2.16                     | 0.45              |
| 17:K:20:VAL:HA   | 17:K:83:GLU:HB3   | 1.99                     | 0.45              |
| 25:S:6:LYS:HD3   | 25:S:6:LYS:N      | 2.31                     | 0.45              |
| 28:a:660:C:N3    | 28:a:661:A:N6     | 2.64                     | 0.45              |
| 28:a:841:G:C5    | 28:a:842:U:C4     | 3.05                     | 0.45              |
| 28:a:2296:U:O2'  | 28:a:2333:A:N6    | 2.47                     | 0.45              |
| 28:a:2370:G:H2'  | 28:a:2371:G:C8    | 2.51                     | 0.45              |
| 34:g:19:ILE:N    | 34:g:19:ILE:HD12  | 2.32                     | 0.45              |
| 36:i:55:ILE:HG22 | 36:i:56:VAL:N     | 2.31                     | 0.45              |
| 44:q:1:MET:HB2   | 44:q:43:ASN:CG    | 2.42                     | 0.45              |
| 48:u:83:LYS:CB   | 48:u:85:LYS:HG3   | 2.43                     | 0.45              |
| 2:l:25:LYS:HE2   | 28:a:1367:A:O2'   | 2.17                     | 0.45              |
| 7:A:78:A:H2'     | 7:A:79:G:C8       | 2.52                     | 0.45              |
| 7:A:89:C:C4      | 7:A:90:C:N4       | 2.85                     | 0.45              |
| 7:A:255:G:H2'    | 7:A:256:U:C6      | 2.51                     | 0.45              |
| 7:A:738:C:OP2    | 12:F:91:ARG:NH2   | 2.50                     | 0.45              |
| 7:A:1448:A:H3'   | 7:A:1449:C:C6     | 2.52                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:A:1517:2MG:N2   | 7:A:1520:MA6:OP2   | 2.48                     | 0.45              |
| 12:F:42:TRP:CE3   | 12:F:102:MET:HE2   | 2.52                     | 0.45              |
| 28:a:52:A:H2'     | 28:a:53:A:C8       | 2.52                     | 0.45              |
| 28:a:155:A:H2'    | 28:a:156:A:C8      | 2.52                     | 0.45              |
| 28:a:621:A:OP2    | 38:k:99:ASN:ND2    | 2.50                     | 0.45              |
| 28:a:634:C:H2'    | 28:a:635:C:O4'     | 2.17                     | 0.45              |
| 28:a:1862:G:H1    | 28:a:1880:U:H3     | 1.64                     | 0.45              |
| 28:a:1873:G:H2'   | 28:a:1874:C:H6     | 1.82                     | 0.45              |
| 28:a:2251:OMG:H1' | 28:a:2251:OMG:HM23 | 1.56                     | 0.45              |
| 28:a:2280:G:H1'   | 28:a:2327:A:C2     | 2.51                     | 0.45              |
| 28:a:2298:A:H3'   | 28:a:2299:U:C6     | 2.52                     | 0.45              |
| 28:a:2526:G:C6    | 28:a:2538:C:C4     | 3.04                     | 0.45              |
| 31:d:36:GLN:O     | 31:d:48:ILE:HA     | 2.16                     | 0.45              |
| 33:f:30:ARG:O     | 33:f:159:THR:OG1   | 2.25                     | 0.45              |
| 36:i:32:LEU:HD23  | 36:i:32:LEU:HA     | 1.85                     | 0.45              |
| 41:n:52:SER:OG    | 41:n:53:THR:N      | 2.48                     | 0.45              |
| 7:A:219:C:H2'     | 7:A:220:G:C8       | 2.52                     | 0.45              |
| 7:A:500:G:H2'     | 7:A:501:C:H6       | 1.82                     | 0.45              |
| 7:A:1024:G:H2'    | 7:A:1025:U:C4'     | 2.47                     | 0.45              |
| 7:A:1110:A:H3'    | 7:A:1111:A:H8      | 1.83                     | 0.45              |
| 9:C:183:ASP:N     | 9:C:183:ASP:OD1    | 2.50                     | 0.45              |
| 13:G:101:MET:O    | 13:G:105:VAL:HG23  | 2.17                     | 0.45              |
| 15:I:43:THR:O     | 15:I:47:VAL:HG22   | 2.17                     | 0.45              |
| 28:a:155:A:H2'    | 28:a:156:A:H8      | 1.82                     | 0.45              |
| 28:a:2625:G:C2    | 28:a:2626:C:C2     | 3.05                     | 0.45              |
| 56:a:6219:SPD:H22 | 56:a:6219:SPD:H51  | 1.78                     | 0.45              |
| 31:d:103:ASP:OD2  | 31:d:103:ASP:N     | 2.50                     | 0.45              |
| 33:f:123:ASP:OD2  | 33:f:127:ASN:HB2   | 2.16                     | 0.45              |
| 33:f:170:LEU:HB3  | 33:f:175:PHE:CG    | 2.52                     | 0.45              |
| 41:n:111:ARG:HH21 | 41:n:117:PHE:C     | 2.23                     | 0.45              |
| 47:t:24:LYS:HB3   | 47:t:24:LYS:HZ2    | 1.82                     | 0.45              |
| 7:A:74:A:H61      | 7:A:95:G:P         | 2.39                     | 0.44              |
| 7:A:532:A:N6      | 7:A:1207:G:O2'     | 2.47                     | 0.44              |
| 7:A:764:C:C2      | 7:A:765:G:H8       | 2.35                     | 0.44              |
| 9:C:190:HIS:CE1   | 9:C:195:VAL:HG13   | 2.52                     | 0.44              |
| 18:L:25:GLU:O     | 18:L:25:GLU:OE2    | 2.35                     | 0.44              |
| 22:P:75:ILE:HD12  | 22:P:76:LYS:N      | 2.31                     | 0.44              |
| 28:a:918:A:O2'    | 29:b:79:G:N2       | 2.50                     | 0.44              |
| 28:a:1048:A:H62   | 28:a:1110:G:H21    | 1.65                     | 0.44              |
| 28:a:1184:U:H2'   | 28:a:1185:G:H5'    | 1.99                     | 0.44              |
| 28:a:1856:U:H2'   | 28:a:1857:G:O4'    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 28:a:2298:A:H5''  | 33:f:72:LYS:HE2  | 1.99                     | 0.44              |
| 28:a:2419:U:O2'   | 28:a:2420:C:H5'  | 2.18                     | 0.44              |
| 28:a:2528:U:C2    | 28:a:2536:G:N1   | 2.84                     | 0.44              |
| 49:v:46:HIS:O     | 49:v:79:PHE:HA   | 2.16                     | 0.44              |
| 7:A:868:C:H2'     | 7:A:869:G:O4'    | 2.17                     | 0.44              |
| 7:A:1014:A:H3'    | 7:A:1015:G:C8    | 2.53                     | 0.44              |
| 7:A:1035:A:O2'    | 7:A:1036:G:H5''  | 2.17                     | 0.44              |
| 13:G:17:LYS:HE2   | 15:I:46:MET:SD   | 2.57                     | 0.44              |
| 13:G:63:GLU:HA    | 13:G:66:LEU:HD23 | 1.99                     | 0.44              |
| 13:G:124:LEU:HD23 | 13:G:124:LEU:O   | 2.17                     | 0.44              |
| 15:I:129:LYS:C    | 15:I:129:LYS:HD3 | 2.41                     | 0.44              |
| 25:S:16:LEU:HA    | 25:S:19:VAL:HB   | 1.99                     | 0.44              |
| 26:T:69:LYS:H     | 26:T:69:LYS:CD   | 2.26                     | 0.44              |
| 28:a:897:C:H2'    | 28:a:898:C:H6    | 1.82                     | 0.44              |
| 28:a:2333:A:OP1   | 49:v:77:ARG:NH1  | 2.49                     | 0.44              |
| 28:a:2579:C:OP1   | 56:a:6220:SPD:N1 | 2.50                     | 0.44              |
| 28:a:2751:G:P     | 34:g:3:ARG:HH11  | 2.40                     | 0.44              |
| 7:A:69:G:H1       | 7:A:98:G:N2      | 2.14                     | 0.44              |
| 7:A:836:G:H2'     | 7:A:837:U:H5'    | 1.99                     | 0.44              |
| 7:A:1402:G:H2'    | 7:A:1403:4OC:O4' | 2.17                     | 0.44              |
| 13:G:38:THR:O     | 13:G:41:SER:OG   | 2.28                     | 0.44              |
| 16:J:18:ILE:O     | 16:J:18:ILE:HG13 | 2.17                     | 0.44              |
| 17:K:84:VAL:O     | 17:K:110:ILE:HA  | 2.18                     | 0.44              |
| 20:N:90:ARG:NH2   | 20:N:92:GLU:OE2  | 2.49                     | 0.44              |
| 21:O:9:ALA:HA     | 21:O:12:VAL:HG12 | 1.99                     | 0.44              |
| 26:T:85:LYS:HD2   | 26:T:85:LYS:O    | 2.17                     | 0.44              |
| 28:a:284:U:O4     | 28:a:356:G:O6    | 2.35                     | 0.44              |
| 28:a:1019:U:OP1   | 28:a:1036:G:H4'  | 2.18                     | 0.44              |
| 28:a:1581:G:H2'   | 28:a:1582:C:H6   | 1.79                     | 0.44              |
| 28:a:2295:C:OP2   | 41:n:10:ARG:HG3  | 2.18                     | 0.44              |
| 28:a:2327:A:H2'   | 28:a:2328:A:O4'  | 2.17                     | 0.44              |
| 28:a:2478:A:C6    | 28:a:2479:U:C4   | 3.05                     | 0.44              |
| 28:a:2533:U:C4    | 28:a:2534:A:H1'  | 2.53                     | 0.44              |
| 29:b:45:A:H8      | 29:b:45:A:O5'    | 1.99                     | 0.44              |
| 29:b:66:A:N6      | 29:b:107:G:H3'   | 2.32                     | 0.44              |
| 32:e:148:ILE:HA   | 32:e:187:VAL:O   | 2.18                     | 0.44              |
| 34:g:30:ASN:CG    | 34:g:136:ALA:HB2 | 2.41                     | 0.44              |
| 34:g:87:LEU:HD22  | 34:g:148:LEU:CB  | 2.41                     | 0.44              |
| 43:p:94:ILE:HD12  | 44:q:4:VAL:HG21  | 1.99                     | 0.44              |
| 48:u:48:MET:CE    | 48:u:85:LYS:HA   | 2.48                     | 0.44              |
| 7:A:449:G:N3      | 7:A:449:G:H2'    | 2.31                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:C:82:GLU:CG     | 9:C:83:ASP:H      | 2.31                     | 0.44              |
| 11:E:112:ARG:O    | 11:E:113:ALA:C    | 2.61                     | 0.44              |
| 12:F:55:HIS:O     | 12:F:55:HIS:ND1   | 2.51                     | 0.44              |
| 19:M:39:ILE:HG22  | 19:M:40:ALA:H     | 1.82                     | 0.44              |
| 28:a:272:A:H2'    | 28:a:273:G:H8     | 1.82                     | 0.44              |
| 28:a:2758:A:H1'   | 34:g:35:ARG:NH2   | 2.33                     | 0.44              |
| 33:f:57:LEU:HA    | 33:f:60:ILE:HG12  | 1.99                     | 0.44              |
| 34:g:90:VAL:HG12  | 34:g:160:LYS:HG2  | 1.99                     | 0.44              |
| 38:k:100:ILE:HD12 | 38:k:101:ILE:HG23 | 1.99                     | 0.44              |
| 40:m:79:LEU:HD12  | 40:m:83:LEU:HD12  | 1.99                     | 0.44              |
| 44:q:64:VAL:HG22  | 44:q:95:ASP:O     | 2.17                     | 0.44              |
| 7:A:422:C:H1'     | 7:A:423:G:C2      | 2.52                     | 0.44              |
| 7:A:973:G:OP1     | 16:J:59:LYS:HD3   | 2.18                     | 0.44              |
| 7:A:996:A:OP2     | 7:A:1217:A:H4'    | 2.17                     | 0.44              |
| 10:D:26:ARG:HB2   | 10:D:27:ALA:H     | 1.59                     | 0.44              |
| 10:D:183:LYS:HB2  | 10:D:184:ARG:HD3  | 1.99                     | 0.44              |
| 23:Q:36:LYS:HB3   | 23:Q:36:LYS:HE3   | 1.83                     | 0.44              |
| 28:a:2419:U:C2    | 28:a:2420:C:C5    | 3.06                     | 0.44              |
| 28:a:2742:G:H2'   | 28:a:2743:U:C1'   | 2.47                     | 0.44              |
| 34:g:54:PRO:HB3   | 34:g:61:GLY:CA    | 2.47                     | 0.44              |
| 37:j:108:ARG:HA   | 37:j:108:ARG:HD2  | 1.61                     | 0.44              |
| 7:A:436:C:H2'     | 7:A:437:U:C6      | 2.53                     | 0.44              |
| 7:A:513:C:H2'     | 7:A:514:C:C6      | 2.53                     | 0.44              |
| 7:A:1256:G:H5''   | 7:A:1357:A:H4'    | 2.00                     | 0.44              |
| 7:A:1320:A:H1'    | 7:A:1321:C:OP1    | 2.18                     | 0.44              |
| 10:D:167:LYS:HE3  | 10:D:167:LYS:HB3  | 1.69                     | 0.44              |
| 12:F:39:LEU:HD22  | 12:F:39:LEU:HA    | 1.84                     | 0.44              |
| 12:F:54:LEU:HD22  | 12:F:56:LYS:O     | 2.18                     | 0.44              |
| 14:H:18:GLN:OE1   | 14:H:70:ALA:HA    | 2.17                     | 0.44              |
| 15:I:87:LEU:HD22  | 15:I:98:LEU:HD11  | 1.99                     | 0.44              |
| 28:a:2296:U:C2'   | 28:a:2333:A:H61   | 2.30                     | 0.44              |
| 36:i:17:VAL:HB    | 36:i:55:ILE:HB    | 1.99                     | 0.44              |
| 39:l:111:GLU:O    | 39:l:114:ARG:HB2  | 2.18                     | 0.44              |
| 41:n:28:VAL:HG11  | 41:n:103:VAL:HG23 | 2.00                     | 0.44              |
| 43:p:78:LYS:HG3   | 43:p:117:LEU:HD13 | 1.99                     | 0.44              |
| 49:v:19:LYS:HB3   | 49:v:19:LYS:HE2   | 1.77                     | 0.44              |
| 7:A:410:G:N2      | 7:A:432:A:H62     | 2.15                     | 0.44              |
| 7:A:892:A:H2'     | 7:A:893:C:C6      | 2.52                     | 0.44              |
| 11:E:33:PHE:CG    | 11:E:57:PRO:HB3   | 2.52                     | 0.44              |
| 11:E:99:ALA:HB2   | 11:E:124:LEU:HD12 | 1.99                     | 0.44              |
| 15:I:50:GLN:N     | 15:I:51:PRO:HD2   | 2.33                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:T:70:ASN:O    | 26:T:74:ARG:HG3   | 2.18                     | 0.44              |
| 28:a:463:G:N2    | 28:a:466:A:OP2    | 2.39                     | 0.44              |
| 28:a:475:C:O2    | 28:a:479:A:N6     | 2.51                     | 0.44              |
| 28:a:1020:A:N6   | 28:a:1141:U:O2    | 2.41                     | 0.44              |
| 28:a:1916:A:H2'  | 28:a:1917:PSU:C6  | 2.52                     | 0.44              |
| 28:a:2473:U:OP1  | 28:a:2474:U:H5    | 2.01                     | 0.44              |
| 28:a:2672:U:H2'  | 28:a:2673:G:H4'   | 1.99                     | 0.44              |
| 29:b:14:U:C4'    | 29:b:69:G:H22     | 2.28                     | 0.44              |
| 48:u:20:LEU:O    | 48:u:25:LYS:N     | 2.50                     | 0.44              |
| 52:y:11:ARG:HB2  | 52:y:54:MET:HB2   | 1.98                     | 0.44              |
| 3:2:15:LYS:HZ1   | 3:2:23:LYS:HD3    | 1.81                     | 0.44              |
| 3:2:43:HIS:NE2   | 28:a:2351:G:N7    | 2.66                     | 0.44              |
| 5:4:56:ARG:NH2   | 25:S:64:ASP:HB3   | 2.33                     | 0.44              |
| 7:A:204:G:O2'    | 7:A:214:C:O2      | 2.29                     | 0.44              |
| 7:A:235:C:H2'    | 7:A:236:A:C8      | 2.53                     | 0.44              |
| 7:A:661:G:O2'    | 7:A:662:U:H5'     | 2.18                     | 0.44              |
| 7:A:736:C:OP1    | 24:R:61:ARG:NH2   | 2.50                     | 0.44              |
| 10:D:117:LEU:O   | 10:D:122:ALA:HB3  | 2.18                     | 0.44              |
| 28:a:630:G:C2    | 28:a:632:A:OP2    | 2.70                     | 0.44              |
| 28:a:861:A:C2    | 29:b:99:A:H2      | 2.36                     | 0.44              |
| 38:k:95:LEU:HA   | 38:k:100:ILE:HD11 | 1.99                     | 0.44              |
| 39:l:53:MET:HA   | 39:l:116:ALA:HB1  | 2.00                     | 0.44              |
| 43:p:62:ILE:HA   | 43:p:65:ILE:HG22  | 1.99                     | 0.44              |
| 52:y:6:LYS:HA    | 52:y:6:LYS:HE3    | 2.00                     | 0.44              |
| 7:A:1318:C:H5'   | 7:A:1319:A:OP2    | 2.18                     | 0.44              |
| 8:B:10:LEU:HA    | 8:B:14:VAL:HG12   | 1.98                     | 0.44              |
| 9:C:157:LEU:HD12 | 9:C:164:ARG:HB2   | 1.99                     | 0.44              |
| 15:I:9:THR:HG22  | 15:I:85:ARG:HH21  | 1.82                     | 0.44              |
| 19:M:34:LEU:CD1  | 19:M:39:ILE:HB    | 2.48                     | 0.44              |
| 20:N:28:LYS:HA   | 20:N:31:ILE:HG22  | 1.99                     | 0.44              |
| 28:a:596:U:C2    | 28:a:662:G:N2     | 2.86                     | 0.44              |
| 28:a:597:G:N1    | 28:a:661:A:N6     | 2.66                     | 0.44              |
| 28:a:627:A:H62   | 38:k:112:LEU:H    | 1.64                     | 0.44              |
| 28:a:728:G:OP2   | 56:a:6215:SPD:N1  | 2.50                     | 0.44              |
| 28:a:973:A:H5'   | 28:a:1188:U:H1'   | 2.00                     | 0.44              |
| 28:a:1110:G:HO2' | 28:a:1111:A:H8    | 1.58                     | 0.44              |
| 28:a:1880:U:N3   | 28:a:1881:C:N4    | 2.65                     | 0.44              |
| 32:e:111:GLU:HG2 | 32:e:114:ARG:HH21 | 1.83                     | 0.44              |
| 32:e:128:ALA:O   | 32:e:130:LYS:N    | 2.51                     | 0.44              |
| 36:i:1:MET:HE3   | 44:q:12:HIS:HA    | 1.99                     | 0.44              |
| 39:l:33:LEU:HD12 | 39:l:129:THR:O    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:l:34:LYS:HG3   | 39:l:131:VAL:HG11 | 1.99                     | 0.44              |
| 43:p:79:PHE:HA    | 43:p:113:ALA:HB1  | 2.00                     | 0.44              |
| 4:3:4:ARG:O       | 4:3:37:GLN:HA     | 2.18                     | 0.43              |
| 7:A:120:A:H2'     | 7:A:122:G:C8      | 2.44                     | 0.43              |
| 13:G:127:ALA:O    | 13:G:131:LYS:N    | 2.49                     | 0.43              |
| 14:H:9:ASP:N      | 14:H:9:ASP:OD1    | 2.49                     | 0.43              |
| 18:L:83:ARG:HE    | 18:L:83:ARG:HB3   | 1.68                     | 0.43              |
| 19:M:52:GLN:HG3   | 19:M:56:LEU:HB3   | 2.00                     | 0.43              |
| 28:a:661:A:C6     | 28:a:662:G:C8     | 3.06                     | 0.43              |
| 28:a:2478:A:C6    | 28:a:2479:U:C5    | 3.05                     | 0.43              |
| 28:a:2766:A:H2'   | 28:a:2766:A:N3    | 2.33                     | 0.43              |
| 3:2:8:ARG:HD2     | 3:2:8:ARG:HA      | 1.70                     | 0.43              |
| 7:A:1028:C:H1'    | 7:A:1035:A:H61    | 1.82                     | 0.43              |
| 8:B:8:ASP:CG      | 8:B:9:MET:H       | 2.26                     | 0.43              |
| 8:B:9:MET:HB2     | 8:B:208:ARG:HH21  | 1.82                     | 0.43              |
| 14:H:36:ILE:HG22  | 14:H:40:LEU:HD23  | 2.01                     | 0.43              |
| 23:Q:30:LYS:HE3   | 23:Q:30:LYS:HB3   | 1.62                     | 0.43              |
| 27:U:12:PHE:O     | 27:U:15:ALA:HB3   | 2.18                     | 0.43              |
| 28:a:279:A:H62    | 28:a:361:G:N2     | 2.15                     | 0.43              |
| 32:e:194:LYS:HE2  | 32:e:194:LYS:N    | 2.33                     | 0.43              |
| 34:g:101:ASN:CA   | 34:g:117:LEU:HB2  | 2.48                     | 0.43              |
| 36:i:60:ASP:OD1   | 36:i:60:ASP:N     | 2.35                     | 0.43              |
| 38:k:14:LYS:HB2   | 38:k:14:LYS:HE3   | 1.82                     | 0.43              |
| 40:m:8:ARG:HD2    | 40:m:43:GLU:HG2   | 2.00                     | 0.43              |
| 43:p:57:PHE:O     | 43:p:61:TRP:CD1   | 2.71                     | 0.43              |
| 44:q:43:ASN:HD22  | 44:q:103:ALA:HB2  | 1.82                     | 0.43              |
| 7:A:378:G:HO2'    | 7:A:379:C:H6      | 1.62                     | 0.43              |
| 11:E:110:ALA:O    | 11:E:111:MET:C    | 2.61                     | 0.43              |
| 13:G:10:ARG:HG3   | 13:G:11:LYS:N     | 2.32                     | 0.43              |
| 17:K:128:ARG:HH11 | 17:K:128:ARG:HG3  | 1.82                     | 0.43              |
| 21:O:88:ARG:NH2   | 21:O:89:ARG:HH22  | 2.17                     | 0.43              |
| 28:a:268:C:H2'    | 28:a:269:C:H5'    | 1.99                     | 0.43              |
| 28:a:548:G:H2'    | 28:a:549:G:C8     | 2.53                     | 0.43              |
| 28:a:634:C:N3     | 28:a:635:C:C4     | 2.86                     | 0.43              |
| 28:a:1018:U:H4'   | 28:a:1036:G:O2'   | 2.18                     | 0.43              |
| 28:a:1023:U:C4    | 28:a:1024:G:C5    | 3.07                     | 0.43              |
| 28:a:1045:C:N4    | 28:a:1111:A:H5''  | 2.33                     | 0.43              |
| 28:a:1799:G:OP1   | 30:c:258:ARG:NH1  | 2.47                     | 0.43              |
| 28:a:2280:G:H4'   | 28:a:2327:A:N3    | 2.34                     | 0.43              |
| 28:a:2357:G:H5'   | 28:a:2358:A:OP2   | 2.19                     | 0.43              |
| 28:a:2369:A:H2'   | 28:a:2370:G:C8    | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:a:2740:A:C8   | 28:a:2741:A:N7    | 2.85                     | 0.43              |
| 28:a:2743:U:H5'  | 28:a:2744:G:OP2   | 2.18                     | 0.43              |
| 28:a:2748:A:H1'  | 28:a:2757:A:H61   | 1.83                     | 0.43              |
| 29:b:80:U:C2     | 29:b:96:G:O6      | 2.71                     | 0.43              |
| 33:f:57:LEU:HA   | 33:f:60:ILE:CG1   | 2.48                     | 0.43              |
| 33:f:63:GLN:HE21 | 33:f:95:ARG:CZ    | 2.31                     | 0.43              |
| 38:k:123:ARG:HG2 | 38:k:124:GLY:N    | 2.34                     | 0.43              |
| 7:A:166:U:H2'    | 7:A:167:G:C8      | 2.52                     | 0.43              |
| 7:A:982:U:OP1    | 7:A:982:U:H6      | 2.01                     | 0.43              |
| 7:A:1369:G:C2'   | 7:A:1370:C:H5'    | 2.49                     | 0.43              |
| 7:A:1402:G:H3'   | 7:A:1403:4OC:H6   | 2.00                     | 0.43              |
| 13:G:35:LYS:HB3  | 13:G:35:LYS:HE2   | 1.77                     | 0.43              |
| 24:R:72:ASP:HB3  | 27:U:3:VAL:CG2    | 2.49                     | 0.43              |
| 25:S:14:HIS:CD2  | 25:S:15:LEU:HD23  | 2.53                     | 0.43              |
| 25:S:50:ALA:HB1  | 25:S:57:HIS:HB3   | 2.00                     | 0.43              |
| 28:a:839:U:C2    | 28:a:840:C:C5     | 3.06                     | 0.43              |
| 28:a:1027:A:C5   | 28:a:1126:A:N6    | 2.86                     | 0.43              |
| 28:a:1593:A:H2'  | 28:a:1594:U:C6    | 2.54                     | 0.43              |
| 28:a:2029:G:H2'  | 28:a:2031:A:OP1   | 2.18                     | 0.43              |
| 28:a:2303:G:O2'  | 33:f:129:SER:HB2  | 2.19                     | 0.43              |
| 30:c:261:LYS:HA  | 30:c:264:ASP:OD2  | 2.19                     | 0.43              |
| 33:f:160:ALA:HB1 | 33:f:165:GLU:HB2  | 2.00                     | 0.43              |
| 34:g:97:ALA:O    | 34:g:104:ASN:N    | 2.47                     | 0.43              |
| 41:n:33:ARG:HG3  | 41:n:34:HIS:CE1   | 2.53                     | 0.43              |
| 7:A:108:G:H5'    | 7:A:109:A:C3'     | 2.49                     | 0.43              |
| 7:A:239:U:C3'    | 7:A:240:G:H5''    | 2.49                     | 0.43              |
| 10:D:91:LEU:O    | 10:D:95:GLU:HB2   | 2.18                     | 0.43              |
| 15:I:118:LEU:CD2 | 15:I:124:ARG:HG2  | 2.48                     | 0.43              |
| 17:K:109:ASN:C   | 17:K:110:ILE:HD12 | 2.43                     | 0.43              |
| 28:a:848:C:H2'   | 28:a:849:A:C8     | 2.50                     | 0.43              |
| 28:a:937:C:N4    | 28:a:938:G:C5     | 2.86                     | 0.43              |
| 28:a:938:G:N1    | 28:a:939:G:N7     | 2.66                     | 0.43              |
| 28:a:1416:G:HO2' | 28:a:1417:C:P     | 2.38                     | 0.43              |
| 28:a:2361:G:H2'  | 28:a:2362:C:O4'   | 2.18                     | 0.43              |
| 28:a:2812:G:H2'  | 28:a:2813:A:C8    | 2.53                     | 0.43              |
| 34:g:3:ARG:HB2   | 34:g:6:LYS:HE3    | 2.00                     | 0.43              |
| 36:i:54:ILE:HG23 | 36:i:122:LEU:CA   | 2.46                     | 0.43              |
| 43:p:90:ILE:HG13 | 43:p:90:ILE:H     | 1.49                     | 0.43              |
| 10:D:145:ILE:CG2 | 10:D:146:ARG:N    | 2.81                     | 0.43              |
| 11:E:159:LYS:HE3 | 14:H:43:GLU:HA    | 2.00                     | 0.43              |
| 17:K:64:GLN:O    | 17:K:68:GLU:HG2   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:M:104:THR:OG1 | 19:M:105:ASN:N    | 2.51                     | 0.43              |
| 20:N:41:ARG:C    | 20:N:43:ASN:H     | 2.26                     | 0.43              |
| 21:O:18:ASP:HB2  | 21:O:19:ALA:H     | 1.61                     | 0.43              |
| 21:O:27:VAL:O    | 21:O:31:LEU:HD12  | 2.19                     | 0.43              |
| 25:S:13:LEU:O    | 25:S:17:LYS:HG2   | 2.18                     | 0.43              |
| 28:a:85:G:C6     | 28:a:98:G:N1      | 2.87                     | 0.43              |
| 28:a:598:U:H2'   | 28:a:599:A:C8     | 2.53                     | 0.43              |
| 28:a:1000:A:H2'  | 28:a:1001:A:C8    | 2.54                     | 0.43              |
| 28:a:1865:U:C6   | 28:a:1875:G:N1    | 2.86                     | 0.43              |
| 28:a:2316:G:H2'  | 28:a:2317:A:C8    | 2.53                     | 0.43              |
| 28:a:2739:U:C2   | 28:a:2764:A:N6    | 2.82                     | 0.43              |
| 29:b:42:C:H6     | 33:f:66:LEU:HD21  | 1.83                     | 0.43              |
| 31:d:35:THR:HA   | 31:d:93:GLY:H     | 1.83                     | 0.43              |
| 33:f:4:LEU:HD23  | 33:f:4:LEU:HA     | 1.78                     | 0.43              |
| 34:g:18:LYS:HD3  | 34:g:19:ILE:N     | 2.34                     | 0.43              |
| 37:j:5:GLN:HA    | 37:j:20:MET:HE3   | 2.00                     | 0.43              |
| 53:z:31:ASP:HB3  | 53:z:35:GLY:H     | 1.82                     | 0.43              |
| 4:3:32:LYS:HD3   | 28:a:2478:A:OP1   | 2.19                     | 0.43              |
| 7:A:1442:A:N6    | 7:A:1461:C:C2     | 2.87                     | 0.43              |
| 7:A:1464:U:H2'   | 7:A:1465:U:C6     | 2.54                     | 0.43              |
| 15:I:22:LYS:H    | 15:I:62:ASP:HB2   | 1.84                     | 0.43              |
| 28:a:1023:U:C5   | 28:a:1024:G:N7    | 2.86                     | 0.43              |
| 28:a:1412:U:H2'  | 28:a:1413:A:C8    | 2.54                     | 0.43              |
| 28:a:2523:G:H21  | 28:a:2764:A:C1'   | 2.18                     | 0.43              |
| 28:a:2680:U:O2'  | 28:a:2681:C:H5'   | 2.19                     | 0.43              |
| 29:b:90:C:C4     | 29:b:91:C:H5      | 2.37                     | 0.43              |
| 30:c:146:MET:SD  | 30:c:154:LEU:HD11 | 2.58                     | 0.43              |
| 34:g:35:ARG:HG3  | 34:g:36:THR:N     | 2.33                     | 0.43              |
| 37:j:7:MET:HE3   | 37:j:7:MET:HB3    | 1.81                     | 0.43              |
| 38:k:75:ALA:O    | 38:k:108:ALA:HB1  | 2.18                     | 0.43              |
| 42:o:43:PHE:CE1  | 42:o:63:LYS:HD3   | 2.53                     | 0.43              |
| 48:u:71:LYS:HB3  | 48:u:73:LYS:NZ    | 2.34                     | 0.43              |
| 7:A:536:C:O2'    | 7:A:537:G:H8      | 2.02                     | 0.43              |
| 7:A:536:C:O2'    | 7:A:537:G:O5'     | 2.25                     | 0.43              |
| 7:A:1392:U:H2'   | 7:A:1393:G:C8     | 2.53                     | 0.43              |
| 7:A:1452:U:H1'   | 7:A:1453:C:OP2    | 2.18                     | 0.43              |
| 9:C:4:LYS:HB2    | 9:C:4:LYS:HE2     | 1.74                     | 0.43              |
| 11:E:81:LEU:HB2  | 11:E:98:PRO:HG3   | 2.01                     | 0.43              |
| 14:H:7:ILE:HD11  | 14:H:32:LEU:HD13  | 1.99                     | 0.43              |
| 19:M:82:ASP:OD1  | 19:M:83:LEU:HD23  | 2.19                     | 0.43              |
| 25:S:28:LYS:O    | 25:S:29:LYS:HB2   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 28:a:760:G:H2'   | 28:a:761:A:O4'   | 2.19                     | 0.43              |
| 28:a:2247:A:H2'  | 28:a:2248:C:H6   | 1.84                     | 0.43              |
| 28:a:2419:U:H2'  | 28:a:2420:C:C6   | 2.53                     | 0.43              |
| 28:a:2527:C:H5'' | 28:a:2528:U:OP2  | 2.18                     | 0.43              |
| 29:b:26:C:H2'    | 29:b:27:C:O4'    | 2.18                     | 0.43              |
| 29:b:70:C:C2     | 29:b:71:C:C5     | 3.06                     | 0.43              |
| 33:f:126:GLY:HA2 | 33:f:163:ASP:HA  | 2.00                     | 0.43              |
| 36:i:5:THR:HG23  | 36:i:45:THR:HG21 | 1.99                     | 0.43              |
| 41:n:26:LEU:HD13 | 41:n:39:VAL:HG22 | 2.00                     | 0.43              |
| 48:u:48:MET:HG2  | 48:u:51:GLN:HE22 | 1.82                     | 0.43              |
| 49:v:65:GLY:HA3  | 49:v:85:GLU:H    | 1.84                     | 0.43              |
| 7:A:377:G:H22    | 7:A:386:C:H5     | 1.67                     | 0.43              |
| 9:C:50:ALA:O     | 9:C:70:THR:OG1   | 2.37                     | 0.43              |
| 16:J:34:ALA:HB1  | 16:J:36:VAL:H    | 1.84                     | 0.43              |
| 28:a:58:G:H2'    | 28:a:59:U:C6     | 2.54                     | 0.43              |
| 28:a:839:U:H2'   | 28:a:840:C:C6    | 2.54                     | 0.43              |
| 28:a:1027:A:O2'  | 28:a:1028:A:H5'  | 2.19                     | 0.43              |
| 28:a:1165:A:N3   | 28:a:1166:G:N7   | 2.67                     | 0.43              |
| 28:a:1183:U:H2'  | 28:a:1184:U:O4'  | 2.19                     | 0.43              |
| 28:a:2740:A:C8   | 28:a:2764:A:N6   | 2.87                     | 0.43              |
| 28:a:2741:A:O2'  | 28:a:2742:G:H5'  | 2.19                     | 0.43              |
| 30:c:80:ARG:NH1  | 30:c:82:GLU:OE2  | 2.52                     | 0.43              |
| 34:g:156:PRO:HB2 | 34:g:172:LYS:NZ  | 2.33                     | 0.43              |
| 37:j:76:VAL:HG22 | 42:o:73:VAL:HG13 | 2.00                     | 0.43              |
| 43:p:80:ILE:HA   | 43:p:83:LEU:HG   | 1.99                     | 0.43              |
| 7:A:215:C:O4'    | 7:A:466:A:N6     | 2.52                     | 0.43              |
| 7:A:377:G:H1     | 7:A:386:C:H41    | 1.67                     | 0.43              |
| 7:A:492:C:H2'    | 7:A:493:A:H8     | 1.81                     | 0.43              |
| 7:A:555:U:H2'    | 7:A:556:C:C6     | 2.54                     | 0.43              |
| 7:A:1086:U:H3    | 7:A:1099:G:N2    | 2.17                     | 0.43              |
| 7:A:1253:A:H62   | 7:A:1286:A:H62   | 1.67                     | 0.43              |
| 7:A:1317:G:N2    | 7:A:1319:A:H3'   | 2.34                     | 0.43              |
| 7:A:1474:G:H2'   | 7:A:1475:U:C6    | 2.54                     | 0.43              |
| 10:D:146:ARG:HB3 | 10:D:152:GLN:HG2 | 2.01                     | 0.43              |
| 11:E:64:MET:HE3  | 11:E:64:MET:HB3  | 1.58                     | 0.43              |
| 22:P:39:PHE:CZ   | 22:P:74:LEU:HB2  | 2.54                     | 0.43              |
| 24:R:12:ARG:HD3  | 24:R:12:ARG:HA   | 1.72                     | 0.43              |
| 28:a:1416:G:O2'  | 28:a:1417:C:P    | 2.77                     | 0.43              |
| 28:a:1794:A:H2'  | 28:a:1795:C:C6   | 2.54                     | 0.43              |
| 28:a:2074:U:H2'  | 28:a:2075:U:C6   | 2.54                     | 0.43              |
| 28:a:2297:A:N6   | 28:a:2319:G:H21  | 2.05                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 28:a:2356:U:H4'  | 49:v:20:ARG:NE   | 2.18                     | 0.43              |
| 34:g:52:PHE:CG   | 34:g:69:ARG:HA   | 2.54                     | 0.43              |
| 42:o:36:SER:O    | 42:o:36:SER:OG   | 2.33                     | 0.43              |
| 47:t:100:SER:O   | 47:t:100:SER:OG  | 2.27                     | 0.43              |
| 50:w:18:ARG:HA   | 50:w:23:ASN:O    | 2.17                     | 0.43              |
| 1:0:10:LYS:HG2   | 1:0:54:ILE:HA    | 2.00                     | 0.42              |
| 4:3:12:ARG:NH2   | 4:3:13:ASN:HA    | 2.34                     | 0.42              |
| 7:A:599:C:H2'    | 7:A:600:A:C8     | 2.40                     | 0.42              |
| 7:A:1347:A:H2'   | 13:G:10:ARG:NH2  | 2.34                     | 0.42              |
| 7:A:1533:U:H1'   | 7:A:1534:C:H3'   | 2.01                     | 0.42              |
| 8:B:152:LYS:NZ   | 8:B:153:ASP:OD1  | 2.37                     | 0.42              |
| 16:J:32:THR:HG21 | 16:J:83:THR:HG22 | 2.01                     | 0.42              |
| 28:a:145:C:H2'   | 28:a:146:A:H8    | 1.84                     | 0.42              |
| 28:a:1027:A:O2'  | 28:a:1028:A:O4'  | 2.29                     | 0.42              |
| 28:a:2280:G:H4'  | 28:a:2327:A:H1'  | 2.01                     | 0.42              |
| 28:a:2294:G:OP2  | 41:n:10:ARG:HD2  | 2.18                     | 0.42              |
| 28:a:2364:C:H5'' | 28:a:2365:G:OP2  | 2.19                     | 0.42              |
| 28:a:2386:A:H5'' | 49:v:55:ARG:HH22 | 1.84                     | 0.42              |
| 28:a:2753:A:OP2  | 28:a:2754:U:H5   | 2.02                     | 0.42              |
| 29:b:91:C:H3'    | 29:b:92:C:C6     | 2.54                     | 0.42              |
| 29:b:109:A:H2'   | 29:b:110:C:O4'   | 2.19                     | 0.42              |
| 32:e:187:VAL:C   | 32:e:188:MET:HE3 | 2.44                     | 0.42              |
| 34:g:7:ALA:HA    | 34:g:8:PRO:HD3   | 1.91                     | 0.42              |
| 34:g:15:VAL:HG11 | 34:g:79:VAL:HB   | 2.01                     | 0.42              |
| 36:i:74:TYR:O    | 36:i:86:GLN:HA   | 2.19                     | 0.42              |
| 44:q:4:VAL:HA    | 44:q:12:HIS:O    | 2.19                     | 0.42              |
| 50:w:59:ILE:HG12 | 50:w:67:VAL:HG21 | 2.01                     | 0.42              |
| 3:2:30:ARG:O     | 28:a:2419:U:H5   | 2.02                     | 0.42              |
| 5:4:36:VAL:HG11  | 33:f:110:ARG:HA  | 2.01                     | 0.42              |
| 7:A:62:U:H2'     | 7:A:63:C:C5      | 2.53                     | 0.42              |
| 7:A:178:C:C2     | 7:A:179:A:C8     | 3.08                     | 0.42              |
| 7:A:1126:U:H1'   | 7:A:1127:G:H2'   | 2.00                     | 0.42              |
| 7:A:1259:G:H2'   | 7:A:1260:C:C6    | 2.53                     | 0.42              |
| 7:A:1288:A:H2    | 7:A:1354:G:H1'   | 1.84                     | 0.42              |
| 8:B:36:ASN:OD1   | 8:B:36:ASN:O     | 2.37                     | 0.42              |
| 8:B:96:TRP:HE1   | 8:B:175:GLU:CD   | 2.27                     | 0.42              |
| 9:C:110:GLU:HG2  | 9:C:144:LEU:HD13 | 2.00                     | 0.42              |
| 10:D:151:LYS:HZ3 | 10:D:154:ARG:HD3 | 1.84                     | 0.42              |
| 14:H:54:ASP:C    | 14:H:56:LYS:H    | 2.27                     | 0.42              |
| 16:J:57:VAL:O    | 16:J:58:ASN:HB2  | 2.19                     | 0.42              |
| 18:L:50:ARG:HB2  | 18:L:90:LEU:HD11 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 20:N:92:GLU:OE1   | 20:N:92:GLU:N    | 2.52                     | 0.42              |
| 28:a:5:A:H2'      | 28:a:6:A:C8      | 2.54                     | 0.42              |
| 28:a:711:G:O6     | 28:a:721:A:N6    | 2.52                     | 0.42              |
| 28:a:1042:G:H1    | 28:a:1113:U:H3   | 0.65                     | 0.42              |
| 28:a:2530:A:O2'   | 28:a:2535:G:O6   | 2.33                     | 0.42              |
| 32:e:148:ILE:CG2  | 32:e:169:VAL:HA  | 2.49                     | 0.42              |
| 43:p:70:ARG:HA    | 43:p:74:ILE:O    | 2.18                     | 0.42              |
| 48:u:25:LYS:HD2   | 48:u:25:LYS:HA   | 1.68                     | 0.42              |
| 48:u:30:ILE:HG22  | 48:u:40:ILE:HD13 | 2.01                     | 0.42              |
| 1:0:10:LYS:HE3    | 1:0:54:ILE:HA    | 1.99                     | 0.42              |
| 4:3:31:PRO:HB2    | 28:a:2527:C:H4'  | 2.00                     | 0.42              |
| 5:4:28:VAL:HG21   | 5:4:32:LEU:HD22  | 2.01                     | 0.42              |
| 10:D:50:ASP:O     | 10:D:54:GLN:HG3  | 2.19                     | 0.42              |
| 10:D:65:TYR:O     | 10:D:67:VAL:HG12 | 2.20                     | 0.42              |
| 23:Q:38:ILE:H     | 23:Q:38:ILE:HG13 | 1.68                     | 0.42              |
| 28:a:84:A:H3'     | 47:t:7:ARG:NH2   | 2.27                     | 0.42              |
| 28:a:1281:G:H2'   | 28:a:1282:U:C6   | 2.54                     | 0.42              |
| 28:a:1864:U:H2'   | 28:a:1865:U:N3   | 2.34                     | 0.42              |
| 28:a:2303:G:O3'   | 33:f:121:SER:HA  | 2.19                     | 0.42              |
| 29:b:9:G:C6       | 29:b:111:U:O2    | 2.70                     | 0.42              |
| 29:b:100:G:H2'    | 29:b:101:A:O4'   | 2.18                     | 0.42              |
| 33:f:5:HIS:O      | 33:f:9:LYS:HG2   | 2.20                     | 0.42              |
| 39:l:62:LYS:HG2   | 39:l:64:TRP:CH2  | 2.54                     | 0.42              |
| 40:m:38:LEU:HD13  | 40:m:111:ALA:HB2 | 2.02                     | 0.42              |
| 47:t:83:VAL:HG22  | 47:t:96:PHE:CD1  | 2.54                     | 0.42              |
| 48:u:42:LEU:HA    | 48:u:42:LEU:HD22 | 1.83                     | 0.42              |
| 7:A:132:U:H2'     | 7:A:133:U:C6     | 2.54                     | 0.42              |
| 7:A:383:A:N7      | 7:A:455:U:H5'    | 2.33                     | 0.42              |
| 7:A:427:U:H2'     | 7:A:428:G:N2     | 2.35                     | 0.42              |
| 7:A:533:A:O2'     | 7:A:536:C:N4     | 2.52                     | 0.42              |
| 7:A:599:C:H4'     | 14:H:122:GLY:O   | 2.19                     | 0.42              |
| 7:A:1067:A:C4     | 7:A:1109:C:H5''  | 2.55                     | 0.42              |
| 10:D:8:LYS:C      | 10:D:10:LYS:H    | 2.27                     | 0.42              |
| 17:K:110:ILE:HG22 | 27:U:19:PHE:CD1  | 2.55                     | 0.42              |
| 20:N:24:ARG:HG3   | 20:N:51:LEU:HD12 | 2.00                     | 0.42              |
| 20:N:76:LYS:HG3   | 20:N:77:PHE:N    | 2.34                     | 0.42              |
| 28:a:273:G:C6     | 28:a:274:C:N4    | 2.86                     | 0.42              |
| 28:a:630:G:H2'    | 28:a:631:A:H3'   | 2.01                     | 0.42              |
| 28:a:1326:U:H2'   | 28:a:1327:A:H8   | 1.83                     | 0.42              |
| 28:a:1597:A:H5''  | 28:a:1598:A:H5'  | 2.02                     | 0.42              |
| 43:p:109:LEU:HD23 | 44:q:49:ILE:HD13 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 44:q:26:ASP:O    | 44:q:27:ILE:HD12  | 2.20                     | 0.42              |
| 47:t:18:ASP:HB3  | 47:t:21:LYS:HD3   | 2.01                     | 0.42              |
| 49:v:45:PHE:HA   | 49:v:78:LYS:O     | 2.19                     | 0.42              |
| 53:z:55:ILE:C    | 53:z:55:ILE:HD12  | 2.45                     | 0.42              |
| 7:A:122:G:H3'    | 7:A:123:C:H6      | 1.85                     | 0.42              |
| 7:A:609:A:H1'    | 7:A:610:G:OP1     | 2.19                     | 0.42              |
| 13:G:25:LYS:HD2  | 13:G:25:LYS:HA    | 1.88                     | 0.42              |
| 13:G:50:LEU:O    | 13:G:54:SER:HB2   | 2.19                     | 0.42              |
| 13:G:60:GLU:O    | 13:G:64:VAL:HG23  | 2.19                     | 0.42              |
| 15:I:98:LEU:HD23 | 15:I:98:LEU:HA    | 1.80                     | 0.42              |
| 15:I:114:LYS:HG2 | 15:I:120:LYS:O    | 2.20                     | 0.42              |
| 17:K:80:LYS:HE2  | 17:K:80:LYS:HB2   | 1.71                     | 0.42              |
| 20:N:61:ARG:HA   | 20:N:61:ARG:HD3   | 1.95                     | 0.42              |
| 25:S:11:ILE:HG23 | 25:S:38:SER:HA    | 2.01                     | 0.42              |
| 25:S:29:LYS:HA   | 25:S:29:LYS:HD2   | 1.87                     | 0.42              |
| 28:a:661:A:C2'   | 28:a:662:G:H5'    | 2.43                     | 0.42              |
| 28:a:851:C:H2'   | 28:a:852:U:C6     | 2.54                     | 0.42              |
| 28:a:2384:U:O2'  | 28:a:2385:C:H5'   | 2.20                     | 0.42              |
| 28:a:2528:U:H2'  | 28:a:2530:A:H8    | 1.85                     | 0.42              |
| 32:e:22:ASP:CG   | 32:e:23:PHE:H     | 2.27                     | 0.42              |
| 32:e:194:LYS:HA  | 32:e:194:LYS:HD3  | 1.83                     | 0.42              |
| 33:f:4:LEU:HG    | 33:f:101:GLU:HB2  | 2.02                     | 0.42              |
| 43:p:94:ILE:HD12 | 44:q:4:VAL:CG2    | 2.50                     | 0.42              |
| 44:q:59:ILE:CG2  | 44:q:98:ILE:HD12  | 2.50                     | 0.42              |
| 7:A:222:U:O2'    | 7:A:223:A:OP1     | 2.32                     | 0.42              |
| 7:A:437:U:O4'    | 10:D:154:ARG:NH2  | 2.45                     | 0.42              |
| 7:A:488:C:O2'    | 7:A:489:C:H5'     | 2.19                     | 0.42              |
| 7:A:596:A:C5     | 7:A:597:G:C2      | 3.07                     | 0.42              |
| 13:G:131:LYS:HA  | 13:G:135:VAL:HG11 | 2.01                     | 0.42              |
| 16:J:17:LEU:HD12 | 16:J:17:LEU:HA    | 1.70                     | 0.42              |
| 19:M:12:HIS:CD2  | 19:M:12:HIS:C     | 2.97                     | 0.42              |
| 27:U:51:SER:O    | 27:U:55:ARG:HG3   | 2.19                     | 0.42              |
| 28:a:268:C:C2    | 28:a:425:G:N2     | 2.88                     | 0.42              |
| 28:a:636:G:OP1   | 38:k:129:LYS:HG3  | 2.19                     | 0.42              |
| 28:a:2379:G:H5'  | 41:n:21:LEU:HD21  | 2.01                     | 0.42              |
| 28:a:2741:A:H2'  | 28:a:2742:G:O4'   | 2.20                     | 0.42              |
| 28:a:2820:A:N3   | 28:a:2820:A:H2'   | 2.34                     | 0.42              |
| 33:f:73:SER:HB3  | 33:f:80:ARG:HH21  | 1.83                     | 0.42              |
| 33:f:164:GLU:OE2 | 33:f:165:GLU:HG2  | 2.20                     | 0.42              |
| 43:p:69:ALA:HB2  | 43:p:106:PHE:CZ   | 2.48                     | 0.42              |
| 44:q:25:LEU:HD21 | 44:q:33:VAL:HG21  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 48:u:40:ILE:HD11 | 48:u:91:PHE:CD2   | 2.54                     | 0.42              |
| 49:v:81:SER:OG   | 49:v:82:ILE:N     | 2.52                     | 0.42              |
| 7:A:539:A:H2'    | 7:A:540:G:C8      | 2.55                     | 0.42              |
| 7:A:778:G:HO2'   | 7:A:779:C:P       | 2.42                     | 0.42              |
| 7:A:1028:C:H2'   | 7:A:1029:U:C6     | 2.55                     | 0.42              |
| 8:B:109:GLN:H    | 8:B:109:GLN:HG3   | 1.64                     | 0.42              |
| 11:E:66:LYS:HB3  | 11:E:66:LYS:HE2   | 1.82                     | 0.42              |
| 19:M:64:VAL:O    | 19:M:69:LEU:HG    | 2.19                     | 0.42              |
| 28:a:660:C:N3    | 28:a:661:A:C6     | 2.87                     | 0.42              |
| 28:a:722:A:H2'   | 28:a:723:C:C6     | 2.54                     | 0.42              |
| 28:a:1021:A:O3'  | 28:a:1022:G:H4'   | 2.19                     | 0.42              |
| 28:a:1864:U:H2'  | 28:a:1865:U:C4    | 2.55                     | 0.42              |
| 28:a:2327:A:C2   | 28:a:2328:A:C8    | 3.08                     | 0.42              |
| 28:a:2747:G:H5'  | 34:g:138:LYS:HZ3  | 1.84                     | 0.42              |
| 33:f:95:ARG:HB3  | 33:f:95:ARG:HE    | 1.77                     | 0.42              |
| 49:v:46:HIS:HB2  | 49:v:79:PHE:CD1   | 2.54                     | 0.42              |
| 52:y:38:ARG:HA   | 52:y:38:ARG:HE    | 1.84                     | 0.42              |
| 7:A:193:C:H2'    | 7:A:194:C:C6      | 2.55                     | 0.42              |
| 7:A:1109:C:H2'   | 7:A:1110:A:O4'    | 2.20                     | 0.42              |
| 7:A:1188:G:OP1   | 7:A:1188:G:H4'    | 2.20                     | 0.42              |
| 7:A:1228:A:P     | 19:M:95:LEU:HD21  | 2.59                     | 0.42              |
| 17:K:26:SER:OG   | 17:K:27:PHE:N     | 2.52                     | 0.42              |
| 19:M:17:ILE:O    | 19:M:41:GLU:HG3   | 2.19                     | 0.42              |
| 21:O:70:LEU:HD12 | 21:O:70:LEU:HA    | 1.88                     | 0.42              |
| 21:O:71:LYS:HB2  | 21:O:78:TYR:CD1   | 2.55                     | 0.42              |
| 28:a:696:G:O6    | 57:a:6221:SPM:H81 | 2.18                     | 0.42              |
| 28:a:721:A:H2'   | 28:a:722:A:C8     | 2.55                     | 0.42              |
| 28:a:1050:A:N6   | 28:a:1109:C:H42   | 2.18                     | 0.42              |
| 31:d:36:GLN:N    | 31:d:49:GLN:O     | 2.52                     | 0.42              |
| 36:i:15:TRP:CD1  | 36:i:53:TYR:HB2   | 2.55                     | 0.42              |
| 36:i:119:PHE:CD1 | 36:i:122:LEU:HB3  | 2.55                     | 0.42              |
| 37:j:44:LYS:HA   | 37:j:44:LYS:HD2   | 1.77                     | 0.42              |
| 38:k:20:GLY:HA2  | 38:k:28:GLY:HA2   | 2.01                     | 0.42              |
| 43:p:68:ALA:C    | 43:p:106:PHE:HE2  | 2.28                     | 0.42              |
| 49:v:72:LYS:CG   | 49:v:79:PHE:HB2   | 2.50                     | 0.42              |
| 7:A:447:G:O2'    | 7:A:448:A:OP1     | 2.29                     | 0.42              |
| 7:A:1104:G:P     | 7:A:1104:G:O4'    | 2.78                     | 0.42              |
| 7:A:1161:G:C6    | 7:A:1162:C:C5     | 3.08                     | 0.42              |
| 9:C:74:GLY:C     | 9:C:76:VAL:H      | 2.26                     | 0.42              |
| 10:D:19:LEU:HB3  | 10:D:21:LEU:HG    | 2.02                     | 0.42              |
| 11:E:112:ARG:H   | 11:E:112:ARG:HG2  | 1.32                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:G:126:ASP:O   | 13:G:131:LYS:HD3 | 2.20                     | 0.42              |
| 16:J:7:ARG:HG2   | 16:J:101:SER:HB2 | 2.01                     | 0.42              |
| 17:K:93:ARG:O    | 17:K:97:ILE:HG12 | 2.20                     | 0.42              |
| 19:M:54:ASP:HA   | 19:M:57:ARG:NE   | 2.25                     | 0.42              |
| 22:P:46:LYS:HE2  | 22:P:46:LYS:HB2  | 1.79                     | 0.42              |
| 24:R:50:LYS:HA   | 24:R:53:ARG:HH12 | 1.85                     | 0.42              |
| 28:a:424:G:N3    | 28:a:425:G:H1'   | 2.34                     | 0.42              |
| 28:a:841:G:C4    | 28:a:842:U:C6    | 3.07                     | 0.42              |
| 28:a:1019:U:O2'  | 28:a:1020:A:H5'  | 2.20                     | 0.42              |
| 28:a:2293:G:H4'  | 41:n:98:GLN:OE1  | 2.19                     | 0.42              |
| 28:a:2404:U:H2'  | 28:a:2405:G:O4'  | 2.20                     | 0.42              |
| 30:c:124:ILE:O   | 30:c:125:LYS:HG3 | 2.20                     | 0.42              |
| 48:u:57:TYR:O    | 48:u:74:ALA:HB3  | 2.19                     | 0.42              |
| 1:0:20:PHE:CE2   | 28:a:2419:U:H1'  | 2.55                     | 0.42              |
| 4:3:25:VAL:O     | 4:3:34:LYS:HA    | 2.20                     | 0.42              |
| 7:A:609:A:H8     | 7:A:609:A:OP2    | 2.02                     | 0.42              |
| 7:A:1192:A:OP2   | 9:C:4:LYS:HG3    | 2.19                     | 0.42              |
| 8:B:115:LYS:HG3  | 8:B:116:ASP:N    | 2.35                     | 0.42              |
| 9:C:19:ASN:O     | 9:C:20:SER:OG    | 2.32                     | 0.42              |
| 10:D:99:ASP:OD2  | 10:D:115:ARG:HG2 | 2.20                     | 0.42              |
| 28:a:2355:G:H2'  | 28:a:2356:U:N1   | 2.35                     | 0.42              |
| 28:a:2514:U:H2'  | 28:a:2515:C:C6   | 2.55                     | 0.42              |
| 28:a:2647:U:H2'  | 28:a:2648:G:H8   | 1.85                     | 0.42              |
| 28:a:2742:G:H2'  | 28:a:2743:U:O4'  | 2.20                     | 0.42              |
| 29:b:24:G:N3     | 29:b:26:C:N4     | 2.68                     | 0.42              |
| 31:d:139:SER:O   | 31:d:139:SER:OG  | 2.34                     | 0.42              |
| 32:e:23:PHE:HE2  | 32:e:25:GLU:HG3  | 1.85                     | 0.42              |
| 38:k:135:ILE:O   | 38:k:140:GLY:N   | 2.37                     | 0.42              |
| 41:n:31:THR:HB   | 41:n:34:HIS:O    | 2.19                     | 0.42              |
| 48:u:25:LYS:HE2  | 48:u:41:GLU:O    | 2.20                     | 0.42              |
| 4:3:23:ILE:O     | 4:3:37:GLN:HG3   | 2.20                     | 0.41              |
| 7:A:1027:C:H2'   | 7:A:1028:C:C6    | 2.55                     | 0.41              |
| 8:B:165:ASP:HA   | 8:B:204:ASP:OD1  | 2.20                     | 0.41              |
| 9:C:62:LYS:N     | 9:C:62:LYS:HD3   | 2.34                     | 0.41              |
| 13:G:15:ASP:HA   | 13:G:16:PRO:HD3  | 1.83                     | 0.41              |
| 13:G:149:LYS:HD2 | 13:G:149:LYS:HA  | 1.87                     | 0.41              |
| 15:I:54:LEU:H    | 15:I:54:LEU:HG   | 1.53                     | 0.41              |
| 15:I:95:ARG:HD3  | 15:I:95:ARG:H    | 1.84                     | 0.41              |
| 18:L:89:D2T:H7   | 18:L:89:D2T:H4   | 1.91                     | 0.41              |
| 28:a:172:A:H2'   | 28:a:173:A:H8    | 1.85                     | 0.41              |
| 28:a:844:A:C2    | 28:a:935:C:C2    | 3.08                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:a:1027:A:N6   | 28:a:1126:A:C6    | 2.88                     | 0.41              |
| 28:a:2271:G:H5'  | 49:v:20:ARG:HD3   | 2.00                     | 0.41              |
| 28:a:2327:A:C6   | 28:a:2388:A:N1    | 2.88                     | 0.41              |
| 29:b:94:A:P      | 48:u:19:ARG:HH21  | 2.42                     | 0.41              |
| 29:b:112:G:H2'   | 29:b:113:C:C6     | 2.55                     | 0.41              |
| 34:g:4:VAL:O     | 34:g:69:ARG:HG2   | 2.20                     | 0.41              |
| 34:g:50:LEU:HD12 | 34:g:52:PHE:CZ    | 2.55                     | 0.41              |
| 35:h:12:LEU:O    | 35:h:12:LEU:HD13  | 2.20                     | 0.41              |
| 43:p:92:ARG:HA   | 43:p:95:LEU:HD12  | 2.00                     | 0.41              |
| 49:v:65:GLY:CA   | 49:v:85:GLU:H     | 2.32                     | 0.41              |
| 52:y:56:LYS:HB3  | 52:y:56:LYS:HE2   | 1.73                     | 0.41              |
| 1:0:38:LYS:C     | 1:0:46:HIS:HD2    | 2.28                     | 0.41              |
| 7:A:690:G:OP2    | 17:K:29:ASN:ND2   | 2.40                     | 0.41              |
| 7:A:1071:C:H2'   | 7:A:1072:G:C8     | 2.54                     | 0.41              |
| 7:A:1411:A:H2'   | 7:A:1412:C:C6     | 2.55                     | 0.41              |
| 9:C:90:VAL:O     | 9:C:94:ILE:HD12   | 2.19                     | 0.41              |
| 11:E:59:ALA:O    | 11:E:61:GLN:HG2   | 2.20                     | 0.41              |
| 16:J:51:VAL:HG11 | 20:N:84:VAL:HG21  | 2.02                     | 0.41              |
| 25:S:30:PRO:HD3  | 25:S:48:THR:HB    | 2.02                     | 0.41              |
| 28:a:270:A:C2    | 28:a:370:G:C4     | 3.08                     | 0.41              |
| 28:a:1023:U:C5   | 28:a:1024:G:C8    | 3.08                     | 0.41              |
| 28:a:1108:U:C4   | 28:a:1109:C:H5    | 2.39                     | 0.41              |
| 28:a:2047:C:H2'  | 28:a:2048:G:H8    | 1.85                     | 0.41              |
| 28:a:2243:U:H2'  | 28:a:2244:U:C6    | 2.55                     | 0.41              |
| 28:a:2557:G:H2'  | 28:a:2558:C:H6    | 1.85                     | 0.41              |
| 29:b:91:C:H3'    | 29:b:92:C:H6      | 1.85                     | 0.41              |
| 32:e:1:MET:SD    | 32:e:1:MET:N      | 2.81                     | 0.41              |
| 7:A:143:A:N1     | 7:A:220:G:O6      | 2.53                     | 0.41              |
| 7:A:259:G:C5     | 7:A:260:G:H1'     | 2.55                     | 0.41              |
| 7:A:373:A:N6     | 7:A:391:G:H1'     | 2.34                     | 0.41              |
| 7:A:1017:C:H5''  | 7:A:1017:C:C6     | 2.56                     | 0.41              |
| 9:C:40:ARG:NH1   | 20:N:92:GLU:HG3   | 2.35                     | 0.41              |
| 9:C:112:ASP:O    | 9:C:114:LYS:N     | 2.54                     | 0.41              |
| 12:F:29:ILE:HG12 | 12:F:34:GLY:HA3   | 2.02                     | 0.41              |
| 13:G:140:ASP:CB  | 13:G:143:ARG:HH21 | 2.33                     | 0.41              |
| 17:K:75:LYS:HD2  | 17:K:75:LYS:HA    | 1.73                     | 0.41              |
| 19:M:86:TYR:HD1  | 19:M:86:TYR:HA    | 1.80                     | 0.41              |
| 25:S:66:MET:O    | 25:S:66:MET:HG2   | 2.19                     | 0.41              |
| 28:a:86:G:N3     | 28:a:87:U:C5      | 2.88                     | 0.41              |
| 28:a:641:U:H3'   | 28:a:642:U:C6     | 2.55                     | 0.41              |
| 28:a:842:U:C2    | 28:a:843:G:C8     | 3.08                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:a:1862:G:C2   | 28:a:1863:G:N7    | 2.89                     | 0.41              |
| 28:a:1923:U:H2'  | 28:a:1924:C:C6    | 2.55                     | 0.41              |
| 33:f:52:ASN:ND2  | 33:f:147:ASP:OD2  | 2.49                     | 0.41              |
| 34:g:72:LEU:O    | 34:g:76:VAL:HG22  | 2.20                     | 0.41              |
| 44:q:48:LYS:HE3  | 44:q:48:LYS:HB3   | 1.84                     | 0.41              |
| 48:u:79:ARG:HA   | 48:u:87:GLN:N     | 2.34                     | 0.41              |
| 5:4:12:ILE:HG12  | 5:4:26:SER:OG     | 2.20                     | 0.41              |
| 7:A:131:A:N6     | 7:A:232:G:H21     | 2.18                     | 0.41              |
| 7:A:718:A:H2     | 24:R:38:LYS:NZ    | 2.17                     | 0.41              |
| 7:A:1080:A:OP2   | 11:E:50:TYR:OH    | 2.32                     | 0.41              |
| 10:D:64:ILE:HG22 | 10:D:65:TYR:CD1   | 2.55                     | 0.41              |
| 22:P:6:LEU:HD11  | 22:P:39:PHE:CD2   | 2.56                     | 0.41              |
| 28:a:6:A:H2'     | 28:a:7:G:C8       | 2.55                     | 0.41              |
| 28:a:1049:C:H5   | 28:a:1110:G:N2    | 2.19                     | 0.41              |
| 28:a:1126:A:H4'  | 28:a:1127:A:O4'   | 2.20                     | 0.41              |
| 28:a:2324:U:H5'' | 28:a:2326:C:OP2   | 2.20                     | 0.41              |
| 28:a:2343:U:HO2' | 28:a:2374:C:H4'   | 1.85                     | 0.41              |
| 28:a:2355:G:C2   | 28:a:2363:G:C6    | 3.08                     | 0.41              |
| 28:a:2419:U:N3   | 28:a:2420:C:C4    | 2.88                     | 0.41              |
| 29:b:33:G:O5'    | 29:b:33:G:H8      | 2.03                     | 0.41              |
| 32:e:125:SER:OG  | 32:e:126:VAL:N    | 2.54                     | 0.41              |
| 34:g:152:ARG:HG3 | 34:g:162:VAL:HG13 | 2.02                     | 0.41              |
| 35:h:14:SER:HB3  | 35:h:15:LEU:H     | 1.74                     | 0.41              |
| 37:j:58:LEU:HD12 | 37:j:86:LEU:HD13  | 2.00                     | 0.41              |
| 47:t:58:ILE:HD12 | 47:t:58:ILE:C     | 2.46                     | 0.41              |
| 2:1:4:THR:HG22   | 28:a:687:C:H1'    | 2.01                     | 0.41              |
| 3:2:17:THR:HA    | 28:a:629:G:OP2    | 2.20                     | 0.41              |
| 4:3:34:LYS:HB3   | 4:3:34:LYS:HE2    | 1.92                     | 0.41              |
| 7:A:183:C:H5'    | 7:A:184:C:OP1     | 2.20                     | 0.41              |
| 7:A:1059:C:H4'   | 20:N:85:ARG:HH21  | 1.82                     | 0.41              |
| 7:A:1264:A:N6    | 7:A:1274:G:H1'    | 2.33                     | 0.41              |
| 8:B:184:PHE:CB   | 8:B:198:PHE:HB2   | 2.47                     | 0.41              |
| 17:K:52:PHE:HA   | 17:K:56:ARG:NH1   | 2.35                     | 0.41              |
| 18:L:3:THR:OG1   | 18:L:6:GLN:HG3    | 2.20                     | 0.41              |
| 28:a:7:G:H4'     | 36:i:15:TRP:HZ2   | 1.85                     | 0.41              |
| 28:a:1432:G:H2'  | 28:a:1433:A:C8    | 2.55                     | 0.41              |
| 28:a:1486:U:H2'  | 28:a:1487:U:H6    | 1.85                     | 0.41              |
| 28:a:1570:A:H2'  | 28:a:1571:A:C8    | 2.55                     | 0.41              |
| 28:a:2295:C:O2'  | 28:a:2296:U:H5'   | 2.20                     | 0.41              |
| 28:a:2299:U:O5'  | 28:a:2299:U:H6    | 2.03                     | 0.41              |
| 28:a:2419:U:N3   | 28:a:2420:C:C5    | 2.89                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:a:2469:A:H4'   | 39:l:55:ARG:HD3   | 2.00                     | 0.41              |
| 28:a:2519:U:C4    | 28:a:2541:A:C6    | 3.08                     | 0.41              |
| 36:i:1:MET:CE     | 44:q:13:ARG:H     | 2.29                     | 0.41              |
| 7:A:473:A:H5''    | 22:P:76:LYS:NZ    | 2.36                     | 0.41              |
| 8:B:66:LYS:HD2    | 8:B:66:LYS:N      | 2.36                     | 0.41              |
| 9:C:140:ASN:OD1   | 9:C:143:ARG:NH1   | 2.53                     | 0.41              |
| 11:E:87:GLY:N     | 11:E:94:VAL:HG12  | 2.36                     | 0.41              |
| 15:I:52:LEU:H     | 15:I:52:LEU:HD12  | 1.84                     | 0.41              |
| 17:K:111:THR:HG22 | 17:K:112:ASP:H    | 1.85                     | 0.41              |
| 20:N:31:ILE:HD12  | 20:N:41:ARG:HE    | 1.86                     | 0.41              |
| 22:P:19:VAL:HG23  | 22:P:39:PHE:HB2   | 2.02                     | 0.41              |
| 25:S:25:SER:O     | 25:S:25:SER:OG    | 2.33                     | 0.41              |
| 28:a:639:U:H2'    | 28:a:640:C:C6     | 2.55                     | 0.41              |
| 28:a:934:U:H2'    | 28:a:935:C:C6     | 2.54                     | 0.41              |
| 28:a:1715:G:O2'   | 28:a:1743:G:O6    | 2.28                     | 0.41              |
| 28:a:2345:G:C2    | 28:a:2382:G:N7    | 2.89                     | 0.41              |
| 28:a:2365:G:H5'   | 49:v:58:THR:HG21  | 2.03                     | 0.41              |
| 29:b:22:U:O2      | 29:b:61:G:O6      | 2.39                     | 0.41              |
| 29:b:29:A:H2'     | 29:b:30:C:C6      | 2.55                     | 0.41              |
| 32:e:147:LEU:O    | 32:e:187:VAL:HG12 | 2.20                     | 0.41              |
| 33:f:117:LEU:O    | 33:f:178:ARG:HG2  | 2.20                     | 0.41              |
| 36:i:32:LEU:HD13  | 36:i:54:ILE:HD11  | 2.02                     | 0.41              |
| 39:l:36:VAL:HG13  | 48:u:82:TYR:O     | 2.20                     | 0.41              |
| 43:p:64:ARG:HD3   | 43:p:100:VAL:HG21 | 2.02                     | 0.41              |
| 43:p:83:LEU:HA    | 43:p:112:LYS:HZ2  | 1.85                     | 0.41              |
| 44:q:16:GLU:CD    | 44:q:16:GLU:H     | 2.28                     | 0.41              |
| 48:u:50:MET:HE2   | 48:u:50:MET:N     | 2.35                     | 0.41              |
| 1:0:26:ASN:ND2    | 1:0:29:THR:OG1    | 2.54                     | 0.41              |
| 7:A:1162:C:C2'    | 7:A:1163:C:H5'    | 2.50                     | 0.41              |
| 7:A:1458:G:C2     | 7:A:1459:G:C8     | 3.09                     | 0.41              |
| 9:C:100:GLN:HB3   | 9:C:102:ASN:OD1   | 2.20                     | 0.41              |
| 10:D:168:PRO:HB2  | 10:D:170:TRP:CE2  | 2.56                     | 0.41              |
| 11:E:41:ASP:OD1   | 11:E:41:ASP:C     | 2.63                     | 0.41              |
| 14:H:11:LEU:HD22  | 14:H:75:ILE:HG12  | 2.02                     | 0.41              |
| 19:M:98:ARG:HD3   | 19:M:99:GLY:N     | 2.36                     | 0.41              |
| 21:O:78:TYR:O     | 21:O:82:ILE:HG23  | 2.21                     | 0.41              |
| 25:S:10:PHE:CD1   | 25:S:11:ILE:HB    | 2.56                     | 0.41              |
| 25:S:64:ASP:HB3   | 25:S:65:GLU:H     | 1.74                     | 0.41              |
| 28:a:2044:C:H2'   | 28:a:2045:C:O4'   | 2.21                     | 0.41              |
| 28:a:2351:G:N2    | 28:a:2366:A:H5''  | 2.34                     | 0.41              |
| 28:a:2527:C:H3'   | 28:a:2528:U:C5    | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 29:b:92:C:P      | 48:u:18:ARG:HH22 | 2.34                     | 0.41              |
| 29:b:94:A:H5''   | 48:u:19:ARG:NH2  | 2.35                     | 0.41              |
| 31:d:46:ARG:NH2  | 31:d:86:GLU:O    | 2.54                     | 0.41              |
| 33:f:60:ILE:O    | 33:f:102:ARG:NH2 | 2.52                     | 0.41              |
| 36:i:102:GLU:HA  | 36:i:102:GLU:OE2 | 2.20                     | 0.41              |
| 39:l:112:LEU:O   | 39:l:115:GLU:HB3 | 2.21                     | 0.41              |
| 7:A:285:C:H2'    | 7:A:286:C:C6     | 2.56                     | 0.41              |
| 7:A:414:A:N6     | 7:A:431:A:N3     | 2.69                     | 0.41              |
| 7:A:1010:G:H1    | 7:A:1019:C:H42   | 1.69                     | 0.41              |
| 7:A:1013:G:O6    | 7:A:1017:C:H5'   | 2.20                     | 0.41              |
| 7:A:1037:C:H4'   | 7:A:1038:U:H5'   | 2.03                     | 0.41              |
| 7:A:1279:G:H5'   | 7:A:1280:A:H5'   | 2.02                     | 0.41              |
| 9:C:12:LEU:HD13  | 9:C:12:LEU:HA    | 1.91                     | 0.41              |
| 9:C:147:LYS:HB2  | 9:C:203:PHE:CE2  | 2.56                     | 0.41              |
| 10:D:183:LYS:N   | 10:D:183:LYS:HD2 | 2.35                     | 0.41              |
| 14:H:113:ASP:N   | 14:H:113:ASP:OD1 | 2.45                     | 0.41              |
| 19:M:113:ARG:HD3 | 19:M:113:ARG:N   | 2.31                     | 0.41              |
| 28:a:75:G:N3     | 28:a:75:G:H2'    | 2.36                     | 0.41              |
| 28:a:359:G:C5    | 28:a:360:U:C4    | 3.09                     | 0.41              |
| 28:a:635:C:O2'   | 28:a:639:U:H5'   | 2.20                     | 0.41              |
| 28:a:1866:A:C5   | 28:a:1867:G:H1'  | 2.55                     | 0.41              |
| 28:a:2801:G:H2'  | 28:a:2802:G:C8   | 2.55                     | 0.41              |
| 29:b:66:A:H2'    | 29:b:66:A:N3     | 2.35                     | 0.41              |
| 31:d:47:ALA:HB2  | 31:d:83:ARG:HD2  | 2.01                     | 0.41              |
| 33:f:78:LYS:HE2  | 33:f:78:LYS:HB2  | 1.91                     | 0.41              |
| 43:p:79:PHE:CE1  | 43:p:109:LEU:HB3 | 2.56                     | 0.41              |
| 3:2:32:ILE:HA    | 28:a:2420:C:OP2  | 2.21                     | 0.41              |
| 4:3:2:LYS:HB2    | 4:3:35:GLN:HG2   | 2.02                     | 0.41              |
| 5:4:34:LEU:HD12  | 5:4:34:LEU:HA    | 1.95                     | 0.41              |
| 5:4:41:HIS:NE2   | 33:f:114:PHE:HB3 | 2.36                     | 0.41              |
| 7:A:91:U:H5'     | 7:A:92:U:C6      | 2.56                     | 0.41              |
| 7:A:229:U:H2'    | 7:A:230:A:O4'    | 2.21                     | 0.41              |
| 7:A:378:G:O2'    | 7:A:379:C:H6     | 2.04                     | 0.41              |
| 7:A:490:U:C2     | 7:A:491:A:C8     | 3.08                     | 0.41              |
| 7:A:621:A:H2'    | 7:A:622:A:C8     | 2.56                     | 0.41              |
| 7:A:707:U:H4'    | 17:K:22:HIS:CD2  | 2.56                     | 0.41              |
| 7:A:877:G:HO2'   | 7:A:878:A:H8     | 1.68                     | 0.41              |
| 7:A:1149:U:O2'   | 7:A:1150:C:O5'   | 2.37                     | 0.41              |
| 7:A:1219:U:OP2   | 20:N:9:ARG:NH1   | 2.54                     | 0.41              |
| 7:A:1350:A:H5''  | 15:I:123:ARG:HB2 | 2.03                     | 0.41              |
| 7:A:1437:C:H2'   | 7:A:1438:A:H8    | 1.86                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:B:177:ASN:OD1  | 8:B:178:ASN:N     | 2.53                     | 0.41              |
| 10:D:8:LYS:HG3   | 10:D:9:LEU:N      | 2.36                     | 0.41              |
| 10:D:171:LEU:HA  | 10:D:181:THR:O    | 2.21                     | 0.41              |
| 12:F:25:TYR:HD1  | 12:F:25:TYR:HA    | 1.70                     | 0.41              |
| 12:F:42:TRP:CZ3  | 12:F:102:MET:HE2  | 2.56                     | 0.41              |
| 12:F:44:ARG:NH1  | 12:F:58:HIS:HD2   | 2.18                     | 0.41              |
| 12:F:68:GLN:OE1  | 12:F:68:GLN:N     | 2.54                     | 0.41              |
| 17:K:97:ILE:HD12 | 27:U:12:PHE:CE1   | 2.55                     | 0.41              |
| 19:M:33:ILE:HD11 | 19:M:59:GLU:O     | 2.21                     | 0.41              |
| 22:P:52:LEU:HG   | 22:P:75:ILE:HG22  | 2.03                     | 0.41              |
| 24:R:29:LEU:O    | 24:R:33:ILE:HG23  | 2.21                     | 0.41              |
| 28:a:274:C:H2'   | 28:a:275:C:O4'    | 2.20                     | 0.41              |
| 28:a:280:U:C4    | 28:a:361:G:N2     | 2.89                     | 0.41              |
| 28:a:356:G:H2'   | 28:a:357:C:C6     | 2.56                     | 0.41              |
| 28:a:633:A:N7    | 28:a:634:C:C2     | 2.89                     | 0.41              |
| 28:a:634:C:N4    | 28:a:635:C:N4     | 2.69                     | 0.41              |
| 28:a:937:C:C2    | 28:a:938:G:H1'    | 2.56                     | 0.41              |
| 28:a:938:G:N1    | 28:a:939:G:C5     | 2.89                     | 0.41              |
| 28:a:948:C:H1'   | 28:a:984:A:C8     | 2.56                     | 0.41              |
| 28:a:1036:G:O6   | 28:a:1119:U:C2    | 2.71                     | 0.41              |
| 28:a:1149:G:H2'  | 28:a:1150:C:C6    | 2.55                     | 0.41              |
| 28:a:1319:C:O2'  | 28:a:1320:C:H5'   | 2.21                     | 0.41              |
| 28:a:1880:U:N3   | 28:a:1881:C:C5    | 2.88                     | 0.41              |
| 28:a:2356:U:N3   | 28:a:2357:G:C8    | 2.89                     | 0.41              |
| 28:a:2567:G:H2'  | 28:a:2568:U:C6    | 2.56                     | 0.41              |
| 28:a:2741:A:C2'  | 28:a:2742:G:C8    | 2.99                     | 0.41              |
| 28:a:2747:G:C6   | 28:a:2756:U:OP1   | 2.73                     | 0.41              |
| 28:a:2897:U:H2'  | 28:a:2898:U:C6    | 2.56                     | 0.41              |
| 29:b:78:A:H62    | 29:b:98:G:H21     | 0.51                     | 0.41              |
| 31:d:51:THR:HA   | 31:d:80:TRP:CZ3   | 2.56                     | 0.41              |
| 33:f:29:PRO:HB2  | 33:f:169:LEU:HD22 | 2.02                     | 0.41              |
| 34:g:25:THR:HA   | 34:g:34:THR:HA    | 2.02                     | 0.41              |
| 34:g:54:PRO:HG3  | 34:g:62:TRP:CG    | 2.56                     | 0.41              |
| 34:g:118:PRO:HB2 | 34:g:121:ILE:HD13 | 2.03                     | 0.41              |
| 34:g:154:PRO:HA  | 34:g:160:LYS:O    | 2.20                     | 0.41              |
| 36:i:1:MET:SD    | 36:i:1:MET:C      | 3.04                     | 0.41              |
| 36:i:88:THR:OG1  | 36:i:91:GLU:OE2   | 2.28                     | 0.41              |
| 37:j:90:ASN:OD1  | 37:j:90:ASN:N     | 2.54                     | 0.41              |
| 41:n:31:THR:HG22 | 41:n:34:HIS:H     | 1.86                     | 0.41              |
| 43:p:79:PHE:HE1  | 43:p:109:LEU:C    | 2.29                     | 0.41              |
| 1:0:14:SER:N     | 1:0:48:ILE:O      | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:47:VAL:HG23   | 1:O:49:TYR:CE1    | 2.56                     | 0.41              |
| 7:A:1254:G:H22    | 7:A:1356:A:H4'    | 1.85                     | 0.41              |
| 7:A:1493:A:H3'    | 7:A:1494:A:C8     | 2.55                     | 0.41              |
| 8:B:13:GLY:HA2    | 8:B:16:PHE:HD2    | 1.85                     | 0.41              |
| 8:B:100:MET:HE2   | 8:B:100:MET:HB3   | 1.96                     | 0.41              |
| 17:K:97:ILE:CD1   | 27:U:16:LEU:HB3   | 2.51                     | 0.41              |
| 23:Q:29:VAL:CG2   | 23:Q:40:ARG:HH22  | 2.33                     | 0.41              |
| 26:T:28:MET:O     | 26:T:32:ILE:HG13  | 2.21                     | 0.41              |
| 28:a:2419:U:C4    | 28:a:2420:C:N4    | 2.89                     | 0.41              |
| 28:a:2849:U:H4'   | 28:a:2868:A:C2    | 2.56                     | 0.41              |
| 33:f:29:PRO:HG3   | 33:f:165:GLU:HB3  | 2.02                     | 0.41              |
| 40:m:24:MET:HE2   | 40:m:24:MET:HB2   | 1.91                     | 0.41              |
| 44:q:41:ILE:HD13  | 44:q:103:ALA:HB1  | 2.03                     | 0.41              |
| 47:t:7:ARG:C      | 47:t:8:ASP:OD1    | 2.64                     | 0.41              |
| 49:v:46:HIS:HB2   | 49:v:79:PHE:CE2   | 2.56                     | 0.41              |
| 7:A:61:G:H22      | 7:A:105:G:N2      | 2.18                     | 0.40              |
| 7:A:500:G:H5''    | 18:L:121:ARG:HH12 | 1.87                     | 0.40              |
| 7:A:836:G:OP1     | 24:R:51:TYR:OH    | 2.38                     | 0.40              |
| 7:A:1067:A:C6     | 7:A:1109:C:H5''   | 2.56                     | 0.40              |
| 9:C:107:ARG:NE    | 9:C:107:ARG:HA    | 2.37                     | 0.40              |
| 18:L:74:LEU:HD12  | 18:L:74:LEU:HA    | 1.85                     | 0.40              |
| 20:N:76:LYS:HG3   | 20:N:77:PHE:H     | 1.85                     | 0.40              |
| 26:T:79:LEU:HD13  | 26:T:79:LEU:HA    | 1.90                     | 0.40              |
| 28:a:2291:U:H4'   | 28:a:2379:G:H21   | 1.87                     | 0.40              |
| 28:a:2487:G:H2'   | 28:a:2488:G:C8    | 2.56                     | 0.40              |
| 28:a:2661:G:H8    | 28:a:2661:G:OP2   | 2.03                     | 0.40              |
| 28:a:2758:A:N3    | 34:g:35:ARG:CZ    | 2.84                     | 0.40              |
| 29:b:60:C:O5'     | 29:b:60:C:H6      | 2.04                     | 0.40              |
| 32:e:23:PHE:HB2   | 32:e:111:GLU:OE1  | 2.20                     | 0.40              |
| 32:e:119:ILE:O    | 32:e:119:ILE:HG13 | 2.21                     | 0.40              |
| 34:g:134:LYS:NZ   | 34:g:134:LYS:HB3  | 2.36                     | 0.40              |
| 36:i:124:VAL:HG12 | 36:i:125:TYR:N    | 2.36                     | 0.40              |
| 47:t:51:ALA:O     | 47:t:52:LEU:HD13  | 2.22                     | 0.40              |
| 48:u:83:LYS:C     | 48:u:85:LYS:H     | 2.29                     | 0.40              |
| 50:w:2:SER:HB2    | 50:w:3:ARG:H      | 1.59                     | 0.40              |
| 7:A:143:A:H2      | 7:A:220:G:H22     | 1.69                     | 0.40              |
| 7:A:465:A:N6      | 7:A:466:A:N3      | 2.70                     | 0.40              |
| 7:A:715:A:H2'     | 7:A:716:A:C8      | 2.57                     | 0.40              |
| 7:A:1134:C:H2'    | 7:A:1135:G:C8     | 2.55                     | 0.40              |
| 7:A:1187:G:OP1    | 15:I:115:LYS:NZ   | 2.30                     | 0.40              |
| 10:D:56:ARG:HA    | 10:D:56:ARG:HD3   | 1.72                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:G:63:GLU:HA   | 13:G:66:LEU:CD2   | 2.51                     | 0.40              |
| 15:I:90:TYR:C    | 15:I:90:TYR:CD2   | 3.00                     | 0.40              |
| 16:J:37:ARG:HD3  | 16:J:37:ARG:HA    | 1.76                     | 0.40              |
| 19:M:18:ALA:HB1  | 19:M:19:LEU:HD22  | 2.03                     | 0.40              |
| 21:O:17:ARG:HE   | 21:O:17:ARG:HB3   | 1.55                     | 0.40              |
| 28:a:627:A:H2    | 28:a:636:G:H2'    | 1.86                     | 0.40              |
| 28:a:851:C:H2'   | 28:a:852:U:H6     | 1.86                     | 0.40              |
| 28:a:1419:A:O2'  | 28:a:1421:G:N7    | 2.49                     | 0.40              |
| 28:a:1583:A:HO2' | 28:a:1585:C:N4    | 2.08                     | 0.40              |
| 28:a:2323:G:H2'  | 28:a:2324:U:O4'   | 2.21                     | 0.40              |
| 28:a:2537:U:H2'  | 28:a:2538:C:H6    | 1.86                     | 0.40              |
| 30:c:175:ARG:NH1 | 30:c:181:MET:HE1  | 2.36                     | 0.40              |
| 31:d:17:GLU:CD   | 31:d:17:GLU:N     | 2.79                     | 0.40              |
| 33:f:26:MET:N    | 33:f:26:MET:SD    | 2.93                     | 0.40              |
| 41:n:7:ARG:HG2   | 41:n:96:GLY:HA3   | 2.03                     | 0.40              |
| 49:v:37:ILE:HG22 | 49:v:38:VAL:HG13  | 2.01                     | 0.40              |
| 2:1:1:MET:HE3    | 2:1:1:MET:H1      | 1.85                     | 0.40              |
| 4:3:25:VAL:N     | 4:3:35:GLN:O      | 2.46                     | 0.40              |
| 7:A:22:G:O2'     | 7:A:885:G:H8      | 2.04                     | 0.40              |
| 7:A:411:A:H5''   | 7:A:411:A:H8      | 1.87                     | 0.40              |
| 7:A:1002:A:H2'   | 7:A:1002:A:N3     | 2.36                     | 0.40              |
| 7:A:1350:A:P     | 15:I:121:ALA:HB3  | 2.61                     | 0.40              |
| 12:F:90:MET:SD   | 12:F:91:ARG:N     | 2.94                     | 0.40              |
| 16:J:6:ILE:HG22  | 16:J:102:LEU:HA   | 2.04                     | 0.40              |
| 16:J:39:PRO:HA   | 16:J:73:LEU:O     | 2.22                     | 0.40              |
| 19:M:56:LEU:C    | 19:M:58:ASP:H     | 2.29                     | 0.40              |
| 27:U:66:ARG:HD3  | 27:U:67:ARG:HH12  | 1.87                     | 0.40              |
| 28:a:269:C:C5    | 28:a:424:G:N1     | 2.90                     | 0.40              |
| 28:a:897:C:H2'   | 28:a:898:C:C6     | 2.55                     | 0.40              |
| 28:a:2273:A:H2'  | 28:a:2274:A:C8    | 2.57                     | 0.40              |
| 31:d:29:VAL:O    | 31:d:185:ASN:HB3  | 2.21                     | 0.40              |
| 39:l:126:ILE:H   | 39:l:126:ILE:HG13 | 1.83                     | 0.40              |
| 41:n:64:TYR:HD1  | 41:n:65:THR:H     | 1.69                     | 0.40              |
| 43:p:61:TRP:CZ2  | 43:p:93:LYS:HB2   | 2.56                     | 0.40              |
| 44:q:4:VAL:HG12  | 44:q:5:PHE:N      | 2.36                     | 0.40              |
| 47:t:39:ILE:HD13 | 47:t:39:ILE:HA    | 1.85                     | 0.40              |
| 48:u:45:ASP:O    | 48:u:49:ASN:ND2   | 2.54                     | 0.40              |
| 48:u:72:VAL:HA   | 48:u:92:VAL:O     | 2.21                     | 0.40              |
| 7:A:86:G:OP2     | 7:A:86:G:H3'      | 2.22                     | 0.40              |
| 7:A:462:G:H3'    | 7:A:463:C:C6      | 2.56                     | 0.40              |
| 7:A:1012:G:H3'   | 7:A:1014:A:O3'    | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:28:LYS:N      | 8:B:29:PRO:HD2    | 2.37                     | 0.40              |
| 9:C:37:PHE:CE2    | 20:N:66:GLN:HG2   | 2.56                     | 0.40              |
| 10:D:35:GLU:HB3   | 10:D:36:GLN:H     | 1.57                     | 0.40              |
| 10:D:164:GLN:O    | 10:D:165:ARG:HG3  | 2.21                     | 0.40              |
| 12:F:53:LYS:HE2   | 12:F:53:LYS:HB2   | 1.61                     | 0.40              |
| 17:K:84:VAL:HB    | 17:K:110:ILE:HG13 | 2.03                     | 0.40              |
| 19:M:3:ARG:HB3    | 19:M:54:ASP:CG    | 2.46                     | 0.40              |
| 28:a:660:C:C2     | 28:a:661:A:C5     | 3.09                     | 0.40              |
| 28:a:1183:U:H4'   | 52:y:30:ARG:HD2   | 2.03                     | 0.40              |
| 28:a:2455:G:H2'   | 28:a:2456:C:C6    | 2.57                     | 0.40              |
| 28:a:2488:G:H2'   | 28:a:2489:U:C6    | 2.56                     | 0.40              |
| 28:a:2741:A:C2'   | 28:a:2742:G:H5'   | 2.51                     | 0.40              |
| 33:f:35:THR:C     | 33:f:36:LEU:HD13  | 2.47                     | 0.40              |
| 33:f:170:LEU:HD13 | 33:f:175:PHE:CE2  | 2.56                     | 0.40              |
| 34:g:22:GLN:NE2   | 34:g:39:ASP:O     | 2.54                     | 0.40              |
| 34:g:44:LYS:CG    | 34:g:45:HIS:H     | 2.33                     | 0.40              |
| 34:g:89:LEU:HB2   | 34:g:94:TYR:HD2   | 1.87                     | 0.40              |
| 34:g:103:ILE:N    | 34:g:115:HIS:O    | 2.39                     | 0.40              |
| 37:j:113:MET:H    | 37:j:113:MET:HE3  | 1.86                     | 0.40              |
| 43:p:95:LEU:O     | 43:p:98:ILE:HB    | 2.22                     | 0.40              |
| 43:p:108:ALA:HB2  | 44:q:47:VAL:HG21  | 2.03                     | 0.40              |
| 44:q:38:VAL:HG22  | 44:q:59:ILE:HD11  | 2.04                     | 0.40              |
| 48:u:26:PHE:CE2   | 48:u:86:LEU:HB2   | 2.57                     | 0.40              |
| 5:4:9:TYR:HB3     | 5:4:25:ARG:NE     | 2.36                     | 0.40              |
| 7:A:524:G:H2'     | 7:A:525:C:C6      | 2.57                     | 0.40              |
| 9:C:167:TRP:CZ3   | 9:C:169:ARG:HG3   | 2.55                     | 0.40              |
| 10:D:189:SER:C    | 10:D:191:LEU:H    | 2.30                     | 0.40              |
| 12:F:15:SER:HB2   | 12:F:44:ARG:HH22  | 1.87                     | 0.40              |
| 14:H:55:THR:O     | 14:H:56:LYS:HG3   | 2.22                     | 0.40              |
| 15:I:46:MET:HE3   | 15:I:46:MET:HB3   | 1.81                     | 0.40              |
| 16:J:87:LEU:HA    | 16:J:90:LEU:HD23  | 2.03                     | 0.40              |
| 19:M:57:ARG:O     | 19:M:59:GLU:N     | 2.54                     | 0.40              |
| 28:a:96:C:H2'     | 28:a:97:C:C6      | 2.56                     | 0.40              |
| 28:a:984:A:H2'    | 28:a:984:A:N3     | 2.37                     | 0.40              |
| 28:a:1028:A:N3    | 28:a:2487:G:H4'   | 2.36                     | 0.40              |
| 28:a:1029:A:H2'   | 28:a:1030:C:H6    | 1.86                     | 0.40              |
| 28:a:1418:G:H2'   | 28:a:1419:A:H5''  | 2.03                     | 0.40              |
| 28:a:1790:C:H2'   | 28:a:1791:A:N7    | 2.36                     | 0.40              |
| 28:a:2747:G:N2    | 28:a:2757:A:H62   | 2.20                     | 0.40              |
| 28:a:2757:A:H2    | 34:g:64:GLN:HA    | 1.87                     | 0.40              |
| 33:f:105:THR:O    | 33:f:106:ILE:HD13 | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:g:44:LYS:HD2  | 34:g:51:THR:N    | 2.33                     | 0.40              |
| 34:g:67:THR:O    | 34:g:71:LEU:HG   | 2.21                     | 0.40              |
| 36:i:125:TYR:HB2 | 36:i:130:HIS:CD2 | 2.55                     | 0.40              |
| 43:p:57:PHE:HD2  | 43:p:61:TRP:HE1  | 1.68                     | 0.40              |
| 43:p:82:GLY:O    | 43:p:86:ALA:HB3  | 2.22                     | 0.40              |
| 45:r:23:LEU:HD12 | 45:r:23:LEU:HA   | 1.91                     | 0.40              |
| 48:u:4:ILE:HD13  | 48:u:4:ILE:HA    | 1.97                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | 0     | 49/55 (89%)   | 47 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 2   | 1     | 44/46 (96%)   | 43 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 3   | 2     | 62/65 (95%)   | 56 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 4   | 3     | 36/38 (95%)   | 30 (83%)  | 6 (17%)  | 0        | 100         | 100 |
| 5   | 4     | 56/70 (80%)   | 49 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 8   | B     | 222/241 (92%) | 196 (88%) | 24 (11%) | 2 (1%)   | 14          | 48  |
| 9   | C     | 204/233 (88%) | 159 (78%) | 40 (20%) | 5 (2%)   | 4           | 23  |
| 10  | D     | 203/206 (98%) | 150 (74%) | 41 (20%) | 12 (6%)  | 1           | 7   |
| 11  | E     | 154/167 (92%) | 129 (84%) | 24 (16%) | 1 (1%)   | 21          | 56  |
| 12  | F     | 101/135 (75%) | 91 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 13  | G     | 151/179 (84%) | 130 (86%) | 21 (14%) | 0        | 100         | 100 |
| 14  | H     | 127/130 (98%) | 106 (84%) | 21 (16%) | 0        | 100         | 100 |
| 15  | I     | 125/130 (96%) | 103 (82%) | 22 (18%) | 0        | 100         | 100 |
| 16  | J     | 96/103 (93%)  | 81 (84%)  | 12 (12%) | 3 (3%)   | 3           | 19  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 17  | K     | 113/129 (88%) | 106 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 18  | L     | 119/124 (96%) | 102 (86%) | 17 (14%) | 0        | 100         | 100 |
| 19  | M     | 113/118 (96%) | 81 (72%)  | 30 (26%) | 2 (2%)   | 6           | 31  |
| 20  | N     | 98/101 (97%)  | 88 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 21  | O     | 86/89 (97%)   | 81 (94%)  | 3 (4%)   | 2 (2%)   | 5           | 25  |
| 22  | P     | 79/82 (96%)   | 59 (75%)  | 18 (23%) | 2 (2%)   | 4           | 23  |
| 23  | Q     | 77/84 (92%)   | 67 (87%)  | 10 (13%) | 0        | 100         | 100 |
| 24  | R     | 64/75 (85%)   | 55 (86%)  | 9 (14%)  | 0        | 100         | 100 |
| 25  | S     | 82/92 (89%)   | 57 (70%)  | 23 (28%) | 2 (2%)   | 4           | 24  |
| 26  | T     | 84/87 (97%)   | 83 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 27  | U     | 68/71 (96%)   | 63 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 30  | c     | 269/273 (98%) | 259 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 31  | d     | 206/209 (99%) | 189 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 32  | e     | 199/201 (99%) | 190 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 33  | f     | 175/179 (98%) | 158 (90%) | 17 (10%) | 0        | 100         | 100 |
| 34  | g     | 174/177 (98%) | 150 (86%) | 23 (13%) | 1 (1%)   | 21          | 56  |
| 35  | h     | 39/149 (26%)  | 34 (87%)  | 5 (13%)  | 0        | 100         | 100 |
| 36  | i     | 140/142 (99%) | 131 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 37  | j     | 121/123 (98%) | 117 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 38  | k     | 142/144 (99%) | 135 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 39  | l     | 132/136 (97%) | 127 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | m     | 116/127 (91%) | 108 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 41  | n     | 114/117 (97%) | 107 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 42  | o     | 112/115 (97%) | 109 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 43  | p     | 115/118 (98%) | 106 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 44  | q     | 101/103 (98%) | 89 (88%)  | 12 (12%) | 0        | 100         | 100 |
| 45  | r     | 108/110 (98%) | 105 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 46  | s     | 91/100 (91%)  | 83 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 47  | t     | 100/104 (96%) | 92 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 48  | u     | 92/94 (98%)   | 83 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 49  | v     | 76/85 (89%)   | 65 (86%)  | 11 (14%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 50  | w     | 75/78 (96%)     | 74 (99%)   | 1 (1%)    | 0        | 100         | 100 |
| 51  | x     | 60/63 (95%)     | 58 (97%)   | 2 (3%)    | 0        | 100         | 100 |
| 52  | y     | 56/59 (95%)     | 55 (98%)   | 1 (2%)    | 0        | 100         | 100 |
| 53  | z     | 54/57 (95%)     | 54 (100%)  | 0         | 0        | 100         | 100 |
| All | All   | 5480/5913 (93%) | 4890 (89%) | 558 (10%) | 32 (1%)  | 23          | 56  |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 154 | MET  |
| 9   | C     | 26  | THR  |
| 10  | D     | 34  | ILE  |
| 10  | D     | 36  | GLN  |
| 10  | D     | 40  | GLN  |
| 10  | D     | 45  | LYS  |
| 19  | M     | 13  | LYS  |
| 22  | P     | 16  | PHE  |
| 9   | C     | 82  | GLU  |
| 10  | D     | 27  | ALA  |
| 10  | D     | 44  | ARG  |
| 10  | D     | 123 | ILE  |
| 19  | M     | 42  | ASP  |
| 9   | C     | 3   | GLN  |
| 10  | D     | 35  | GLU  |
| 10  | D     | 165 | ARG  |
| 21  | O     | 18  | ASP  |
| 25  | S     | 12  | ASP  |
| 34  | g     | 47  | ASP  |
| 16  | J     | 54  | SER  |
| 21  | O     | 17  | ARG  |
| 8   | B     | 74  | ARG  |
| 9   | C     | 60  | PRO  |
| 9   | C     | 196 | ILE  |
| 10  | D     | 43  | ALA  |
| 10  | D     | 85  | ASN  |
| 10  | D     | 129 | VAL  |
| 11  | E     | 90  | THR  |
| 16  | J     | 78  | GLU  |
| 22  | P     | 42  | ILE  |
| 16  | J     | 57  | VAL  |
| 25  | S     | 29  | LYS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 1   | 0     | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 45          | 74  |
| 2   | 1     | 38/38 (100%)  | 38 (100%) | 0        | 100         | 100 |
| 3   | 2     | 51/52 (98%)   | 47 (92%)  | 4 (8%)   | 11          | 39  |
| 4   | 3     | 34/34 (100%)  | 30 (88%)  | 4 (12%)  | 5           | 22  |
| 5   | 4     | 55/62 (89%)   | 53 (96%)  | 2 (4%)   | 31          | 65  |
| 8   | B     | 186/199 (94%) | 169 (91%) | 17 (9%)  | 9           | 33  |
| 9   | C     | 170/190 (90%) | 155 (91%) | 15 (9%)  | 9           | 35  |
| 10  | D     | 171/173 (99%) | 152 (89%) | 19 (11%) | 6           | 25  |
| 11  | E     | 119/126 (94%) | 108 (91%) | 11 (9%)  | 8           | 33  |
| 12  | F     | 90/116 (78%)  | 83 (92%)  | 7 (8%)   | 11          | 39  |
| 13  | G     | 126/147 (86%) | 112 (89%) | 14 (11%) | 6           | 25  |
| 14  | H     | 104/105 (99%) | 99 (95%)  | 5 (5%)   | 23          | 57  |
| 15  | I     | 105/107 (98%) | 98 (93%)  | 7 (7%)   | 15          | 46  |
| 16  | J     | 86/90 (96%)   | 73 (85%)  | 13 (15%) | 3           | 14  |
| 17  | K     | 89/98 (91%)   | 87 (98%)  | 2 (2%)   | 45          | 74  |
| 18  | L     | 102/103 (99%) | 87 (85%)  | 15 (15%) | 3           | 15  |
| 19  | M     | 93/96 (97%)   | 86 (92%)  | 7 (8%)   | 12          | 41  |
| 20  | N     | 83/84 (99%)   | 77 (93%)  | 6 (7%)   | 13          | 43  |
| 21  | O     | 76/77 (99%)   | 68 (90%)  | 8 (10%)  | 6           | 27  |
| 22  | P     | 65/65 (100%)  | 60 (92%)  | 5 (8%)   | 12          | 40  |
| 23  | Q     | 73/78 (94%)   | 61 (84%)  | 12 (16%) | 2           | 12  |
| 24  | R     | 57/65 (88%)   | 56 (98%)  | 1 (2%)   | 51          | 77  |
| 25  | S     | 72/79 (91%)   | 59 (82%)  | 13 (18%) | 2           | 9   |
| 26  | T     | 65/66 (98%)   | 61 (94%)  | 4 (6%)   | 16          | 49  |
| 27  | U     | 60/61 (98%)   | 58 (97%)  | 2 (3%)   | 33          | 67  |
| 30  | c     | 216/218 (99%) | 204 (94%) | 12 (6%)  | 19          | 52  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 31  | d     | 163/163 (100%)  | 152 (93%)  | 11 (7%)  | 15          | 46  |
| 32  | e     | 165/165 (100%)  | 157 (95%)  | 8 (5%)   | 23          | 57  |
| 33  | f     | 148/150 (99%)   | 142 (96%)  | 6 (4%)   | 27          | 61  |
| 34  | g     | 137/138 (99%)   | 121 (88%)  | 16 (12%) | 5           | 23  |
| 35  | h     | 32/114 (28%)    | 32 (100%)  | 0        | 100         | 100 |
| 36  | i     | 116/116 (100%)  | 109 (94%)  | 7 (6%)   | 17          | 50  |
| 37  | j     | 104/104 (100%)  | 96 (92%)   | 8 (8%)   | 12          | 40  |
| 38  | k     | 103/103 (100%)  | 98 (95%)   | 5 (5%)   | 22          | 56  |
| 39  | l     | 107/107 (100%)  | 103 (96%)  | 4 (4%)   | 30          | 64  |
| 40  | m     | 98/103 (95%)    | 93 (95%)   | 5 (5%)   | 21          | 55  |
| 41  | n     | 86/87 (99%)     | 80 (93%)   | 6 (7%)   | 14          | 44  |
| 42  | o     | 99/100 (99%)    | 93 (94%)   | 6 (6%)   | 17          | 49  |
| 43  | p     | 89/90 (99%)     | 81 (91%)   | 8 (9%)   | 9           | 34  |
| 44  | q     | 84/84 (100%)    | 80 (95%)   | 4 (5%)   | 23          | 57  |
| 45  | r     | 93/93 (100%)    | 90 (97%)   | 3 (3%)   | 34          | 67  |
| 46  | s     | 80/84 (95%)     | 73 (91%)   | 7 (9%)   | 9           | 35  |
| 47  | t     | 83/85 (98%)     | 77 (93%)   | 6 (7%)   | 13          | 43  |
| 48  | u     | 78/78 (100%)    | 73 (94%)   | 5 (6%)   | 16          | 48  |
| 49  | v     | 58/63 (92%)     | 53 (91%)   | 5 (9%)   | 10          | 36  |
| 50  | w     | 67/68 (98%)     | 59 (88%)   | 8 (12%)  | 5           | 22  |
| 51  | x     | 54/55 (98%)     | 51 (94%)   | 3 (6%)   | 19          | 52  |
| 52  | y     | 48/49 (98%)     | 46 (96%)   | 2 (4%)   | 26          | 61  |
| 53  | z     | 47/48 (98%)     | 45 (96%)   | 2 (4%)   | 26          | 60  |
| All | All   | 4571/4825 (95%) | 4230 (92%) | 341 (8%) | 14          | 41  |

All (341) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 35  | GLU  |
| 3   | 2     | 6   | THR  |
| 3   | 2     | 29  | LEU  |
| 3   | 2     | 32  | ILE  |
| 3   | 2     | 38  | THR  |
| 4   | 3     | 16  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 17  | VAL  |
| 4   | 3     | 26  | ILE  |
| 4   | 3     | 28  | SER  |
| 5   | 4     | 6   | HIS  |
| 5   | 4     | 36  | VAL  |
| 8   | B     | 14  | VAL  |
| 8   | B     | 38  | VAL  |
| 8   | B     | 47  | VAL  |
| 8   | B     | 60  | ILE  |
| 8   | B     | 64  | LYS  |
| 8   | B     | 88  | ASP  |
| 8   | B     | 92  | VAL  |
| 8   | B     | 101 | LEU  |
| 8   | B     | 130 | THR  |
| 8   | B     | 140 | GLU  |
| 8   | B     | 159 | ASP  |
| 8   | B     | 163 | VAL  |
| 8   | B     | 183 | VAL  |
| 8   | B     | 191 | SER  |
| 8   | B     | 197 | ASP  |
| 8   | B     | 207 | ILE  |
| 8   | B     | 223 | GLU  |
| 9   | C     | 12  | LEU  |
| 9   | C     | 14  | ILE  |
| 9   | C     | 22  | TRP  |
| 9   | C     | 27  | LYS  |
| 9   | C     | 33  | LEU  |
| 9   | C     | 57  | ILE  |
| 9   | C     | 63  | SER  |
| 9   | C     | 67  | THR  |
| 9   | C     | 69  | HIS  |
| 9   | C     | 112 | ASP  |
| 9   | C     | 176 | HIS  |
| 9   | C     | 177 | THR  |
| 9   | C     | 183 | ASP  |
| 9   | C     | 187 | SER  |
| 9   | C     | 195 | VAL  |
| 10  | D     | 12  | SER  |
| 10  | D     | 22  | LYS  |
| 10  | D     | 25  | VAL  |
| 10  | D     | 26  | ARG  |
| 10  | D     | 31  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | D     | 33  | LYS  |
| 10  | D     | 35  | GLU  |
| 10  | D     | 36  | GLN  |
| 10  | D     | 40  | GLN  |
| 10  | D     | 41  | HIS  |
| 10  | D     | 45  | LYS  |
| 10  | D     | 47  | ARG  |
| 10  | D     | 62  | ARG  |
| 10  | D     | 117 | LEU  |
| 10  | D     | 119 | SER  |
| 10  | D     | 185 | LYS  |
| 10  | D     | 187 | GLU  |
| 10  | D     | 188 | ARG  |
| 10  | D     | 195 | ILE  |
| 11  | E     | 21  | VAL  |
| 11  | E     | 30  | ILE  |
| 11  | E     | 39  | VAL  |
| 11  | E     | 76  | LEU  |
| 11  | E     | 100 | SER  |
| 11  | E     | 103 | THR  |
| 11  | E     | 111 | MET  |
| 11  | E     | 112 | ARG  |
| 11  | E     | 132 | ASN  |
| 11  | E     | 142 | ASP  |
| 11  | E     | 156 | LYS  |
| 12  | F     | 22  | ILE  |
| 12  | F     | 39  | LEU  |
| 12  | F     | 60  | VAL  |
| 12  | F     | 61  | LEU  |
| 12  | F     | 62  | MET  |
| 12  | F     | 96  | VAL  |
| 12  | F     | 103 | VAL  |
| 13  | G     | 12  | ILE  |
| 13  | G     | 17  | LYS  |
| 13  | G     | 29  | ILE  |
| 13  | G     | 42  | ILE  |
| 13  | G     | 45  | SER  |
| 13  | G     | 47  | LEU  |
| 13  | G     | 49  | THR  |
| 13  | G     | 66  | LEU  |
| 13  | G     | 70  | ARG  |
| 13  | G     | 72  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | G     | 77  | SER  |
| 13  | G     | 87  | VAL  |
| 13  | G     | 94  | VAL  |
| 13  | G     | 138 | ARG  |
| 14  | H     | 2   | SER  |
| 14  | H     | 40  | LEU  |
| 14  | H     | 41  | LYS  |
| 14  | H     | 64  | LYS  |
| 14  | H     | 101 | ILE  |
| 15  | I     | 11  | ARG  |
| 15  | I     | 28  | ILE  |
| 15  | I     | 54  | LEU  |
| 15  | I     | 72  | ILE  |
| 15  | I     | 93  | SER  |
| 15  | I     | 110 | GLN  |
| 15  | I     | 114 | LYS  |
| 16  | J     | 17  | LEU  |
| 16  | J     | 28  | THR  |
| 16  | J     | 40  | ILE  |
| 16  | J     | 63  | ASP  |
| 16  | J     | 64  | GLN  |
| 16  | J     | 70  | HIS  |
| 16  | J     | 75  | ASP  |
| 16  | J     | 76  | ILE  |
| 16  | J     | 77  | VAL  |
| 16  | J     | 80  | THR  |
| 16  | J     | 81  | GLU  |
| 16  | J     | 85  | ASP  |
| 16  | J     | 100 | ILE  |
| 17  | K     | 33  | THR  |
| 17  | K     | 81  | ASN  |
| 18  | L     | 8   | VAL  |
| 18  | L     | 18  | LYS  |
| 18  | L     | 35  | THR  |
| 18  | L     | 39  | THR  |
| 18  | L     | 41  | THR  |
| 18  | L     | 47  | SER  |
| 18  | L     | 51  | LYS  |
| 18  | L     | 77  | HIS  |
| 18  | L     | 79  | VAL  |
| 18  | L     | 93  | VAL  |
| 18  | L     | 94  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | L     | 107 | VAL  |
| 18  | L     | 108 | LYS  |
| 18  | L     | 111 | LYS  |
| 18  | L     | 112 | GLN  |
| 19  | M     | 4   | ILE  |
| 19  | M     | 14  | HIS  |
| 19  | M     | 48  | LEU  |
| 19  | M     | 54  | ASP  |
| 19  | M     | 65  | VAL  |
| 19  | M     | 85  | CYS  |
| 19  | M     | 113 | ARG  |
| 20  | N     | 4   | GLN  |
| 20  | N     | 39  | GLU  |
| 20  | N     | 45  | VAL  |
| 20  | N     | 69  | ARG  |
| 20  | N     | 90  | ARG  |
| 20  | N     | 100 | SER  |
| 21  | O     | 14  | GLU  |
| 21  | O     | 18  | ASP  |
| 21  | O     | 20  | ASN  |
| 21  | O     | 21  | ASP  |
| 21  | O     | 27  | VAL  |
| 21  | O     | 52  | SER  |
| 21  | O     | 67  | LEU  |
| 21  | O     | 77  | ARG  |
| 22  | P     | 12  | LYS  |
| 22  | P     | 31  | ARG  |
| 22  | P     | 61  | VAL  |
| 22  | P     | 71  | VAL  |
| 22  | P     | 76  | LYS  |
| 23  | Q     | 27  | ARG  |
| 23  | Q     | 29  | VAL  |
| 23  | Q     | 30  | LYS  |
| 23  | Q     | 40  | ARG  |
| 23  | Q     | 41  | THR  |
| 23  | Q     | 42  | THR  |
| 23  | Q     | 51  | ASN  |
| 23  | Q     | 52  | GLU  |
| 23  | Q     | 55  | ILE  |
| 23  | Q     | 57  | ASP  |
| 23  | Q     | 61  | ILE  |
| 23  | Q     | 70  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | R     | 28  | THR  |
| 25  | S     | 13  | LEU  |
| 25  | S     | 25  | SER  |
| 25  | S     | 34  | TRP  |
| 25  | S     | 38  | SER  |
| 25  | S     | 39  | THR  |
| 25  | S     | 40  | ILE  |
| 25  | S     | 45  | ILE  |
| 25  | S     | 51  | VAL  |
| 25  | S     | 56  | GLN  |
| 25  | S     | 63  | THR  |
| 25  | S     | 66  | MET  |
| 25  | S     | 67  | VAL  |
| 25  | S     | 83  | HIS  |
| 26  | T     | 6   | SER  |
| 26  | T     | 23  | SER  |
| 26  | T     | 36  | TYR  |
| 26  | T     | 79  | LEU  |
| 27  | U     | 6   | VAL  |
| 27  | U     | 13  | ASP  |
| 30  | c     | 10  | SER  |
| 30  | c     | 35  | GLU  |
| 30  | c     | 69  | ARG  |
| 30  | c     | 78  | VAL  |
| 30  | c     | 90  | ASN  |
| 30  | c     | 129 | THR  |
| 30  | c     | 139 | SER  |
| 30  | c     | 140 | THR  |
| 30  | c     | 157 | SER  |
| 30  | c     | 164 | ILE  |
| 30  | c     | 194 | GLU  |
| 30  | c     | 204 | VAL  |
| 31  | d     | 14  | ILE  |
| 31  | d     | 24  | VAL  |
| 31  | d     | 29  | VAL  |
| 31  | d     | 51  | THR  |
| 31  | d     | 79  | LEU  |
| 31  | d     | 94  | GLN  |
| 31  | d     | 121 | THR  |
| 31  | d     | 131 | ASP  |
| 31  | d     | 137 | SER  |
| 31  | d     | 193 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | d     | 199 | SER  |
| 32  | e     | 14  | VAL  |
| 32  | e     | 43  | THR  |
| 32  | e     | 75  | SER  |
| 32  | e     | 105 | LEU  |
| 32  | e     | 116 | ASP  |
| 32  | e     | 119 | ILE  |
| 32  | e     | 121 | VAL  |
| 32  | e     | 150 | THR  |
| 33  | f     | 5   | HIS  |
| 33  | f     | 36  | LEU  |
| 33  | f     | 89  | VAL  |
| 33  | f     | 108 | VAL  |
| 33  | f     | 130 | MET  |
| 33  | f     | 132 | VAL  |
| 34  | g     | 4   | VAL  |
| 34  | g     | 9   | VAL  |
| 34  | g     | 15  | VAL  |
| 34  | g     | 20  | ASN  |
| 34  | g     | 24  | ILE  |
| 34  | g     | 25  | THR  |
| 34  | g     | 44  | LYS  |
| 34  | g     | 60  | ASP  |
| 34  | g     | 67  | THR  |
| 34  | g     | 89  | LEU  |
| 34  | g     | 122 | THR  |
| 34  | g     | 125 | CYS  |
| 34  | g     | 127 | THR  |
| 34  | g     | 134 | LYS  |
| 34  | g     | 140 | VAL  |
| 34  | g     | 157 | TYR  |
| 36  | i     | 45  | THR  |
| 36  | i     | 53  | TYR  |
| 36  | i     | 54  | ILE  |
| 36  | i     | 64  | VAL  |
| 36  | i     | 65  | THR  |
| 36  | i     | 131 | ASN  |
| 36  | i     | 139 | VAL  |
| 37  | j     | 8   | LEU  |
| 37  | j     | 20  | MET  |
| 37  | j     | 28  | SER  |
| 37  | j     | 63  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | j     | 69  | VAL  |
| 37  | j     | 76  | VAL  |
| 37  | j     | 91  | SER  |
| 37  | j     | 110 | GLU  |
| 38  | k     | 13  | LYS  |
| 38  | k     | 23  | ILE  |
| 38  | k     | 67  | THR  |
| 38  | k     | 77  | ILE  |
| 38  | k     | 105 | ILE  |
| 39  | l     | 3   | GLN  |
| 39  | l     | 78  | LEU  |
| 39  | l     | 89  | VAL  |
| 39  | l     | 114 | ARG  |
| 40  | m     | 10  | LEU  |
| 40  | m     | 15  | SER  |
| 40  | m     | 20  | MET  |
| 40  | m     | 33  | ILE  |
| 40  | m     | 98  | LEU  |
| 41  | n     | 49  | VAL  |
| 41  | n     | 52  | SER  |
| 41  | n     | 64  | TYR  |
| 41  | n     | 74  | VAL  |
| 41  | n     | 83  | LEU  |
| 41  | n     | 106 | LEU  |
| 42  | o     | 4   | ILE  |
| 42  | o     | 12  | GLN  |
| 42  | o     | 27  | GLU  |
| 42  | o     | 28  | VAL  |
| 42  | o     | 47  | VAL  |
| 42  | o     | 73  | VAL  |
| 43  | p     | 22  | LYS  |
| 43  | p     | 52  | GLN  |
| 43  | p     | 57  | PHE  |
| 43  | p     | 75  | SER  |
| 43  | p     | 78  | LYS  |
| 43  | p     | 90  | ILE  |
| 43  | p     | 91  | ASP  |
| 43  | p     | 104 | VAL  |
| 44  | q     | 37  | GLU  |
| 44  | q     | 72  | VAL  |
| 44  | q     | 96  | VAL  |
| 44  | q     | 101 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | r     | 13  | SER  |
| 45  | r     | 99  | ARG  |
| 45  | r     | 107 | VAL  |
| 46  | s     | 24  | MET  |
| 46  | s     | 25  | GLU  |
| 46  | s     | 28  | ASN  |
| 46  | s     | 50  | LEU  |
| 46  | s     | 55  | VAL  |
| 46  | s     | 78  | SER  |
| 46  | s     | 79  | ASP  |
| 47  | t     | 15  | THR  |
| 47  | t     | 29  | LEU  |
| 47  | t     | 43  | LYS  |
| 47  | t     | 49  | VAL  |
| 47  | t     | 70  | VAL  |
| 47  | t     | 94  | ARG  |
| 48  | u     | 20  | LEU  |
| 48  | u     | 25  | LYS  |
| 48  | u     | 30  | ILE  |
| 48  | u     | 41  | GLU  |
| 48  | u     | 42  | LEU  |
| 49  | v     | 10  | THR  |
| 49  | v     | 21  | LEU  |
| 49  | v     | 30  | SER  |
| 49  | v     | 58  | THR  |
| 49  | v     | 78  | LYS  |
| 50  | w     | 2   | SER  |
| 50  | w     | 11  | ARG  |
| 50  | w     | 28  | ARG  |
| 50  | w     | 35  | SER  |
| 50  | w     | 40  | VAL  |
| 50  | w     | 42  | SER  |
| 50  | w     | 48  | THR  |
| 50  | w     | 65  | ASP  |
| 51  | x     | 38  | GLN  |
| 51  | x     | 40  | SER  |
| 51  | x     | 53  | VAL  |
| 52  | y     | 12  | SER  |
| 52  | y     | 37  | GLU  |
| 53  | z     | 26  | THR  |
| 53  | z     | 44  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 26  | HIS  |
| 3   | 2     | 31  | HIS  |
| 4   | 3     | 33  | HIS  |
| 9   | C     | 32  | ASN  |
| 9   | C     | 190 | HIS  |
| 10  | D     | 131 | ASN  |
| 11  | E     | 43  | ASN  |
| 11  | E     | 97  | GLN  |
| 13  | G     | 97  | ASN  |
| 13  | G     | 142 | HIS  |
| 15  | I     | 31  | ASN  |
| 16  | J     | 15  | HIS  |
| 17  | K     | 40  | ASN  |
| 17  | K     | 101 | ASN  |
| 18  | L     | 59  | ASN  |
| 19  | M     | 12  | HIS  |
| 20  | N     | 4   | GLN  |
| 20  | N     | 62  | ASN  |
| 21  | O     | 42  | HIS  |
| 25  | S     | 14  | HIS  |
| 30  | c     | 153 | GLN  |
| 30  | c     | 239 | ASN  |
| 31  | d     | 140 | HIS  |
| 31  | d     | 185 | ASN  |
| 32  | e     | 30  | GLN  |
| 34  | g     | 104 | ASN  |
| 35  | h     | 2   | GLN  |
| 35  | h     | 20  | ASN  |
| 36  | i     | 40  | HIS  |
| 36  | i     | 58  | ASN  |
| 36  | i     | 86  | GLN  |
| 36  | i     | 132 | HIS  |
| 37  | j     | 3   | GLN  |
| 37  | j     | 82  | ASN  |
| 39  | l     | 45  | GLN  |
| 41  | n     | 98  | GLN  |
| 42  | o     | 56  | HIS  |
| 44  | q     | 43  | ASN  |
| 45  | r     | 60  | HIS  |
| 47  | t     | 74  | ASN  |
| 49  | v     | 57  | HIS  |
| 51  | x     | 31  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | x     | 58  | ASN  |
| 53  | z     | 19  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 28  | a     | 2747/2904 (94%) | 427 (15%)         | 0               |
| 29  | b     | 118/120 (98%)   | 36 (30%)          | 0               |
| 6   | 5     | 1/2 (50%)       | 1 (100%)          | 0               |
| 7   | A     | 1513/1517 (99%) | 564 (37%)         | 59 (3%)         |
| All | All   | 4379/4543 (96%) | 1028 (23%)        | 59 (1%)         |

All (1028) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 5     | 76  | A    |
| 7   | A     | 4   | U    |
| 7   | A     | 6   | G    |
| 7   | A     | 7   | A    |
| 7   | A     | 8   | A    |
| 7   | A     | 9   | G    |
| 7   | A     | 10  | A    |
| 7   | A     | 11  | G    |
| 7   | A     | 15  | G    |
| 7   | A     | 17  | U    |
| 7   | A     | 18  | C    |
| 7   | A     | 22  | G    |
| 7   | A     | 32  | A    |
| 7   | A     | 35  | G    |
| 7   | A     | 37  | U    |
| 7   | A     | 39  | G    |
| 7   | A     | 41  | G    |
| 7   | A     | 42  | G    |
| 7   | A     | 43  | C    |
| 7   | A     | 47  | C    |
| 7   | A     | 48  | C    |
| 7   | A     | 51  | A    |
| 7   | A     | 62  | U    |
| 7   | A     | 63  | C    |
| 7   | A     | 65  | A    |
| 7   | A     | 66  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 73  | C    |
| 7   | A     | 75  | C    |
| 7   | A     | 76  | A    |
| 7   | A     | 78  | A    |
| 7   | A     | 79  | G    |
| 7   | A     | 82  | A    |
| 7   | A     | 83  | C    |
| 7   | A     | 84  | U    |
| 7   | A     | 85  | U    |
| 7   | A     | 86  | G    |
| 7   | A     | 87  | U    |
| 7   | A     | 88  | U    |
| 7   | A     | 89  | C    |
| 7   | A     | 90  | C    |
| 7   | A     | 91  | U    |
| 7   | A     | 92  | U    |
| 7   | A     | 93  | G    |
| 7   | A     | 94  | G    |
| 7   | A     | 95  | G    |
| 7   | A     | 96  | U    |
| 7   | A     | 99  | C    |
| 7   | A     | 100 | G    |
| 7   | A     | 106 | C    |
| 7   | A     | 109 | A    |
| 7   | A     | 116 | A    |
| 7   | A     | 120 | A    |
| 7   | A     | 121 | U    |
| 7   | A     | 122 | G    |
| 7   | A     | 123 | C    |
| 7   | A     | 131 | A    |
| 7   | A     | 132 | U    |
| 7   | A     | 134 | G    |
| 7   | A     | 144 | G    |
| 7   | A     | 145 | G    |
| 7   | A     | 146 | G    |
| 7   | A     | 154 | C    |
| 7   | A     | 157 | U    |
| 7   | A     | 162 | A    |
| 7   | A     | 171 | A    |
| 7   | A     | 173 | U    |
| 7   | A     | 177 | G    |
| 7   | A     | 181 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 182 | A    |
| 7   | A     | 183 | C    |
| 7   | A     | 184 | C    |
| 7   | A     | 186 | C    |
| 7   | A     | 193 | C    |
| 7   | A     | 195 | A    |
| 7   | A     | 196 | A    |
| 7   | A     | 197 | A    |
| 7   | A     | 198 | G    |
| 7   | A     | 199 | C    |
| 7   | A     | 200 | A    |
| 7   | A     | 215 | C    |
| 7   | A     | 216 | U    |
| 7   | A     | 222 | U    |
| 7   | A     | 223 | A    |
| 7   | A     | 228 | A    |
| 7   | A     | 239 | U    |
| 7   | A     | 240 | G    |
| 7   | A     | 245 | U    |
| 7   | A     | 247 | G    |
| 7   | A     | 251 | G    |
| 7   | A     | 259 | G    |
| 7   | A     | 260 | G    |
| 7   | A     | 261 | U    |
| 7   | A     | 262 | A    |
| 7   | A     | 266 | G    |
| 7   | A     | 267 | C    |
| 7   | A     | 268 | U    |
| 7   | A     | 274 | A    |
| 7   | A     | 280 | C    |
| 7   | A     | 281 | G    |
| 7   | A     | 283 | U    |
| 7   | A     | 289 | G    |
| 7   | A     | 295 | C    |
| 7   | A     | 299 | G    |
| 7   | A     | 300 | A    |
| 7   | A     | 301 | G    |
| 7   | A     | 306 | A    |
| 7   | A     | 325 | A    |
| 7   | A     | 326 | G    |
| 7   | A     | 327 | A    |
| 7   | A     | 328 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 330 | C    |
| 7   | A     | 332 | G    |
| 7   | A     | 334 | C    |
| 7   | A     | 338 | A    |
| 7   | A     | 344 | A    |
| 7   | A     | 348 | G    |
| 7   | A     | 351 | G    |
| 7   | A     | 352 | C    |
| 7   | A     | 354 | G    |
| 7   | A     | 367 | U    |
| 7   | A     | 372 | C    |
| 7   | A     | 373 | A    |
| 7   | A     | 377 | G    |
| 7   | A     | 378 | G    |
| 7   | A     | 379 | C    |
| 7   | A     | 381 | C    |
| 7   | A     | 382 | A    |
| 7   | A     | 383 | A    |
| 7   | A     | 384 | G    |
| 7   | A     | 385 | C    |
| 7   | A     | 386 | C    |
| 7   | A     | 397 | A    |
| 7   | A     | 406 | A    |
| 7   | A     | 407 | U    |
| 7   | A     | 410 | G    |
| 7   | A     | 411 | A    |
| 7   | A     | 412 | C    |
| 7   | A     | 413 | A    |
| 7   | A     | 414 | A    |
| 7   | A     | 415 | A    |
| 7   | A     | 422 | C    |
| 7   | A     | 423 | G    |
| 7   | A     | 424 | G    |
| 7   | A     | 428 | G    |
| 7   | A     | 429 | U    |
| 7   | A     | 435 | A    |
| 7   | A     | 436 | C    |
| 7   | A     | 437 | U    |
| 7   | A     | 438 | U    |
| 7   | A     | 440 | C    |
| 7   | A     | 442 | G    |
| 7   | A     | 445 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 446 | G    |
| 7   | A     | 448 | A    |
| 7   | A     | 449 | G    |
| 7   | A     | 450 | G    |
| 7   | A     | 451 | A    |
| 7   | A     | 452 | A    |
| 7   | A     | 455 | U    |
| 7   | A     | 458 | U    |
| 7   | A     | 460 | A    |
| 7   | A     | 463 | C    |
| 7   | A     | 465 | A    |
| 7   | A     | 466 | A    |
| 7   | A     | 467 | U    |
| 7   | A     | 468 | A    |
| 7   | A     | 470 | C    |
| 7   | A     | 474 | A    |
| 7   | A     | 475 | U    |
| 7   | A     | 476 | C    |
| 7   | A     | 477 | A    |
| 7   | A     | 480 | U    |
| 7   | A     | 483 | C    |
| 7   | A     | 484 | G    |
| 7   | A     | 485 | U    |
| 7   | A     | 486 | U    |
| 7   | A     | 489 | C    |
| 7   | A     | 490 | U    |
| 7   | A     | 497 | G    |
| 7   | A     | 498 | A    |
| 7   | A     | 499 | A    |
| 7   | A     | 500 | G    |
| 7   | A     | 502 | A    |
| 7   | A     | 505 | G    |
| 7   | A     | 507 | C    |
| 7   | A     | 508 | U    |
| 7   | A     | 511 | C    |
| 7   | A     | 512 | U    |
| 7   | A     | 513 | C    |
| 7   | A     | 516 | PSU  |
| 7   | A     | 518 | C    |
| 7   | A     | 521 | G    |
| 7   | A     | 524 | G    |
| 7   | A     | 527 | G7M  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 532 | A    |
| 7   | A     | 533 | A    |
| 7   | A     | 534 | U    |
| 7   | A     | 536 | C    |
| 7   | A     | 537 | G    |
| 7   | A     | 539 | A    |
| 7   | A     | 540 | G    |
| 7   | A     | 543 | U    |
| 7   | A     | 544 | G    |
| 7   | A     | 547 | A    |
| 7   | A     | 548 | G    |
| 7   | A     | 549 | C    |
| 7   | A     | 550 | G    |
| 7   | A     | 559 | A    |
| 7   | A     | 564 | C    |
| 7   | A     | 573 | A    |
| 7   | A     | 575 | G    |
| 7   | A     | 576 | C    |
| 7   | A     | 577 | G    |
| 7   | A     | 586 | U    |
| 7   | A     | 589 | U    |
| 7   | A     | 592 | G    |
| 7   | A     | 596 | A    |
| 7   | A     | 598 | U    |
| 7   | A     | 599 | C    |
| 7   | A     | 600 | A    |
| 7   | A     | 602 | A    |
| 7   | A     | 607 | A    |
| 7   | A     | 608 | A    |
| 7   | A     | 609 | A    |
| 7   | A     | 610 | G    |
| 7   | A     | 611 | C    |
| 7   | A     | 612 | C    |
| 7   | A     | 613 | C    |
| 7   | A     | 615 | G    |
| 7   | A     | 616 | G    |
| 7   | A     | 617 | G    |
| 7   | A     | 622 | A    |
| 7   | A     | 626 | G    |
| 7   | A     | 632 | C    |
| 7   | A     | 633 | G    |
| 7   | A     | 637 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 638 | U    |
| 7   | A     | 639 | G    |
| 7   | A     | 642 | A    |
| 7   | A     | 643 | C    |
| 7   | A     | 644 | U    |
| 7   | A     | 652 | U    |
| 7   | A     | 653 | A    |
| 7   | A     | 662 | U    |
| 7   | A     | 663 | A    |
| 7   | A     | 665 | A    |
| 7   | A     | 687 | A    |
| 7   | A     | 695 | A    |
| 7   | A     | 707 | U    |
| 7   | A     | 720 | C    |
| 7   | A     | 721 | G    |
| 7   | A     | 723 | U    |
| 7   | A     | 724 | G    |
| 7   | A     | 738 | C    |
| 7   | A     | 747 | A    |
| 7   | A     | 749 | A    |
| 7   | A     | 755 | A    |
| 7   | A     | 777 | A    |
| 7   | A     | 779 | C    |
| 7   | A     | 781 | A    |
| 7   | A     | 787 | A    |
| 7   | A     | 793 | U    |
| 7   | A     | 794 | A    |
| 7   | A     | 799 | G    |
| 7   | A     | 802 | A    |
| 7   | A     | 815 | A    |
| 7   | A     | 817 | C    |
| 7   | A     | 818 | G    |
| 7   | A     | 819 | A    |
| 7   | A     | 820 | U    |
| 7   | A     | 821 | G    |
| 7   | A     | 825 | A    |
| 7   | A     | 827 | U    |
| 7   | A     | 831 | A    |
| 7   | A     | 832 | G    |
| 7   | A     | 836 | G    |
| 7   | A     | 838 | G    |
| 7   | A     | 839 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 847 | G    |
| 7   | A     | 848 | C    |
| 7   | A     | 850 | U    |
| 7   | A     | 851 | G    |
| 7   | A     | 860 | A    |
| 7   | A     | 872 | A    |
| 7   | A     | 878 | A    |
| 7   | A     | 881 | G    |
| 7   | A     | 887 | G    |
| 7   | A     | 890 | G    |
| 7   | A     | 891 | U    |
| 7   | A     | 892 | A    |
| 7   | A     | 908 | A    |
| 7   | A     | 909 | A    |
| 7   | A     | 912 | C    |
| 7   | A     | 913 | A    |
| 7   | A     | 914 | A    |
| 7   | A     | 922 | G    |
| 7   | A     | 926 | G    |
| 7   | A     | 927 | G    |
| 7   | A     | 934 | C    |
| 7   | A     | 935 | A    |
| 7   | A     | 938 | A    |
| 7   | A     | 953 | G    |
| 7   | A     | 957 | U    |
| 7   | A     | 958 | A    |
| 7   | A     | 959 | A    |
| 7   | A     | 960 | U    |
| 7   | A     | 962 | C    |
| 7   | A     | 963 | G    |
| 7   | A     | 965 | U    |
| 7   | A     | 966 | 2MG  |
| 7   | A     | 967 | 5MC  |
| 7   | A     | 969 | A    |
| 7   | A     | 972 | C    |
| 7   | A     | 973 | G    |
| 7   | A     | 974 | A    |
| 7   | A     | 975 | A    |
| 7   | A     | 976 | G    |
| 7   | A     | 978 | A    |
| 7   | A     | 979 | C    |
| 7   | A     | 981 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 982  | U    |
| 7   | A     | 989  | U    |
| 7   | A     | 991  | U    |
| 7   | A     | 992  | U    |
| 7   | A     | 993  | G    |
| 7   | A     | 994  | A    |
| 7   | A     | 995  | C    |
| 7   | A     | 996  | A    |
| 7   | A     | 997  | U    |
| 7   | A     | 998  | C    |
| 7   | A     | 999  | C    |
| 7   | A     | 1000 | A    |
| 7   | A     | 1001 | G    |
| 7   | A     | 1002 | A    |
| 7   | A     | 1003 | G    |
| 7   | A     | 1004 | A    |
| 7   | A     | 1005 | A    |
| 7   | A     | 1006 | U    |
| 7   | A     | 1008 | U    |
| 7   | A     | 1009 | A    |
| 7   | A     | 1010 | G    |
| 7   | A     | 1011 | C    |
| 7   | A     | 1012 | G    |
| 7   | A     | 1013 | G    |
| 7   | A     | 1014 | A    |
| 7   | A     | 1015 | G    |
| 7   | A     | 1016 | A    |
| 7   | A     | 1017 | C    |
| 7   | A     | 1018 | G    |
| 7   | A     | 1021 | G    |
| 7   | A     | 1022 | G    |
| 7   | A     | 1023 | A    |
| 7   | A     | 1024 | G    |
| 7   | A     | 1025 | U    |
| 7   | A     | 1026 | G    |
| 7   | A     | 1027 | C    |
| 7   | A     | 1028 | C    |
| 7   | A     | 1030 | U    |
| 7   | A     | 1031 | C    |
| 7   | A     | 1032 | G    |
| 7   | A     | 1034 | G    |
| 7   | A     | 1035 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1036 | G    |
| 7   | A     | 1037 | C    |
| 7   | A     | 1038 | U    |
| 7   | A     | 1039 | C    |
| 7   | A     | 1040 | U    |
| 7   | A     | 1041 | G    |
| 7   | A     | 1042 | A    |
| 7   | A     | 1043 | G    |
| 7   | A     | 1044 | A    |
| 7   | A     | 1045 | C    |
| 7   | A     | 1046 | A    |
| 7   | A     | 1047 | G    |
| 7   | A     | 1048 | G    |
| 7   | A     | 1049 | U    |
| 7   | A     | 1050 | G    |
| 7   | A     | 1057 | G    |
| 7   | A     | 1059 | C    |
| 7   | A     | 1065 | U    |
| 7   | A     | 1067 | A    |
| 7   | A     | 1080 | A    |
| 7   | A     | 1081 | A    |
| 7   | A     | 1090 | U    |
| 7   | A     | 1094 | G    |
| 7   | A     | 1095 | U    |
| 7   | A     | 1099 | G    |
| 7   | A     | 1100 | C    |
| 7   | A     | 1101 | A    |
| 7   | A     | 1102 | A    |
| 7   | A     | 1104 | G    |
| 7   | A     | 1108 | G    |
| 7   | A     | 1109 | C    |
| 7   | A     | 1110 | A    |
| 7   | A     | 1113 | C    |
| 7   | A     | 1114 | C    |
| 7   | A     | 1115 | U    |
| 7   | A     | 1116 | U    |
| 7   | A     | 1119 | C    |
| 7   | A     | 1120 | C    |
| 7   | A     | 1122 | U    |
| 7   | A     | 1123 | G    |
| 7   | A     | 1124 | U    |
| 7   | A     | 1125 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1126 | U    |
| 7   | A     | 1127 | G    |
| 7   | A     | 1130 | A    |
| 7   | A     | 1131 | G    |
| 7   | A     | 1133 | A    |
| 7   | A     | 1134 | C    |
| 7   | A     | 1135 | G    |
| 7   | A     | 1136 | U    |
| 7   | A     | 1138 | A    |
| 7   | A     | 1140 | G    |
| 7   | A     | 1141 | G    |
| 7   | A     | 1142 | U    |
| 7   | A     | 1143 | G    |
| 7   | A     | 1146 | A    |
| 7   | A     | 1147 | A    |
| 7   | A     | 1149 | U    |
| 7   | A     | 1150 | C    |
| 7   | A     | 1151 | C    |
| 7   | A     | 1153 | G    |
| 7   | A     | 1156 | A    |
| 7   | A     | 1157 | G    |
| 7   | A     | 1158 | A    |
| 7   | A     | 1159 | C    |
| 7   | A     | 1160 | U    |
| 7   | A     | 1161 | G    |
| 7   | A     | 1163 | C    |
| 7   | A     | 1168 | A    |
| 7   | A     | 1169 | U    |
| 7   | A     | 1170 | A    |
| 7   | A     | 1176 | G    |
| 7   | A     | 1177 | A    |
| 7   | A     | 1179 | G    |
| 7   | A     | 1180 | A    |
| 7   | A     | 1181 | A    |
| 7   | A     | 1182 | G    |
| 7   | A     | 1183 | G    |
| 7   | A     | 1184 | U    |
| 7   | A     | 1185 | G    |
| 7   | A     | 1186 | G    |
| 7   | A     | 1187 | G    |
| 7   | A     | 1188 | G    |
| 7   | A     | 1190 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1191 | G    |
| 7   | A     | 1192 | A    |
| 7   | A     | 1193 | C    |
| 7   | A     | 1197 | A    |
| 7   | A     | 1198 | A    |
| 7   | A     | 1199 | G    |
| 7   | A     | 1200 | U    |
| 7   | A     | 1201 | C    |
| 7   | A     | 1202 | A    |
| 7   | A     | 1203 | U    |
| 7   | A     | 1212 | U    |
| 7   | A     | 1213 | U    |
| 7   | A     | 1214 | A    |
| 7   | A     | 1215 | C    |
| 7   | A     | 1216 | G    |
| 7   | A     | 1226 | A    |
| 7   | A     | 1227 | C    |
| 7   | A     | 1228 | A    |
| 7   | A     | 1235 | C    |
| 7   | A     | 1239 | A    |
| 7   | A     | 1241 | U    |
| 7   | A     | 1242 | G    |
| 7   | A     | 1243 | G    |
| 7   | A     | 1244 | C    |
| 7   | A     | 1246 | U    |
| 7   | A     | 1247 | A    |
| 7   | A     | 1249 | A    |
| 7   | A     | 1250 | C    |
| 7   | A     | 1251 | A    |
| 7   | A     | 1253 | A    |
| 7   | A     | 1254 | G    |
| 7   | A     | 1256 | G    |
| 7   | A     | 1257 | C    |
| 7   | A     | 1258 | A    |
| 7   | A     | 1259 | G    |
| 7   | A     | 1275 | G    |
| 7   | A     | 1276 | A    |
| 7   | A     | 1277 | G    |
| 7   | A     | 1280 | A    |
| 7   | A     | 1281 | A    |
| 7   | A     | 1282 | U    |
| 7   | A     | 1283 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1284 | U    |
| 7   | A     | 1286 | A    |
| 7   | A     | 1287 | C    |
| 7   | A     | 1288 | A    |
| 7   | A     | 1293 | A    |
| 7   | A     | 1299 | U    |
| 7   | A     | 1301 | G    |
| 7   | A     | 1303 | C    |
| 7   | A     | 1306 | G    |
| 7   | A     | 1307 | A    |
| 7   | A     | 1311 | G    |
| 7   | A     | 1312 | A    |
| 7   | A     | 1313 | G    |
| 7   | A     | 1314 | U    |
| 7   | A     | 1317 | G    |
| 7   | A     | 1318 | C    |
| 7   | A     | 1320 | A    |
| 7   | A     | 1321 | C    |
| 7   | A     | 1322 | U    |
| 7   | A     | 1323 | C    |
| 7   | A     | 1329 | C    |
| 7   | A     | 1330 | A    |
| 7   | A     | 1332 | G    |
| 7   | A     | 1336 | U    |
| 7   | A     | 1337 | C    |
| 7   | A     | 1347 | A    |
| 7   | A     | 1348 | G    |
| 7   | A     | 1349 | U    |
| 7   | A     | 1351 | A    |
| 7   | A     | 1354 | G    |
| 7   | A     | 1361 | A    |
| 7   | A     | 1362 | G    |
| 7   | A     | 1364 | A    |
| 7   | A     | 1365 | U    |
| 7   | A     | 1370 | C    |
| 7   | A     | 1371 | G    |
| 7   | A     | 1373 | U    |
| 7   | A     | 1379 | C    |
| 7   | A     | 1380 | G    |
| 7   | A     | 1381 | U    |
| 7   | A     | 1382 | U    |
| 7   | A     | 1395 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1399 | A    |
| 7   | A     | 1402 | G    |
| 7   | A     | 1403 | 4OC  |
| 7   | A     | 1404 | C    |
| 7   | A     | 1420 | A    |
| 7   | A     | 1429 | A    |
| 7   | A     | 1433 | G    |
| 7   | A     | 1440 | G    |
| 7   | A     | 1442 | A    |
| 7   | A     | 1443 | G    |
| 7   | A     | 1444 | U    |
| 7   | A     | 1447 | A    |
| 7   | A     | 1448 | A    |
| 7   | A     | 1449 | C    |
| 7   | A     | 1452 | U    |
| 7   | A     | 1453 | C    |
| 7   | A     | 1454 | G    |
| 7   | A     | 1457 | A    |
| 7   | A     | 1461 | C    |
| 7   | A     | 1462 | G    |
| 7   | A     | 1493 | A    |
| 7   | A     | 1494 | A    |
| 7   | A     | 1496 | U    |
| 7   | A     | 1498 | G    |
| 7   | A     | 1500 | A    |
| 7   | A     | 1504 | A    |
| 7   | A     | 1507 | U    |
| 7   | A     | 1512 | C    |
| 7   | A     | 1518 | G    |
| 7   | A     | 1519 | MA6  |
| 7   | A     | 1528 | C    |
| 7   | A     | 1530 | G    |
| 7   | A     | 1531 | G    |
| 7   | A     | 1532 | A    |
| 7   | A     | 1534 | C    |
| 28  | a     | 10   | A    |
| 28  | a     | 12   | U    |
| 28  | a     | 34   | U    |
| 28  | a     | 51   | G    |
| 28  | a     | 71   | A    |
| 28  | a     | 74   | A    |
| 28  | a     | 75   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | a     | 84  | A    |
| 28  | a     | 85  | G    |
| 28  | a     | 86  | G    |
| 28  | a     | 87  | U    |
| 28  | a     | 100 | U    |
| 28  | a     | 101 | A    |
| 28  | a     | 102 | U    |
| 28  | a     | 118 | A    |
| 28  | a     | 119 | A    |
| 28  | a     | 120 | U    |
| 28  | a     | 125 | A    |
| 28  | a     | 139 | U    |
| 28  | a     | 142 | A    |
| 28  | a     | 163 | C    |
| 28  | a     | 181 | A    |
| 28  | a     | 196 | A    |
| 28  | a     | 199 | A    |
| 28  | a     | 215 | G    |
| 28  | a     | 216 | A    |
| 28  | a     | 221 | A    |
| 28  | a     | 222 | A    |
| 28  | a     | 228 | C    |
| 28  | a     | 233 | A    |
| 28  | a     | 248 | G    |
| 28  | a     | 264 | C    |
| 28  | a     | 265 | A    |
| 28  | a     | 268 | C    |
| 28  | a     | 269 | C    |
| 28  | a     | 270 | A    |
| 28  | a     | 271 | G    |
| 28  | a     | 272 | A    |
| 28  | a     | 276 | U    |
| 28  | a     | 278 | A    |
| 28  | a     | 282 | A    |
| 28  | a     | 285 | G    |
| 28  | a     | 287 | G    |
| 28  | a     | 311 | A    |
| 28  | a     | 329 | G    |
| 28  | a     | 330 | A    |
| 28  | a     | 345 | A    |
| 28  | a     | 361 | G    |
| 28  | a     | 362 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | a     | 385 | C    |
| 28  | a     | 386 | G    |
| 28  | a     | 396 | G    |
| 28  | a     | 404 | A    |
| 28  | a     | 405 | U    |
| 28  | a     | 406 | G    |
| 28  | a     | 411 | G    |
| 28  | a     | 416 | U    |
| 28  | a     | 420 | C    |
| 28  | a     | 425 | G    |
| 28  | a     | 456 | C    |
| 28  | a     | 481 | G    |
| 28  | a     | 490 | C    |
| 28  | a     | 491 | G    |
| 28  | a     | 504 | A    |
| 28  | a     | 505 | A    |
| 28  | a     | 509 | C    |
| 28  | a     | 510 | C    |
| 28  | a     | 530 | G    |
| 28  | a     | 531 | C    |
| 28  | a     | 532 | A    |
| 28  | a     | 545 | U    |
| 28  | a     | 546 | U    |
| 28  | a     | 549 | G    |
| 28  | a     | 551 | G    |
| 28  | a     | 563 | A    |
| 28  | a     | 573 | U    |
| 28  | a     | 574 | A    |
| 28  | a     | 575 | A    |
| 28  | a     | 599 | A    |
| 28  | a     | 600 | G    |
| 28  | a     | 601 | C    |
| 28  | a     | 602 | A    |
| 28  | a     | 615 | U    |
| 28  | a     | 627 | A    |
| 28  | a     | 628 | G    |
| 28  | a     | 629 | G    |
| 28  | a     | 631 | A    |
| 28  | a     | 632 | A    |
| 28  | a     | 636 | G    |
| 28  | a     | 637 | A    |
| 28  | a     | 644 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | a     | 645 | C    |
| 28  | a     | 647 | G    |
| 28  | a     | 654 | A    |
| 28  | a     | 655 | A    |
| 28  | a     | 656 | G    |
| 28  | a     | 661 | A    |
| 28  | a     | 663 | G    |
| 28  | a     | 686 | U    |
| 28  | a     | 696 | G    |
| 28  | a     | 717 | C    |
| 28  | a     | 730 | A    |
| 28  | a     | 736 | C    |
| 28  | a     | 738 | G    |
| 28  | a     | 746 | PSU  |
| 28  | a     | 747 | 5MU  |
| 28  | a     | 764 | A    |
| 28  | a     | 775 | G    |
| 28  | a     | 776 | G    |
| 28  | a     | 782 | A    |
| 28  | a     | 784 | G    |
| 28  | a     | 785 | G    |
| 28  | a     | 792 | A    |
| 28  | a     | 805 | G    |
| 28  | a     | 806 | C    |
| 28  | a     | 812 | C    |
| 28  | a     | 827 | U    |
| 28  | a     | 828 | U    |
| 28  | a     | 845 | A    |
| 28  | a     | 846 | U    |
| 28  | a     | 847 | U    |
| 28  | a     | 859 | G    |
| 28  | a     | 864 | G    |
| 28  | a     | 883 | G    |
| 28  | a     | 884 | U    |
| 28  | a     | 888 | C    |
| 28  | a     | 890 | C    |
| 28  | a     | 891 | G    |
| 28  | a     | 893 | C    |
| 28  | a     | 895 | U    |
| 28  | a     | 896 | A    |
| 28  | a     | 897 | C    |
| 28  | a     | 910 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | a     | 934  | U    |
| 28  | a     | 936  | A    |
| 28  | a     | 938  | G    |
| 28  | a     | 939  | G    |
| 28  | a     | 946  | C    |
| 28  | a     | 961  | C    |
| 28  | a     | 971  | G    |
| 28  | a     | 974  | G    |
| 28  | a     | 983  | A    |
| 28  | a     | 996  | A    |
| 28  | a     | 1009 | A    |
| 28  | a     | 1011 | G    |
| 28  | a     | 1012 | U    |
| 28  | a     | 1013 | C    |
| 28  | a     | 1022 | G    |
| 28  | a     | 1023 | U    |
| 28  | a     | 1024 | G    |
| 28  | a     | 1025 | G    |
| 28  | a     | 1026 | G    |
| 28  | a     | 1028 | A    |
| 28  | a     | 1029 | A    |
| 28  | a     | 1032 | A    |
| 28  | a     | 1033 | U    |
| 28  | a     | 1047 | G    |
| 28  | a     | 1048 | A    |
| 28  | a     | 1110 | G    |
| 28  | a     | 1111 | A    |
| 28  | a     | 1112 | G    |
| 28  | a     | 1116 | G    |
| 28  | a     | 1127 | A    |
| 28  | a     | 1130 | U    |
| 28  | a     | 1132 | U    |
| 28  | a     | 1135 | C    |
| 28  | a     | 1136 | G    |
| 28  | a     | 1141 | U    |
| 28  | a     | 1142 | A    |
| 28  | a     | 1168 | G    |
| 28  | a     | 1169 | A    |
| 28  | a     | 1179 | G    |
| 28  | a     | 1180 | U    |
| 28  | a     | 1184 | U    |
| 28  | a     | 1185 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | a     | 1186 | G    |
| 28  | a     | 1206 | G    |
| 28  | a     | 1212 | G    |
| 28  | a     | 1250 | G    |
| 28  | a     | 1253 | A    |
| 28  | a     | 1255 | U    |
| 28  | a     | 1256 | G    |
| 28  | a     | 1271 | G    |
| 28  | a     | 1272 | A    |
| 28  | a     | 1300 | G    |
| 28  | a     | 1301 | A    |
| 28  | a     | 1313 | U    |
| 28  | a     | 1365 | A    |
| 28  | a     | 1379 | U    |
| 28  | a     | 1383 | A    |
| 28  | a     | 1415 | U    |
| 28  | a     | 1416 | G    |
| 28  | a     | 1417 | C    |
| 28  | a     | 1428 | C    |
| 28  | a     | 1429 | G    |
| 28  | a     | 1452 | G    |
| 28  | a     | 1453 | A    |
| 28  | a     | 1458 | U    |
| 28  | a     | 1482 | G    |
| 28  | a     | 1493 | C    |
| 28  | a     | 1510 | G    |
| 28  | a     | 1515 | A    |
| 28  | a     | 1524 | G    |
| 28  | a     | 1535 | A    |
| 28  | a     | 1536 | C    |
| 28  | a     | 1537 | G    |
| 28  | a     | 1566 | A    |
| 28  | a     | 1569 | A    |
| 28  | a     | 1578 | U    |
| 28  | a     | 1583 | A    |
| 28  | a     | 1584 | U    |
| 28  | a     | 1585 | C    |
| 28  | a     | 1608 | A    |
| 28  | a     | 1609 | A    |
| 28  | a     | 1622 | G    |
| 28  | a     | 1646 | C    |
| 28  | a     | 1647 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | a     | 1648 | U    |
| 28  | a     | 1654 | A    |
| 28  | a     | 1674 | G    |
| 28  | a     | 1675 | C    |
| 28  | a     | 1676 | A    |
| 28  | a     | 1715 | G    |
| 28  | a     | 1729 | U    |
| 28  | a     | 1730 | C    |
| 28  | a     | 1733 | G    |
| 28  | a     | 1738 | G    |
| 28  | a     | 1764 | C    |
| 28  | a     | 1773 | A    |
| 28  | a     | 1800 | C    |
| 28  | a     | 1801 | A    |
| 28  | a     | 1808 | A    |
| 28  | a     | 1816 | C    |
| 28  | a     | 1829 | A    |
| 28  | a     | 1839 | G    |
| 28  | a     | 1847 | A    |
| 28  | a     | 1848 | A    |
| 28  | a     | 1858 | A    |
| 28  | a     | 1865 | U    |
| 28  | a     | 1866 | A    |
| 28  | a     | 1870 | C    |
| 28  | a     | 1871 | A    |
| 28  | a     | 1872 | A    |
| 28  | a     | 1883 | U    |
| 28  | a     | 1905 | C    |
| 28  | a     | 1906 | G    |
| 28  | a     | 1913 | A    |
| 28  | a     | 1929 | G    |
| 28  | a     | 1930 | G    |
| 28  | a     | 1936 | A    |
| 28  | a     | 1937 | A    |
| 28  | a     | 1955 | U    |
| 28  | a     | 1967 | C    |
| 28  | a     | 1970 | A    |
| 28  | a     | 1971 | U    |
| 28  | a     | 1972 | G    |
| 28  | a     | 1991 | U    |
| 28  | a     | 1993 | U    |
| 28  | a     | 2007 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | a     | 2023 | C    |
| 28  | a     | 2027 | G    |
| 28  | a     | 2030 | 6MZ  |
| 28  | a     | 2031 | A    |
| 28  | a     | 2033 | A    |
| 28  | a     | 2035 | G    |
| 28  | a     | 2036 | C    |
| 28  | a     | 2043 | C    |
| 28  | a     | 2046 | G    |
| 28  | a     | 2055 | C    |
| 28  | a     | 2056 | G    |
| 28  | a     | 2060 | A    |
| 28  | a     | 2061 | G    |
| 28  | a     | 2062 | A    |
| 28  | a     | 2069 | G7M  |
| 28  | a     | 2077 | A    |
| 28  | a     | 2093 | G    |
| 28  | a     | 2198 | A    |
| 28  | a     | 2199 | A    |
| 28  | a     | 2203 | U    |
| 28  | a     | 2204 | G    |
| 28  | a     | 2211 | A    |
| 28  | a     | 2212 | A    |
| 28  | a     | 2225 | A    |
| 28  | a     | 2238 | G    |
| 28  | a     | 2239 | G    |
| 28  | a     | 2279 | G    |
| 28  | a     | 2283 | C    |
| 28  | a     | 2287 | A    |
| 28  | a     | 2288 | A    |
| 28  | a     | 2292 | U    |
| 28  | a     | 2305 | U    |
| 28  | a     | 2307 | G    |
| 28  | a     | 2308 | G    |
| 28  | a     | 2312 | U    |
| 28  | a     | 2317 | A    |
| 28  | a     | 2318 | G    |
| 28  | a     | 2319 | G    |
| 28  | a     | 2320 | U    |
| 28  | a     | 2322 | A    |
| 28  | a     | 2324 | U    |
| 28  | a     | 2325 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | a     | 2326 | C    |
| 28  | a     | 2327 | A    |
| 28  | a     | 2331 | G    |
| 28  | a     | 2333 | A    |
| 28  | a     | 2334 | U    |
| 28  | a     | 2335 | A    |
| 28  | a     | 2336 | A    |
| 28  | a     | 2338 | C    |
| 28  | a     | 2339 | C    |
| 28  | a     | 2345 | G    |
| 28  | a     | 2347 | C    |
| 28  | a     | 2348 | U    |
| 28  | a     | 2349 | G    |
| 28  | a     | 2351 | G    |
| 28  | a     | 2352 | A    |
| 28  | a     | 2357 | G    |
| 28  | a     | 2358 | A    |
| 28  | a     | 2361 | G    |
| 28  | a     | 2362 | C    |
| 28  | a     | 2363 | G    |
| 28  | a     | 2364 | C    |
| 28  | a     | 2366 | A    |
| 28  | a     | 2367 | G    |
| 28  | a     | 2372 | U    |
| 28  | a     | 2376 | A    |
| 28  | a     | 2379 | G    |
| 28  | a     | 2381 | A    |
| 28  | a     | 2382 | G    |
| 28  | a     | 2383 | G    |
| 28  | a     | 2385 | C    |
| 28  | a     | 2388 | A    |
| 28  | a     | 2389 | G    |
| 28  | a     | 2402 | U    |
| 28  | a     | 2403 | C    |
| 28  | a     | 2406 | A    |
| 28  | a     | 2417 | C    |
| 28  | a     | 2418 | A    |
| 28  | a     | 2421 | G    |
| 28  | a     | 2425 | A    |
| 28  | a     | 2429 | G    |
| 28  | a     | 2441 | U    |
| 28  | a     | 2448 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | a     | 2459 | A    |
| 28  | a     | 2470 | G    |
| 28  | a     | 2476 | A    |
| 28  | a     | 2478 | A    |
| 28  | a     | 2480 | C    |
| 28  | a     | 2488 | G    |
| 28  | a     | 2491 | U    |
| 28  | a     | 2498 | OMC  |
| 28  | a     | 2502 | G    |
| 28  | a     | 2505 | G    |
| 28  | a     | 2513 | A    |
| 28  | a     | 2518 | A    |
| 28  | a     | 2520 | C    |
| 28  | a     | 2528 | U    |
| 28  | a     | 2530 | A    |
| 28  | a     | 2531 | A    |
| 28  | a     | 2534 | A    |
| 28  | a     | 2535 | G    |
| 28  | a     | 2542 | A    |
| 28  | a     | 2543 | G    |
| 28  | a     | 2547 | A    |
| 28  | a     | 2566 | A    |
| 28  | a     | 2567 | G    |
| 28  | a     | 2582 | G    |
| 28  | a     | 2585 | U    |
| 28  | a     | 2586 | U    |
| 28  | a     | 2602 | A    |
| 28  | a     | 2603 | G    |
| 28  | a     | 2609 | U    |
| 28  | a     | 2613 | U    |
| 28  | a     | 2615 | U    |
| 28  | a     | 2624 | G    |
| 28  | a     | 2628 | C    |
| 28  | a     | 2629 | U    |
| 28  | a     | 2646 | C    |
| 28  | a     | 2649 | C    |
| 28  | a     | 2651 | C    |
| 28  | a     | 2652 | C    |
| 28  | a     | 2653 | U    |
| 28  | a     | 2661 | G    |
| 28  | a     | 2667 | C    |
| 28  | a     | 2670 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | a     | 2673 | G    |
| 28  | a     | 2674 | G    |
| 28  | a     | 2682 | A    |
| 28  | a     | 2689 | U    |
| 28  | a     | 2690 | U    |
| 28  | a     | 2703 | C    |
| 28  | a     | 2714 | G    |
| 28  | a     | 2726 | A    |
| 28  | a     | 2733 | A    |
| 28  | a     | 2739 | U    |
| 28  | a     | 2742 | G    |
| 28  | a     | 2743 | U    |
| 28  | a     | 2744 | G    |
| 28  | a     | 2746 | U    |
| 28  | a     | 2747 | G    |
| 28  | a     | 2751 | G    |
| 28  | a     | 2752 | C    |
| 28  | a     | 2755 | C    |
| 28  | a     | 2756 | U    |
| 28  | a     | 2757 | A    |
| 28  | a     | 2763 | G    |
| 28  | a     | 2764 | A    |
| 28  | a     | 2765 | A    |
| 28  | a     | 2766 | A    |
| 28  | a     | 2776 | A    |
| 28  | a     | 2777 | G    |
| 28  | a     | 2778 | A    |
| 28  | a     | 2790 | U    |
| 28  | a     | 2791 | G    |
| 28  | a     | 2798 | U    |
| 28  | a     | 2799 | A    |
| 28  | a     | 2820 | A    |
| 28  | a     | 2821 | A    |
| 28  | a     | 2835 | A    |
| 28  | a     | 2849 | U    |
| 28  | a     | 2861 | U    |
| 28  | a     | 2873 | A    |
| 28  | a     | 2880 | C    |
| 28  | a     | 2884 | U    |
| 28  | a     | 2893 | A    |
| 28  | a     | 2896 | C    |
| 28  | a     | 2899 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | b     | 9   | G    |
| 29  | b     | 12  | C    |
| 29  | b     | 14  | U    |
| 29  | b     | 15  | A    |
| 29  | b     | 24  | G    |
| 29  | b     | 25  | U    |
| 29  | b     | 33  | G    |
| 29  | b     | 35  | C    |
| 29  | b     | 36  | C    |
| 29  | b     | 37  | C    |
| 29  | b     | 41  | G    |
| 29  | b     | 43  | C    |
| 29  | b     | 44  | G    |
| 29  | b     | 45  | A    |
| 29  | b     | 47  | C    |
| 29  | b     | 50  | A    |
| 29  | b     | 53  | A    |
| 29  | b     | 56  | G    |
| 29  | b     | 57  | A    |
| 29  | b     | 68  | C    |
| 29  | b     | 73  | A    |
| 29  | b     | 75  | G    |
| 29  | b     | 77  | U    |
| 29  | b     | 81  | G    |
| 29  | b     | 89  | U    |
| 29  | b     | 90  | C    |
| 29  | b     | 91  | C    |
| 29  | b     | 94  | A    |
| 29  | b     | 95  | U    |
| 29  | b     | 96  | G    |
| 29  | b     | 99  | A    |
| 29  | b     | 100 | G    |
| 29  | b     | 104 | A    |
| 29  | b     | 105 | G    |
| 29  | b     | 108 | A    |
| 29  | b     | 109 | A    |

All (59) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | A     | 64  | G    |
| 7   | A     | 87  | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 93   | G    |
| 7   | A     | 195  | A    |
| 7   | A     | 198  | G    |
| 7   | A     | 222  | U    |
| 7   | A     | 239  | U    |
| 7   | A     | 280  | C    |
| 7   | A     | 326  | G    |
| 7   | A     | 435  | A    |
| 7   | A     | 447  | G    |
| 7   | A     | 450  | G    |
| 7   | A     | 454  | G    |
| 7   | A     | 467  | U    |
| 7   | A     | 484  | G    |
| 7   | A     | 489  | C    |
| 7   | A     | 506  | G    |
| 7   | A     | 538  | G    |
| 7   | A     | 539  | A    |
| 7   | A     | 548  | G    |
| 7   | A     | 588  | G    |
| 7   | A     | 599  | C    |
| 7   | A     | 609  | A    |
| 7   | A     | 778  | G    |
| 7   | A     | 880  | C    |
| 7   | A     | 964  | A    |
| 7   | A     | 994  | A    |
| 7   | A     | 995  | C    |
| 7   | A     | 996  | A    |
| 7   | A     | 999  | C    |
| 7   | A     | 1004 | A    |
| 7   | A     | 1010 | G    |
| 7   | A     | 1012 | G    |
| 7   | A     | 1017 | C    |
| 7   | A     | 1036 | G    |
| 7   | A     | 1040 | U    |
| 7   | A     | 1043 | G    |
| 7   | A     | 1044 | A    |
| 7   | A     | 1066 | C    |
| 7   | A     | 1100 | C    |
| 7   | A     | 1115 | U    |
| 7   | A     | 1122 | U    |
| 7   | A     | 1133 | A    |
| 7   | A     | 1156 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | A     | 1160 | U    |
| 7   | A     | 1180 | A    |
| 7   | A     | 1190 | C    |
| 7   | A     | 1191 | G    |
| 7   | A     | 1243 | G    |
| 7   | A     | 1306 | G    |
| 7   | A     | 1320 | A    |
| 7   | A     | 1321 | C    |
| 7   | A     | 1347 | A    |
| 7   | A     | 1348 | G    |
| 7   | A     | 1370 | C    |
| 7   | A     | 1448 | A    |
| 7   | A     | 1452 | U    |
| 7   | A     | 1453 | C    |
| 7   | A     | 1506 | G    |

## 5.4 Non-standard residues in protein, DNA, RNA chains

40 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$ |
| 28  | PSU  | a     | 1911 | 28    | 18,21,22     | 0.95 | 1 (5%)      | 21,30,33    | 1.98 | 4 (19%)     |
| 7   | 2MG  | A     | 1208 | 7     | 23,26,27     | 0.78 | 0           | 33,38,41    | 2.19 | 10 (30%)    |
| 28  | 6MZ  | a     | 2030 | 28    | 22,25,26     | 1.16 | 2 (9%)      | 29,36,39    | 2.21 | 9 (31%)     |
| 28  | PSU  | a     | 746  | 55,28 | 18,21,22     | 1.15 | 3 (16%)     | 21,30,33    | 1.94 | 4 (19%)     |
| 28  | OMU  | a     | 2552 | 28    | 19,22,23     | 1.11 | 3 (15%)     | 25,31,34    | 2.06 | 6 (24%)     |
| 7   | 5MC  | A     | 1408 | 7     | 19,22,23     | 1.37 | 2 (10%)     | 26,32,35    | 1.15 | 3 (11%)     |
| 7   | 4OC  | A     | 1403 | 7     | 20,23,24     | 0.36 | 0           | 25,32,35    | 0.65 | 1 (4%)      |
| 28  | 1MG  | a     | 745  | 28    | 23,26,27     | 1.05 | 1 (4%)      | 33,39,42    | 1.76 | 6 (18%)     |
| 28  | H2U  | a     | 2449 | 28    | 18,21,22     | 0.49 | 0           | 19,30,33    | 1.09 | 1 (5%)      |
| 28  | PSU  | a     | 2604 | 28    | 18,21,22     | 1.10 | 3 (16%)     | 21,30,33    | 2.02 | 4 (19%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | G7M  | a     | 2069 | 28    | 23,26,27     | 0.58 | 0        | 34,39,42    | 0.93 | 2 (5%)   |
| 7   | MA6  | A     | 1520 | 7     | 23,26,27     | 2.51 | 5 (21%)  | 33,38,41    | 2.78 | 7 (21%)  |
| 28  | 3TD  | a     | 1915 | -     | 19,22,23     | 1.10 | 2 (10%)  | 23,32,35    | 1.95 | 3 (13%)  |
| 28  | 6MZ  | a     | 1618 | 28    | 22,25,26     | 1.11 | 2 (9%)   | 29,36,39    | 2.29 | 9 (31%)  |
| 28  | OMC  | a     | 2498 | 55,28 | 19,22,23     | 1.00 | 1 (5%)   | 25,31,34    | 1.28 | 2 (8%)   |
| 28  | 2MG  | a     | 1835 | 28    | 23,26,27     | 0.80 | 1 (4%)   | 33,38,41    | 2.30 | 11 (33%) |
| 28  | PSU  | a     | 2580 | 28    | 18,21,22     | 1.22 | 3 (16%)  | 21,30,33    | 2.21 | 5 (23%)  |
| 7   | G7M  | A     | 527  | 7     | 23,26,27     | 0.51 | 0        | 34,39,42    | 0.94 | 1 (2%)   |
| 28  | PSU  | a     | 1917 | 28    | 18,21,22     | 1.00 | 1 (5%)   | 21,30,33    | 1.98 | 5 (23%)  |
| 28  | 5MU  | a     | 1939 | 28    | 19,22,23     | 1.21 | 4 (21%)  | 27,32,35    | 2.19 | 6 (22%)  |
| 28  | 5MU  | a     | 747  | 28    | 19,22,23     | 1.13 | 3 (15%)  | 27,32,35    | 2.16 | 7 (25%)  |
| 39  | MS6  | l     | 82   | 39    | 5,7,8        | 0.59 | 0        | 2,7,9       | 1.09 | 0        |
| 7   | 2MG  | A     | 1517 | 7     | 23,26,27     | 0.79 | 0        | 33,38,41    | 2.28 | 11 (33%) |
| 28  | PSU  | a     | 2504 | 28    | 18,21,22     | 1.01 | 1 (5%)   | 21,30,33    | 1.92 | 4 (19%)  |
| 28  | PSU  | a     | 2457 | 28    | 18,21,22     | 1.14 | 4 (22%)  | 21,30,33    | 2.14 | 5 (23%)  |
| 7   | PSU  | A     | 516  | 7     | 18,21,22     | 0.99 | 1 (5%)   | 21,30,33    | 2.00 | 5 (23%)  |
| 18  | D2T  | L     | 89   | 18    | 8,9,10       | 1.78 | 2 (25%)  | 6,11,13     | 1.80 | 2 (33%)  |
| 39  | 4D4  | l     | 81   | 39    | 9,11,12      | 2.10 | 2 (22%)  | 7,13,15     | 2.19 | 3 (42%)  |
| 7   | 5MC  | A     | 967  | 7     | 19,22,23     | 1.28 | 2 (10%)  | 26,32,35    | 1.08 | 2 (7%)   |
| 31  | MEQ  | d     | 150  | 31    | 8,9,10       | 0.83 | 0        | 5,10,12     | 0.37 | 0        |
| 17  | BH2  | K     | 119  | 17    | 5,6,9        | 0.93 | 0        | 1,6,12      | 0.62 | 0        |
| 28  | OMG  | a     | 2251 | 28    | 23,26,27     | 0.77 | 1 (4%)   | 32,38,41    | 1.99 | 9 (28%)  |
| 28  | 2MG  | a     | 2445 | 28    | 23,26,27     | 0.91 | 2 (8%)   | 33,38,41    | 2.23 | 9 (27%)  |
| 28  | 2MA  | a     | 2503 | 55,28 | 22,25,26     | 1.30 | 3 (13%)  | 32,37,40    | 2.07 | 7 (21%)  |
| 28  | 5MC  | a     | 1962 | 28    | 19,22,23     | 1.53 | 2 (10%)  | 26,32,35    | 1.20 | 2 (7%)   |
| 7   | 2MG  | A     | 966  | 7     | 23,26,27     | 0.74 | 1 (4%)   | 33,38,41    | 2.21 | 10 (30%) |
| 7   | UR3  | A     | 1499 | 7     | 19,22,23     | 3.89 | 6 (31%)  | 26,32,35    | 4.65 | 11 (42%) |
| 7   | MA6  | A     | 1519 | 7     | 23,26,27     | 2.53 | 5 (21%)  | 33,38,41    | 2.80 | 7 (21%)  |
| 28  | PSU  | a     | 2605 | 28    | 18,21,22     | 1.13 | 2 (11%)  | 21,30,33    | 1.97 | 3 (14%)  |
| 28  | PSU  | a     | 955  | 28    | 18,21,22     | 1.16 | 3 (16%)  | 21,30,33    | 2.08 | 4 (19%)  |

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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 28  | PSU  | a     | 1911 | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 7   | 2MG  | A     | 1208 | 7     | -       | 0/9/27/28  | 0/3/3/3 |
| 28  | 6MZ  | a     | 2030 | 28    | -       | 2/9/27/28  | 0/3/3/3 |
| 28  | PSU  | a     | 746  | 55,28 | -       | 1/7/25/26  | 0/2/2/2 |
| 28  | OMU  | a     | 2552 | 28    | -       | 0/9/27/28  | 0/2/2/2 |
| 7   | 5MC  | A     | 1408 | 7     | -       | 0/7/25/26  | 0/2/2/2 |
| 7   | 4OC  | A     | 1403 | 7     | -       | 2/9/29/30  | 0/2/2/2 |
| 28  | 1MG  | a     | 745  | 28    | -       | 0/7/25/26  | 0/3/3/3 |
| 28  | H2U  | a     | 2449 | 28    | -       | 0/7/38/39  | 0/2/2/2 |
| 28  | PSU  | a     | 2604 | 28    | -       | 1/7/25/26  | 0/2/2/2 |
| 28  | G7M  | a     | 2069 | 28    | -       | 2/7/25/26  | 0/3/3/3 |
| 7   | MA6  | A     | 1520 | 7     | -       | 2/11/29/30 | 0/3/3/3 |
| 28  | 3TD  | a     | 1915 | -     | -       | 4/7/25/26  | 0/2/2/2 |
| 28  | 6MZ  | a     | 1618 | 28    | -       | 0/9/27/28  | 0/3/3/3 |
| 28  | OMC  | a     | 2498 | 55,28 | -       | 3/9/27/28  | 0/2/2/2 |
| 28  | 2MG  | a     | 1835 | 28    | -       | 0/9/27/28  | 0/3/3/3 |
| 28  | PSU  | a     | 2580 | 28    | -       | 1/7/25/26  | 0/2/2/2 |
| 7   | G7M  | A     | 527  | 7     | -       | 2/7/25/26  | 0/3/3/3 |
| 28  | PSU  | a     | 1917 | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | 5MU  | a     | 1939 | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | 5MU  | a     | 747  | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | MS6  | l     | 82   | 39    | -       | 2/4/6/8    | -       |
| 7   | 2MG  | A     | 1517 | 7     | -       | 0/9/27/28  | 0/3/3/3 |
| 28  | PSU  | a     | 2504 | 28    | -       | 2/7/25/26  | 0/2/2/2 |
| 28  | PSU  | a     | 2457 | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 7   | PSU  | A     | 516  | 7     | -       | 1/7/25/26  | 0/2/2/2 |
| 18  | D2T  | L     | 89   | 18    | -       | 5/7/12/14  | -       |
| 39  | 4D4  | l     | 81   | 39    | -       | 2/11/12/14 | -       |
| 7   | 5MC  | A     | 967  | 7     | -       | 1/7/25/26  | 0/2/2/2 |
| 31  | MEQ  | d     | 150  | 31    | -       | 3/8/9/11   | -       |
| 17  | BH2  | K     | 119  | 17    | 1/1/1/4 | 1/4/5/12   | -       |
| 28  | OMG  | a     | 2251 | 28    | -       | 1/9/27/28  | 0/3/3/3 |
| 28  | 2MG  | a     | 2445 | 28    | -       | 0/9/27/28  | 0/3/3/3 |
| 28  | 2MA  | a     | 2503 | 55,28 | -       | 2/7/25/26  | 0/3/3/3 |
| 28  | 5MC  | a     | 1962 | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 7   | 2MG  | A     | 966  | 7     | -       | 0/9/27/28  | 0/3/3/3 |
| 7   | UR3  | A     | 1499 | 7     | -       | 2/7/25/26  | 0/2/2/2 |
| 7   | MA6  | A     | 1519 | 7     | -       | 3/11/29/30 | 0/3/3/3 |
| 28  | PSU  | a     | 2605 | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | PSU  | a     | 955  | 28    | -       | 0/7/25/26  | 0/2/2/2 |

All (74) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | A     | 1499 | UR3  | C2-N1   | 13.96 | 1.57        | 1.38     |
| 7   | A     | 1520 | MA6  | C5-N7   | 7.70  | 1.53        | 1.39     |
| 7   | A     | 1519 | MA6  | C5-N7   | 7.66  | 1.53        | 1.39     |
| 7   | A     | 1499 | UR3  | C6-N1   | 6.20  | 1.52        | 1.38     |
| 7   | A     | 1499 | UR3  | C2-N3   | 5.71  | 1.50        | 1.39     |
| 7   | A     | 1519 | MA6  | C8-N9   | -5.59 | 1.28        | 1.37     |
| 7   | A     | 1520 | MA6  | C8-N9   | -5.46 | 1.28        | 1.37     |
| 28  | a     | 1962 | 5MC  | C5-C4   | -5.35 | 1.40        | 1.44     |
| 7   | A     | 1519 | MA6  | C4-N9   | -5.29 | 1.26        | 1.37     |
| 39  | l     | 81   | 4D4  | CZ-NE   | 5.23  | 1.43        | 1.33     |
| 7   | A     | 1520 | MA6  | C4-N9   | -5.07 | 1.27        | 1.37     |
| 7   | A     | 1408 | 5MC  | C5-C4   | -4.35 | 1.40        | 1.44     |
| 7   | A     | 967  | 5MC  | C5-C4   | -4.14 | 1.41        | 1.44     |
| 28  | a     | 2503 | 2MA  | C6-N1   | 3.72  | 1.40        | 1.35     |
| 28  | a     | 2030 | 6MZ  | C6-N6   | 3.56  | 1.38        | 1.34     |
| 18  | L     | 89   | D2T  | CB-CA   | -3.42 | 1.53        | 1.54     |
| 28  | a     | 1618 | 6MZ  | C6-N6   | 3.35  | 1.38        | 1.34     |
| 7   | A     | 1520 | MA6  | C6-N6   | 3.28  | 1.45        | 1.36     |
| 7   | A     | 1519 | MA6  | C6-N6   | 3.21  | 1.45        | 1.36     |
| 7   | A     | 1499 | UR3  | C6-C5   | -3.19 | 1.27        | 1.35     |
| 7   | A     | 1519 | MA6  | C8-N7   | 3.12  | 1.37        | 1.31     |
| 7   | A     | 1520 | MA6  | C8-N7   | 3.12  | 1.37        | 1.31     |
| 28  | a     | 2503 | 2MA  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 28  | a     | 745  | 1MG  | C6-N1   | -2.84 | 1.34        | 1.40     |
| 39  | l     | 81   | 4D4  | CZ-NH1  | 2.83  | 1.44        | 1.34     |
| 7   | A     | 1408 | 5MC  | C2-N1   | -2.81 | 1.34        | 1.40     |
| 28  | a     | 1939 | 5MU  | C2-N1   | -2.76 | 1.34        | 1.38     |
| 28  | a     | 1962 | 5MC  | C2-N1   | -2.73 | 1.34        | 1.40     |
| 28  | a     | 1915 | 3TD  | C4-N3   | -2.72 | 1.34        | 1.40     |
| 28  | a     | 2552 | OMU  | C2-N1   | -2.69 | 1.34        | 1.38     |
| 28  | a     | 747  | 5MU  | C2-N1   | -2.66 | 1.34        | 1.38     |
| 7   | A     | 967  | 5MC  | C2-N1   | -2.58 | 1.34        | 1.40     |
| 28  | a     | 2498 | OMC  | C2-N1   | -2.56 | 1.34        | 1.40     |
| 28  | a     | 2580 | PSU  | C2-N1   | -2.54 | 1.33        | 1.36     |
| 28  | a     | 2605 | PSU  | C2-N3   | -2.49 | 1.33        | 1.37     |
| 28  | a     | 746  | PSU  | O4'-C1' | -2.47 | 1.40        | 1.43     |
| 28  | a     | 955  | PSU  | C4-N3   | -2.42 | 1.34        | 1.38     |
| 28  | a     | 2580 | PSU  | O4'-C1' | -2.42 | 1.40        | 1.43     |
| 28  | a     | 2445 | 2MG  | C6-N1   | -2.38 | 1.34        | 1.38     |
| 28  | a     | 2552 | OMU  | C4-N3   | -2.38 | 1.34        | 1.38     |
| 28  | a     | 2604 | PSU  | C4-N3   | -2.37 | 1.34        | 1.38     |
| 28  | a     | 2605 | PSU  | C4-N3   | -2.36 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 28  | a     | 1939 | 5MU  | C4-C5   | -2.35 | 1.41        | 1.44     |
| 28  | a     | 1939 | 5MU  | C4-N3   | -2.32 | 1.34        | 1.38     |
| 28  | a     | 2580 | PSU  | C4-N3   | -2.31 | 1.34        | 1.38     |
| 28  | a     | 2503 | 2MA  | C5-C6   | 2.27  | 1.47        | 1.41     |
| 28  | a     | 1939 | 5MU  | C2-N3   | -2.27 | 1.34        | 1.38     |
| 28  | a     | 2552 | OMU  | C2-N3   | -2.27 | 1.34        | 1.38     |
| 28  | a     | 747  | 5MU  | C4-C5   | -2.26 | 1.41        | 1.44     |
| 28  | a     | 746  | PSU  | C4-N3   | -2.26 | 1.34        | 1.38     |
| 28  | a     | 747  | 5MU  | C4-N3   | -2.25 | 1.34        | 1.38     |
| 28  | a     | 1915 | 3TD  | C4-C5   | -2.23 | 1.42        | 1.47     |
| 28  | a     | 2457 | PSU  | C4-N3   | -2.22 | 1.34        | 1.38     |
| 28  | a     | 2604 | PSU  | C2-N3   | -2.21 | 1.33        | 1.37     |
| 28  | a     | 2030 | 6MZ  | C5-N7   | -2.20 | 1.35        | 1.39     |
| 28  | a     | 2457 | PSU  | C2-N1   | -2.20 | 1.33        | 1.36     |
| 28  | a     | 955  | PSU  | C2-N3   | -2.17 | 1.33        | 1.37     |
| 28  | a     | 2457 | PSU  | O4'-C1' | -2.13 | 1.40        | 1.43     |
| 28  | a     | 2504 | PSU  | C4-N3   | -2.13 | 1.34        | 1.38     |
| 28  | a     | 2251 | OMG  | C6-N1   | -2.12 | 1.34        | 1.38     |
| 28  | a     | 2604 | PSU  | C2-N1   | -2.11 | 1.33        | 1.36     |
| 7   | A     | 1499 | UR3  | O4-C4   | -2.11 | 1.19        | 1.23     |
| 7   | A     | 516  | PSU  | C4-N3   | -2.10 | 1.34        | 1.38     |
| 28  | a     | 1917 | PSU  | C4-N3   | -2.10 | 1.34        | 1.38     |
| 28  | a     | 1835 | 2MG  | C6-N1   | -2.09 | 1.34        | 1.38     |
| 7   | A     | 1499 | UR3  | O2-C2   | -2.08 | 1.18        | 1.22     |
| 28  | a     | 1618 | 6MZ  | C5-N7   | -2.08 | 1.35        | 1.39     |
| 28  | a     | 1911 | PSU  | C4-N3   | -2.07 | 1.35        | 1.38     |
| 28  | a     | 2457 | PSU  | C2-N3   | -2.05 | 1.34        | 1.37     |
| 7   | A     | 966  | 2MG  | C2-N2   | 2.05  | 1.37        | 1.33     |
| 18  | L     | 89   | D2T  | CB1-SB  | -2.05 | 1.75        | 1.79     |
| 28  | a     | 955  | PSU  | C2-N1   | -2.04 | 1.34        | 1.36     |
| 28  | a     | 2445 | 2MG  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 28  | a     | 746  | PSU  | C2-N3   | -2.00 | 1.34        | 1.37     |

All (200) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 7   | A     | 1499 | UR3  | C6-N1-C2 | -14.80 | 109.71      | 121.80   |
| 7   | A     | 1499 | UR3  | C4-N3-C2 | -14.23 | 113.13      | 124.58   |
| 7   | A     | 1519 | MA6  | C4-N9-C8 | 13.53  | 119.95      | 105.74   |
| 7   | A     | 1520 | MA6  | C4-N9-C8 | 13.38  | 119.79      | 105.74   |
| 28  | a     | 1835 | 2MG  | C2-N3-C4 | 7.68   | 121.60      | 112.00   |
| 7   | A     | 1499 | UR3  | C5-C4-N3 | 7.55   | 124.99      | 115.04   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 7   | A     | 1517 | 2MG  | C2-N3-C4  | 7.53  | 121.42      | 112.00   |
| 7   | A     | 966  | 2MG  | C2-N3-C4  | 7.42  | 121.29      | 112.00   |
| 7   | A     | 1208 | 2MG  | C2-N3-C4  | 7.34  | 121.18      | 112.00   |
| 28  | a     | 2445 | 2MG  | C2-N3-C4  | 7.34  | 121.18      | 112.00   |
| 28  | a     | 1915 | 3TD  | N1-C2-N3  | 6.52  | 120.87      | 116.13   |
| 28  | a     | 2503 | 2MA  | C5-C4-N3  | -6.29 | 120.56      | 127.18   |
| 28  | a     | 2580 | PSU  | N1-C2-N3  | 6.10  | 121.60      | 115.17   |
| 28  | a     | 2457 | PSU  | N1-C2-N3  | 5.89  | 121.38      | 115.17   |
| 28  | a     | 2251 | OMG  | C5-C4-N3  | -5.82 | 119.13      | 128.39   |
| 28  | a     | 955  | PSU  | N1-C2-N3  | 5.68  | 121.16      | 115.17   |
| 28  | a     | 2604 | PSU  | N1-C2-N3  | 5.64  | 121.12      | 115.17   |
| 28  | a     | 1618 | 6MZ  | C5-C4-N3  | -5.63 | 118.96      | 126.72   |
| 28  | a     | 2445 | 2MG  | C5-C4-N3  | -5.60 | 119.47      | 128.39   |
| 28  | a     | 2552 | OMU  | C4-N3-C2  | -5.60 | 119.67      | 126.61   |
| 28  | a     | 745  | 1MG  | C5-C4-N3  | -5.57 | 119.52      | 128.39   |
| 28  | a     | 1939 | 5MU  | C4-N3-C2  | -5.56 | 120.05      | 127.34   |
| 28  | a     | 1835 | 2MG  | C5-C4-N3  | -5.56 | 119.54      | 128.39   |
| 7   | A     | 1517 | 2MG  | C5-C4-N3  | -5.53 | 119.59      | 128.39   |
| 7   | A     | 1208 | 2MG  | C5-C4-N3  | -5.53 | 119.59      | 128.39   |
| 28  | a     | 1917 | PSU  | N1-C2-N3  | 5.49  | 120.96      | 115.17   |
| 7   | A     | 966  | 2MG  | C5-C4-N3  | -5.47 | 119.68      | 128.39   |
| 28  | a     | 1911 | PSU  | N1-C2-N3  | 5.47  | 120.94      | 115.17   |
| 28  | a     | 2030 | 6MZ  | C5-C4-N3  | -5.45 | 119.22      | 126.72   |
| 28  | a     | 746  | PSU  | N1-C2-N3  | 5.42  | 120.89      | 115.17   |
| 28  | a     | 2504 | PSU  | N1-C2-N3  | 5.36  | 120.82      | 115.17   |
| 28  | a     | 2552 | OMU  | N3-C2-N1  | 5.32  | 121.82      | 114.89   |
| 7   | A     | 516  | PSU  | N1-C2-N3  | 5.32  | 120.78      | 115.17   |
| 28  | a     | 747  | 5MU  | C4-N3-C2  | -5.28 | 120.42      | 127.34   |
| 28  | a     | 2605 | PSU  | N1-C2-N3  | 5.21  | 120.67      | 115.17   |
| 28  | a     | 2251 | OMG  | C2-N3-C4  | 5.17  | 121.20      | 112.30   |
| 28  | a     | 1939 | 5MU  | N3-C2-N1  | 4.97  | 121.36      | 114.89   |
| 28  | a     | 955  | PSU  | C4-N3-C2  | -4.95 | 119.55      | 126.37   |
| 28  | a     | 2503 | 2MA  | N3-C4-N9  | 4.95  | 133.27      | 126.99   |
| 28  | a     | 2605 | PSU  | C4-N3-C2  | -4.93 | 119.57      | 126.37   |
| 7   | A     | 1499 | UR3  | C1'-N1-C2 | 4.85  | 124.97      | 117.04   |
| 28  | a     | 2457 | PSU  | C4-N3-C2  | -4.77 | 119.80      | 126.37   |
| 28  | a     | 1618 | 6MZ  | C9-N6-C6  | -4.75 | 118.44      | 122.85   |
| 28  | a     | 747  | 5MU  | N3-C2-N1  | 4.71  | 121.02      | 114.89   |
| 28  | a     | 2604 | PSU  | C4-N3-C2  | -4.70 | 119.90      | 126.37   |
| 28  | a     | 746  | PSU  | C4-N3-C2  | -4.67 | 119.94      | 126.37   |
| 28  | a     | 2580 | PSU  | C4-N3-C2  | -4.63 | 120.00      | 126.37   |
| 28  | a     | 1911 | PSU  | C4-N3-C2  | -4.62 | 120.01      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 28  | a     | 1939 | 5MU  | C5-C4-N3  | 4.59  | 119.31      | 115.32   |
| 28  | a     | 2445 | 2MG  | N9-C4-N3  | 4.57  | 135.08      | 125.95   |
| 28  | a     | 747  | 5MU  | C5-C4-N3  | 4.55  | 119.27      | 115.32   |
| 28  | a     | 1618 | 6MZ  | N3-C4-N9  | 4.53  | 134.87      | 127.17   |
| 28  | a     | 1917 | PSU  | C4-N3-C2  | -4.52 | 120.15      | 126.37   |
| 28  | a     | 2251 | OMG  | N9-C4-N3  | 4.42  | 134.80      | 125.95   |
| 28  | a     | 2504 | PSU  | C4-N3-C2  | -4.38 | 120.34      | 126.37   |
| 28  | a     | 2030 | 6MZ  | N3-C4-N9  | 4.37  | 134.60      | 127.17   |
| 7   | A     | 516  | PSU  | C4-N3-C2  | -4.37 | 120.35      | 126.37   |
| 28  | a     | 747  | 5MU  | O4-C4-C5  | -4.24 | 120.06      | 124.92   |
| 7   | A     | 1208 | 2MG  | N9-C4-N3  | 4.18  | 134.32      | 125.95   |
| 28  | a     | 1939 | 5MU  | O4-C4-C5  | -4.17 | 120.15      | 124.92   |
| 7   | A     | 1517 | 2MG  | N9-C4-N3  | 4.15  | 134.26      | 125.95   |
| 28  | a     | 2503 | 2MA  | N6-C6-N1  | 4.14  | 122.62      | 117.03   |
| 28  | a     | 745  | 1MG  | C2-N3-C4  | 4.12  | 121.25      | 111.98   |
| 7   | A     | 966  | 2MG  | N9-C4-N3  | 4.12  | 134.19      | 125.95   |
| 28  | a     | 1618 | 6MZ  | N1-C2-N3  | -4.10 | 122.37      | 128.58   |
| 7   | A     | 1499 | UR3  | C3U-N3-C4 | 4.08  | 123.53      | 117.87   |
| 28  | a     | 2580 | PSU  | O2-C2-N1  | -4.06 | 118.60      | 122.79   |
| 28  | a     | 745  | 1MG  | N9-C4-N3  | 4.06  | 134.06      | 125.95   |
| 28  | a     | 1835 | 2MG  | N9-C4-N3  | 4.05  | 134.06      | 125.95   |
| 7   | A     | 1519 | MA6  | N9-C8-N7  | -4.05 | 108.19      | 113.94   |
| 7   | A     | 1520 | MA6  | N9-C8-N7  | -3.96 | 108.32      | 113.94   |
| 28  | a     | 1915 | 3TD  | C4-N3-C2  | -3.93 | 120.45      | 124.61   |
| 28  | a     | 2445 | 2MG  | C2-N1-C6  | -3.90 | 119.84      | 124.55   |
| 28  | a     | 2030 | 6MZ  | C5-N7-C8  | 3.87  | 109.53      | 103.45   |
| 28  | a     | 2030 | 6MZ  | N1-C2-N3  | -3.86 | 122.74      | 128.58   |
| 28  | a     | 2503 | 2MA  | C5-N7-C8  | 3.85  | 109.49      | 103.45   |
| 39  | l     | 81   | 4D4  | NE-CZ-NH2 | 3.79  | 127.19      | 120.67   |
| 7   | A     | 1517 | 2MG  | C2-N1-C6  | -3.77 | 119.99      | 124.55   |
| 28  | a     | 2030 | 6MZ  | C9-N6-C6  | -3.77 | 119.36      | 122.85   |
| 28  | a     | 1835 | 2MG  | C2-N1-C6  | -3.76 | 120.01      | 124.55   |
| 28  | a     | 1618 | 6MZ  | C5-N7-C8  | 3.74  | 109.33      | 103.45   |
| 28  | a     | 1618 | 6MZ  | C2-N3-C4  | 3.73  | 120.93      | 111.83   |
| 28  | a     | 2457 | PSU  | O2-C2-N1  | -3.72 | 118.96      | 122.79   |
| 28  | a     | 1962 | 5MC  | C5-C6-N1  | -3.70 | 119.29      | 123.31   |
| 7   | A     | 1519 | MA6  | C4-C5-N7  | -3.68 | 106.37      | 110.58   |
| 28  | a     | 2449 | H2U  | C5-C4-N3  | -3.65 | 112.81      | 116.69   |
| 7   | A     | 1408 | 5MC  | C5-C6-N1  | -3.60 | 119.40      | 123.31   |
| 28  | a     | 1939 | 5MU  | C5-C6-N1  | -3.57 | 119.43      | 123.31   |
| 7   | A     | 1208 | 2MG  | C2-N1-C6  | -3.57 | 120.23      | 124.55   |
| 28  | a     | 2030 | 6MZ  | C2-N3-C4  | 3.56  | 120.54      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | a     | 1915 | 3TD  | C1'-C5-C4   | 3.54  | 122.98      | 117.61   |
| 7   | A     | 967  | 5MC  | C5-C6-N1    | -3.54 | 119.47      | 123.31   |
| 39  | l     | 81   | 4D4  | O-C-CA      | -3.53 | 115.68      | 124.77   |
| 7   | A     | 966  | 2MG  | C2-N1-C6    | -3.52 | 120.30      | 124.55   |
| 7   | A     | 1520 | MA6  | C4-C5-N7    | -3.52 | 106.56      | 110.58   |
| 7   | A     | 1499 | UR3  | C3U-N3-C2   | 3.45  | 123.34      | 117.33   |
| 28  | a     | 2552 | OMU  | C5-C4-N3    | 3.40  | 119.57      | 114.80   |
| 28  | a     | 2503 | 2MA  | N9-C8-N7    | -3.34 | 109.19      | 113.94   |
| 7   | A     | 1519 | MA6  | C1'-N9-C8   | -3.33 | 119.71      | 127.09   |
| 28  | a     | 2604 | PSU  | O2-C2-N1    | -3.32 | 119.36      | 122.79   |
| 7   | A     | 1520 | MA6  | C1'-N9-C8   | -3.30 | 119.77      | 127.09   |
| 28  | a     | 2552 | OMU  | CM2-O2'-C2' | -3.30 | 106.01      | 114.47   |
| 28  | a     | 2504 | PSU  | O2-C2-N1    | -3.26 | 119.43      | 122.79   |
| 7   | A     | 1517 | 2MG  | N1-C2-N2    | 3.25  | 119.88      | 116.56   |
| 7   | A     | 516  | PSU  | O2-C2-N1    | -3.25 | 119.44      | 122.79   |
| 28  | a     | 2498 | OMC  | CM2-O2'-C2' | -3.24 | 106.15      | 114.47   |
| 7   | A     | 527  | G7M  | C8-N7-C5    | -3.22 | 103.76      | 107.78   |
| 28  | a     | 746  | PSU  | O2-C2-N1    | -3.15 | 119.54      | 122.79   |
| 28  | a     | 2030 | 6MZ  | C4-C5-N7    | -3.14 | 107.00      | 110.58   |
| 28  | a     | 1911 | PSU  | O2-C2-N1    | -3.14 | 119.56      | 122.79   |
| 28  | a     | 2498 | OMC  | O2-C2-N3    | -3.13 | 117.40      | 122.33   |
| 28  | a     | 2069 | G7M  | C8-N7-C5    | -3.13 | 103.87      | 107.78   |
| 28  | a     | 955  | PSU  | O2-C2-N1    | -3.12 | 119.57      | 122.79   |
| 28  | a     | 1917 | PSU  | O2-C2-N1    | -3.11 | 119.58      | 122.79   |
| 28  | a     | 1835 | 2MG  | N1-C2-N2    | 3.09  | 119.71      | 116.56   |
| 28  | a     | 1618 | 6MZ  | C4-C5-N7    | -3.01 | 107.14      | 110.58   |
| 28  | a     | 2580 | PSU  | C6-N1-C2    | -2.99 | 119.91      | 122.69   |
| 28  | a     | 2030 | 6MZ  | N9-C8-N7    | -2.94 | 109.77      | 113.94   |
| 28  | a     | 2251 | OMG  | C2-N1-C6    | -2.92 | 119.81      | 125.11   |
| 28  | a     | 747  | 5MU  | C5-C6-N1    | -2.91 | 120.15      | 123.31   |
| 18  | L     | 89   | D2T  | O-C-CA      | -2.88 | 117.37      | 124.77   |
| 7   | A     | 1208 | 2MG  | C8-N7-C5    | 2.87  | 109.37      | 104.26   |
| 28  | a     | 745  | 1MG  | C8-N7-C5    | 2.81  | 109.27      | 104.26   |
| 28  | a     | 2605 | PSU  | O2-C2-N1    | -2.80 | 119.91      | 122.79   |
| 7   | A     | 966  | 2MG  | C8-N7-C5    | 2.79  | 109.24      | 104.26   |
| 28  | a     | 2251 | OMG  | C8-N7-C5    | 2.78  | 109.21      | 104.26   |
| 28  | a     | 2445 | 2MG  | C8-N7-C5    | 2.77  | 109.20      | 104.26   |
| 28  | a     | 1835 | 2MG  | C8-N7-C5    | 2.76  | 109.17      | 104.26   |
| 28  | a     | 2552 | OMU  | O2-C2-N1    | -2.76 | 119.21      | 122.80   |
| 7   | A     | 966  | 2MG  | N1-C2-N2    | 2.74  | 119.36      | 116.56   |
| 7   | A     | 1517 | 2MG  | C8-N7-C5    | 2.74  | 109.14      | 104.26   |
| 28  | a     | 1939 | 5MU  | O2-C2-N1    | -2.70 | 119.28      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | A     | 1519 | MA6  | C4-N9-C1'   | -2.69 | 120.34      | 126.63   |
| 28  | a     | 1618 | 6MZ  | N9-C8-N7    | -2.69 | 110.12      | 113.94   |
| 28  | a     | 2503 | 2MA  | C4-C5-N7    | -2.66 | 107.53      | 110.58   |
| 7   | A     | 1520 | MA6  | C4-N9-C1'   | -2.65 | 120.43      | 126.63   |
| 7   | A     | 1519 | MA6  | C6-C5-N7    | 2.65  | 137.66      | 133.43   |
| 28  | a     | 2503 | 2MA  | C5-C6-N1    | -2.63 | 114.81      | 118.90   |
| 28  | a     | 2552 | OMU  | O4-C4-C5    | -2.59 | 120.70      | 125.16   |
| 28  | a     | 2457 | PSU  | C6-N1-C2    | -2.55 | 120.32      | 122.69   |
| 7   | A     | 1519 | MA6  | C2-N1-C6    | 2.52  | 117.98      | 111.83   |
| 7   | A     | 516  | PSU  | O4'-C1'-C2' | 2.48  | 108.59      | 105.15   |
| 7   | A     | 1520 | MA6  | C2-N1-C6    | 2.44  | 117.79      | 111.83   |
| 28  | a     | 747  | 5MU  | C1'-N1-C2   | 2.43  | 121.95      | 117.59   |
| 7   | A     | 1499 | UR3  | O4-C4-C5    | -2.39 | 117.56      | 124.35   |
| 7   | A     | 516  | PSU  | C6-N1-C2    | -2.39 | 120.47      | 122.69   |
| 28  | a     | 1835 | 2MG  | O6-C6-C5    | -2.38 | 120.24      | 126.53   |
| 7   | A     | 1499 | UR3  | O2-C2-N3    | -2.38 | 118.04      | 121.33   |
| 28  | a     | 1835 | 2MG  | CM2-N2-C2   | -2.38 | 118.54      | 123.65   |
| 28  | a     | 1917 | PSU  | C6-N1-C2    | -2.36 | 120.50      | 122.69   |
| 28  | a     | 2030 | 6MZ  | C6-C5-N7    | 2.35  | 134.99      | 132.43   |
| 7   | A     | 1517 | 2MG  | O6-C6-C5    | -2.35 | 120.33      | 126.53   |
| 28  | a     | 2251 | OMG  | CM2-O2'-C2' | -2.35 | 108.45      | 114.47   |
| 7   | A     | 1520 | MA6  | C6-C5-N7    | 2.32  | 137.13      | 133.43   |
| 28  | a     | 745  | 1MG  | C6-C5-N7    | 2.31  | 134.50      | 129.36   |
| 28  | a     | 1618 | 6MZ  | C6-C5-N7    | 2.31  | 134.95      | 132.43   |
| 28  | a     | 1835 | 2MG  | C6-C5-N7    | 2.30  | 134.48      | 130.29   |
| 7   | A     | 1408 | 5MC  | C5-C4-N3    | -2.27 | 119.43      | 121.75   |
| 28  | a     | 745  | 1MG  | C4-C5-N7    | -2.26 | 107.09      | 110.67   |
| 7   | A     | 966  | 2MG  | O6-C6-C5    | -2.25 | 120.59      | 126.53   |
| 28  | a     | 2580 | PSU  | O4'-C1'-C2' | 2.25  | 108.26      | 105.15   |
| 18  | L     | 89   | D2T  | CB-CA-N     | 2.22  | 113.60      | 109.10   |
| 28  | a     | 2445 | 2MG  | C5-C6-N1    | 2.22  | 118.89      | 113.25   |
| 28  | a     | 2445 | 2MG  | O6-C6-C5    | -2.21 | 120.69      | 126.53   |
| 39  | l     | 81   | 4D4  | NH1-CZ-NE   | -2.21 | 114.24      | 119.27   |
| 7   | A     | 1517 | 2MG  | CM2-N2-C2   | -2.21 | 118.90      | 123.65   |
| 7   | A     | 1208 | 2MG  | N1-C2-N2    | 2.21  | 118.82      | 116.56   |
| 28  | a     | 2457 | PSU  | O4'-C1'-C2' | 2.21  | 108.21      | 105.15   |
| 28  | a     | 1835 | 2MG  | C5-C6-N1    | 2.19  | 118.83      | 113.25   |
| 28  | a     | 1835 | 2MG  | C4-C5-N7    | -2.19 | 107.21      | 110.67   |
| 28  | a     | 2504 | PSU  | C6-N1-C2    | -2.18 | 120.67      | 122.69   |
| 7   | A     | 1208 | 2MG  | O6-C6-C5    | -2.18 | 120.79      | 126.53   |
| 28  | a     | 2445 | 2MG  | N9-C8-N7    | -2.17 | 109.37      | 113.40   |
| 7   | A     | 1499 | UR3  | C6-C5-C4    | 2.17  | 124.88      | 120.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | A     | 1499 | UR3  | O2-C2-N1    | -2.16 | 117.97      | 122.78   |
| 7   | A     | 966  | 2MG  | C4-C5-N7    | -2.14 | 107.28      | 110.67   |
| 28  | a     | 2445 | 2MG  | CM2-N2-C2   | -2.14 | 119.05      | 123.65   |
| 7   | A     | 1208 | 2MG  | C4-C5-N7    | -2.14 | 107.29      | 110.67   |
| 28  | a     | 1917 | PSU  | O4'-C1'-C2' | 2.13  | 108.10      | 105.15   |
| 28  | a     | 2604 | PSU  | C6-N1-C2    | -2.13 | 120.72      | 122.69   |
| 28  | a     | 1911 | PSU  | C6-N1-C2    | -2.13 | 120.72      | 122.69   |
| 7   | A     | 1499 | UR3  | C1'-N1-C6   | 2.12  | 125.31      | 120.78   |
| 28  | a     | 955  | PSU  | C6-N1-C2    | -2.12 | 120.72      | 122.69   |
| 28  | a     | 1962 | 5MC  | O2-C2-N3    | -2.11 | 119.01      | 122.33   |
| 28  | a     | 2251 | OMG  | O6-C6-C5    | -2.11 | 120.97      | 126.53   |
| 7   | A     | 1517 | 2MG  | C5-C6-N1    | 2.11  | 118.62      | 113.25   |
| 7   | A     | 1408 | 5MC  | O2-C2-N3    | -2.10 | 119.01      | 122.33   |
| 7   | A     | 966  | 2MG  | C6-C5-N7    | 2.10  | 134.11      | 130.29   |
| 7   | A     | 1208 | 2MG  | C6-C5-N7    | 2.10  | 134.10      | 130.29   |
| 28  | a     | 2251 | OMG  | C4-C5-N7    | -2.08 | 107.38      | 110.67   |
| 28  | a     | 747  | 5MU  | O2-C2-N1    | -2.07 | 120.10      | 122.80   |
| 7   | A     | 1517 | 2MG  | C4-C5-N7    | -2.06 | 107.41      | 110.67   |
| 7   | A     | 967  | 5MC  | C5-C4-N3    | -2.06 | 119.65      | 121.75   |
| 7   | A     | 1208 | 2MG  | C5-C6-N1    | 2.05  | 118.48      | 113.25   |
| 28  | a     | 2251 | OMG  | C5-C6-N1    | 2.05  | 118.48      | 113.25   |
| 28  | a     | 2069 | G7M  | CN7-N7-C8   | 2.05  | 127.90      | 124.79   |
| 7   | A     | 1517 | 2MG  | C6-C5-N7    | 2.04  | 134.01      | 130.29   |
| 7   | A     | 1403 | 4OC  | O4'-C4'-C3' | -2.04 | 101.11      | 105.15   |
| 7   | A     | 966  | 2MG  | C5-C6-N1    | 2.02  | 118.40      | 113.25   |
| 28  | a     | 746  | PSU  | C6-N1-C2    | -2.01 | 120.82      | 122.69   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 17  | K     | 119 | BH2  | CB   |

All (45) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | L     | 89   | D2T  | O-C-CA-CB       |
| 18  | L     | 89   | D2T  | CG-CB-SB-CB1    |
| 7   | A     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 17  | K     | 119  | BH2  | CA-CB-CG-OD1    |
| 28  | a     | 1915 | 3TD  | O4'-C1'-C5-C4   |
| 28  | a     | 1915 | 3TD  | O4'-C1'-C5-C6   |
| 28  | a     | 2251 | OMG  | C1'-C2'-O2'-CM2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 7   | A     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 7   | A     | 1403 | 4OC  | C3'-C4'-C5'-O5' |
| 28  | a     | 2498 | OMC  | O4'-C4'-C5'-O5' |
| 39  | l     | 82   | MS6  | CA-CB-CG-SD     |
| 7   | A     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 28  | a     | 1915 | 3TD  | C3'-C4'-C5'-O5' |
| 28  | a     | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 28  | a     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 31  | d     | 150  | MEQ  | CA-CB-CG-CD     |
| 28  | a     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 28  | a     | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 7   | A     | 516  | PSU  | C4'-C5'-O5'-P   |
| 28  | a     | 2498 | OMC  | C3'-C4'-C5'-O5' |
| 7   | A     | 1520 | MA6  | C5-C6-N6-C10    |
| 7   | A     | 1499 | UR3  | O4'-C4'-C5'-O5' |
| 39  | l     | 82   | MS6  | CB-CG-SD-CE     |
| 31  | d     | 150  | MEQ  | OE1-CD-CG-CB    |
| 7   | A     | 1403 | 4OC  | O4'-C4'-C5'-O5' |
| 31  | d     | 150  | MEQ  | NE2-CD-CG-CB    |
| 28  | a     | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 39  | l     | 81   | 4D4  | CA-CB-CG-CD     |
| 18  | L     | 89   | D2T  | SB-CB-CG-OD1    |
| 7   | A     | 1520 | MA6  | O4'-C4'-C5'-O5' |
| 39  | l     | 81   | 4D4  | OB-CB-CG-CD     |
| 28  | a     | 2069 | G7M  | C4'-C5'-O5'-P   |
| 7   | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 7   | A     | 1499 | UR3  | C3'-C4'-C5'-O5' |
| 7   | A     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 7   | A     | 967  | 5MC  | C4'-C5'-O5'-P   |
| 28  | a     | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 28  | a     | 2580 | PSU  | O4'-C4'-C5'-O5' |
| 18  | L     | 89   | D2T  | SB-CB-CG-OD2    |
| 28  | a     | 2503 | 2MA  | C3'-C4'-C5'-O5' |
| 28  | a     | 2604 | PSU  | O4'-C4'-C5'-O5' |
| 28  | a     | 746  | PSU  | O4'-C1'-C5-C6   |
| 18  | L     | 89   | D2T  | CA-CB-CG-OD2    |
| 28  | a     | 2498 | OMC  | C2'-C1'-N1-C2   |
| 28  | a     | 2069 | G7M  | O4'-C4'-C5'-O5' |

There are no ring outliers.

8 monomers are involved in 10 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 7   | A     | 1403 | 4OC  | 3       | 0            |
| 7   | A     | 1520 | MA6  | 1       | 0            |
| 28  | a     | 1917 | PSU  | 1       | 0            |
| 7   | A     | 1517 | 2MG  | 1       | 0            |
| 18  | L     | 89   | D2T  | 1       | 0            |
| 7   | A     | 967  | 5MC  | 2       | 0            |
| 28  | a     | 2251 | OMG  | 1       | 0            |
| 7   | A     | 1519 | MA6  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 289 ligands modelled in this entry, 274 are monoatomic - leaving 15 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 57  | SPM  | a     | 6221 | -    | 13,13,13     | 0.34 | 0           | 12,12,12    | 0.90 | 0           |
| 56  | SPD  | a     | 6211 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.76 | 0           |
| 56  | SPD  | a     | 6219 | -    | 9,9,9        | 0.36 | 0           | 8,8,8       | 0.82 | 0           |
| 56  | SPD  | a     | 6210 | -    | 9,9,9        | 0.31 | 0           | 8,8,8       | 0.85 | 0           |
| 56  | SPD  | a     | 6213 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.83 | 0           |
| 56  | SPD  | a     | 6209 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.70 | 0           |
| 56  | SPD  | a     | 6214 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.96 | 0           |
| 56  | SPD  | a     | 6215 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.82 | 0           |
| 56  | SPD  | a     | 6220 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.79 | 0           |
| 56  | SPD  | a     | 6208 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.77 | 0           |
| 56  | SPD  | a     | 6212 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.81 | 0           |
| 56  | SPD  | a     | 6218 | -    | 9,9,9        | 0.29 | 0           | 8,8,8       | 0.83 | 0           |
| 56  | SPD  | a     | 6216 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.83 | 0           |
| 56  | SPD  | a     | 6217 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.83 | 0           |
| 56  | SPD  | a     | 6207 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.81 | 0           |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 57  | SPM  | a     | 6221 | -    | -       | 3/11/11/11 | -     |
| 56  | SPD  | a     | 6211 | -    | -       | 0/7/7/7    | -     |
| 56  | SPD  | a     | 6219 | -    | -       | 2/7/7/7    | -     |
| 56  | SPD  | a     | 6210 | -    | -       | 0/7/7/7    | -     |
| 56  | SPD  | a     | 6213 | -    | -       | 1/7/7/7    | -     |
| 56  | SPD  | a     | 6209 | -    | -       | 2/7/7/7    | -     |
| 56  | SPD  | a     | 6214 | -    | -       | 1/7/7/7    | -     |
| 56  | SPD  | a     | 6215 | -    | -       | 2/7/7/7    | -     |
| 56  | SPD  | a     | 6220 | -    | -       | 1/7/7/7    | -     |
| 56  | SPD  | a     | 6208 | -    | -       | 3/7/7/7    | -     |
| 56  | SPD  | a     | 6212 | -    | -       | 2/7/7/7    | -     |
| 56  | SPD  | a     | 6218 | -    | -       | 1/7/7/7    | -     |
| 56  | SPD  | a     | 6216 | -    | -       | 2/7/7/7    | -     |
| 56  | SPD  | a     | 6217 | -    | -       | 3/7/7/7    | -     |
| 56  | SPD  | a     | 6207 | -    | -       | 3/7/7/7    | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 57  | a     | 6221 | SPM  | N10-C11-C12-C13 |
| 56  | a     | 6209 | SPD  | C8-C7-N6-C5     |
| 56  | a     | 6215 | SPD  | C8-C7-N6-C5     |
| 57  | a     | 6221 | SPM  | N5-C6-C7-C8     |
| 56  | a     | 6208 | SPD  | C4-C5-N6-C7     |
| 56  | a     | 6208 | SPD  | N1-C2-C3-C4     |
| 56  | a     | 6208 | SPD  | C2-C3-C4-C5     |
| 56  | a     | 6207 | SPD  | N6-C7-C8-C9     |
| 56  | a     | 6216 | SPD  | N1-C2-C3-C4     |
| 56  | a     | 6212 | SPD  | N1-C2-C3-C4     |
| 56  | a     | 6214 | SPD  | C2-C3-C4-C5     |
| 56  | a     | 6216 | SPD  | C2-C3-C4-C5     |
| 56  | a     | 6217 | SPD  | N6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 56  | a     | 6213 | SPD  | N1-C2-C3-C4     |
| 56  | a     | 6217 | SPD  | C7-C8-C9-N10    |
| 57  | a     | 6221 | SPM  | C11-C12-C13-N14 |
| 56  | a     | 6217 | SPD  | N1-C2-C3-C4     |
| 56  | a     | 6218 | SPD  | N6-C7-C8-C9     |
| 56  | a     | 6212 | SPD  | C2-C3-C4-C5     |
| 56  | a     | 6220 | SPD  | C2-C3-C4-C5     |
| 56  | a     | 6215 | SPD  | C2-C3-C4-C5     |
| 56  | a     | 6207 | SPD  | C4-C5-N6-C7     |
| 56  | a     | 6209 | SPD  | C4-C5-N6-C7     |
| 56  | a     | 6219 | SPD  | C2-C3-C4-C5     |
| 56  | a     | 6207 | SPD  | N1-C2-C3-C4     |
| 56  | a     | 6219 | SPD  | C7-C8-C9-N10    |

There are no ring outliers.

10 monomers are involved in 13 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57  | a     | 6221 | SPM  | 1       | 0            |
| 56  | a     | 6211 | SPD  | 2       | 0            |
| 56  | a     | 6219 | SPD  | 1       | 0            |
| 56  | a     | 6210 | SPD  | 2       | 0            |
| 56  | a     | 6214 | SPD  | 2       | 0            |
| 56  | a     | 6215 | SPD  | 1       | 0            |
| 56  | a     | 6220 | SPD  | 1       | 0            |
| 56  | a     | 6208 | SPD  | 1       | 0            |
| 56  | a     | 6218 | SPD  | 1       | 0            |
| 56  | a     | 6217 | SPD  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 7   | A     | 3                |
| 28  | a     | 2                |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 18  | L     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1267:G    | O3'    | 1271:G    | P      | 15.18        |
| 1     | A     | 840:C     | O3'    | 846:G     | P      | 13.53        |
| 1     | A     | 204:G     | O3'    | 214:C     | P      | 10.50        |
| 1     | a     | 1914:C    | O3'    | 1915:3TD  | P      | 5.23         |
| 1     | a     | 1915:3TD  | O3'    | 1916:A    | P      | 4.29         |
| 1     | L     | 89:D2T    | C      | 90:LEU    | N      | 3.30         |

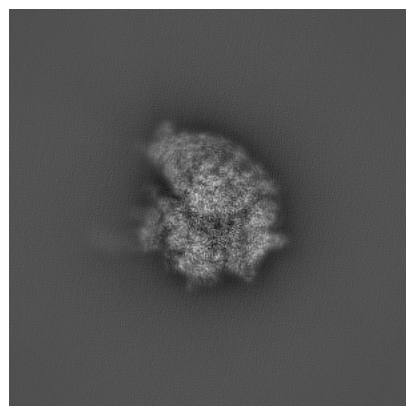
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75634. These allow visual inspection of the internal detail of the map and identification of artifacts.

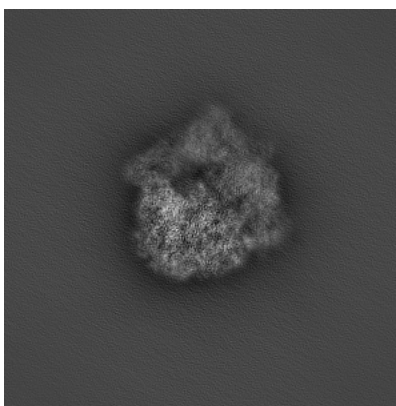
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

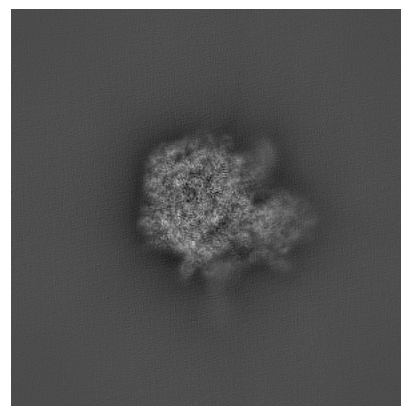
#### 6.1.1 Primary map



X

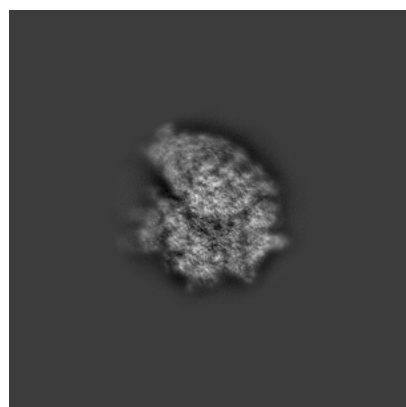


Y

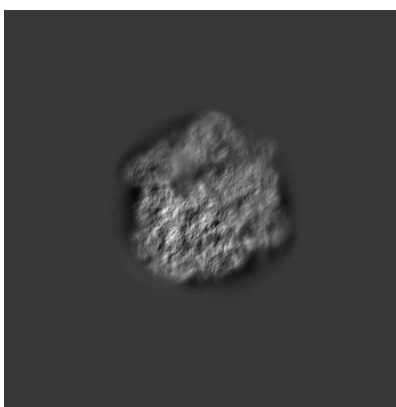


Z

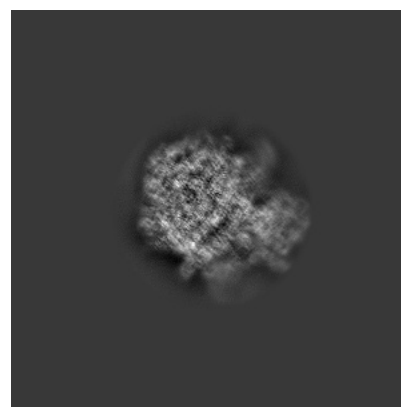
#### 6.1.2 Raw map



X



Y

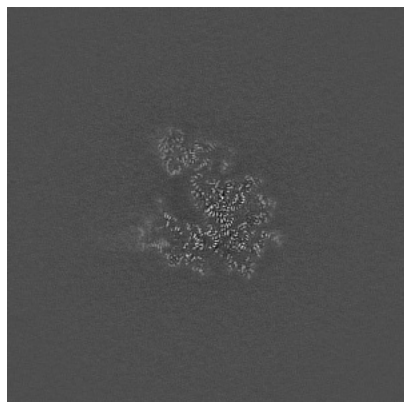


Z

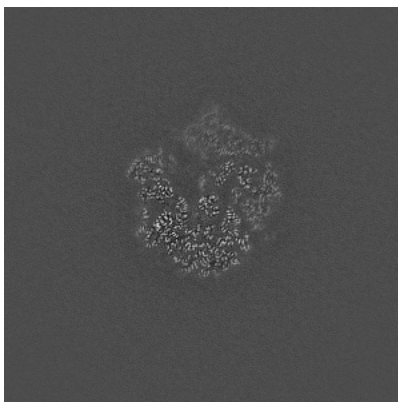
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

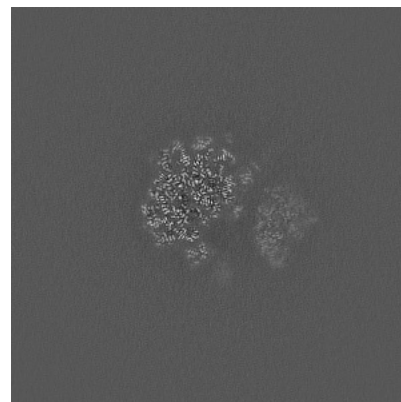
### 6.2.1 Primary map



X Index: 240

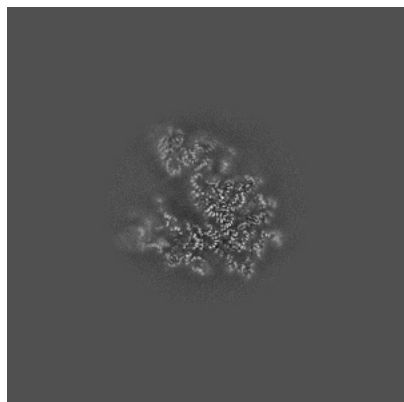


Y Index: 240

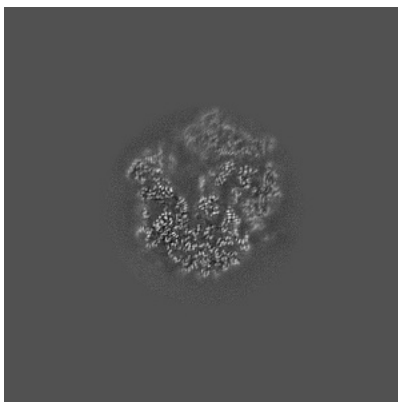


Z Index: 240

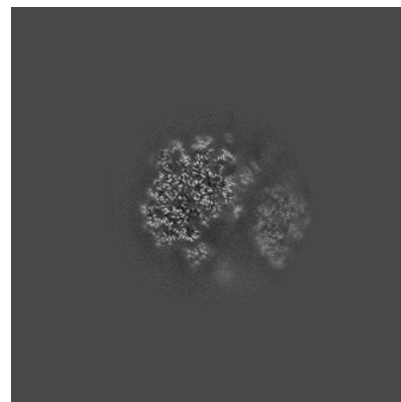
### 6.2.2 Raw map



X Index: 240



Y Index: 240

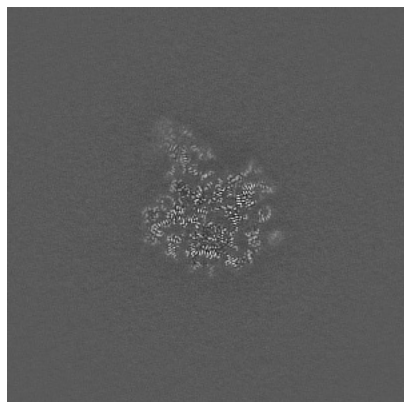


Z Index: 240

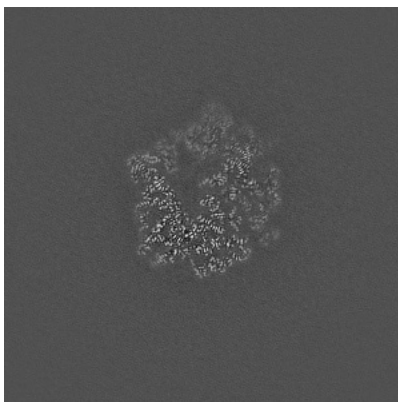
The images above show central slices of the map in three orthogonal directions.

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

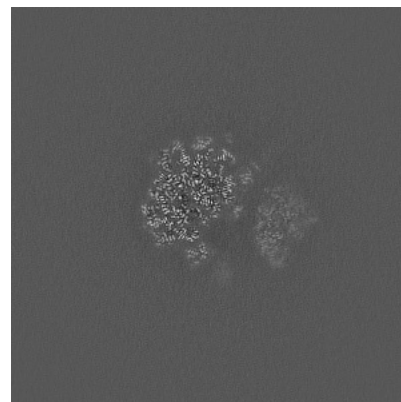
### 6.3.1 Primary map



X Index: 218

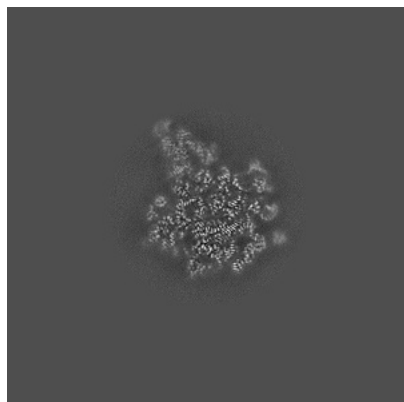


Y Index: 234

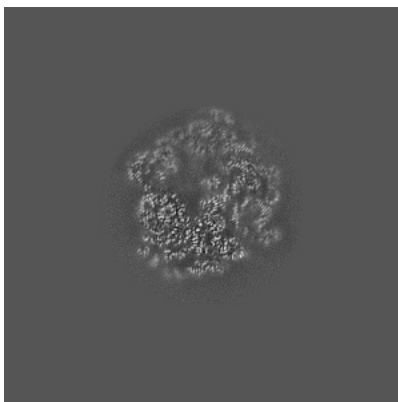


Z Index: 240

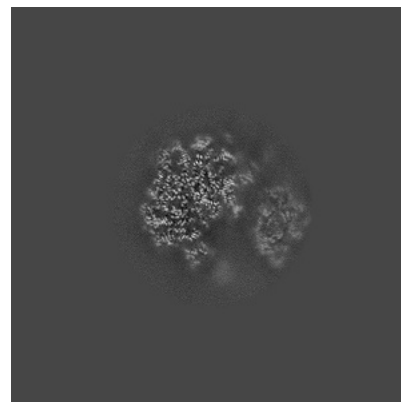
### 6.3.2 Raw map



X Index: 224



Y Index: 229

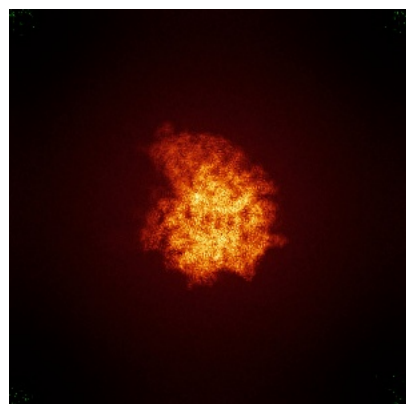


Z Index: 239

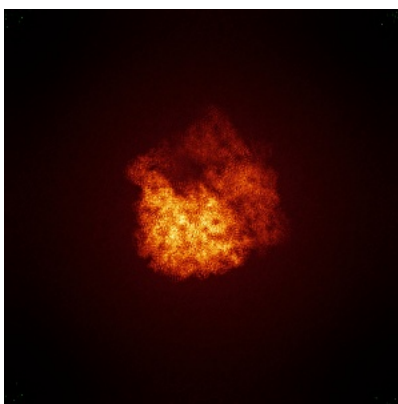
The images above show the largest variance slices of the map in three orthogonal directions.

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

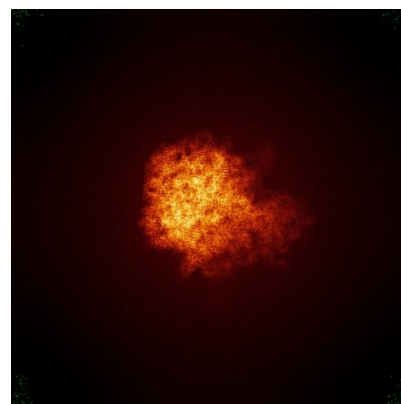
### 6.4.1 Primary map



X

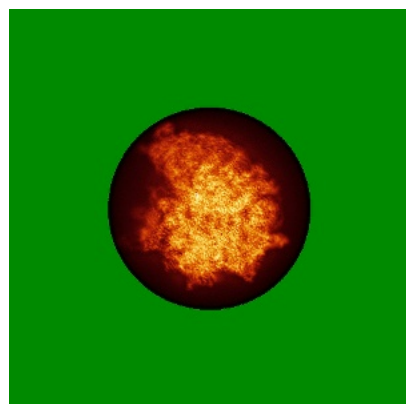


Y

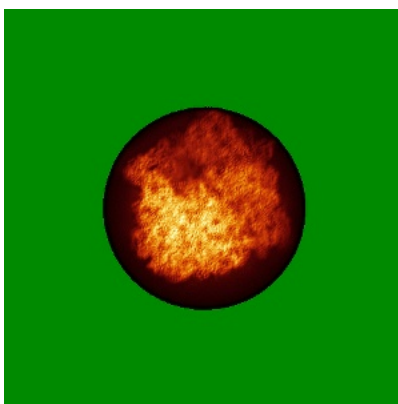


Z

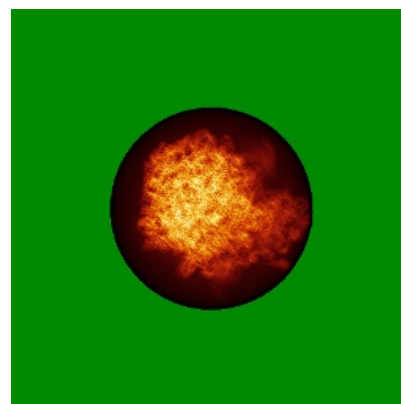
### 6.4.2 Raw map



X



Y



Z

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

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

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

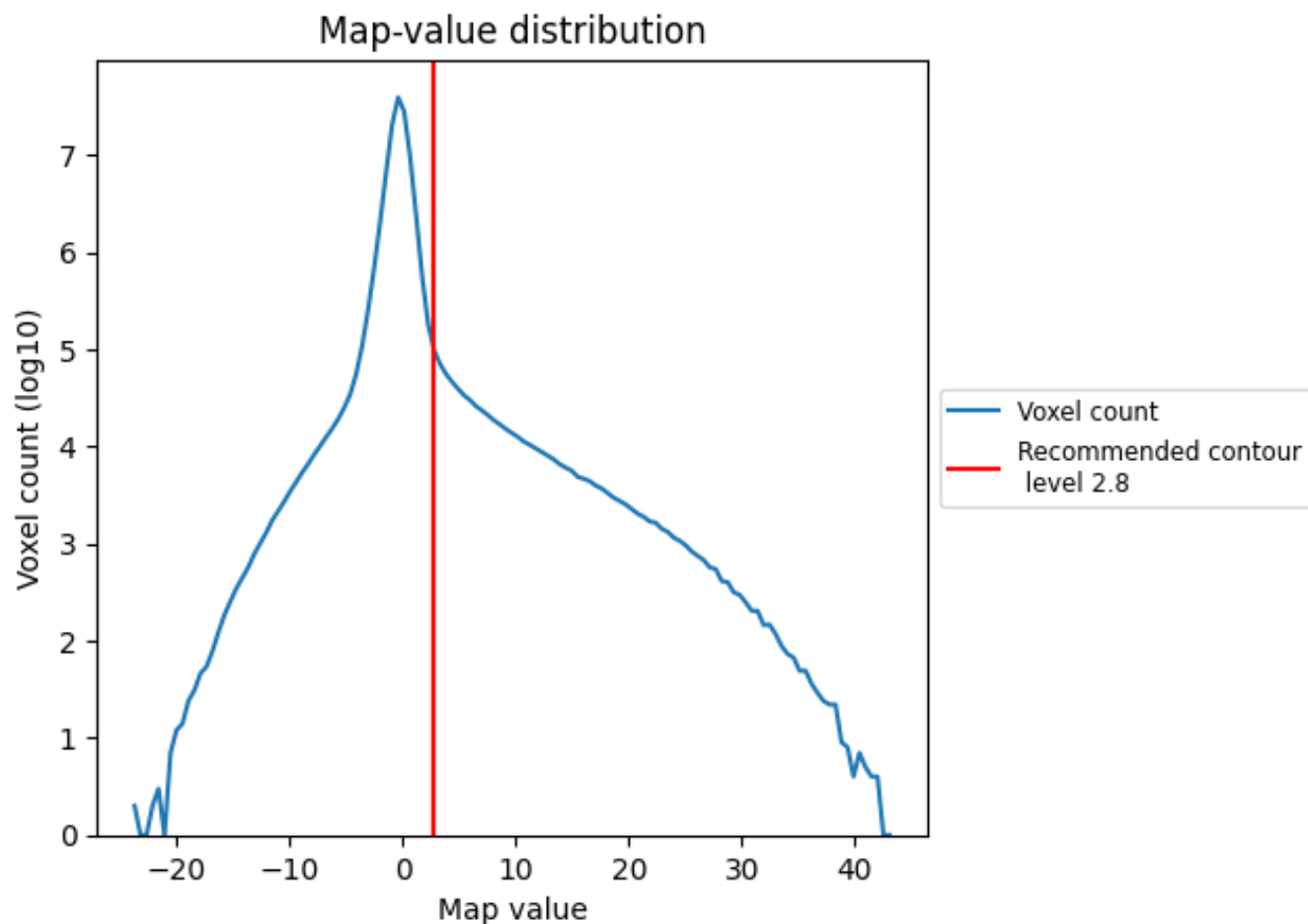
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

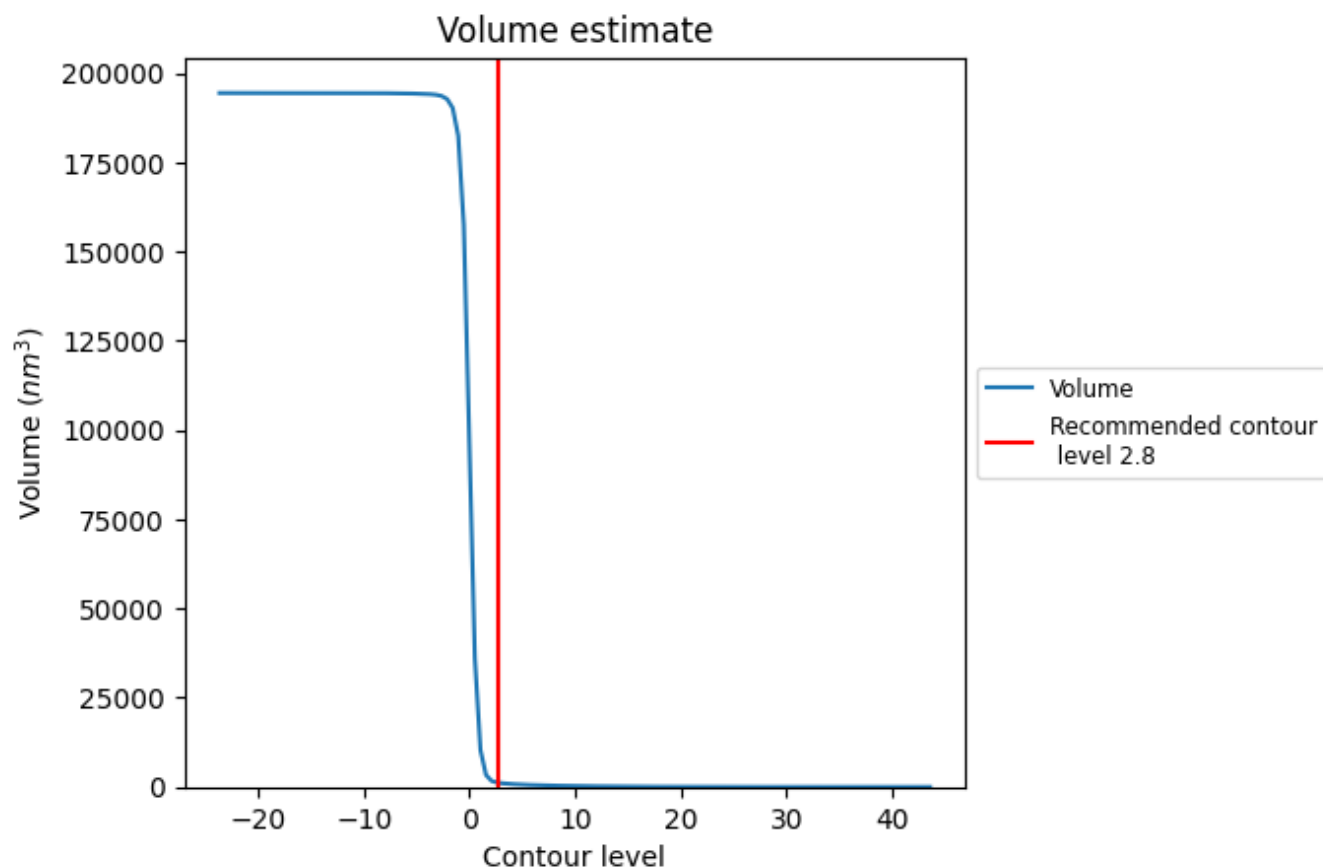
This section contains the results of statistical analysis of the map.

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



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

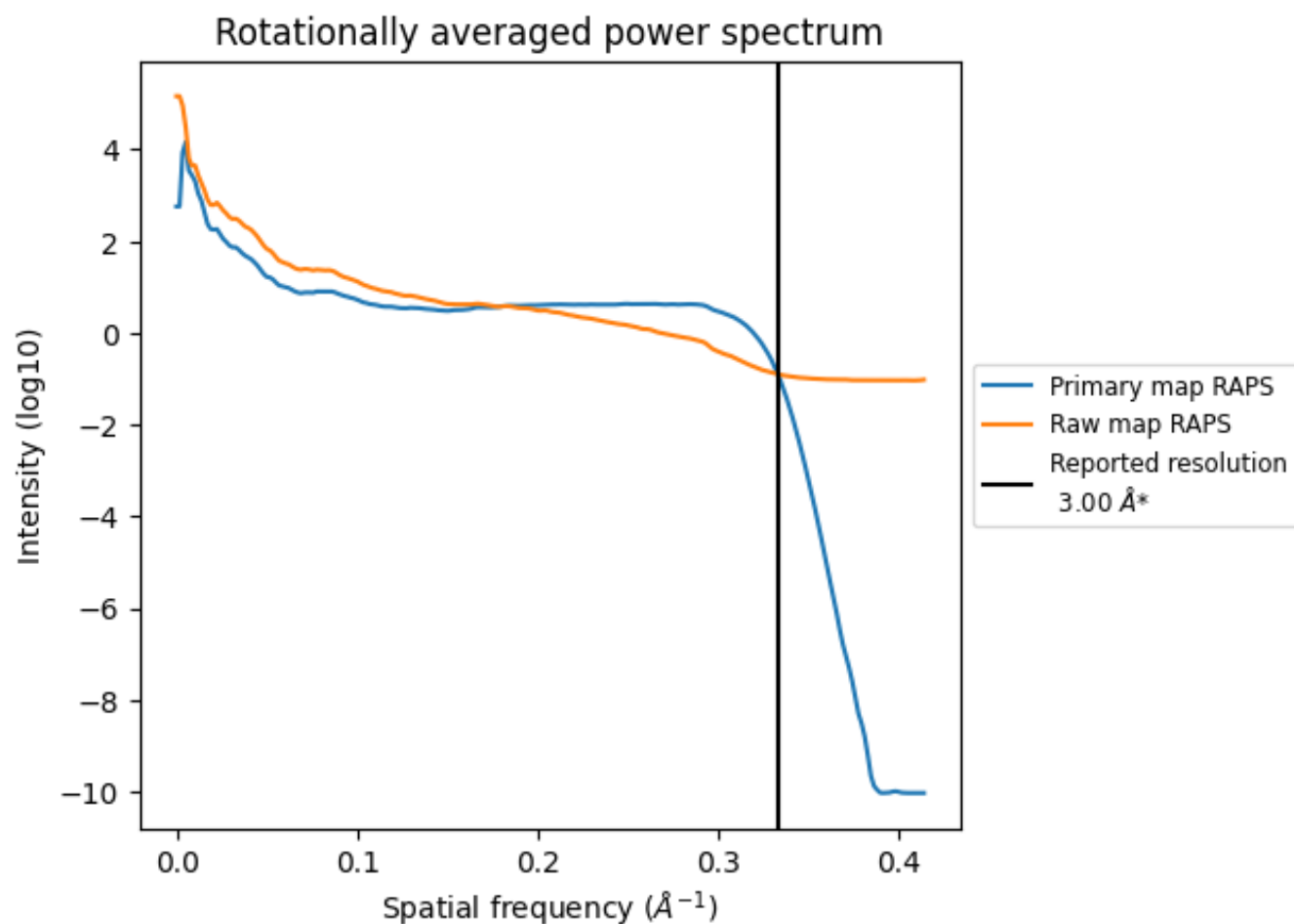
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1155  $\text{nm}^3$ ; this corresponds to an approximate mass of 1044 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 ⓘ

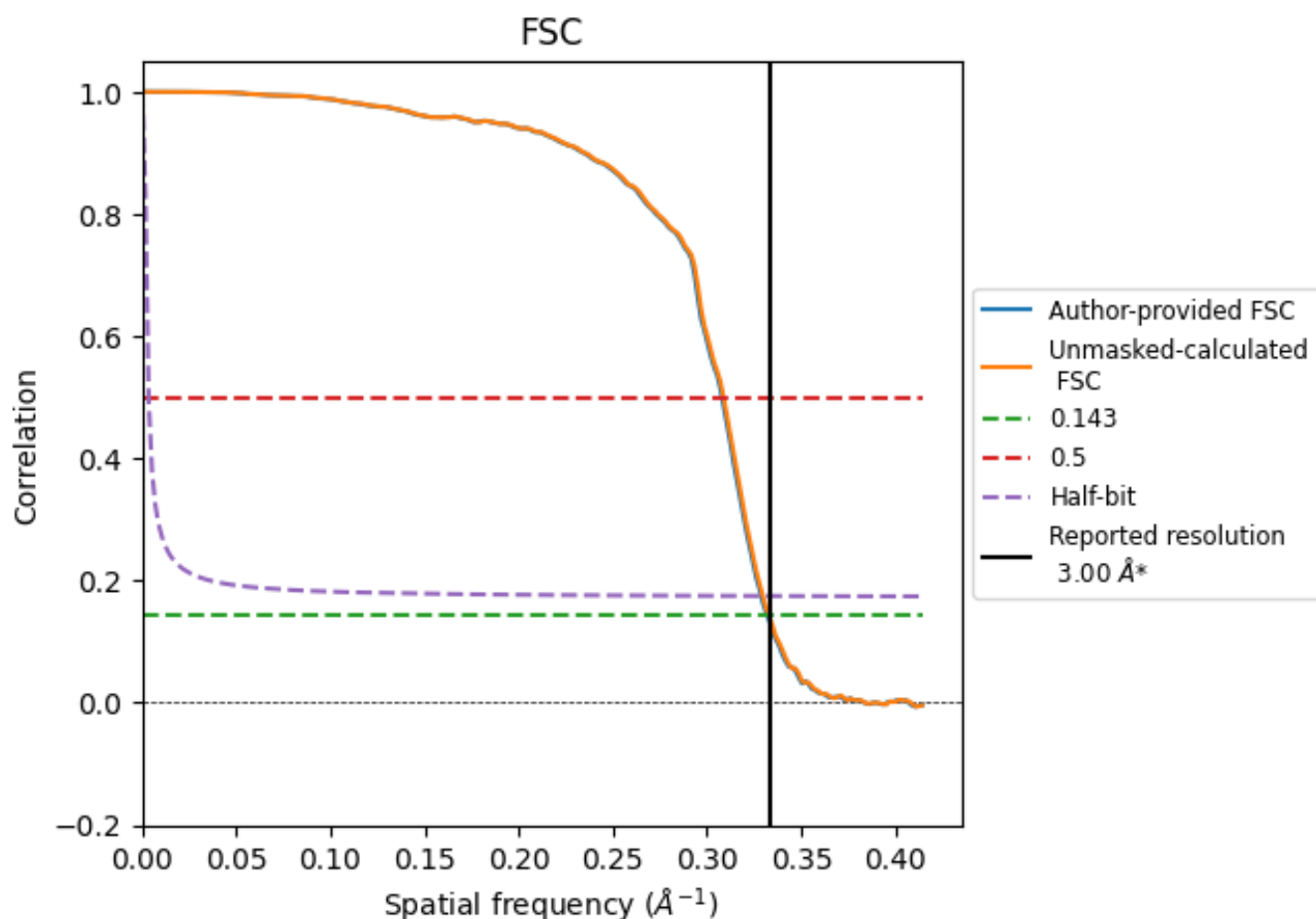


\*Reported resolution corresponds to spatial frequency of 0.333  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

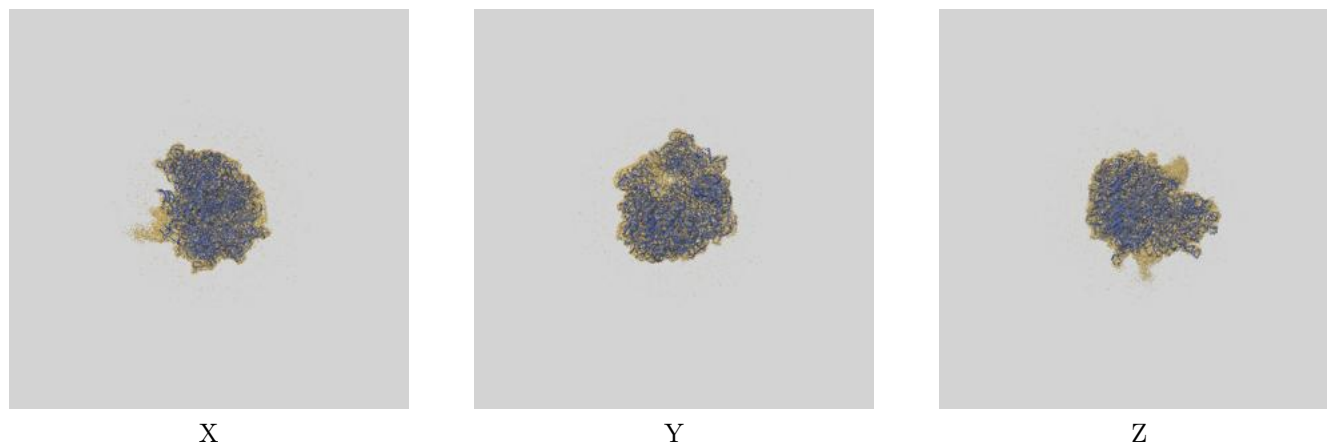
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.00                               | -    | -        |
| Author-provided FSC curve | 3.01                               | 3.25 | 3.04     |
| Unmasked-calculated*      | 3.00                               | 3.24 | 3.03     |

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

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

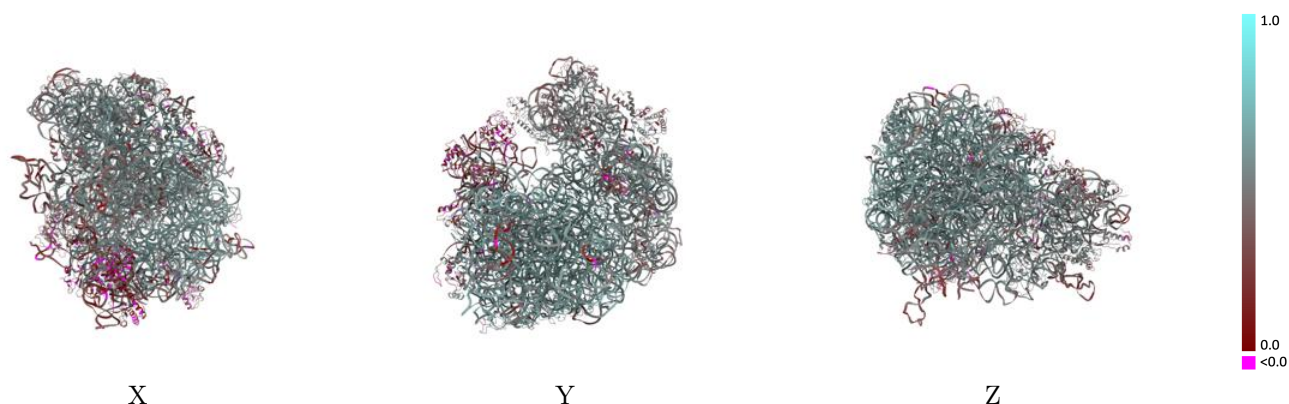
This section contains information regarding the fit between EMDB map EMD-75634 and PDB model 11DG. Per-residue inclusion information can be found in section 3 on page 17.

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



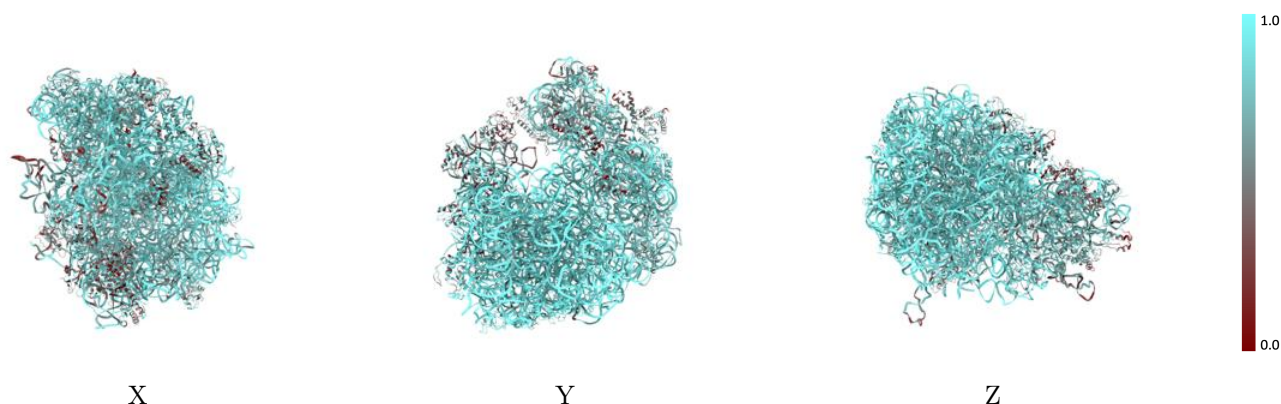
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



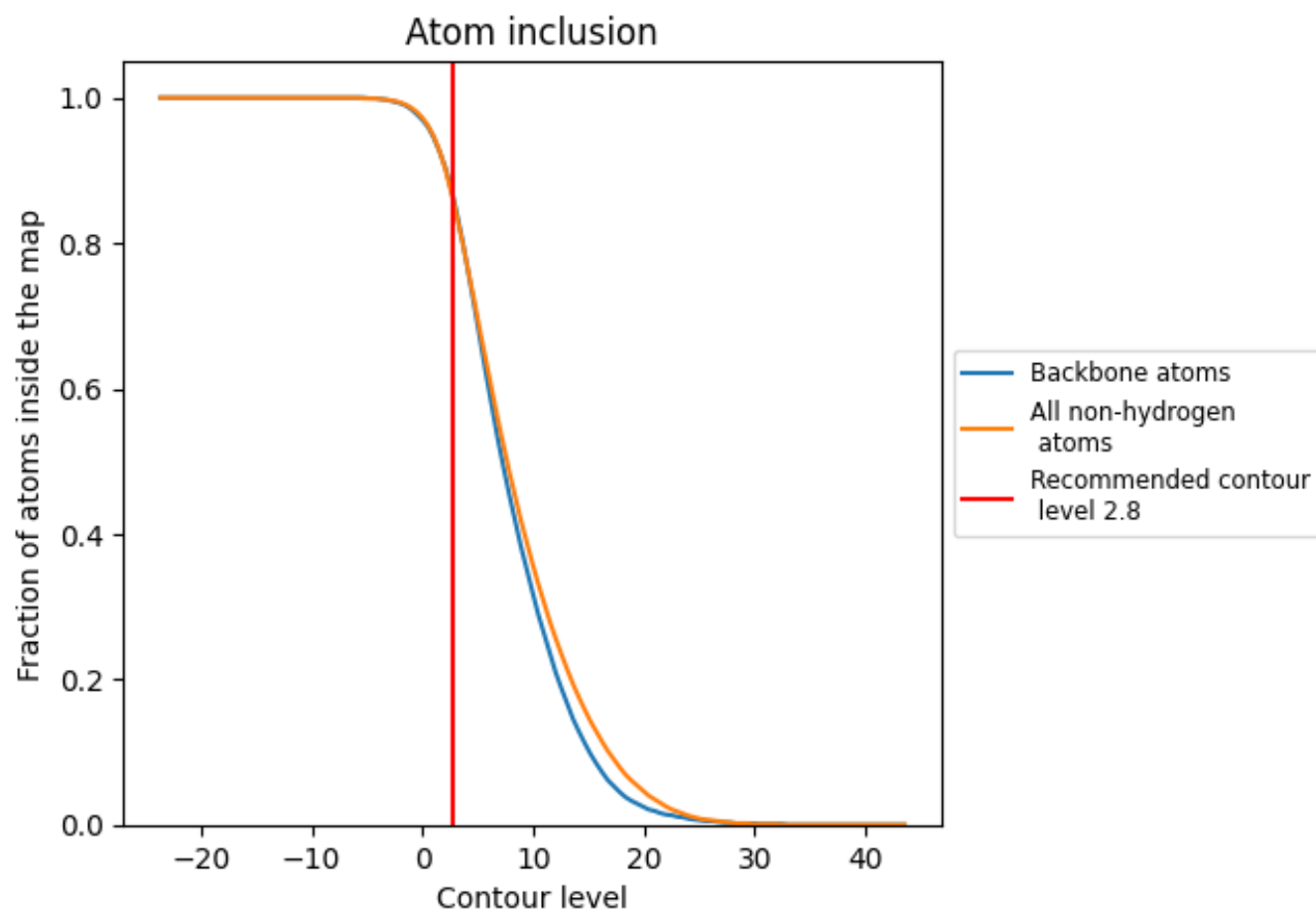
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.8).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (2.8) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8590   |  0.5060   |
| 0     |  0.5280   |  0.2890   |
| 1     |  0.9270   |  0.6130   |
| 2     |  0.8900   |  0.5760   |
| 3     |  0.6210   |  0.2870   |
| 4     |  0.4700   |  0.2220   |
| 5     |  0.5950   |  0.5370   |
| A     |  0.8880   |  0.5080   |
| B     |  0.5610   |  0.4390   |
| C     |  0.6610   |  0.4910   |
| D     |  0.6900   |  0.4990   |
| E     |  0.8300   |  0.5460   |
| F     |  0.5260   |  0.2720   |
| G     |  0.4750   |  0.4070   |
| H     |  0.8370  |  0.5570  |
| I     |  0.7250 |  0.4660 |
| J     |  0.5270 |  0.4340 |
| K     |  0.8120 |  0.5110 |
| L     |  0.8450 |  0.5510 |
| M     |  0.5470 |  0.3970 |
| N     |  0.7430 |  0.5010 |
| O     |  0.7670 |  0.4440 |
| P     |  0.7810 |  0.5160 |
| Q     |  0.7870 |  0.5260 |
| R     |  0.7250 |  0.3960 |
| S     |  0.5910 |  0.4310 |
| T     |  0.7940 |  0.5150 |
| U     |  0.3560 |  0.3510 |
| a     |  0.9390 |  0.5480 |
| b     |  0.6440 |  0.2780 |
| c     |  0.9470 |  0.6030 |
| d     |  0.8730 |  0.5300 |
| e     |  0.8300 |  0.4840 |
| f     |  0.4530 |  0.1560 |
| g     |  0.5260 |  0.2010 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| h     |  0.7770   |  0.4560   |
| i     |  0.8360   |  0.4950   |
| j     |  0.8980   |  0.5870   |
| k     |  0.8070   |  0.4540   |
| l     |  0.8740   |  0.5310   |
| m     |  0.9590   |  0.5990   |
| n     |  0.4790   |  0.1840   |
| o     |  0.9060   |  0.5830   |
| p     |  0.8140   |  0.4450   |
| q     |  0.7590   |  0.4290   |
| r     |  0.8950   |  0.5820   |
| s     |  0.9040   |  0.5680   |
| t     |  0.8630   |  0.5180   |
| u     |  0.5150   |  0.1950   |
| v     |  0.7900   |  0.4710   |
| w     |  0.9270   |  0.5860   |
| x     |  0.8610   |  0.5300   |
| y     |  0.8720  |  0.5210  |
| z     |  0.9040 |  0.5920 |