



## Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 08:10 AM UTC

PDB ID : 9FY2 / pdb\_00009fy2  
EMDB ID : EMD-50856  
Title : Structure of CliM-stalled Bacillus subtilis 70S ribosome with empty A-site  
Authors : Gersteuer, F.; Wilson, D.N.  
Deposited on : 2024-07-02  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
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) : 2.49

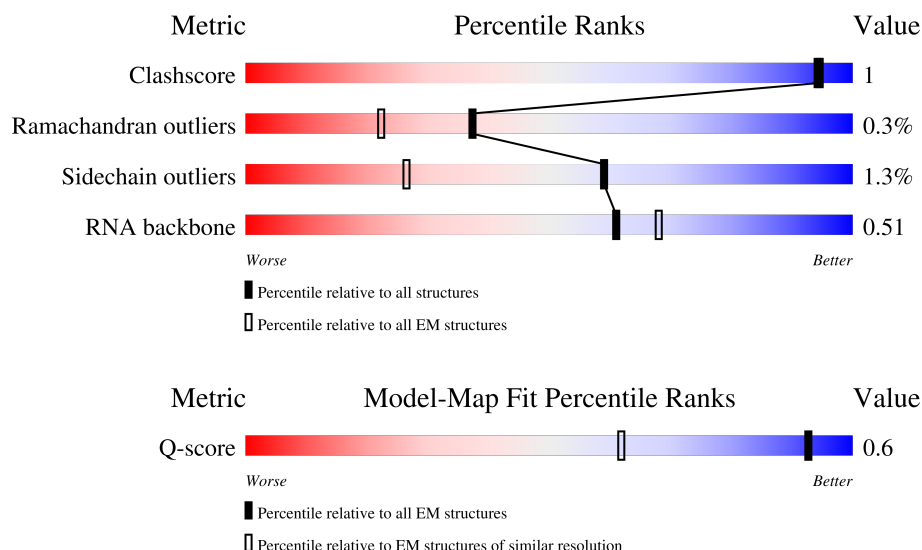
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 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.









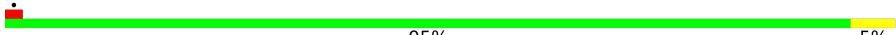




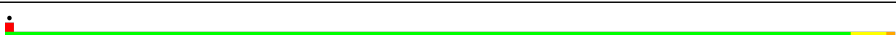

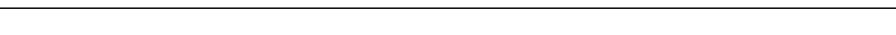
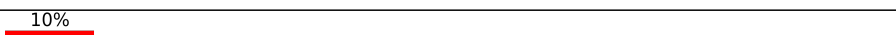
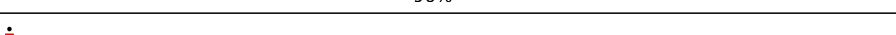
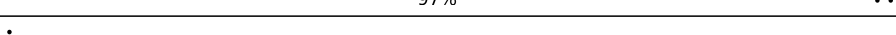
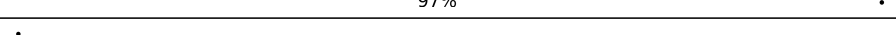
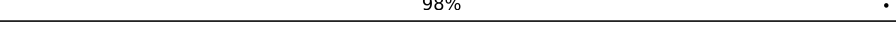

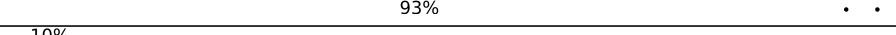
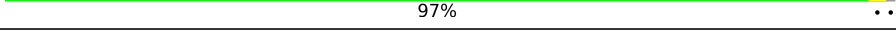


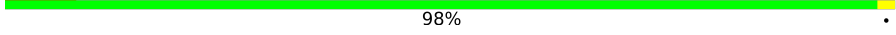
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| RNA backbone          | 8273                        | 3508                        | -  |
| Q-score               | -                           | 25397                       | 4254 ( 1.80 - 2.80 )                                     |

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     | 59     |                  |
| 2   | 1     | 49     |                  |
| 3   | 2     | 44     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | 3     | 66     |    |
| 5   | 4     | 37     |    |
| 6   | 6     | 66     |    |
| 7   | B     | 112    |    |
| 8   | C     | 277    |    |
| 9   | D     | 209    |    |
| 10  | E     | 207    |    |
| 11  | F     | 179    |    |
| 12  | G     | 179    |    |
| 13  | J     | 145    |    |
| 14  | K     | 122    |    |
| 15  | L     | 146    |    |
| 16  | M     | 144    |  |
| 17  | N     | 120    |  |
| 18  | O     | 120    |  |
| 19  | P     | 115    |  |
| 20  | Q     | 119    |  |
| 21  | R     | 102    |  |
| 22  | S     | 113    |  |
| 23  | T     | 95     |  |
| 24  | U     | 103    |  |
| 25  | W     | 94     |  |
| 26  | X     | 62     |  |
| 27  | Y     | 66     |  |
| 28  | Z     | 59     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | c     | 218    |                  |
| 30  | e     | 166    |                  |
| 31  | f     | 95     |                  |
| 32  | g     | 156    |                  |
| 33  | h     | 132    |                  |
| 34  | i     | 130    |                  |
| 35  | j     | 102    |                  |
| 36  | k     | 131    |                  |
| 37  | l     | 138    |                  |
| 38  | m     | 121    |                  |
| 39  | n     | 61     |                  |
| 40  | o     | 89     |                  |
| 41  | p     | 90     |                  |
| 42  | q     | 87     |                  |
| 43  | r     | 79     |                  |
| 44  | t     | 88     |                  |
| 45  | v     | 76     |                  |
| 46  | A     | 2928   |                  |
| 47  | b     | 246    |                  |
| 48  | s     | 92     |                  |
| 49  | 5     | 38     |                  |
| 50  | 7     | 6      |                  |
| 51  | a     | 1554   |                  |
| 52  | d     | 200    |                  |

## 2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 137121 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 Large ribosomal subunit protein bL32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 0     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 432   | 267 | 87 | 72 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 0     | 11      | VAL      | MET    | conflict | UNP O34687 |

- Molecule 2 is a protein called 50S ribosomal protein L33 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 403   | 245 | 81 | 74 | 3 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 368   | 222 | 89 | 55 | 2 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 4   | 3     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 512   | 321 | 107 | 82 | 2 |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 297   | 186 | 60 | 46 | 5 |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | 6     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 356   | 222 | 63 | 66 | 5 |         |       |

- Molecule 7 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 7   | B     | 112      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2392  | 1068 | 435 | 778 | 111 |         |       |

- Molecule 8 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | C     | 273      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2093  | 1301 | 412 | 374 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 216     | VAL      | ILE    | conflict | UNP P42919 |

- Molecule 9 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | D     | 207      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1575  | 988 | 290 | 292 | 5 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | E     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1567  | 983 | 290 | 292 | 2 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | F     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1405  | 893 | 245 | 260 | 7 |         |       |

- Molecule 12 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | G     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1342  | 835 | 248 | 257 | 2 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | J     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1131  | 714 | 207 | 205 | 5 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | K     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 921   | 571 | 173 | 173 | 4 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | L     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1082  | 671 | 207 | 202 | 2 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | M     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1076  | 690 | 205 | 176 | 5 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | N     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 954   | 583 | 186 | 181 | 4 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | O     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 913   | 564 | 176 | 172 | 1 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 19  | P     | 114      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 937   | 595 | 184 | 158 |         |       |

- Molecule 20 is a protein called Large ribosomal subunit protein bL20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | Q     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 597 | 191 | 158 | 4 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | R     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 795   | 506 | 140 | 148 | 1 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | S     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 850   | 530 | 165 | 151 | 4 |         |       |

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | T     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 733   | 458 | 135 | 137 | 3 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | U     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 770   | 482 | 143 | 141 | 4 |         |       |

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 25  | W     | 82       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 629   | 390 | 123 | 116 |         |       |

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.



| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | X     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 467   | 288 | 98 | 79 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| X     | 33      | VAL      | LEU    | conflict | UNP P37807 |

- Molecule 27 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Y     | 66       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 540   | 334 | 104 | 100 | 2 |         |       |

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | Z     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 456   | 281 | 89 | 85 | 1 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29  | c     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1004 | 302 | 299 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| c     | 148     | ILE      | VAL    | conflict | UNP P21465 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1219  | 767 | 225 | 225 | 2 |         |       |

- Molecule 31 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | f     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 482 | 136 | 145 | 2 |         |       |

- Molecule 32 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | g     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1199  | 751 | 225 | 217 | 6 |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1030  | 650 | 190 | 187 | 3 |         |       |

- Molecule 34 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | i     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 618 | 198 | 180 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| i     | 72      | PHE      | LEU    | conflict | UNP P21470 |

- Molecule 35 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | j     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 788   | 497 | 144 | 145 | 2 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | k     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 847   | 520 | 166 | 159 | 2 |         |       |

- Molecule 37 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | l     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1036  | 642 | 208 | 184 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 1     | 2       | ALA      | PRO    | conflict | UNP P21472 |

- Molecule 38 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 38  | m     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 934   | 573 | 192 | 169 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| m     | 33      | ILE      | VAL    | conflict | UNP P20282 |

- Molecule 39 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | n     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 498   | 317 | 98 | 78 | 5 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | o     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 730   | 448 | 149 | 132 | 1 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | p     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 691   | 439 | 127 | 123 | 2 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | q     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 438 | 128 | 125 | 2 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | r     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 522   | 334 | 97 | 89 | 2 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | t     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 658   | 402 | 134 | 121 | 1 |         |       |

- Molecule 45 is a RNA chain called P-site tRNA-Phe.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 45  | v     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1622  | 723 | 290 | 533 | 76 |         |       |

- Molecule 46 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 46  | A     | 2729     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 58630 | 26158 | 10860 | 18885 | 2727 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | b     | 195      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1564  | 996 | 277 | 285 | 6 |         |       |

- Molecule 48 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | s     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 680   | 435 | 126 | 117 | 2 |         |       |

- Molecule 49 is a protein called Nascent Chain CliM.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | 5     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 346   | 232 | 56 | 57 | 1 |         |       |

- Molecule 50 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 50  | 7     | 6        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 123   | 55 | 15 | 47 | 6 |         |       |

- Molecule 51 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 51  | a     | 1509     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32391 | 14444 | 5959 | 10479 | 1509 |         |       |

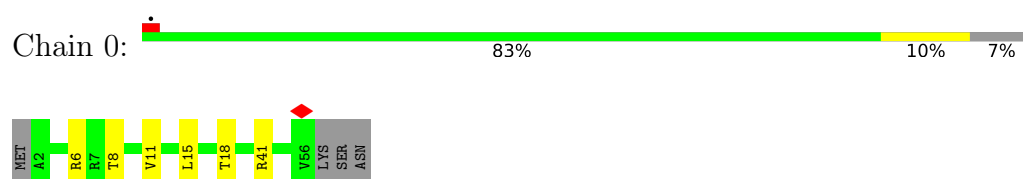
- Molecule 52 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | d     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1604  | 1013 | 298 | 291 | 2 |         |       |

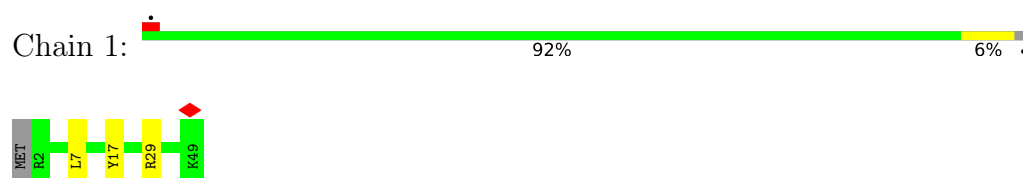
### 3 Residue-property plots [i](#)

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.

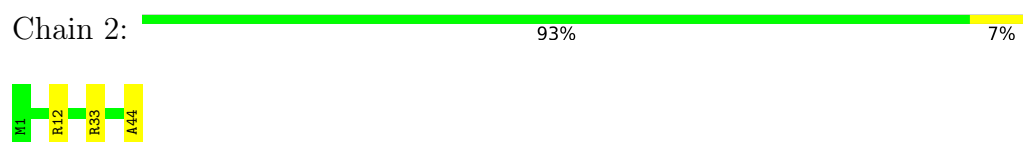
- Molecule 1: Large ribosomal subunit protein bL32



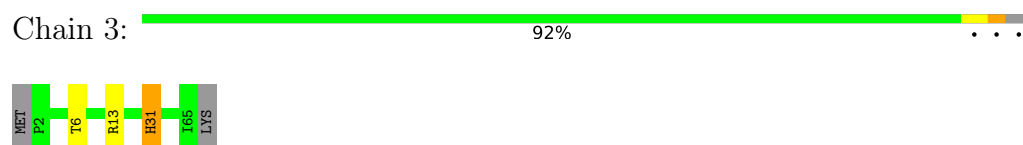
- Molecule 2: 50S ribosomal protein L33 1



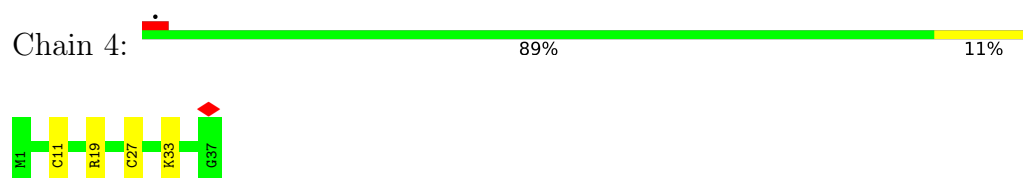
- Molecule 3: 50S ribosomal protein L34



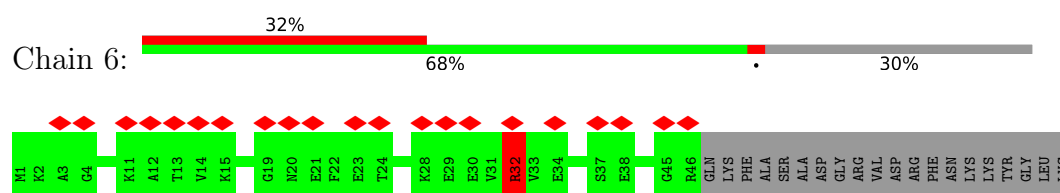
- Molecule 4: 50S ribosomal protein L35



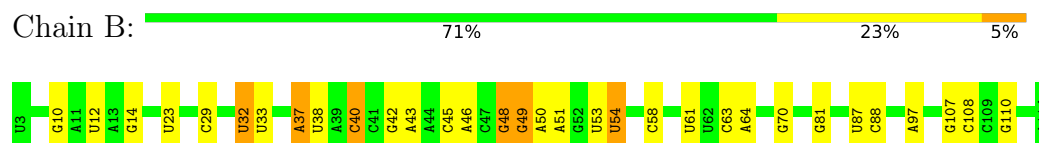
- Molecule 5: 50S ribosomal protein L36



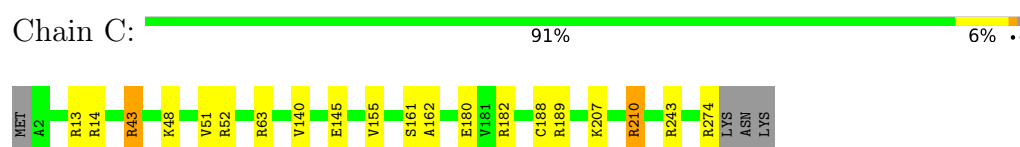
- Molecule 6: 50S ribosomal protein L31



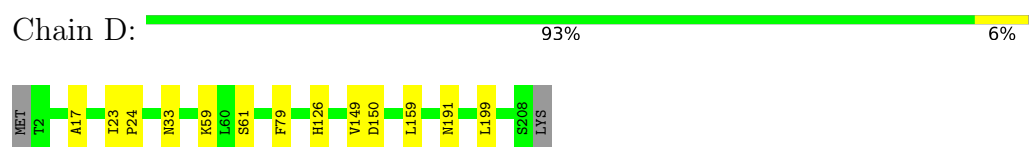
- Molecule 7: 5S rRNA



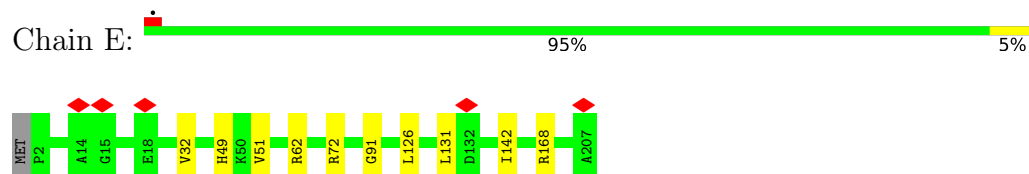
- Molecule 8: Large ribosomal subunit protein uL2



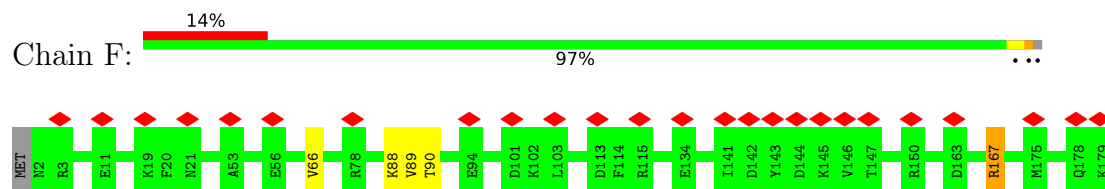
- Molecule 9: 50S ribosomal protein L3



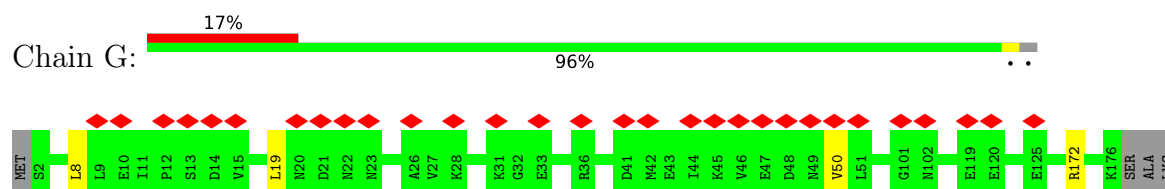
- Molecule 10: 50S ribosomal protein L4



- Molecule 11: 50S ribosomal protein L5



- Molecule 12: Large ribosomal subunit protein uL6



- Molecule 13: 50S ribosomal protein L13

Chain J:  96% ..



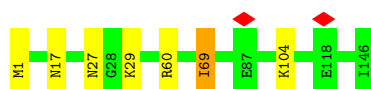
- Molecule 14: 50S ribosomal protein L14

Chain K:  91% 9%



- Molecule 15: 50S ribosomal protein L15

Chain L:  95% ..




- Molecule 16: 50S ribosomal protein L16

Chain M:  89% 5% 6%



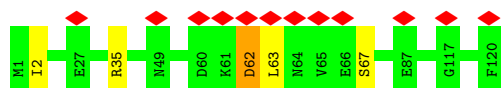
- Molecule 17: 50S ribosomal protein L17

Chain N:  88% 10% ..



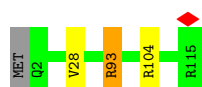
- Molecule 18: 50S ribosomal protein L18

Chain O:  10% 96% ..



- Molecule 19: 50S ribosomal protein L19

Chain P:  97% ...





- Molecule 20: Large ribosomal subunit protein bL20

Chain Q:  97% ..



- Molecule 21: 50S ribosomal protein L21

Chain R:  98% .

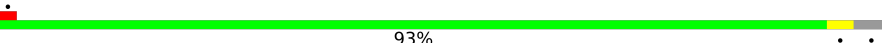


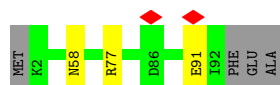
- Molecule 22: 50S ribosomal protein L22

Chain S:  89% 7% ..



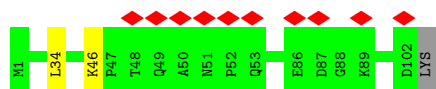
- Molecule 23: Large ribosomal subunit protein uL23

Chain T:  93% ..




- Molecule 24: 50S ribosomal protein L24

Chain U:  10% 97% ..



- Molecule 25: Large ribosomal subunit protein bL27

Chain W:  80% 7% 13%

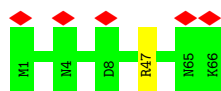


- Molecule 26: Large ribosomal subunit protein bL28

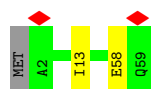
Chain X:  92% 6% .



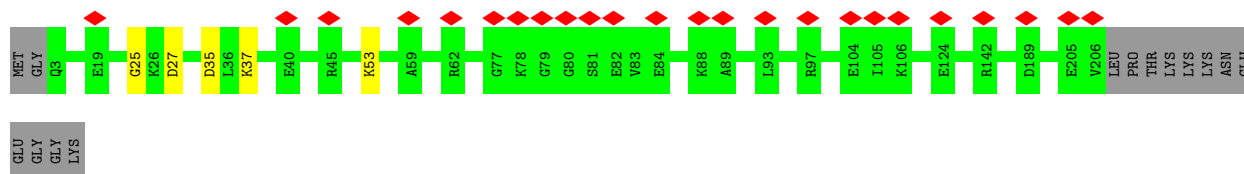
- Molecule 27: 50S ribosomal protein L29



- Molecule 28: Large ribosomal subunit protein uL30



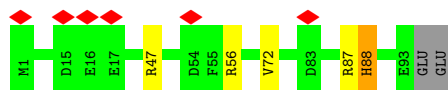
- Molecule 29: Small ribosomal subunit protein uS3



- Molecule 30: 30S ribosomal protein S5

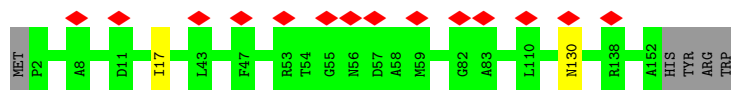


- Molecule 31: 30S ribosomal protein S6



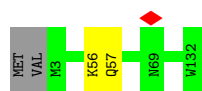
- Molecule 32: Small ribosomal subunit protein uS7





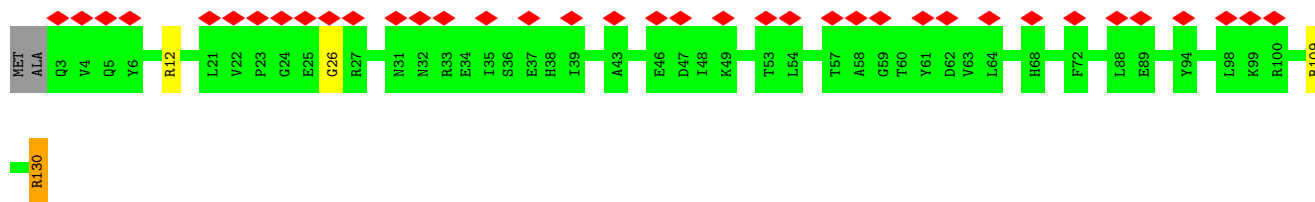
- Molecule 33: 30S ribosomal protein S8

Chain h: 97%



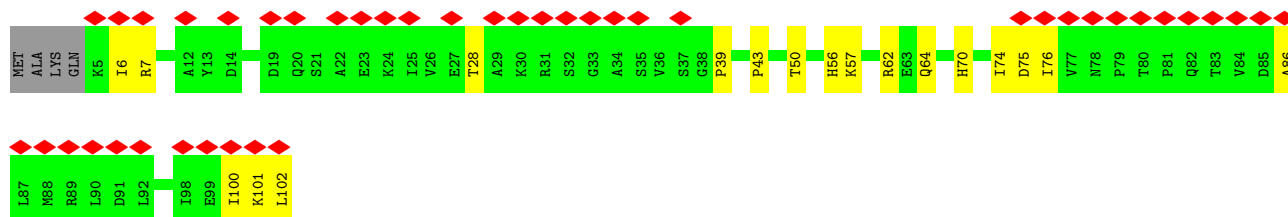
- Molecule 34: Small ribosomal subunit protein uS9

Chain i: 28% 95%



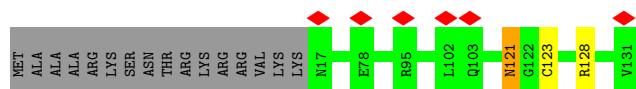
- Molecule 35: 30S ribosomal protein S10

Chain j: 42% 78% 18%



- Molecule 36: 30S ribosomal protein S11

Chain k: 5% 85% 12%

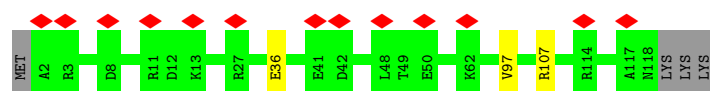


- Molecule 37: Small ribosomal subunit protein uS12

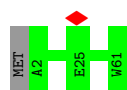
Chain l: 96%



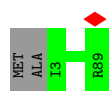
- Molecule 38: Small ribosomal subunit protein uS13



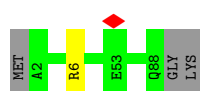
- Molecule 39: 30S ribosomal protein S14



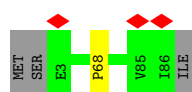
- Molecule 40: 30S ribosomal protein S15



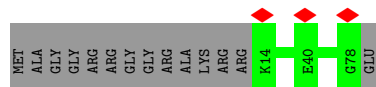
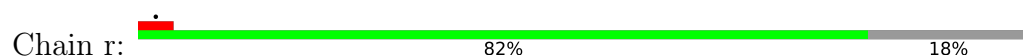
- Molecule 41: 30S ribosomal protein S16



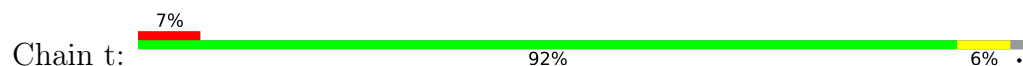
- Molecule 42: 30S ribosomal protein S17

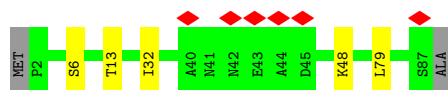


- Molecule 43: 30S ribosomal protein S18

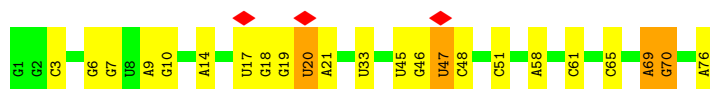


- Molecule 44: 30S ribosomal protein S20

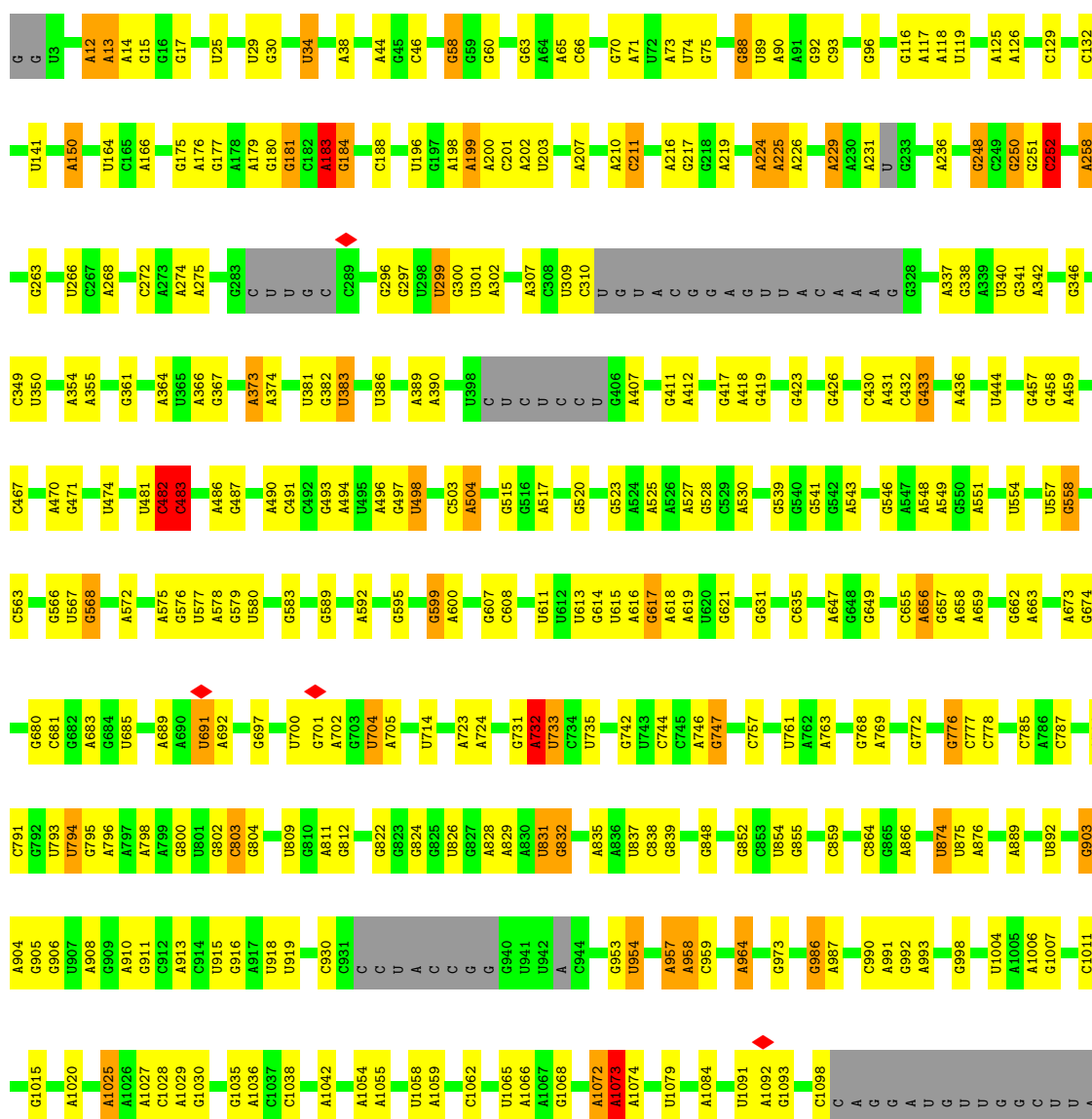




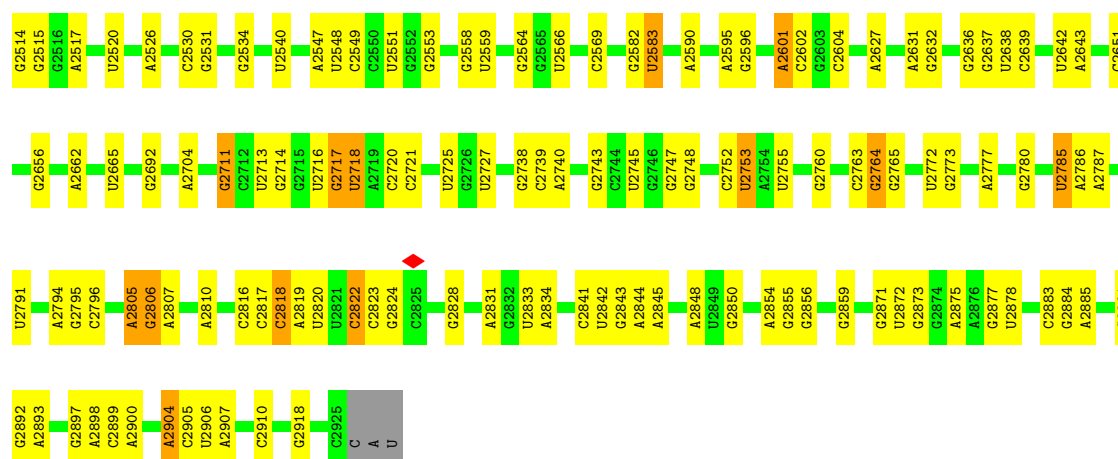
• Molecule 45: P-site tRNA-Phe



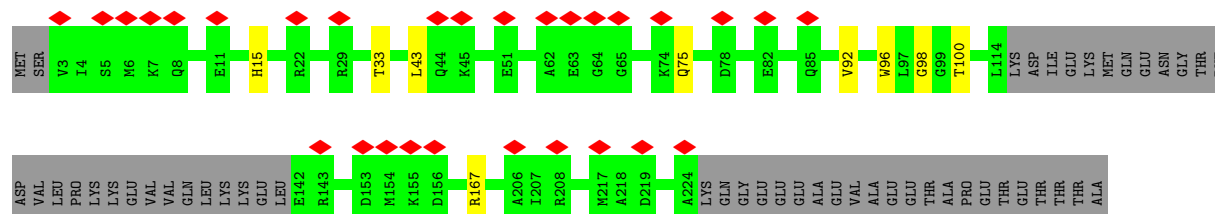
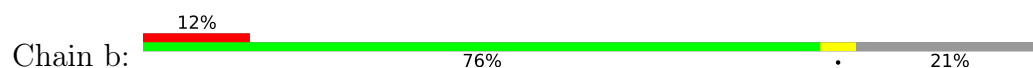
• Molecule 46: 23S rRNA



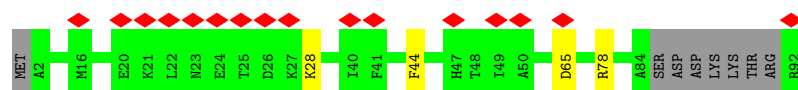
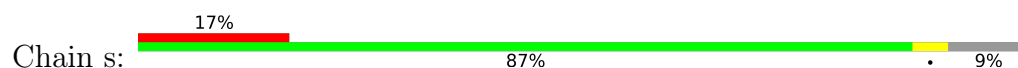
|       |       |   |   |       |       |       |       |   |       |       |       |       |   |
|-------|-------|---|---|-------|-------|-------|-------|---|-------|-------|-------|-------|---|
| G2412 | A2315 | A | C | U2057 | G1939 | G1801 | G1690 | A | A1485 | G1378 | G1300 | G1185 | G |
| G2413 | A2316 | C | A | G2058 | U1940 | G1802 | A1691 | A | U1489 | U1379 | G1301 | C1186 | A |
| G2414 | A2317 | U | G | A2059 | A1941 | A1802 | U1692 | A | A1490 | A1381 | U1301 | U1187 | A |
| U2415 | C2322 | A | G | A2060 | C1942 | G1805 | C1693 | U | U1488 | U1382 | U1306 | A1188 | G |
| U2416 | C2323 | C | G | G2061 | U1943 | U1806 | G1694 | A | U1499 | U1383 | G1307 | A1189 | C |
| A2417 | C2324 | U | U | A2062 | C1944 | U1807 | A1695 | U | U1500 | G1384 | A1308 | A1190 | A |
| G2418 | C2327 | C | G | U2063 | U1945 | U1807 | U1695 | A | U1501 | G1385 | G1309 | C1196 | G |
| U2421 | G2328 | G | G | C2064 | U1946 | G1810 | U1704 | U | G1502 | G1386 | C1310 | A1197 | C |
| U2422 | G2329 | U | U | C2065 | G1958 | C1811 | U1707 | A | G1507 | G1387 | G1311 | C1199 | C |
| C2423 | G2330 | C | A | A2066 | G1959 | C1812 | U1708 | A | U1506 | G1388 | A1312 | G1200 | C |
| C2424 | G2331 | U | G | C2067 | A1966 | A1814 | A1709 | G | U1507 | A1389 | G1315 | A1201 | C |
| G2425 | U2334 | G | G | C2073 | A1967 | A1815 | A1710 | U | C1508 | C1390 | A1316 | A1202 | A |
| U2431 | U2335 | U | C | G2074 | U1984 | A1816 | G1711 | U | U1512 | U1391 | G1317 | G1203 | U |
| C2432 | G2336 | C | C | G2075 | U1984 | C1817 | G1712 | U | G1513 | G1392 | U1318 | U1204 | U |
| U2433 | G2337 | C | U | C2076 | G1988 | U1825 | A1713 | U | C1514 | G1393 | G1319 | U1205 | U |
| C2434 | U2338 | U | U | A2077 | G1989 | U1826 | C1715 | U | A1515 | A1404 | G1322 | G1209 | A |
| U2435 | G2339 | C | G | C2078 | U1992 | U1827 | G1719 | U | A1516 | U1411 | A1323 | G1216 | A |
| C2436 | A2340 | C | G | A2079 | C1993 | G1828 | A1722 | U | C1516 | U1412 | G1324 | U     | G |
| U2437 | U2341 | U | A | C2080 | G1994 | C1829 | A1723 | U | U1517 | U1413 | A1325 | C     | U |
| G2438 | C2342 | A | A | U2081 | A1995 | U1830 | A1724 | U | G1525 | G1414 | A1326 | G1220 | G |
| G2439 | C2343 | C | C | G2082 | C1996 | A1831 | A1725 | U | G1526 | A1417 | U1327 | G     | C |
| A2440 | C2344 | U | U | A2083 | C1997 | G1832 | G1740 | U | G1527 | U1418 | C1328 | G     | G |
| U2441 | G2345 | C | C | C2084 | G1998 | U1833 | G1741 | U | C1528 | U1419 | A1335 | G1228 | U |
| C2442 | A2346 | C | G | G2085 | A1999 | A1834 | G1742 | U | G1529 | A1423 | C1336 | U1229 | A |
| U2443 | U2347 | U | U | A2086 | C1999 | U1835 | G1743 | U | G1530 | A1424 | C1337 | A1230 | U |
| G2444 | C2348 | C | C | C2087 | G2001 | A1836 | G1744 | U | G1531 | A1425 | G1338 | A1235 | U |
| C2445 | G2349 | U | U | A2088 | G2002 | C1837 | U1750 | U | U1535 | A1426 | A1339 | U1239 | A |
| U2446 | A2350 | C | C | C2089 | G2003 | U1838 | G1751 | U | A1536 | G1427 | A1340 | U1239 | G |
| C2447 | G2351 | C | G | U2090 | A2010 | A1839 | U1752 | U | U1540 | U1428 | U1341 | A1244 | C |
| U2448 | U2352 | U | U | C2091 | U2011 | A1840 | C1755 | U | A1541 | G1429 | C1342 | G1245 | U |
| G2449 | C2353 | C | C | A2092 | U2012 | A1841 | U1756 | U | A1542 | U1430 | C1343 | G1246 | C |
| U2450 | U2354 | U | U | C2093 | U2013 | A1842 | U1757 | U | C1543 | U1431 | U1344 | G1247 | A |
| C2451 | G2355 | C | C | U2094 | U2014 | G1843 | U1758 | U | C1544 | U1432 | A1345 | U     | C |
| U2452 | A2356 | C | C | A2095 | U2015 | U1844 | U1759 | U | A1553 | U1433 | U1346 | G1250 | U |
| G2453 | G2357 | U | U | C2096 | U2016 | A1845 | U1760 | U | U     | U1434 | U1351 | U1251 | G |
| A2454 | U2358 | C | C | U2097 | U2017 | A1846 | U1761 | U | A1554 | U1435 | U1352 | U1251 | A |
| U2455 | C2359 | C | C | C2098 | U2018 | A1847 | U1762 | U | A1555 | U1436 | C1353 | G1256 | G |
| G2456 | G2360 | U | U | U2099 | U2019 | A1848 | G1763 | U | A1556 | U1437 | C1354 | G1257 | U |
| C2457 | A2361 | C | C | C2100 | U2020 | G1849 | U1764 | U | G1557 | U1438 | A1355 | A1258 | C |
| U2458 | U2362 | C | C | A2099 | U2021 | U1850 | U1765 | U | G1558 | A1456 | C1356 | A1266 | G |
| G2459 | G2363 | U | U | C2100 | U2022 | A1851 | C1766 | U | C1559 | U     | C1364 | G1267 | U |
| U2460 | C2364 | C | C | U2101 | C2023 | A1852 | G1767 | U | U1560 | U     | U1365 | U1267 | A |
| C2461 | A2365 | C | C | A2102 | U2024 | G1853 | U1768 | U | G1561 | U     | C1366 | A1277 | G |
| U2462 | G2366 | U | U | C2103 | C2025 | A1854 | U1769 | U | A1562 | U     | U1367 | G1278 | C |
| G2463 | U2367 | C | C | U2104 | A2026 | A1855 | C1770 | U | G1563 | G1460 | U1368 | C1279 | A |
| U2464 | C2368 | C | C | A2105 | A2027 | U1856 | C1771 | U | C1564 | A1465 | C1369 | A1286 | G |
| C2465 | A2369 | U | U | C2106 | U2028 | U1857 | U1772 | U | U1565 | U1466 | C1370 | U1286 | C |
| U2466 | G2370 | C | C | U2107 | A2029 | G1858 | A1773 | U | U1566 | U1467 | G1371 | G1177 | U |
| G2467 | U2371 | C | C | A2108 | U2030 | U1859 | G1774 | U | U1567 | A1473 | C1372 | U1178 | A |
| U2468 | C2372 | U | U | C2109 | U2031 | A1860 | U1775 | U | U1568 | U1474 | U1373 | C1180 | C |
| C2469 | A2373 | C | C | U2110 | A2032 | A1861 | G1776 | U | G1569 | G1475 | C1374 | C1181 | G |
| U2470 | G2374 | C | C | A2111 | U2033 | U1862 | U1777 | U | A1570 | U1476 | A1375 | A1293 | C |
| G2471 | U2375 | U | U | C2112 | C2034 | A1863 | G1778 | U | U1571 | U1477 | U1376 | U1294 | U |
| U2472 | A2376 | C | C | U2113 | U2035 | A1864 | U1779 | U | C1572 | A1481 | G1377 | G1296 | G |
| C2473 | G2377 | C | C | A2114 | U2036 | U1865 | U1780 | U | U1573 | U1482 | U1378 | U1297 | A |
| U2474 | U2378 | U | U | C2115 | A2037 | G1866 | C1781 | U | U1574 | U1483 | C1379 | G1298 | C |
| G2475 | C2379 | C | C | U2116 | U2038 | A1867 | G1782 | U | U1575 | U1484 | U1380 | U1299 | G |
| U2476 | A2380 | C | C | A2117 | U2039 | U1868 | U1783 | U | U1576 | U1485 | C1381 | A1290 | C |
| C2477 | G2381 | U | U | C2118 | U2040 | A1869 | A1774 | U | U1577 | U1486 | G1382 | A1291 | A |
| U2478 | U2382 | C | C | U2119 | A2041 | U1870 | G1775 | U | U1578 | U1487 | C1383 | G1292 | C |
| G2479 | C2383 | C | C | A2120 | U2042 | A1871 | U1776 | U | U1579 | U1488 | U1384 | U1293 | G |
| U2480 | A2384 | U | U | C2121 | C2043 | A1872 | A1777 | U | U1580 | U1489 | C1385 | U1294 | C |
| C2481 | G2385 | C | C | U2122 | U2044 | U1873 | U1778 | U | U1581 | U1490 | U1386 | G1295 | A |
| U2482 | U2386 | C | C | A2123 | A2045 | A1874 | G1779 | U | U1582 | U1491 | C1387 | U1296 | C |
| G2483 | C2387 | U | U | U2124 | U2046 | A1875 | U1780 | U | U1583 | U1492 | U1388 | U1297 | G |
| U2484 | A2388 | C | C | C2125 | U2047 | U1876 | C1781 | U | U1584 | U1493 | C1389 | A1286 | C |
| C2485 | G2389 | C | C | A2126 | U2048 | A1877 | G1782 | U | U1585 | U1494 | G1390 | U1178 | A |
| U2486 | U2390 | U | U | U2127 | A2049 | G1878 | U1774 | U | U1586 | U1495 | C1391 | G1179 | C |
| G2487 | C2391 | C | C | C2128 | U2050 | U1879 | G1775 | U | U1587 | U1496 | C1392 | C1180 | G |
| U2488 | A2392 | C | C | U2129 | A2051 | A1880 | U1776 | U | U1588 | U1497 | U1393 | C1181 | C |
| C2489 | G2393 | U | U | A2130 | U2052 | A1881 | U1777 | U | U1589 | U1498 | C1394 | A1293 | A |
| U2490 | U2394 | C | C | U2131 | U2053 | U1882 | G1778 | U | U1590 | U1499 | U1395 | U1294 | C |
| G2491 | A2395 | C | C | C2132 | U2054 | A1883 | U1779 | U | U1591 | U1500 | G1396 | G1295 | G |
| U2492 | C2396 | U | U | U2133 | U2055 | U1884 | U1780 | U | U1592 | U1501 | C1397 | U1296 | C |
| C2493 | G2397 | C | C | A2134 | U2056 | U1885 | C1781 | U | U1593 | U1502 | U1398 | U1297 | A |
| U2494 | U2398 | C | C | U2135 | U2057 | A1886 | G1782 | U | U1594 | U1503 | C1399 | A1286 | C |
| G2495 | A2399 | U | U | C2136 | U2058 | U1887 | U1783 | U | U1595 | U1504 | G1400 | U1178 | A |
| U2496 | C2400 | C | C | U2137 | U2059 | A1888 | U1784 | U | U1596 | U1505 | C1401 | G1179 | C |
| C2497 | G2401 | C | C | A2137 | U2060 | A1889 | U1785 | U | U1597 | U1506 | U1402 | C1180 | G |
| U2498 | U2402 | U | U | U2138 | U2061 | U1890 | G1786 | U | U1598 | U1507 | U1403 | C1181 | C |
| G2499 | A2403 | C | C | C2139 | A2062 | A1891 | U1787 | U | U1599 | U1508 | C1404 | A1293 | A |
| U2500 | C2404 | C | C | U2140 | U2063 | U1892 | U1788 | U | U1600 | U1509 | U1405 | U1294 | C |
| C2501 | G2405 | U | U | A2141 | U2064 | U1893 | U1789 | U | U1601 | U1510 | C1406 | G1295 | G |
| U2502 | U2406 | C | C | U2142 | U2065 | A1894 | U1790 | U | U1602 | U1511 | U1407 | U1296 | C |
| G2503 | A2407 | C | C | C2143 | U2066 | U1895 | U1791 | U | U1603 | U1512 | C1408 | U1297 | A |
| U2504 | C2408 | C | C | U2144 | U2067 | A1896 | U1792 | U | U1604 | U1513 | U1409 | A1286 | C |
| C2505 | G2409 | U | U | A2145 | U2068 | U1897 | G1793 | U | U1605 | U1514 | C1410 | U1178 | A |
| U2506 | U2410 | C | C | U2146 | U2069 | U1898 | U1794 | U | U1606 | U1515 | U1411 | G1179 | C |
| G2507 | A2411 | C | C | C2147 | U2070 | A1899 | U1795 | U | U1607 | U1516 | U1412 | C1180 | G |
| U2508 | C2412 | U | U | U2148 | U2071 | U1899 | U1796 | U | U1608 | U1517 | C1413 | A1293 | A |
| C2509 | G2413 | C | C | A2149 | U2072 | A1900 | U1797 | U | U1609 | U1518 | U1414 | U1294 | C |
| U2510 | U2414 | C | C | U2150 | U2073 | U1901 | U1798 | U | U1610 | U1519 | C1415 | U1295 | G |
| G2511 | A2415 | C | C | C2151 | U2074 | A1902 | U1799 | U | U1611 | U1520 | U1416 | G1296 | C |
| U2512 | C2416 | U | U | U2152 | U2075 | U1903 | U1800 | U | U1612 | U1521 | C1417 | U1297 | A |
| C2513 | G2417 | C | C | A2153 | U2076 | U1904 | U1801 | U | U1613 | U1522 | U1418 | A1286 | C |
| U2514 | U2418 | C | C | U2154 | U2077 | A1905 | U1802 | U | U1614 | U1523 | C1419 | U1178 | A |
| G2515 | A2419 | C | C | C2155 | U2078 | U1906 | U1803 | U | U1615 | U1524 | U1420 | G1179 | C |
| U2516 | C2420 | U | U | U2156 | U2079 | C1907 | U1804 | U | U1616 | U1525 | C1421 | C1180 | G |
| C2517 | G2421 | C | C | A2157 | U2080 | U1908 | U1805 | U | U1617 | U1526 | U1422 | A1293 | A |
| U2518 | U2422 | C | C | C2158 | U2081 | A1909 | U1806 | U | U1618 | U1527 | U1423 | U1294 | C |
| G2519 | A2423 | C | C | U2159 | U2082 | C1910 | U1807 | U | U1619 | U1528 | C1424 | U1295 | G |
| U2520 | C2424 | U | U | A2160 | U2083 | U1911 | U1808 | U | U1620 | U1529 | U1425 | G1296 | C |
| C2521 |       |   |   |       |       |       |       |   |       |       |       |       |   |



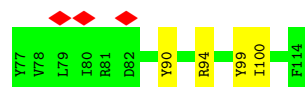
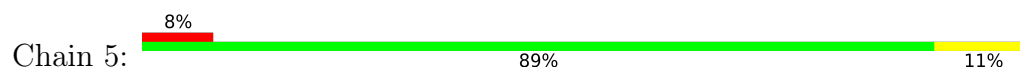
• Molecule 47: 30S ribosomal protein S2



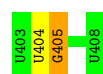
• Molecule 48: Small ribosomal subunit protein uS19



• Molecule 49: Nascent Chain CliM

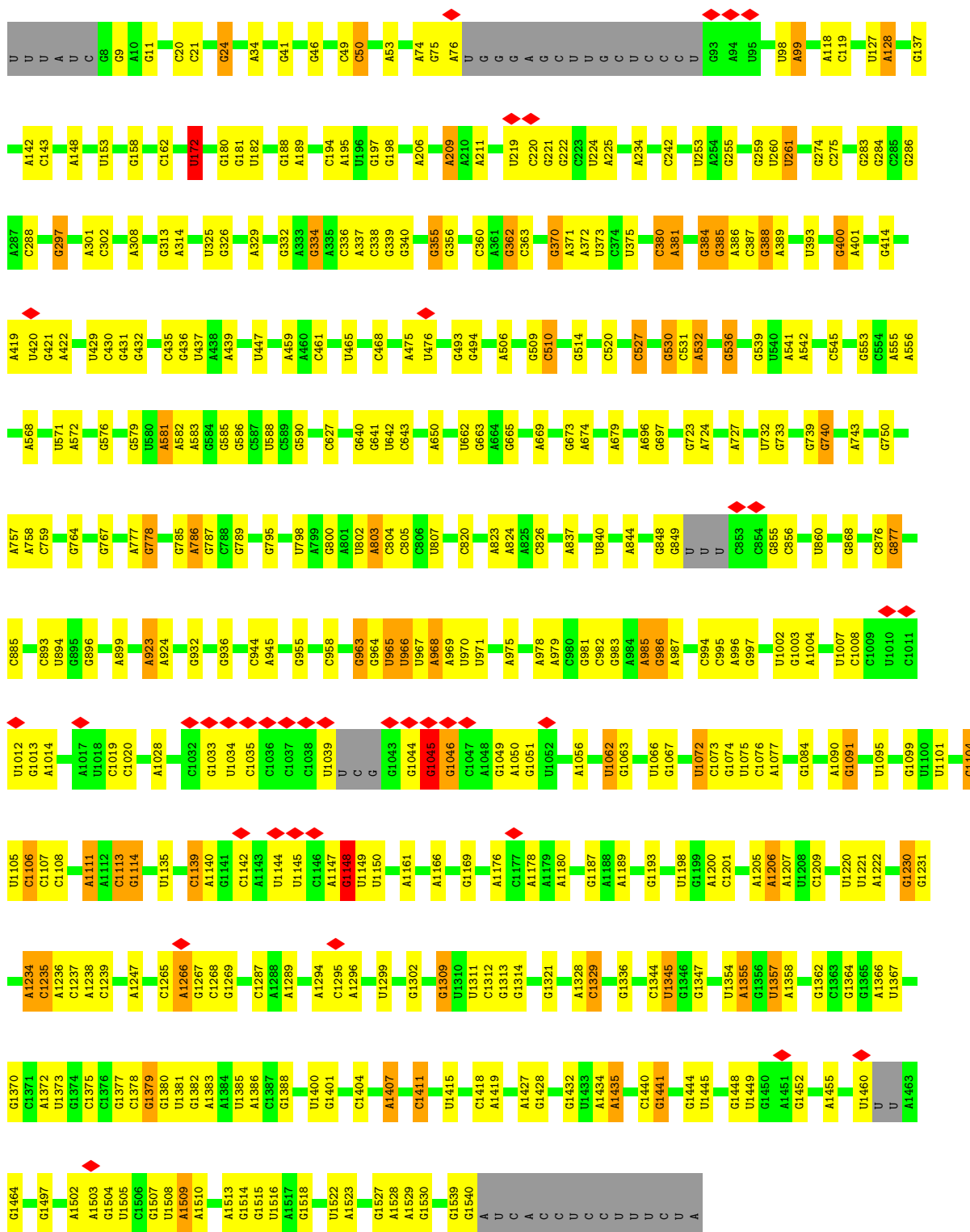


• Molecule 50: mRNA



• Molecule 51: 16S rRNA

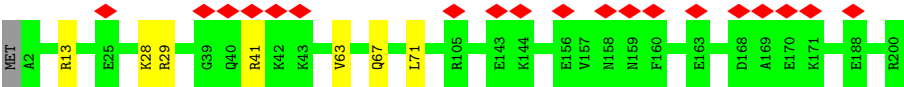




- Molecule 52: 30S ribosomal protein S4







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 368433                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.14                                    | Depositor |
| Minimum defocus (nm)                 | 300                                     | Depositor |
| Maximum defocus (nm)                 | 900                                     | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.060                                   | Depositor |
| Minimum map value                    | -0.016                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.008                                   | Depositor |
| Map size (Å)                         | 319.104, 319.104, 319.104               | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.83100003, 0.83100003, 0.83100003      | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, PSU

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     | 0.64         | 0/439       | 1.16        | 1/584 (0.2%)   |
| 2   | 1     | 0.50         | 0/408       | 0.93        | 0/541          |
| 3   | 2     | 0.65         | 0/371       | 1.05        | 0/483          |
| 4   | 3     | 0.64         | 0/519       | 1.06        | 2/680 (0.3%)   |
| 5   | 4     | 0.52         | 0/300       | 0.99        | 0/393          |
| 6   | 6     | 0.54         | 0/363       | 1.01        | 0/485          |
| 7   | B     | 0.57         | 0/2675      | 1.06        | 13/4170 (0.3%) |
| 8   | C     | 0.59         | 0/2130      | 1.01        | 0/2858         |
| 9   | D     | 0.57         | 0/1597      | 1.00        | 2/2140 (0.1%)  |
| 10  | E     | 0.54         | 0/1586      | 0.98        | 0/2139         |
| 11  | F     | 0.51         | 0/1424      | 1.05        | 0/1910         |
| 12  | G     | 0.52         | 0/1360      | 0.97        | 0/1832         |
| 13  | J     | 0.56         | 0/1154      | 0.96        | 0/1552         |
| 14  | K     | 0.52         | 0/928       | 0.99        | 0/1245         |
| 15  | L     | 0.55         | 0/1094      | 1.01        | 0/1457         |
| 16  | M     | 0.53         | 0/1099      | 1.00        | 0/1468         |
| 17  | N     | 0.57         | 0/961       | 1.16        | 2/1284 (0.2%)  |
| 18  | O     | 0.54         | 0/922       | 1.00        | 0/1236         |
| 19  | P     | 0.53         | 0/950       | 1.01        | 0/1269         |
| 20  | Q     | 0.60         | 0/962       | 1.03        | 0/1277         |
| 21  | R     | 0.48         | 0/806       | 0.90        | 0/1080         |
| 22  | S     | 0.60         | 0/859       | 1.07        | 0/1156         |
| 23  | T     | 0.53         | 0/739       | 1.04        | 0/985          |
| 24  | U     | 0.54         | 0/780       | 0.94        | 0/1043         |
| 25  | W     | 0.54         | 0/637       | 1.06        | 1/846 (0.1%)   |
| 26  | X     | 0.53         | 0/471       | 1.03        | 1/626 (0.2%)   |
| 27  | Y     | 0.46         | 0/541       | 1.06        | 0/718          |
| 28  | Z     | 0.51         | 0/458       | 1.00        | 0/613          |
| 29  | c     | 0.51         | 0/1630      | 1.02        | 0/2193         |
| 30  | e     | 0.52         | 0/1231      | 1.01        | 1/1655 (0.1%)  |
| 31  | f     | 0.46         | 0/776       | 0.96        | 0/1043         |
| 32  | g     | 0.51         | 0/1215      | 1.09        | 0/1629         |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 33  | h     | 0.49         | 0/1042   | 0.93        | 0/1397            |
| 34  | i     | 0.54         | 0/1011   | 1.00        | 0/1356            |
| 35  | j     | 0.54         | 0/800    | 1.08        | 1/1077 (0.1%)     |
| 36  | k     | 0.55         | 0/861    | 0.97        | 0/1164            |
| 37  | l     | 0.50         | 0/1052   | 0.92        | 0/1413            |
| 38  | m     | 0.54         | 0/940    | 1.08        | 0/1257            |
| 39  | n     | 0.51         | 0/508    | 1.00        | 0/672             |
| 40  | o     | 0.48         | 0/738    | 1.07        | 0/985             |
| 41  | p     | 0.48         | 0/704    | 0.97        | 0/945             |
| 42  | q     | 0.46         | 0/701    | 0.90        | 0/936             |
| 43  | r     | 0.48         | 0/530    | 1.01        | 0/710             |
| 44  | t     | 0.49         | 0/661    | 1.17        | 0/882             |
| 45  | v     | 0.58         | 0/1812   | 1.07        | 6/2823 (0.2%)     |
| 46  | A     | 0.56         | 0/65622  | 1.20        | 489/102356 (0.5%) |
| 47  | b     | 0.49         | 0/1586   | 1.07        | 0/2130            |
| 48  | s     | 0.52         | 0/696    | 1.05        | 1/931 (0.1%)      |
| 49  | 5     | 0.52         | 0/356    | 1.04        | 0/481             |
| 50  | 7     | 0.66         | 0/135    | 1.13        | 1/207 (0.5%)      |
| 51  | a     | 0.56         | 0/36267  | 1.06        | 152/56571 (0.3%)  |
| 52  | d     | 0.50         | 0/1635   | 1.01        | 0/2196            |
| All | All   | 0.55         | 0/149042 | 1.12        | 673/223079 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 0     | 0                   | 2                   |
| 2   | 1     | 0                   | 1                   |
| 3   | 2     | 0                   | 1                   |
| 5   | 4     | 0                   | 1                   |
| 6   | 6     | 0                   | 1                   |
| 8   | C     | 0                   | 7                   |
| 10  | E     | 0                   | 3                   |
| 11  | F     | 0                   | 1                   |
| 12  | G     | 0                   | 1                   |
| 15  | L     | 0                   | 1                   |
| 16  | M     | 0                   | 1                   |
| 17  | N     | 0                   | 3                   |
| 18  | O     | 0                   | 1                   |
| 19  | P     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 20  | Q     | 0                   | 1                   |
| 21  | R     | 0                   | 1                   |
| 22  | S     | 0                   | 1                   |
| 26  | X     | 0                   | 1                   |
| 27  | Y     | 0                   | 1                   |
| 30  | e     | 0                   | 2                   |
| 31  | f     | 0                   | 2                   |
| 34  | i     | 0                   | 3                   |
| 35  | j     | 0                   | 1                   |
| 38  | m     | 0                   | 1                   |
| 46  | A     | 0                   | 3                   |
| 47  | b     | 0                   | 1                   |
| 48  | s     | 0                   | 1                   |
| 51  | a     | 0                   | 1                   |
| 52  | d     | 0                   | 2                   |
| All | All   | 0                   | 48                  |

There are no bond length outliers.

All (673) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 46  | A     | 732  | A    | O3'-P-O5'   | -18.09 | 76.87       | 104.00   |
| 46  | A     | 490  | A    | O3'-P-O5'   | -14.84 | 81.74       | 104.00   |
| 46  | A     | 1244 | A    | O3'-P-O5'   | 14.61  | 125.91      | 104.00   |
| 46  | A     | 2904 | A    | C2'-C3'-O3' | 14.52  | 131.28      | 109.50   |
| 46  | A     | 1363 | G    | O3'-P-O5'   | -12.18 | 85.74       | 104.00   |
| 51  | a     | 261  | U    | O3'-P-O5'   | -11.48 | 86.78       | 104.00   |
| 46  | A     | 1707 | U    | O3'-P-O5'   | -11.28 | 87.08       | 104.00   |
| 51  | a     | 20   | C    | O3'-P-O5'   | -11.24 | 87.15       | 104.00   |
| 46  | A     | 354  | A    | O3'-P-O5'   | -11.20 | 87.20       | 104.00   |
| 51  | a     | 387  | C    | O3'-P-O5'   | -11.15 | 87.27       | 104.00   |
| 46  | A     | 2121 | U    | O3'-P-O5'   | -10.89 | 87.67       | 104.00   |
| 46  | A     | 2738 | G    | O3'-P-O5'   | -10.88 | 87.69       | 104.00   |
| 46  | A     | 2739 | C    | O3'-P-O5'   | -10.83 | 87.75       | 104.00   |
| 46  | A     | 207  | A    | O3'-P-O5'   | -10.79 | 87.82       | 104.00   |
| 46  | A     | 1375 | A    | O3'-P-O5'   | -10.34 | 88.49       | 104.00   |
| 46  | A     | 481  | U    | O3'-P-O5'   | 10.26  | 119.39      | 104.00   |
| 46  | A     | 1277 | A    | O3'-P-O5'   | -10.23 | 88.65       | 104.00   |
| 46  | A     | 986  | G    | O3'-P-O5'   | 10.11  | 119.16      | 104.00   |
| 46  | A     | 1810 | G    | O3'-P-O5'   | -10.06 | 88.91       | 104.00   |
| 46  | A     | 1177 | G    | O3'-P-O5'   | -10.01 | 88.98       | 104.00   |
| 51  | a     | 963  | G    | O3'-P-O5'   | -9.99  | 89.01       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 2859 | G    | O3'-P-O5'   | -9.70 | 89.45       | 104.00   |
| 46  | A     | 2711 | G    | O3'-P-O5'   | -9.67 | 89.50       | 104.00   |
| 46  | A     | 1606 | A    | O3'-P-O5'   | -9.59 | 89.62       | 104.00   |
| 46  | A     | 1966 | A    | O3'-P-O5'   | -9.45 | 89.83       | 104.00   |
| 46  | A     | 2740 | A    | O3'-P-O5'   | -9.39 | 89.92       | 104.00   |
| 46  | A     | 2414 | C    | O3'-P-O5'   | -9.38 | 89.92       | 104.00   |
| 46  | A     | 2636 | G    | O3'-P-O5'   | -9.37 | 89.94       | 104.00   |
| 46  | A     | 2074 | C    | O3'-P-O5'   | -9.22 | 90.17       | 104.00   |
| 51  | a     | 785  | G    | O3'-P-O5'   | -9.14 | 90.29       | 104.00   |
| 46  | A     | 2842 | U    | O3'-P-O5'   | -8.94 | 90.59       | 104.00   |
| 46  | A     | 2308 | G    | O3'-P-O5'   | -8.84 | 90.74       | 104.00   |
| 46  | A     | 1318 | G    | O3'-P-O5'   | -8.80 | 90.80       | 104.00   |
| 51  | a     | 789  | G    | O3'-P-O5'   | -8.79 | 90.81       | 104.00   |
| 46  | A     | 482  | C    | C4'-C3'-O3' | 8.77  | 122.56      | 109.40   |
| 46  | A     | 1167 | C    | O3'-P-O5'   | -8.74 | 90.89       | 104.00   |
| 46  | A     | 2457 | G    | O3'-P-O5'   | -8.71 | 90.94       | 104.00   |
| 51  | a     | 1508 | U    | O3'-P-O5'   | -8.63 | 91.06       | 104.00   |
| 46  | A     | 828  | A    | O3'-P-O5'   | -8.59 | 91.12       | 104.00   |
| 46  | A     | 1884 | G    | O3'-P-O5'   | -8.54 | 91.19       | 104.00   |
| 51  | a     | 355  | G    | O3'-P-O5'   | -8.48 | 91.28       | 104.00   |
| 46  | A     | 1180 | C    | O3'-P-O5'   | -8.47 | 91.30       | 104.00   |
| 46  | A     | 1690 | G    | C2'-C3'-O3' | -8.45 | 101.03      | 113.70   |
| 46  | A     | 1004 | U    | O3'-P-O5'   | -8.39 | 91.42       | 104.00   |
| 51  | a     | 786  | A    | O3'-P-O5'   | -8.39 | 91.42       | 104.00   |
| 46  | A     | 1371 | G    | O3'-P-O5'   | -8.35 | 91.47       | 104.00   |
| 46  | A     | 1250 | G    | C4'-C3'-O3' | 8.34  | 121.90      | 109.40   |
| 51  | a     | 127  | U    | O3'-P-O5'   | -8.32 | 91.52       | 104.00   |
| 46  | A     | 874  | U    | C2'-C3'-O3' | -8.21 | 101.39      | 113.70   |
| 46  | A     | 1173 | A    | O3'-P-O5'   | -8.15 | 91.77       | 104.00   |
| 46  | A     | 116  | G    | O3'-P-O5'   | -8.14 | 91.79       | 104.00   |
| 46  | A     | 1939 | G    | O3'-P-O5'   | -8.13 | 91.80       | 104.00   |
| 51  | a     | 896  | G    | O3'-P-O5'   | -8.13 | 91.81       | 104.00   |
| 46  | A     | 1934 | C    | O3'-P-O5'   | -8.11 | 91.84       | 104.00   |
| 46  | A     | 2418 | G    | C4'-C3'-O3' | -8.09 | 100.87      | 113.00   |
| 51  | a     | 696  | A    | O3'-P-O5'   | -8.08 | 91.87       | 104.00   |
| 46  | A     | 1398 | A    | O3'-P-O5'   | -8.05 | 91.92       | 104.00   |
| 46  | A     | 1876 | A    | O3'-P-O5'   | -8.04 | 91.94       | 104.00   |
| 7   | B     | 14   | G    | O3'-P-O5'   | -8.01 | 91.99       | 104.00   |
| 46  | A     | 1940 | U    | O3'-P-O5'   | -7.96 | 92.06       | 104.00   |
| 46  | A     | 2424 | C    | O3'-P-O5'   | -7.93 | 92.10       | 104.00   |
| 46  | A     | 2340 | A    | O3'-P-O5'   | -7.92 | 92.12       | 104.00   |
| 46  | A     | 1751 | U    | O3'-P-O5'   | -7.89 | 92.16       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 383  | U    | O3'-P-O5'   | -7.89 | 92.17       | 104.00   |
| 46  | A     | 2382 | G    | O3'-P-O5'   | -7.88 | 92.18       | 104.00   |
| 46  | A     | 126  | A    | O3'-P-O5'   | -7.87 | 92.19       | 104.00   |
| 51  | a     | 385  | G    | O3'-P-O5'   | -7.87 | 92.20       | 104.00   |
| 51  | a     | 966  | U    | O3'-P-O5'   | -7.87 | 92.20       | 104.00   |
| 46  | A     | 2051 | U    | O3'-P-O5'   | -7.85 | 92.22       | 104.00   |
| 51  | a     | 986  | G    | O3'-P-O5'   | -7.85 | 92.23       | 104.00   |
| 46  | A     | 1417 | A    | C2'-C3'-O3' | 7.85  | 121.27      | 109.50   |
| 46  | A     | 723  | A    | O3'-P-O5'   | -7.83 | 92.26       | 104.00   |
| 51  | a     | 1090 | A    | O3'-P-O5'   | -7.82 | 92.28       | 104.00   |
| 51  | a     | 118  | A    | O3'-P-O5'   | -7.80 | 92.30       | 104.00   |
| 46  | A     | 1751 | U    | C4'-C3'-O3' | 7.80  | 121.09      | 109.40   |
| 46  | A     | 1337 | C    | O3'-P-O5'   | 7.79  | 115.68      | 104.00   |
| 46  | A     | 2334 | U    | O3'-P-O5'   | -7.78 | 92.33       | 104.00   |
| 46  | A     | 225  | A    | O3'-P-O5'   | -7.77 | 92.35       | 104.00   |
| 46  | A     | 1770 | C    | O3'-P-O5'   | -7.77 | 92.35       | 104.00   |
| 46  | A     | 613  | U    | C4'-C3'-O3' | -7.74 | 101.39      | 113.00   |
| 46  | A     | 2831 | A    | O3'-P-O5'   | -7.73 | 92.40       | 104.00   |
| 46  | A     | 66   | C    | O3'-P-O5'   | -7.71 | 92.43       | 104.00   |
| 46  | A     | 1886 | G    | O3'-P-O5'   | -7.70 | 92.45       | 104.00   |
| 46  | A     | 2412 | G    | O3'-P-O5'   | -7.69 | 92.46       | 104.00   |
| 46  | A     | 1181 | C    | C4'-C3'-O3' | -7.68 | 101.48      | 113.00   |
| 46  | A     | 2032 | A    | O3'-P-O5'   | -7.67 | 92.50       | 104.00   |
| 46  | A     | 1708 | U    | C4'-C3'-O3' | -7.64 | 101.54      | 113.00   |
| 46  | A     | 803  | C    | O3'-P-O5'   | -7.64 | 92.54       | 104.00   |
| 46  | A     | 444  | U    | O3'-P-O5'   | -7.61 | 92.58       | 104.00   |
| 51  | a     | 1419 | A    | O3'-P-O5'   | -7.60 | 92.60       | 104.00   |
| 51  | a     | 356  | G    | O3'-P-O5'   | -7.57 | 92.65       | 104.00   |
| 46  | A     | 1179 | A    | O3'-P-O5'   | -7.55 | 92.67       | 104.00   |
| 46  | A     | 13   | A    | O3'-P-O5'   | -7.55 | 92.67       | 104.00   |
| 46  | A     | 2035 | C    | C4'-C3'-O3' | -7.55 | 101.67      | 113.00   |
| 51  | a     | 260  | U    | O3'-P-O5'   | -7.49 | 92.76       | 104.00   |
| 46  | A     | 252  | C    | O3'-P-O5'   | -7.49 | 92.76       | 104.00   |
| 46  | A     | 129  | C    | O3'-P-O5'   | -7.49 | 92.77       | 104.00   |
| 51  | a     | 840  | U    | O3'-P-O5'   | -7.46 | 92.81       | 104.00   |
| 46  | A     | 266  | U    | O3'-P-O5'   | -7.44 | 92.84       | 104.00   |
| 26  | X     | 27   | ARG  | CB-CA-C     | -7.43 | 95.59       | 110.30   |
| 51  | a     | 1382 | G    | O3'-P-O5'   | -7.43 | 92.86       | 104.00   |
| 50  | 7     | 405  | G    | O3'-P-O5'   | -7.42 | 92.87       | 104.00   |
| 46  | A     | 1200 | G    | O3'-P-O5'   | -7.41 | 92.89       | 104.00   |
| 46  | A     | 543  | A    | O3'-P-O5'   | -7.39 | 92.91       | 104.00   |
| 45  | v     | 47   | U    | C2'-C3'-O3' | 7.33  | 120.50      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 2392 | U    | O3'-P-O5'   | -7.32 | 93.03       | 104.00   |
| 46  | A     | 794  | U    | C4'-C3'-O3' | -7.31 | 102.03      | 113.00   |
| 46  | A     | 2054 | C    | O3'-P-O5'   | -7.25 | 93.12       | 104.00   |
| 51  | a     | 981  | G    | O3'-P-O5'   | -7.25 | 93.12       | 104.00   |
| 46  | A     | 1708 | U    | O3'-P-O5'   | -7.23 | 93.16       | 104.00   |
| 46  | A     | 2302 | A    | C4'-C3'-O3' | -7.22 | 102.17      | 113.00   |
| 51  | a     | 795  | G    | O3'-P-O5'   | -7.22 | 93.18       | 104.00   |
| 46  | A     | 746  | A    | O3'-P-O5'   | -7.21 | 93.19       | 104.00   |
| 46  | A     | 1055 | A    | O3'-P-O5'   | -7.18 | 93.23       | 104.00   |
| 46  | A     | 889  | A    | O3'-P-O5'   | -7.17 | 93.25       | 104.00   |
| 46  | A     | 2030 | A    | O3'-P-O5'   | -7.15 | 93.27       | 104.00   |
| 51  | a     | 386  | A    | O3'-P-O5'   | -7.14 | 93.29       | 104.00   |
| 46  | A     | 88   | G    | C2'-C3'-O3' | 7.14  | 124.41      | 113.70   |
| 46  | A     | 2753 | U    | C3'-C2'-O2' | 7.13  | 121.39      | 110.70   |
| 45  | v     | 70   | G    | O3'-P-O5'   | -7.12 | 93.32       | 104.00   |
| 46  | A     | 432  | C    | O3'-P-O5'   | -7.12 | 93.33       | 104.00   |
| 46  | A     | 1339 | A    | C2'-C3'-O3' | 7.11  | 120.16      | 109.50   |
| 46  | A     | 2704 | A    | O3'-P-O5'   | -7.10 | 93.36       | 104.00   |
| 46  | A     | 1740 | G    | O3'-P-O5'   | -7.10 | 93.36       | 104.00   |
| 7   | B     | 54   | U    | O3'-P-O5'   | -7.09 | 93.36       | 104.00   |
| 51  | a     | 994  | C    | O3'-P-O5'   | -7.09 | 93.36       | 104.00   |
| 46  | A     | 1560 | U    | O3'-P-O5'   | -7.09 | 93.37       | 104.00   |
| 51  | a     | 1383 | A    | O3'-P-O5'   | -7.08 | 93.39       | 104.00   |
| 7   | B     | 42   | G    | O3'-P-O5'   | -7.07 | 93.40       | 104.00   |
| 46  | A     | 497  | G    | O3'-P-O5'   | -7.06 | 93.41       | 104.00   |
| 51  | a     | 860  | U    | O3'-P-O5'   | -7.05 | 93.43       | 104.00   |
| 51  | a     | 1091 | G    | C4'-C3'-O3' | -7.05 | 102.43      | 113.00   |
| 46  | A     | 1759 | U    | C4'-C3'-O3' | 7.02  | 119.94      | 109.40   |
| 46  | A     | 1988 | G    | O3'-P-O5'   | -7.01 | 93.48       | 104.00   |
| 46  | A     | 1998 | A    | C4'-C3'-O3' | -7.01 | 102.49      | 113.00   |
| 51  | a     | 372  | A    | C4'-C3'-O3' | 7.01  | 123.51      | 113.00   |
| 46  | A     | 196  | U    | O3'-P-O5'   | -6.98 | 93.53       | 104.00   |
| 46  | A     | 1769 | G    | O3'-P-O5'   | -6.98 | 93.53       | 104.00   |
| 46  | A     | 2805 | A    | O3'-P-O5'   | 6.96  | 114.44      | 104.00   |
| 46  | A     | 1184 | G    | C2'-C3'-O3' | -6.96 | 103.26      | 113.70   |
| 46  | A     | 2091 | A    | O3'-P-O5'   | -6.96 | 93.57       | 104.00   |
| 46  | A     | 217  | G    | O3'-P-O5'   | -6.95 | 93.57       | 104.00   |
| 51  | a     | 1448 | G    | O3'-P-O5'   | -6.95 | 93.58       | 104.00   |
| 46  | A     | 1279 | C    | O3'-P-O5'   | -6.95 | 93.58       | 104.00   |
| 51  | a     | 385  | G    | C4'-C3'-O3' | -6.94 | 102.59      | 113.00   |
| 51  | a     | 1091 | G    | O3'-P-O5'   | -6.94 | 93.59       | 104.00   |
| 46  | A     | 2526 | A    | O3'-P-O5'   | -6.93 | 93.60       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | a     | 885  | C    | O3'-P-O5'   | -6.93 | 93.61       | 104.00   |
| 46  | A     | 349  | C    | O3'-P-O5'   | -6.93 | 93.61       | 104.00   |
| 46  | A     | 2583 | U    | O5'-P-OP1   | -6.91 | 87.28       | 108.00   |
| 46  | A     | 1244 | A    | C2'-C3'-O3' | 6.90  | 124.05      | 113.70   |
| 46  | A     | 1202 | A    | O3'-P-O5'   | 6.89  | 114.34      | 104.00   |
| 46  | A     | 2387 | A    | O3'-P-O5'   | -6.88 | 93.69       | 104.00   |
| 46  | A     | 1196 | C    | O3'-P-O5'   | -6.87 | 93.69       | 104.00   |
| 46  | A     | 539  | G    | O3'-P-O5'   | -6.86 | 93.71       | 104.00   |
| 46  | A     | 1294 | A    | C4'-C3'-O3' | -6.85 | 102.72      | 113.00   |
| 46  | A     | 1600 | G    | O3'-P-O5'   | -6.85 | 93.73       | 104.00   |
| 51  | a     | 965  | U    | C2'-C3'-O3' | 6.84  | 123.97      | 113.70   |
| 46  | A     | 776  | G    | C4'-C3'-O3' | -6.83 | 102.76      | 113.00   |
| 46  | A     | 1174 | A    | O3'-P-O5'   | -6.82 | 93.76       | 104.00   |
| 46  | A     | 1841 | G    | C4'-C3'-O3' | -6.82 | 102.78      | 113.00   |
| 46  | A     | 2639 | C    | O3'-P-O5'   | -6.82 | 93.78       | 104.00   |
| 46  | A     | 342  | A    | O3'-P-O5'   | -6.81 | 93.78       | 104.00   |
| 46  | A     | 831  | U    | C2'-C3'-O3' | -6.80 | 103.50      | 113.70   |
| 51  | a     | 1113 | C    | O3'-P-O5'   | -6.76 | 93.86       | 104.00   |
| 51  | a     | 739  | G    | O3'-P-O5'   | 6.76  | 114.14      | 104.00   |
| 46  | A     | 772  | G    | C4'-C3'-O3' | -6.76 | 102.86      | 113.00   |
| 46  | A     | 2717 | G    | C1'-C2'-O2' | 6.75  | 118.53      | 108.40   |
| 51  | a     | 982  | C    | C4'-C3'-O3' | -6.75 | 102.87      | 113.00   |
| 46  | A     | 481  | U    | C2'-C3'-O3' | 6.73  | 119.59      | 109.50   |
| 7   | B     | 48   | G    | C2'-C3'-O3' | 6.73  | 123.79      | 113.70   |
| 51  | a     | 283  | G    | O3'-P-O5'   | -6.72 | 93.92       | 104.00   |
| 46  | A     | 1480 | A    | O3'-P-O5'   | -6.72 | 93.92       | 104.00   |
| 46  | A     | 2713 | U    | C2'-C3'-O3' | -6.72 | 103.62      | 113.70   |
| 46  | A     | 436  | A    | O3'-P-O5'   | -6.71 | 93.94       | 104.00   |
| 51  | a     | 588  | U    | O3'-P-O5'   | -6.71 | 93.94       | 104.00   |
| 46  | A     | 2747 | G    | C1'-C2'-O2' | 6.70  | 118.45      | 108.40   |
| 46  | A     | 1171 | G    | C4'-C3'-O3' | -6.70 | 102.96      | 113.00   |
| 51  | a     | 641  | G    | C2'-C3'-O3' | 6.68  | 119.52      | 109.50   |
| 46  | A     | 1941 | A    | C2'-C3'-O3' | 6.68  | 119.52      | 109.50   |
| 46  | A     | 1998 | A    | O3'-P-O5'   | -6.68 | 93.99       | 104.00   |
| 46  | A     | 1625 | C    | O3'-P-O5'   | -6.66 | 94.00       | 104.00   |
| 46  | A     | 2452 | U    | O3'-P-O5'   | -6.66 | 94.00       | 104.00   |
| 46  | A     | 1328 | C    | O3'-P-O5'   | -6.65 | 94.02       | 104.00   |
| 46  | A     | 34   | U    | C2'-C3'-O3' | 6.65  | 119.47      | 109.50   |
| 46  | A     | 1672 | A    | C2'-C3'-O3' | 6.64  | 123.66      | 113.70   |
| 46  | A     | 2459 | A    | O4'-C4'-C3' | -6.64 | 99.46       | 106.10   |
| 51  | a     | 1357 | U    | O3'-P-O5'   | -6.64 | 94.04       | 104.00   |
| 46  | A     | 201  | C    | O3'-P-O5'   | -6.63 | 94.06       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | a     | 1200 | A    | O3'-P-O5'   | -6.62 | 94.06       | 104.00   |
| 46  | A     | 1645 | C    | O3'-P-O5'   | -6.62 | 94.08       | 104.00   |
| 46  | A     | 2805 | A    | C4'-C3'-O3' | 6.61  | 119.31      | 109.40   |
| 46  | A     | 1258 | A    | C2'-C3'-O3' | 6.60  | 123.61      | 113.70   |
| 46  | A     | 1481 | G    | O3'-P-O5'   | -6.59 | 94.11       | 104.00   |
| 46  | A     | 2753 | U    | C4'-C3'-O3' | -6.58 | 103.12      | 113.00   |
| 51  | a     | 1364 | G    | O3'-P-O5'   | -6.58 | 94.13       | 104.00   |
| 45  | v     | 69   | A    | O3'-P-O5'   | -6.56 | 94.16       | 104.00   |
| 46  | A     | 25   | U    | O3'-P-O5'   | -6.55 | 94.17       | 104.00   |
| 46  | A     | 1258 | A    | C4'-C3'-O3' | -6.55 | 103.17      | 113.00   |
| 46  | A     | 2416 | U    | O3'-P-O5'   | -6.55 | 94.17       | 104.00   |
| 46  | A     | 1941 | A    | O3'-P-O5'   | -6.54 | 94.18       | 104.00   |
| 51  | a     | 339  | G    | O3'-P-O5'   | -6.54 | 94.19       | 104.00   |
| 46  | A     | 2805 | A    | P-O3'-C3'   | 6.54  | 130.00      | 120.20   |
| 51  | a     | 759  | C    | O3'-P-O5'   | -6.53 | 94.21       | 104.00   |
| 46  | A     | 572  | A    | C4'-C3'-O3' | -6.51 | 103.24      | 113.00   |
| 46  | A     | 1893 | U    | O3'-P-O5'   | -6.51 | 94.24       | 104.00   |
| 46  | A     | 1742 | G    | O3'-P-O5'   | -6.48 | 94.28       | 104.00   |
| 46  | A     | 2842 | U    | C3'-C2'-O2' | 6.48  | 120.42      | 110.70   |
| 46  | A     | 1258 | A    | O3'-P-O5'   | -6.47 | 94.30       | 104.00   |
| 46  | A     | 483  | C    | O3'-P-O5'   | -6.44 | 94.33       | 104.00   |
| 46  | A     | 998  | G    | O3'-P-O5'   | -6.44 | 94.34       | 104.00   |
| 46  | A     | 2548 | U    | O3'-P-O5'   | -6.44 | 94.34       | 104.00   |
| 51  | a     | 553  | G    | O3'-P-O5'   | -6.44 | 94.34       | 104.00   |
| 46  | A     | 1930 | A    | C4'-C3'-O3' | -6.43 | 103.35      | 113.00   |
| 46  | A     | 1286 | A    | O3'-P-O5'   | -6.43 | 94.36       | 104.00   |
| 46  | A     | 2271 | G    | O3'-P-O5'   | -6.43 | 94.36       | 104.00   |
| 46  | A     | 1814 | A    | C4'-C3'-O3' | -6.42 | 103.37      | 113.00   |
| 51  | a     | 572  | A    | O3'-P-O5'   | -6.41 | 94.38       | 104.00   |
| 46  | A     | 2530 | C    | O3'-P-O5'   | -6.40 | 94.41       | 104.00   |
| 51  | a     | 381  | A    | O3'-P-O5'   | -6.39 | 94.41       | 104.00   |
| 7   | B     | 45   | C    | O3'-P-O5'   | -6.38 | 94.43       | 104.00   |
| 46  | A     | 2065 | C    | O3'-P-O5'   | -6.38 | 94.43       | 104.00   |
| 46  | A     | 1188 | A    | O3'-P-O5'   | -6.38 | 94.44       | 104.00   |
| 46  | A     | 2307 | A    | O3'-P-O5'   | -6.38 | 94.44       | 104.00   |
| 51  | a     | 436  | G    | O3'-P-O5'   | -6.37 | 94.45       | 104.00   |
| 51  | a     | 583  | A    | C4'-C3'-O3' | -6.35 | 103.47      | 113.00   |
| 51  | a     | 1077 | A    | O3'-P-O5'   | -6.34 | 94.48       | 104.00   |
| 51  | a     | 261  | U    | C4'-C3'-O3' | -6.34 | 103.49      | 113.00   |
| 46  | A     | 1424 | A    | O3'-P-O5'   | -6.33 | 94.50       | 104.00   |
| 46  | A     | 44   | A    | O3'-P-O5'   | -6.32 | 94.52       | 104.00   |
| 51  | a     | 679  | A    | O3'-P-O5'   | -6.32 | 94.52       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 1704 | U    | O3'-P-O5'   | -6.32 | 94.52       | 104.00   |
| 46  | A     | 1995 | A    | O3'-P-O5'   | -6.31 | 94.54       | 104.00   |
| 46  | A     | 457  | G    | C2'-C3'-O3' | -6.29 | 104.27      | 113.70   |
| 46  | A     | 1776 | A    | O3'-P-O5'   | -6.28 | 94.58       | 104.00   |
| 46  | A     | 918  | U    | O3'-P-O5'   | -6.27 | 94.59       | 104.00   |
| 46  | A     | 1369 | C    | O3'-P-O5'   | -6.27 | 94.60       | 104.00   |
| 7   | B     | 81   | G    | O3'-P-O5'   | -6.26 | 94.61       | 104.00   |
| 46  | A     | 1676 | G    | O3'-P-O5'   | -6.26 | 94.61       | 104.00   |
| 51  | a     | 1201 | C    | O3'-P-O5'   | -6.26 | 94.61       | 104.00   |
| 51  | a     | 1514 | G    | O3'-P-O5'   | -6.26 | 94.61       | 104.00   |
| 46  | A     | 274  | A    | O3'-P-O5'   | -6.25 | 94.62       | 104.00   |
| 46  | A     | 1335 | A    | C4'-C3'-O3' | -6.24 | 103.64      | 113.00   |
| 51  | a     | 1329 | C    | O3'-P-O5'   | -6.24 | 94.64       | 104.00   |
| 46  | A     | 1525 | G    | C2'-C3'-O3' | 6.24  | 123.05      | 113.70   |
| 51  | a     | 1266 | A    | C2'-C3'-O3' | 6.23  | 118.85      | 109.50   |
| 46  | A     | 1300 | G    | O3'-P-O5'   | -6.23 | 94.66       | 104.00   |
| 51  | a     | 805  | C    | O3'-P-O5'   | -6.23 | 94.66       | 104.00   |
| 7   | B     | 70   | G    | O3'-P-O5'   | -6.20 | 94.69       | 104.00   |
| 46  | A     | 958  | A    | O3'-P-O5'   | -6.20 | 94.70       | 104.00   |
| 46  | A     | 1427 | G    | C3'-C2'-O2' | 6.20  | 119.99      | 110.70   |
| 46  | A     | 2601 | A    | O3'-P-O5'   | -6.19 | 94.72       | 104.00   |
| 46  | A     | 2553 | G    | O3'-P-O5'   | -6.18 | 94.72       | 104.00   |
| 51  | a     | 510  | C    | O3'-P-O5'   | -6.18 | 94.73       | 104.00   |
| 46  | A     | 1386 | G    | C4'-C3'-C2' | -6.17 | 96.43       | 102.60   |
| 46  | A     | 1886 | G    | C4'-C3'-O3' | -6.17 | 103.74      | 113.00   |
| 46  | A     | 583  | G    | C4'-C3'-O3' | -6.17 | 103.75      | 113.00   |
| 46  | A     | 1379 | U    | C2'-C3'-O3' | -6.17 | 100.25      | 109.50   |
| 46  | A     | 635  | C    | O3'-P-O5'   | -6.15 | 94.78       | 104.00   |
| 51  | a     | 393  | U    | O3'-P-O5'   | -6.15 | 94.78       | 104.00   |
| 46  | A     | 1565 | U    | C2'-C3'-O3' | 6.14  | 122.90      | 113.70   |
| 46  | A     | 656  | A    | O3'-P-O5'   | -6.12 | 94.82       | 104.00   |
| 51  | a     | 1148 | G    | C2'-C3'-O3' | 6.12  | 118.68      | 109.50   |
| 46  | A     | 2506 | C    | O3'-P-O5'   | -6.12 | 94.82       | 104.00   |
| 46  | A     | 2643 | A    | O3'-P-O5'   | -6.10 | 94.85       | 104.00   |
| 46  | A     | 993  | A    | C4'-C3'-O3' | -6.10 | 103.86      | 113.00   |
| 46  | A     | 1065 | U    | C4'-C3'-O3' | -6.09 | 103.86      | 113.00   |
| 46  | A     | 1181 | C    | O3'-P-O5'   | 6.09  | 113.14      | 104.00   |
| 46  | A     | 1671 | G    | O3'-P-O5'   | -6.09 | 94.86       | 104.00   |
| 46  | A     | 1369 | C    | C4'-C3'-O3' | -6.09 | 103.87      | 113.00   |
| 51  | a     | 1198 | U    | O3'-P-O5'   | -6.08 | 94.88       | 104.00   |
| 46  | A     | 470  | A    | O3'-P-O5'   | -6.07 | 94.89       | 104.00   |
| 51  | a     | 21   | C    | C4'-C3'-O3' | -6.07 | 103.90      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 2290 | C    | O3'-P-O5'   | -6.06 | 94.91       | 104.00   |
| 46  | A     | 2459 | A    | C1'-O4'-C4' | -6.06 | 103.64      | 109.70   |
| 46  | A     | 386  | U    | O3'-P-O5'   | -6.06 | 94.92       | 104.00   |
| 46  | A     | 199  | A    | C1'-C2'-O2' | -6.05 | 102.72      | 111.80   |
| 46  | A     | 1185 | G    | O5'-P-OP2   | -6.05 | 89.86       | 108.00   |
| 46  | A     | 1383 | U    | O3'-P-O5'   | -6.05 | 94.93       | 104.00   |
| 51  | a     | 1377 | G    | O3'-P-O5'   | -6.04 | 94.94       | 104.00   |
| 46  | A     | 2058 | G    | O3'-P-O5'   | -6.04 | 94.94       | 104.00   |
| 46  | A     | 1802 | A    | C2'-C3'-O3' | 6.04  | 122.76      | 113.70   |
| 51  | a     | 837  | A    | O3'-P-O5'   | -6.03 | 94.95       | 104.00   |
| 46  | A     | 1006 | A    | O3'-P-O5'   | 6.03  | 113.04      | 104.00   |
| 46  | A     | 1512 | G    | C1'-C2'-O2' | 6.03  | 117.44      | 108.40   |
| 46  | A     | 1807 | U    | C1'-C2'-O2' | 6.02  | 117.42      | 108.40   |
| 51  | a     | 1235 | C    | O3'-P-O5'   | -6.01 | 94.98       | 104.00   |
| 51  | a     | 576  | G    | O3'-P-O5'   | -6.00 | 94.99       | 104.00   |
| 46  | A     | 1888 | A    | O3'-P-O5'   | -6.00 | 95.00       | 104.00   |
| 51  | a     | 1372 | A    | O3'-P-O5'   | -6.00 | 95.01       | 104.00   |
| 46  | A     | 2748 | G    | O3'-P-O5'   | -5.99 | 95.01       | 104.00   |
| 46  | A     | 1651 | G    | O3'-P-O5'   | -5.99 | 95.02       | 104.00   |
| 46  | A     | 2551 | U    | O3'-P-O5'   | -5.99 | 95.02       | 104.00   |
| 51  | a     | 955  | G    | O3'-P-O5'   | -5.99 | 95.02       | 104.00   |
| 46  | A     | 2383 | A    | C4'-C3'-O3' | -5.97 | 104.04      | 113.00   |
| 46  | A     | 2024 | U    | O3'-P-O5'   | 5.96  | 112.95      | 104.00   |
| 46  | A     | 1771 | C    | O3'-P-O5'   | -5.96 | 95.06       | 104.00   |
| 46  | A     | 1345 | U    | O3'-P-O5'   | -5.96 | 95.07       | 104.00   |
| 46  | A     | 1695 | A    | O3'-P-O5'   | -5.96 | 95.07       | 104.00   |
| 46  | A     | 2025 | C    | O3'-P-O5'   | -5.95 | 95.08       | 104.00   |
| 46  | A     | 125  | A    | C2'-C3'-O3' | -5.94 | 104.78      | 113.70   |
| 46  | A     | 1959 | G    | O3'-P-O5'   | -5.94 | 95.09       | 104.00   |
| 35  | j     | 43   | PRO  | N-CA-C      | 5.94  | 120.40      | 111.14   |
| 51  | a     | 509  | G    | O3'-P-O5'   | -5.93 | 95.11       | 104.00   |
| 51  | a     | 877  | G    | O3'-P-O5'   | -5.93 | 95.11       | 104.00   |
| 46  | A     | 1197 | A    | C2'-C3'-O3' | 5.92  | 122.59      | 113.70   |
| 46  | A     | 1374 | C    | O3'-P-O5'   | -5.92 | 95.12       | 104.00   |
| 46  | A     | 2805 | A    | C2'-C3'-O3' | 5.92  | 118.38      | 109.50   |
| 46  | A     | 2855 | G    | O3'-P-O5'   | -5.91 | 95.14       | 104.00   |
| 51  | a     | 899  | A    | O3'-P-O5'   | -5.91 | 95.14       | 104.00   |
| 46  | A     | 2514 | G    | O3'-P-O5'   | -5.91 | 95.14       | 104.00   |
| 46  | A     | 911  | G    | C3'-C2'-O2' | 5.90  | 119.56      | 110.70   |
| 46  | A     | 575  | A    | O3'-P-O5'   | -5.90 | 95.15       | 104.00   |
| 51  | a     | 581  | A    | O3'-P-O5'   | -5.90 | 95.15       | 104.00   |
| 46  | A     | 30   | G    | C2'-C3'-O3' | -5.89 | 104.86      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 1306 | G    | O3'-P-O5'   | -5.89 | 95.16       | 104.00   |
| 46  | A     | 2311 | G    | O3'-P-O5'   | -5.89 | 95.16       | 104.00   |
| 46  | A     | 2332 | G    | O3'-P-O5'   | -5.89 | 95.17       | 104.00   |
| 46  | A     | 2662 | A    | O3'-P-O5'   | -5.88 | 95.17       | 104.00   |
| 51  | a     | 297  | G    | O3'-P-O5'   | -5.88 | 95.19       | 104.00   |
| 46  | A     | 417  | G    | O3'-P-O5'   | -5.87 | 95.19       | 104.00   |
| 46  | A     | 953  | G    | O3'-P-O5'   | -5.87 | 95.19       | 104.00   |
| 46  | A     | 903  | G    | O3'-P-O5'   | -5.87 | 95.19       | 104.00   |
| 46  | A     | 2358 | A    | C1'-C2'-O2' | 5.87  | 117.21      | 108.40   |
| 46  | A     | 746  | A    | C4'-C3'-O3' | -5.87 | 104.20      | 113.00   |
| 46  | A     | 2910 | C    | O3'-P-O5'   | -5.87 | 95.20       | 104.00   |
| 46  | A     | 338  | G    | O3'-P-O5'   | -5.86 | 95.22       | 104.00   |
| 46  | A     | 828  | A    | C4'-C3'-O3' | -5.85 | 104.22      | 113.00   |
| 46  | A     | 1258 | A    | P-O5'-C5'   | -5.84 | 112.14      | 120.90   |
| 46  | A     | 198  | A    | C4'-C3'-O3' | -5.84 | 104.24      | 113.00   |
| 46  | A     | 621  | G    | O3'-P-O5'   | -5.83 | 95.26       | 104.00   |
| 46  | A     | 1940 | U    | C4'-C3'-O3' | -5.83 | 104.26      | 113.00   |
| 46  | A     | 2418 | G    | O3'-P-O5'   | -5.83 | 95.26       | 104.00   |
| 51  | a     | 1230 | G    | C2'-C3'-O3' | -5.82 | 104.96      | 113.70   |
| 46  | A     | 2103 | U    | C3'-C2'-O2' | 5.82  | 119.43      | 110.70   |
| 51  | a     | 1370 | G    | O3'-P-O5'   | -5.81 | 95.28       | 104.00   |
| 46  | A     | 795  | G    | C4'-C3'-O3' | -5.81 | 104.29      | 113.00   |
| 51  | a     | 334  | G    | O3'-P-O5'   | -5.81 | 95.29       | 104.00   |
| 51  | a     | 128  | A    | O3'-P-O5'   | -5.81 | 95.29       | 104.00   |
| 46  | A     | 2495 | C    | C4'-C3'-O3' | -5.80 | 104.30      | 113.00   |
| 46  | A     | 1648 | A    | O3'-P-O5'   | -5.80 | 95.30       | 104.00   |
| 51  | a     | 1418 | C    | O3'-P-O5'   | -5.80 | 95.31       | 104.00   |
| 46  | A     | 1301 | U    | O3'-P-O5'   | -5.79 | 95.32       | 104.00   |
| 46  | A     | 250  | G    | C4'-C3'-O3' | -5.78 | 104.34      | 113.00   |
| 46  | A     | 1205 | U    | O3'-P-O5'   | -5.78 | 95.33       | 104.00   |
| 46  | A     | 1230 | A    | C4'-C3'-O3' | -5.77 | 104.34      | 113.00   |
| 46  | A     | 1277 | A    | C4'-C3'-O3' | 5.77  | 118.06      | 109.40   |
| 46  | A     | 809  | U    | C1'-C2'-O2' | -5.77 | 103.15      | 111.80   |
| 51  | a     | 1358 | A    | C2'-C3'-O3' | -5.77 | 105.05      | 113.70   |
| 46  | A     | 38   | A    | C4'-C3'-O3' | -5.77 | 104.35      | 113.00   |
| 1   | 0     | 8    | THR  | CA-CB-OG1   | -5.76 | 100.96      | 109.60   |
| 46  | A     | 132  | C    | O3'-P-O5'   | -5.76 | 95.36       | 104.00   |
| 46  | A     | 2415 | U    | O3'-P-O5'   | -5.76 | 95.36       | 104.00   |
| 46  | A     | 1203 | G    | O5'-P-OP1   | -5.76 | 90.73       | 108.00   |
| 46  | A     | 1364 | C    | O5'-P-OP2   | 5.76  | 125.27      | 108.00   |
| 45  | v     | 3    | C    | O3'-P-O5'   | -5.75 | 95.37       | 104.00   |
| 51  | a     | 1101 | U    | O3'-P-O5'   | -5.75 | 95.37       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 1256 | C    | C4'-C3'-O3' | -5.75 | 104.37      | 113.00   |
| 46  | A     | 1388 | A    | P-O5'-C5'   | -5.75 | 112.27      | 120.90   |
| 46  | A     | 1816 | A    | C4'-C3'-O3' | -5.75 | 104.37      | 113.00   |
| 46  | A     | 1543 | U    | O3'-P-O5'   | -5.75 | 95.38       | 104.00   |
| 46  | A     | 1789 | A    | O3'-P-O5'   | -5.74 | 95.39       | 104.00   |
| 46  | A     | 583  | G    | O3'-P-O5'   | -5.73 | 95.40       | 104.00   |
| 46  | A     | 1757 | G    | C1'-O4'-C4' | -5.73 | 103.97      | 109.70   |
| 46  | A     | 1360 | A    | C4'-C3'-O3' | -5.73 | 104.41      | 113.00   |
| 51  | a     | 172  | U    | O3'-P-O5'   | -5.72 | 95.42       | 104.00   |
| 51  | a     | 1427 | A    | O3'-P-O5'   | -5.72 | 95.42       | 104.00   |
| 46  | A     | 373  | A    | O3'-P-O5'   | -5.71 | 95.43       | 104.00   |
| 46  | A     | 1054 | A    | O3'-P-O5'   | -5.71 | 95.43       | 104.00   |
| 46  | A     | 1935 | G    | O3'-P-O5'   | -5.71 | 95.43       | 104.00   |
| 46  | A     | 919  | U    | O3'-P-O5'   | -5.71 | 95.44       | 104.00   |
| 51  | a     | 536  | G    | O3'-P-O5'   | -5.71 | 95.44       | 104.00   |
| 46  | A     | 1055 | A    | C4'-C3'-O3' | -5.71 | 104.44      | 113.00   |
| 46  | A     | 525  | A    | O3'-P-O5'   | -5.70 | 95.45       | 104.00   |
| 46  | A     | 1475 | G    | O3'-P-O5'   | -5.70 | 95.46       | 104.00   |
| 51  | a     | 286  | G    | O3'-P-O5'   | -5.69 | 95.46       | 104.00   |
| 46  | A     | 2582 | G    | C1'-C2'-O2' | 5.69  | 116.94      | 108.40   |
| 46  | A     | 1352 | U    | O4'-C4'-C3' | -5.68 | 98.32       | 104.00   |
| 46  | A     | 2760 | G    | C4'-C3'-O3' | -5.68 | 104.48      | 113.00   |
| 46  | A     | 2872 | U    | C4'-C3'-O3' | -5.68 | 104.48      | 113.00   |
| 46  | A     | 2324 | C    | O3'-P-O5'   | -5.67 | 95.49       | 104.00   |
| 46  | A     | 733  | U    | O5'-P-OP1   | 5.67  | 125.01      | 108.00   |
| 46  | A     | 1239 | U    | O3'-P-O5'   | -5.67 | 95.50       | 104.00   |
| 51  | a     | 1104 | G    | O3'-P-O5'   | -5.67 | 95.50       | 104.00   |
| 46  | A     | 2289 | C    | C4'-C3'-O3' | -5.66 | 104.50      | 113.00   |
| 46  | A     | 1391 | U    | O3'-P-O5'   | -5.66 | 95.52       | 104.00   |
| 46  | A     | 2569 | C    | C4'-C3'-C2' | -5.65 | 96.95       | 102.60   |
| 51  | a     | 590  | G    | O3'-P-O5'   | -5.65 | 95.53       | 104.00   |
| 46  | A     | 778  | C    | O3'-P-O5'   | -5.64 | 95.53       | 104.00   |
| 51  | a     | 198  | G    | O3'-P-O5'   | -5.64 | 95.54       | 104.00   |
| 46  | A     | 1338 | G    | O3'-P-O5'   | -5.64 | 95.54       | 104.00   |
| 9   | D     | 150  | ASP  | CA-CB-CG    | 5.63  | 118.23      | 112.60   |
| 46  | A     | 1750 | G    | O3'-P-O5'   | -5.63 | 95.56       | 104.00   |
| 46  | A     | 2796 | C    | O3'-P-O5'   | -5.63 | 95.56       | 104.00   |
| 46  | A     | 2312 | C    | O3'-P-O5'   | -5.62 | 95.57       | 104.00   |
| 51  | a     | 555  | A    | O3'-P-O5'   | -5.61 | 95.59       | 104.00   |
| 51  | a     | 640  | G    | O3'-P-O5'   | -5.61 | 95.59       | 104.00   |
| 46  | A     | 1631 | A    | C4'-C3'-O3' | 5.60  | 117.80      | 109.40   |
| 51  | a     | 1268 | C    | O3'-P-O5'   | -5.60 | 95.60       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | B     | 37   | A    | C4'-C3'-C2' | -5.60 | 97.00       | 102.60   |
| 46  | A     | 258  | A    | C2'-C3'-O3' | -5.59 | 105.31      | 113.70   |
| 46  | A     | 1911 | C    | O3'-P-O5'   | -5.59 | 95.62       | 104.00   |
| 51  | a     | 868  | G    | O3'-P-O5'   | -5.58 | 95.63       | 104.00   |
| 51  | a     | 1072 | U    | C4'-C3'-O3' | -5.58 | 104.63      | 113.00   |
| 46  | A     | 1186 | C    | O3'-P-O5'   | -5.58 | 95.63       | 104.00   |
| 46  | A     | 1752 | G    | O3'-P-O5'   | -5.58 | 95.63       | 104.00   |
| 51  | a     | 767  | G    | C4'-C3'-O3' | -5.58 | 104.63      | 113.00   |
| 46  | A     | 1616 | G    | O3'-P-O5'   | -5.58 | 95.64       | 104.00   |
| 51  | a     | 206  | A    | O3'-P-O5'   | -5.57 | 95.65       | 104.00   |
| 51  | a     | 982  | C    | O3'-P-O5'   | -5.57 | 95.65       | 104.00   |
| 46  | A     | 835  | A    | O3'-P-O5'   | -5.57 | 95.65       | 104.00   |
| 46  | A     | 2436 | A    | O3'-P-O5'   | -5.56 | 95.66       | 104.00   |
| 46  | A     | 541  | G    | O3'-P-O5'   | -5.56 | 95.66       | 104.00   |
| 46  | A     | 2665 | U    | O3'-P-O5'   | -5.55 | 95.67       | 104.00   |
| 51  | a     | 807  | U    | O3'-P-O5'   | -5.55 | 95.67       | 104.00   |
| 46  | A     | 2753 | U    | C1'-C2'-O2' | -5.55 | 100.07      | 108.40   |
| 51  | a     | 965  | U    | C4'-C3'-C2' | -5.55 | 97.05       | 102.60   |
| 46  | A     | 496  | A    | C3'-C2'-O2' | 5.55  | 119.02      | 110.70   |
| 46  | A     | 1618 | A    | O3'-P-O5'   | -5.54 | 95.69       | 104.00   |
| 46  | A     | 1246 | G    | O4'-C4'-C3' | -5.54 | 98.46       | 104.00   |
| 46  | A     | 1530 | G    | C2'-C3'-O3' | 5.54  | 122.01      | 113.70   |
| 46  | A     | 2049 | A    | O3'-P-O5'   | -5.53 | 95.70       | 104.00   |
| 46  | A     | 2229 | C    | O3'-P-O5'   | -5.53 | 95.70       | 104.00   |
| 46  | A     | 1397 | G    | O3'-P-O5'   | -5.53 | 95.70       | 104.00   |
| 46  | A     | 2023 | C    | C3'-C2'-O2' | 5.53  | 119.00      | 110.70   |
| 17  | N     | 22   | THR  | CA-CB-OG1   | -5.53 | 101.31      | 109.60   |
| 51  | a     | 532  | A    | O3'-P-O5'   | -5.52 | 95.73       | 104.00   |
| 46  | A     | 14   | A    | O3'-P-O5'   | -5.51 | 95.73       | 104.00   |
| 46  | A     | 1419 | G    | C3'-C2'-O2' | 5.51  | 118.97      | 110.70   |
| 46  | A     | 2904 | A    | C4'-C3'-O3' | -5.50 | 101.15      | 109.40   |
| 46  | A     | 1011 | C    | C4'-C3'-O3' | -5.50 | 104.75      | 113.00   |
| 46  | A     | 704  | U    | O3'-P-O5'   | -5.50 | 95.75       | 104.00   |
| 46  | A     | 1267 | G    | C4'-C3'-O3' | -5.50 | 104.75      | 113.00   |
| 46  | A     | 181  | G    | C4'-C3'-O3' | -5.49 | 104.77      | 113.00   |
| 46  | A     | 2727 | U    | C4'-C3'-O3' | -5.49 | 104.77      | 113.00   |
| 46  | A     | 915  | U    | O3'-P-O5'   | -5.48 | 95.78       | 104.00   |
| 46  | A     | 1184 | G    | O3'-P-O5'   | 5.48  | 112.22      | 104.00   |
| 46  | A     | 2872 | U    | O3'-P-O5'   | -5.48 | 95.78       | 104.00   |
| 51  | a     | 436  | G    | C4'-C3'-O3' | 5.48  | 117.62      | 109.40   |
| 46  | A     | 2278 | U    | O3'-P-O5'   | -5.48 | 95.78       | 104.00   |
| 51  | a     | 400  | G    | O3'-P-O5'   | -5.48 | 95.78       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | a     | 848  | G    | C2'-C3'-O3' | 5.48  | 121.92      | 113.70   |
| 46  | A     | 1516 | A    | C4'-C3'-O3' | -5.47 | 104.80      | 113.00   |
| 46  | A     | 2549 | C    | O3'-P-O5'   | -5.46 | 95.81       | 104.00   |
| 7   | B     | 32   | U    | O3'-P-O5'   | -5.46 | 95.81       | 104.00   |
| 46  | A     | 517  | A    | O3'-P-O5'   | -5.46 | 95.81       | 104.00   |
| 51  | a     | 1206 | A    | C4'-C3'-O3' | -5.46 | 104.81      | 113.00   |
| 46  | A     | 29   | U    | O3'-P-O5'   | -5.46 | 95.81       | 104.00   |
| 51  | a     | 1385 | U    | O3'-P-O5'   | -5.46 | 95.81       | 104.00   |
| 46  | A     | 342  | A    | C4'-C3'-O3' | -5.45 | 104.83      | 113.00   |
| 46  | A     | 826  | U    | C2'-C3'-O3' | -5.44 | 105.54      | 113.70   |
| 51  | a     | 669  | A    | O3'-P-O5'   | -5.44 | 95.84       | 104.00   |
| 46  | A     | 296  | G    | O3'-P-O5'   | -5.44 | 95.84       | 104.00   |
| 46  | A     | 2075 | G    | O3'-P-O5'   | -5.44 | 95.84       | 104.00   |
| 46  | A     | 785  | C    | O3'-P-O5'   | 5.44  | 112.15      | 104.00   |
| 46  | A     | 297  | G    | O3'-P-O5'   | -5.43 | 95.85       | 104.00   |
| 17  | N     | 23   | ASP  | CA-CB-CG    | 5.42  | 118.02      | 112.60   |
| 51  | a     | 1313 | G    | O3'-P-O5'   | -5.42 | 95.87       | 104.00   |
| 46  | A     | 2907 | A    | C4'-C3'-O3' | -5.42 | 104.87      | 113.00   |
| 46  | A     | 2059 | A    | O3'-P-O5'   | -5.42 | 95.87       | 104.00   |
| 51  | a     | 1239 | C    | O3'-P-O5'   | -5.41 | 95.88       | 104.00   |
| 46  | A     | 1027 | A    | C2'-C3'-O3' | -5.41 | 105.59      | 113.70   |
| 51  | a     | 1294 | A    | O3'-P-O5'   | -5.41 | 95.89       | 104.00   |
| 46  | A     | 2745 | U    | C4'-C3'-O3' | -5.41 | 104.89      | 113.00   |
| 51  | a     | 1411 | C    | C3'-C2'-O2' | 5.40  | 118.81      | 110.70   |
| 51  | a     | 302  | C    | O3'-P-O5'   | -5.40 | 95.90       | 104.00   |
| 51  | a     | 363  | C    | C4'-C3'-O3' | -5.40 | 104.90      | 113.00   |
| 51  | a     | 362  | G    | C4'-C3'-O3' | -5.39 | 104.91      | 113.00   |
| 46  | A     | 1244 | A    | C4'-C3'-C2' | -5.39 | 97.21       | 102.60   |
| 46  | A     | 1414 | G    | O3'-P-O5'   | -5.39 | 95.92       | 104.00   |
| 46  | A     | 2871 | G    | O3'-P-O5'   | 5.39  | 112.08      | 104.00   |
| 51  | a     | 823  | A    | O3'-P-O5'   | -5.39 | 95.92       | 104.00   |
| 46  | A     | 1774 | A    | O3'-P-O5'   | -5.38 | 95.92       | 104.00   |
| 46  | A     | 2354 | G    | O3'-P-O5'   | -5.38 | 95.92       | 104.00   |
| 46  | A     | 1722 | A    | C2'-C3'-O3' | -5.38 | 105.63      | 113.70   |
| 46  | A     | 802  | G    | O3'-P-O5'   | -5.38 | 95.93       | 104.00   |
| 46  | A     | 1340 | A    | O3'-P-O5'   | -5.38 | 95.93       | 104.00   |
| 46  | A     | 558  | G    | O4'-C1'-N9  | 5.38  | 116.27      | 108.20   |
| 51  | a     | 820  | C    | C4'-C3'-O3' | -5.38 | 104.94      | 113.00   |
| 46  | A     | 731  | G    | O3'-P-O5'   | -5.37 | 95.94       | 104.00   |
| 51  | a     | 380  | C    | O3'-P-O5'   | -5.37 | 95.95       | 104.00   |
| 46  | A     | 691  | U    | O4'-C1'-C2' | -5.37 | 102.23      | 107.60   |
| 7   | B     | 46   | A    | C4'-C3'-O3' | -5.37 | 104.95      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 1485 | A    | O4'-C4'-C3' | -5.37 | 98.64       | 104.00   |
| 46  | A     | 2510 | G    | C4'-C3'-O3' | -5.36 | 104.95      | 113.00   |
| 46  | A     | 2873 | G    | C3'-C2'-O2' | 5.36  | 122.64      | 114.60   |
| 46  | A     | 649  | G    | O3'-P-O5'   | -5.36 | 95.96       | 104.00   |
| 46  | A     | 1863 | U    | C4'-C3'-O3' | -5.35 | 104.97      | 113.00   |
| 46  | A     | 1779 | G    | O3'-P-O5'   | -5.35 | 95.97       | 104.00   |
| 45  | v     | 45   | U    | O3'-P-O5'   | -5.35 | 95.98       | 104.00   |
| 46  | A     | 1073 | A    | C4'-C3'-O3' | -5.34 | 104.98      | 113.00   |
| 46  | A     | 1200 | G    | C2'-C3'-O3' | -5.34 | 105.69      | 113.70   |
| 25  | W     | 46   | TYR  | CB-CA-C     | 5.34  | 118.03      | 110.24   |
| 46  | A     | 381  | U    | O3'-P-O5'   | -5.34 | 95.99       | 104.00   |
| 46  | A     | 1711 | G    | O4'-C4'-C3' | -5.34 | 98.66       | 104.00   |
| 46  | A     | 1390 | C    | C4'-C3'-C2' | -5.34 | 97.26       | 102.60   |
| 46  | A     | 2022 | U    | C4'-C3'-C2' | -5.33 | 97.27       | 102.60   |
| 46  | A     | 527  | A    | O3'-P-O5'   | -5.33 | 96.00       | 104.00   |
| 46  | A     | 88   | G    | O3'-P-O5'   | 5.33  | 112.00      | 104.00   |
| 46  | A     | 224  | A    | O3'-P-O5'   | -5.33 | 96.01       | 104.00   |
| 46  | A     | 1558 | G    | O3'-P-O5'   | -5.33 | 96.01       | 104.00   |
| 46  | A     | 1709 | A    | C4'-C3'-O3' | -5.33 | 105.01      | 113.00   |
| 51  | a     | 995  | C    | O3'-P-O5'   | -5.33 | 96.01       | 104.00   |
| 46  | A     | 916  | G    | O3'-P-O5'   | -5.33 | 96.01       | 104.00   |
| 51  | a     | 384  | G    | O3'-P-O5'   | -5.32 | 96.02       | 104.00   |
| 51  | a     | 1207 | A    | O3'-P-O5'   | -5.32 | 96.02       | 104.00   |
| 51  | a     | 893  | C    | C4'-C3'-O3' | -5.32 | 105.02      | 113.00   |
| 46  | A     | 482  | C    | C4'-C3'-C2' | -5.32 | 97.28       | 102.60   |
| 46  | A     | 1618 | A    | C3'-C2'-O2' | 5.32  | 118.67      | 110.70   |
| 51  | a     | 1404 | C    | O3'-P-O5'   | -5.31 | 96.03       | 104.00   |
| 46  | A     | 263  | G    | O3'-P-O5'   | -5.31 | 96.03       | 104.00   |
| 46  | A     | 504  | A    | O3'-P-O5'   | -5.31 | 96.03       | 104.00   |
| 46  | A     | 1567 | U    | O3'-P-O5'   | -5.31 | 96.04       | 104.00   |
| 46  | A     | 1614 | A    | O3'-P-O5'   | -5.31 | 96.04       | 104.00   |
| 51  | a     | 739  | G    | C2'-C3'-O3' | -5.31 | 105.74      | 113.70   |
| 46  | A     | 1351 | U    | C1'-C2'-O2' | -5.30 | 103.85      | 111.80   |
| 46  | A     | 58   | G    | O3'-P-O5'   | -5.30 | 96.05       | 104.00   |
| 46  | A     | 557  | U    | C4'-C3'-O3' | -5.30 | 105.05      | 113.00   |
| 46  | A     | 1339 | A    | C4'-C3'-O3' | 5.30  | 117.34      | 109.40   |
| 46  | A     | 1801 | G    | C1'-C2'-O2' | 5.29  | 116.34      | 108.40   |
| 51  | a     | 1045 | G    | O3'-P-O5'   | 5.29  | 111.94      | 104.00   |
| 46  | A     | 426  | G    | O3'-P-O5'   | -5.29 | 96.07       | 104.00   |
| 46  | A     | 2816 | C    | O3'-P-O5'   | -5.29 | 96.07       | 104.00   |
| 46  | A     | 1678 | G    | C4'-C3'-O3' | -5.28 | 105.07      | 113.00   |
| 4   | 3     | 6    | THR  | CA-CB-OG1   | -5.28 | 101.68      | 109.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30  | e     | 23   | LYS  | CB-CA-C     | 5.28  | 118.54      | 109.51   |
| 46  | A     | 1867 | C    | O5'-P-OP1   | -5.28 | 92.16       | 108.00   |
| 46  | A     | 2078 | A    | O3'-P-O5'   | -5.28 | 96.08       | 104.00   |
| 46  | A     | 2435 | C    | O3'-P-O5'   | -5.28 | 96.08       | 104.00   |
| 46  | A     | 714  | U    | O3'-P-O5'   | -5.28 | 96.09       | 104.00   |
| 46  | A     | 1366 | C    | C4'-C3'-O3' | -5.28 | 105.09      | 113.00   |
| 46  | A     | 1682 | C    | C1'-C2'-O2' | 5.28  | 116.31      | 108.40   |
| 46  | A     | 2097 | U    | O3'-P-O5'   | 5.28  | 111.91      | 104.00   |
| 46  | A     | 1989 | A    | C4'-C3'-O3' | -5.27 | 105.09      | 113.00   |
| 51  | a     | 1345 | U    | O3'-P-O5'   | -5.27 | 96.09       | 104.00   |
| 46  | A     | 141  | U    | O3'-P-O5'   | -5.27 | 96.09       | 104.00   |
| 46  | A     | 493  | G    | O3'-P-O5'   | -5.27 | 96.09       | 104.00   |
| 46  | A     | 2844 | A    | O3'-P-O5'   | -5.27 | 96.09       | 104.00   |
| 9   | D     | 33   | ASN  | CA-CB-CG    | 5.27  | 117.87      | 112.60   |
| 46  | A     | 2740 | A    | C4'-C3'-O3' | -5.27 | 105.10      | 113.00   |
| 51  | a     | 142  | A    | O3'-P-O5'   | -5.27 | 96.10       | 104.00   |
| 46  | A     | 2791 | U    | O3'-P-O5'   | -5.27 | 96.10       | 104.00   |
| 46  | A     | 1229 | U    | C4'-C3'-O3' | -5.26 | 105.11      | 113.00   |
| 51  | a     | 1147 | A    | O3'-P-O5'   | -5.26 | 96.11       | 104.00   |
| 46  | A     | 1432 | A    | C2'-C3'-O3' | -5.26 | 105.81      | 113.70   |
| 46  | A     | 2721 | C    | C4'-C3'-C2' | -5.26 | 97.34       | 102.60   |
| 46  | A     | 1228 | G    | C4'-C3'-O3' | -5.26 | 105.11      | 113.00   |
| 46  | A     | 787  | C    | C4'-C3'-O3' | -5.25 | 105.12      | 113.00   |
| 51  | a     | 371  | A    | O3'-P-O5'   | -5.25 | 96.12       | 104.00   |
| 46  | A     | 423  | G    | O3'-P-O5'   | -5.25 | 96.13       | 104.00   |
| 46  | A     | 1791 | A    | O3'-P-O5'   | -5.25 | 96.13       | 104.00   |
| 46  | A     | 70   | G    | C1'-C2'-O2' | -5.25 | 103.93      | 111.80   |
| 46  | A     | 769  | A    | O3'-P-O5'   | -5.24 | 96.14       | 104.00   |
| 46  | A     | 1428 | G    | O3'-P-O5'   | -5.24 | 96.14       | 104.00   |
| 46  | A     | 65   | A    | C4'-C3'-O3' | -5.24 | 105.15      | 113.00   |
| 46  | A     | 1382 | G    | C4'-C3'-O3' | 5.24  | 120.86      | 113.00   |
| 46  | A     | 1257 | G    | O3'-P-O5'   | -5.23 | 96.16       | 104.00   |
| 46  | A     | 1591 | G    | O3'-P-O5'   | -5.23 | 96.16       | 104.00   |
| 51  | a     | 1309 | G    | O3'-P-O5'   | -5.23 | 96.15       | 104.00   |
| 46  | A     | 2740 | A    | C3'-C2'-O2' | 5.23  | 118.54      | 110.70   |
| 46  | A     | 2843 | G    | C3'-C2'-O2' | 5.23  | 118.54      | 110.70   |
| 51  | a     | 579  | G    | C4'-C3'-O3' | -5.22 | 105.16      | 113.00   |
| 46  | A     | 1319 | G    | O3'-P-O5'   | -5.22 | 96.17       | 104.00   |
| 46  | A     | 2063 | U    | C4'-C3'-O3' | -5.22 | 105.17      | 113.00   |
| 46  | A     | 2296 | A    | N9-C1'-C2'  | 5.22  | 119.83      | 112.00   |
| 46  | A     | 1542 | A    | C4'-C3'-O3' | 5.22  | 117.22      | 109.40   |
| 51  | a     | 1336 | G    | C4'-C3'-O3' | -5.21 | 105.18      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 1235 | A    | O3'-P-O5'   | -5.21 | 96.18       | 104.00   |
| 51  | a     | 923  | A    | O3'-P-O5'   | -5.21 | 96.18       | 104.00   |
| 46  | A     | 2854 | A    | O3'-P-O5'   | -5.21 | 96.18       | 104.00   |
| 46  | A     | 12   | A    | O3'-P-O5'   | -5.21 | 96.19       | 104.00   |
| 46  | A     | 546  | G    | O3'-P-O5'   | -5.20 | 96.20       | 104.00   |
| 46  | A     | 1613 | C    | O3'-P-O5'   | -5.20 | 96.20       | 104.00   |
| 46  | A     | 2253 | G    | O3'-P-O5'   | -5.20 | 96.20       | 104.00   |
| 51  | a     | 983  | G    | C4'-C3'-O3' | -5.20 | 105.20      | 113.00   |
| 46  | A     | 515  | G    | C4'-C3'-O3' | -5.19 | 105.21      | 113.00   |
| 46  | A     | 747  | G    | C4'-C3'-O3' | -5.19 | 105.22      | 113.00   |
| 46  | A     | 768  | G    | O3'-P-O5'   | -5.19 | 96.21       | 104.00   |
| 46  | A     | 2478 | U    | C1'-C2'-O2' | -5.19 | 104.02      | 111.80   |
| 51  | a     | 740  | G    | O5'-P-OP2   | -5.18 | 92.44       | 108.00   |
| 46  | A     | 1715 | C    | C3'-C2'-O2' | 5.18  | 118.47      | 110.70   |
| 46  | A     | 1934 | C    | C4'-C3'-O3' | -5.18 | 105.23      | 113.00   |
| 46  | A     | 2904 | A    | P-O3'-C3'   | 5.18  | 127.97      | 120.20   |
| 46  | A     | 1782 | G    | C2'-C3'-O3' | 5.18  | 121.47      | 113.70   |
| 46  | A     | 2353 | U    | C4'-C3'-O3' | -5.18 | 105.23      | 113.00   |
| 46  | A     | 2505 | A    | O3'-P-O5'   | 5.18  | 111.76      | 104.00   |
| 46  | A     | 2112 | G    | O3'-P-O5'   | -5.17 | 96.24       | 104.00   |
| 46  | A     | 1036 | A    | O3'-P-O5'   | -5.17 | 96.25       | 104.00   |
| 51  | a     | 844  | A    | O3'-P-O5'   | -5.17 | 96.25       | 104.00   |
| 46  | A     | 1751 | U    | P-O3'-C3'   | 5.17  | 127.95      | 120.20   |
| 46  | A     | 1627 | A    | O3'-P-O5'   | -5.16 | 96.26       | 104.00   |
| 46  | A     | 1380 | U    | C3'-C2'-O2' | -5.16 | 106.86      | 114.60   |
| 51  | a     | 301  | A    | O3'-P-O5'   | -5.16 | 96.26       | 104.00   |
| 46  | A     | 188  | C    | O3'-P-O5'   | -5.16 | 96.27       | 104.00   |
| 46  | A     | 1025 | A    | C4'-C3'-C2' | -5.15 | 97.45       | 102.60   |
| 51  | a     | 1062 | U    | O3'-P-O5'   | -5.15 | 96.27       | 104.00   |
| 46  | A     | 30   | G    | O3'-P-O5'   | -5.15 | 96.28       | 104.00   |
| 46  | A     | 1209 | G    | O3'-P-O5'   | -5.15 | 96.28       | 104.00   |
| 51  | a     | 1528 | A    | C1'-C2'-O2' | 5.15  | 116.12      | 108.40   |
| 46  | A     | 498  | U    | C1'-O4'-C4' | -5.14 | 104.75      | 109.90   |
| 46  | A     | 824  | G    | O3'-P-O5'   | 5.14  | 111.71      | 104.00   |
| 46  | A     | 1651 | G    | C2'-C3'-O3' | -5.14 | 105.99      | 113.70   |
| 46  | A     | 125  | A    | C4'-C3'-O3' | -5.14 | 105.29      | 113.00   |
| 46  | A     | 2520 | U    | C4'-C3'-O3' | -5.14 | 105.30      | 113.00   |
| 46  | A     | 211  | C    | O3'-P-O5'   | -5.13 | 96.30       | 104.00   |
| 7   | B     | 49   | G    | C2'-C3'-O3' | 5.13  | 121.39      | 113.70   |
| 7   | B     | 29   | C    | O3'-P-O5'   | -5.13 | 96.31       | 104.00   |
| 46  | A     | 1424 | A    | C4'-C3'-O3' | 5.13  | 117.09      | 109.40   |
| 46  | A     | 180  | G    | C3'-C2'-O2' | 5.13  | 118.39      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 589  | G    | O3'-P-O5'   | -5.13 | 96.31       | 104.00   |
| 46  | A     | 2272 | U    | C4'-C3'-O3' | -5.12 | 105.31      | 113.00   |
| 46  | A     | 2841 | C    | O3'-P-O5'   | -5.12 | 96.31       | 104.00   |
| 46  | A     | 744  | C    | C4'-C3'-O3' | -5.12 | 105.32      | 113.00   |
| 7   | B     | 37   | A    | C2'-C3'-O3' | 5.12  | 121.38      | 113.70   |
| 46  | A     | 1363 | G    | C2'-C3'-O3' | 5.12  | 117.17      | 109.50   |
| 51  | a     | 388  | G    | O3'-P-O5'   | -5.11 | 96.34       | 104.00   |
| 46  | A     | 1817 | C    | C3'-C2'-O2' | 5.10  | 118.35      | 110.70   |
| 46  | A     | 299  | U    | O3'-P-O5'   | -5.09 | 96.36       | 104.00   |
| 46  | A     | 1877 | A    | O3'-P-O5'   | -5.09 | 96.36       | 104.00   |
| 51  | a     | 789  | G    | C4'-C3'-O3' | -5.09 | 105.36      | 113.00   |
| 46  | A     | 2725 | U    | C3'-C2'-O2' | 5.09  | 118.33      | 110.70   |
| 46  | A     | 1062 | C    | O3'-P-O5'   | -5.09 | 96.37       | 104.00   |
| 46  | A     | 2082 | G    | O4'-C4'-C3' | -5.09 | 98.91       | 104.00   |
| 51  | a     | 326  | G    | C4'-C3'-C2' | -5.09 | 97.51       | 102.60   |
| 46  | A     | 2473 | G    | O3'-P-O5'   | -5.08 | 96.38       | 104.00   |
| 46  | A     | 2473 | G    | C4'-C3'-O3' | -5.08 | 105.38      | 113.00   |
| 51  | a     | 370  | G    | C1'-C2'-O2' | 5.08  | 116.02      | 108.40   |
| 51  | a     | 1509 | A    | C4'-C3'-O3' | -5.08 | 105.38      | 113.00   |
| 46  | A     | 1807 | U    | C4'-C3'-O3' | -5.08 | 105.39      | 113.00   |
| 51  | a     | 740  | G    | O3'-P-O5'   | -5.08 | 96.39       | 104.00   |
| 46  | A     | 2717 | G    | C2'-C3'-O3' | -5.07 | 106.09      | 113.70   |
| 46  | A     | 1351 | U    | C2'-C3'-O3' | 5.07  | 117.11      | 109.50   |
| 46  | A     | 1564 | C    | O3'-P-O5'   | -5.07 | 96.39       | 104.00   |
| 46  | A     | 2468 | A    | C4'-C3'-O3' | 5.07  | 117.01      | 109.40   |
| 46  | A     | 599  | G    | O3'-P-O5'   | -5.07 | 96.40       | 104.00   |
| 46  | A     | 1197 | A    | C4'-C3'-O3' | -5.07 | 105.40      | 113.00   |
| 46  | A     | 2496 | C    | C4'-C3'-O3' | -5.07 | 105.40      | 113.00   |
| 46  | A     | 757  | C    | O3'-P-O5'   | -5.06 | 96.41       | 104.00   |
| 46  | A     | 864  | C    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 46  | A     | 1186 | C    | C4'-C3'-O3' | -5.05 | 105.42      | 113.00   |
| 46  | A     | 2764 | G    | O3'-P-O5'   | -5.05 | 96.42       | 104.00   |
| 46  | A     | 1277 | A    | C2'-C3'-O3' | -5.05 | 101.92      | 109.50   |
| 46  | A     | 1561 | G    | O3'-P-O5'   | -5.05 | 96.42       | 104.00   |
| 46  | A     | 2425 | G    | C4'-C3'-O3' | -5.05 | 105.43      | 113.00   |
| 46  | A     | 724  | A    | C4'-C3'-O3' | -5.04 | 105.43      | 113.00   |
| 46  | A     | 1373 | U    | O3'-P-O5'   | -5.04 | 96.43       | 104.00   |
| 46  | A     | 2225 | C    | O3'-P-O5'   | -5.04 | 96.44       | 104.00   |
| 46  | A     | 1573 | C    | C3'-C2'-O2' | 5.04  | 118.26      | 110.70   |
| 46  | A     | 910  | A    | C4'-C3'-O3' | -5.04 | 105.44      | 113.00   |
| 51  | a     | 530  | G    | C1'-C2'-O2' | 5.03  | 115.95      | 108.40   |
| 46  | A     | 563  | C    | O3'-P-O5'   | -5.03 | 96.45       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | A     | 183  | A    | C1'-C2'-O2' | 5.03  | 115.94      | 108.40   |
| 46  | A     | 274  | A    | C4'-C3'-O3' | -5.03 | 105.45      | 113.00   |
| 51  | a     | 1407 | A    | O3'-P-O5'   | -5.03 | 96.45       | 104.00   |
| 51  | a     | 50   | C    | O3'-P-O5'   | -5.03 | 96.46       | 104.00   |
| 46  | A     | 798  | A    | C2'-C3'-O3' | -5.03 | 106.16      | 113.70   |
| 4   | 3     | 13   | ARG  | CB-CA-C     | -5.02 | 101.27      | 109.56   |
| 51  | a     | 1441 | G    | O3'-P-O5'   | -5.02 | 96.47       | 104.00   |
| 51  | a     | 1381 | U    | O3'-P-O5'   | -5.02 | 96.47       | 104.00   |
| 48  | s     | 44   | PHE  | CA-CB-CG    | 5.02  | 118.82      | 113.80   |
| 46  | A     | 611  | U    | C4'-C3'-O3' | -5.02 | 105.48      | 113.00   |
| 46  | A     | 1386 | G    | C3'-C2'-O2' | 5.01  | 118.22      | 110.70   |
| 51  | a     | 650  | A    | O3'-P-O5'   | -5.01 | 96.48       | 104.00   |
| 46  | A     | 2822 | C    | O3'-P-O5'   | -5.01 | 96.48       | 104.00   |
| 46  | A     | 724  | A    | O3'-P-O5'   | -5.01 | 96.48       | 104.00   |
| 51  | a     | 894  | U    | O3'-P-O5'   | -5.01 | 96.48       | 104.00   |
| 46  | A     | 832  | G    | C4'-C3'-O3' | -5.01 | 105.48      | 113.00   |
| 51  | a     | 778  | G    | C4'-C3'-O3' | -5.01 | 105.49      | 113.00   |
| 46  | A     | 2091 | A    | OP2-P-O3'   | 5.01  | 123.02      | 108.00   |
| 45  | v     | 20   | U    | C2'-C3'-O3' | 5.01  | 117.01      | 109.50   |
| 46  | A     | 1515 | C    | O3'-P-O5'   | -5.01 | 96.49       | 104.00   |
| 46  | A     | 367  | G    | O3'-P-O5'   | -5.00 | 96.49       | 104.00   |
| 51  | a     | 308  | A    | O3'-P-O5'   | -5.00 | 96.50       | 104.00   |

There are no chirality outliers.

All (48) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | 0     | 41   | ARG  | Sidechain |
| 1   | 0     | 6    | ARG  | Sidechain |
| 2   | 1     | 29   | ARG  | Sidechain |
| 3   | 2     | 33   | ARG  | Sidechain |
| 5   | 4     | 19   | ARG  | Sidechain |
| 6   | 6     | 32   | ARG  | Sidechain |
| 46  | A     | 1801 | G    | Sidechain |
| 46  | A     | 2066 | A    | Sidechain |
| 46  | A     | 558  | G    | Sidechain |
| 8   | C     | 13   | ARG  | Sidechain |
| 8   | C     | 14   | ARG  | Sidechain |
| 8   | C     | 189  | ARG  | Sidechain |
| 8   | C     | 210  | ARG  | Sidechain |
| 8   | C     | 274  | ARG  | Sidechain |
| 8   | C     | 43   | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 8   | C     | 52  | ARG  | Sidechain |
| 10  | E     | 168 | ARG  | Sidechain |
| 10  | E     | 62  | ARG  | Sidechain |
| 10  | E     | 72  | ARG  | Sidechain |
| 11  | F     | 167 | ARG  | Sidechain |
| 12  | G     | 172 | ARG  | Sidechain |
| 15  | L     | 60  | ARG  | Sidechain |
| 16  | M     | 119 | ARG  | Sidechain |
| 17  | N     | 107 | ARG  | Sidechain |
| 17  | N     | 108 | ARG  | Sidechain |
| 17  | N     | 59  | ARG  | Sidechain |
| 18  | O     | 35  | ARG  | Sidechain |
| 19  | P     | 104 | ARG  | Sidechain |
| 19  | P     | 93  | ARG  | Sidechain |
| 20  | Q     | 51  | ARG  | Sidechain |
| 21  | R     | 67  | ARG  | Sidechain |
| 22  | S     | 41  | ARG  | Sidechain |
| 26  | X     | 3   | ARG  | Sidechain |
| 27  | Y     | 47  | ARG  | Sidechain |
| 51  | a     | 370 | G    | Sidechain |
| 47  | b     | 167 | ARG  | Sidechain |
| 52  | d     | 13  | ARG  | Sidechain |
| 52  | d     | 29  | ARG  | Sidechain |
| 30  | e     | 29  | ARG  | Sidechain |
| 30  | e     | 30  | ARG  | Sidechain |
| 31  | f     | 47  | ARG  | Sidechain |
| 31  | f     | 56  | ARG  | Sidechain |
| 34  | i     | 109 | ARG  | Sidechain |
| 34  | i     | 12  | ARG  | Sidechain |
| 34  | i     | 130 | ARG  | Sidechain |
| 35  | j     | 62  | ARG  | Sidechain |
| 38  | m     | 107 | ARG  | Sidechain |
| 48  | s     | 78  | ARG  | Sidechain |

## 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     | 432   | 0        | 454      | 3       | 0            |
| 2   | 1     | 403   | 0        | 414      | 1       | 0            |
| 3   | 2     | 368   | 0        | 410      | 1       | 0            |
| 4   | 3     | 512   | 0        | 564      | 1       | 0            |
| 5   | 4     | 297   | 0        | 342      | 2       | 0            |
| 6   | 6     | 356   | 0        | 350      | 1       | 0            |
| 7   | B     | 2392  | 0        | 1213     | 1       | 0            |
| 8   | C     | 2093  | 0        | 2179     | 10      | 0            |
| 9   | D     | 1575  | 0        | 1642     | 7       | 0            |
| 10  | E     | 1567  | 0        | 1652     | 2       | 0            |
| 11  | F     | 1405  | 0        | 1467     | 2       | 0            |
| 12  | G     | 1342  | 0        | 1388     | 1       | 0            |
| 13  | J     | 1131  | 0        | 1169     | 2       | 0            |
| 14  | K     | 921   | 0        | 977      | 4       | 0            |
| 15  | L     | 1082  | 0        | 1132     | 2       | 0            |
| 16  | M     | 1076  | 0        | 1145     | 3       | 0            |
| 17  | N     | 954   | 0        | 983      | 6       | 0            |
| 18  | O     | 913   | 0        | 947      | 0       | 0            |
| 19  | P     | 937   | 0        | 1008     | 0       | 0            |
| 20  | Q     | 950   | 0        | 1018     | 1       | 0            |
| 21  | R     | 795   | 0        | 838      | 1       | 0            |
| 22  | S     | 850   | 0        | 911      | 4       | 0            |
| 23  | T     | 733   | 0        | 781      | 2       | 0            |
| 24  | U     | 770   | 0        | 825      | 1       | 0            |
| 25  | W     | 629   | 0        | 644      | 3       | 0            |
| 26  | X     | 467   | 0        | 512      | 2       | 0            |
| 27  | Y     | 540   | 0        | 581      | 0       | 0            |
| 28  | Z     | 456   | 0        | 491      | 1       | 0            |
| 29  | c     | 1608  | 0        | 1646     | 0       | 0            |
| 30  | e     | 1219  | 0        | 1300     | 1       | 0            |
| 31  | f     | 765   | 0        | 765      | 0       | 0            |
| 32  | g     | 1199  | 0        | 1256     | 0       | 0            |
| 33  | h     | 1030  | 0        | 1086     | 0       | 0            |
| 34  | i     | 997   | 0        | 1033     | 1       | 0            |
| 35  | j     | 788   | 0        | 832      | 8       | 0            |
| 36  | k     | 847   | 0        | 860      | 1       | 0            |
| 37  | l     | 1036  | 0        | 1091     | 0       | 0            |
| 38  | m     | 934   | 0        | 995      | 0       | 0            |
| 39  | n     | 498   | 0        | 533      | 0       | 0            |
| 40  | o     | 730   | 0        | 759      | 0       | 0            |
| 41  | p     | 691   | 0        | 718      | 1       | 0            |
| 42  | q     | 693   | 0        | 734      | 1       | 0            |
| 43  | r     | 522   | 0        | 558      | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44  | t     | 658    | 0        | 715      | 1       | 0            |
| 45  | v     | 1622   | 0        | 820      | 1       | 0            |
| 46  | A     | 58630  | 0        | 29517    | 151     | 0            |
| 47  | b     | 1564   | 0        | 1625     | 2       | 0            |
| 48  | s     | 680    | 0        | 694      | 0       | 0            |
| 49  | 5     | 346    | 0        | 345      | 2       | 0            |
| 50  | 7     | 123    | 0        | 62       | 0       | 0            |
| 51  | a     | 32391  | 0        | 16310    | 51      | 0            |
| 52  | d     | 1604   | 0        | 1638     | 1       | 0            |
| All | All   | 137121 | 0        | 91929    | 248     | 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 1.

All (248) 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) |
|------------------|------------------|--------------------------|-------------------|
| 46:A:2806:G:OP2  | 46:A:2810:A:O2'  | 2.07                     | 0.73              |
| 46:A:2231:C:O2'  | 46:A:2233:C:OP1  | 2.09                     | 0.70              |
| 46:A:1367:G:H2'  | 46:A:1369:C:C5   | 2.26                     | 0.70              |
| 46:A:1887:G:O2'  | 46:A:1912:G:N2   | 2.33                     | 0.61              |
| 46:A:1359:G:C2   | 46:A:1368:U:H5'' | 2.35                     | 0.61              |
| 46:A:790:A:O2'   | 46:A:1704:U:OP1  | 2.18                     | 0.60              |
| 51:a:673:G:H22   | 51:a:750:G:H1    | 1.50                     | 0.59              |
| 15:L:17:ASN:HD21 | 15:L:27:ASN:HD22 | 1.50                     | 0.59              |
| 23:T:58:ASN:ND2  | 23:T:77:ARG:HH11 | 2.00                     | 0.59              |
| 36:k:121:ASN:HB2 | 51:a:727:A:H5'   | 1.85                     | 0.58              |
| 46:A:2092:C:O2   | 46:A:2479:A:N1   | 2.36                     | 0.58              |
| 46:A:1542:A:O2'  | 46:A:1544:C:N4   | 2.36                     | 0.58              |
| 35:j:28:THR:HG22 | 35:j:86:ALA:HB1  | 1.87                     | 0.57              |
| 46:A:2009:G:O2'  | 46:A:2011:U:OP2  | 2.23                     | 0.56              |
| 51:a:969:A:C2    | 51:a:1231:G:O4'  | 2.58                     | 0.56              |
| 46:A:1377:G:O2'  | 46:A:1432:A:N1   | 2.38                     | 0.56              |
| 46:A:1379:U:C5   | 46:A:1648:A:C8   | 2.93                     | 0.56              |
| 25:W:67:LEU:HD13 | 25:W:87:VAL:HG12 | 1.88                     | 0.56              |
| 22:S:29:VAL:HG22 | 22:S:55:ILE:HD11 | 1.86                     | 0.56              |
| 51:a:1400:U:H2'  | 51:a:1401:G:C8   | 2.40                     | 0.56              |
| 9:D:24:PRO:HB3   | 46:A:2711:G:C2   | 2.41                     | 0.55              |
| 46:A:2229:C:O2   | 46:A:2255:C:N4   | 2.39                     | 0.55              |
| 46:A:747:G:O2'   | 46:A:1677:A:N3   | 2.37                     | 0.55              |
| 46:A:567:U:O2'   | 46:A:568:G:N7    | 2.36                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:A:1366:C:C4    | 46:A:1367:G:C6    | 2.95                     | 0.54              |
| 46:A:1367:G:H2'   | 46:A:1369:C:C4    | 2.42                     | 0.54              |
| 51:a:1107:C:H2'   | 51:a:1108:C:C6    | 2.42                     | 0.54              |
| 46:A:1074:A:N3    | 46:A:2515:G:O2'   | 2.41                     | 0.54              |
| 22:S:21:MET:HE2   | 22:S:103:ILE:HG23 | 1.88                     | 0.54              |
| 51:a:778:G:H4'    | 51:a:1523:A:H4'   | 1.88                     | 0.54              |
| 51:a:985:A:N1     | 51:a:1375:C:O2'   | 2.34                     | 0.54              |
| 51:a:1444:G:H2'   | 51:a:1445:U:C6    | 2.43                     | 0.53              |
| 46:A:2417:A:N7    | 46:A:2418:G:C6    | 2.76                     | 0.53              |
| 14:K:23:LYS:NZ    | 46:A:2590:A:N3    | 2.56                     | 0.53              |
| 46:A:523:G:H4'    | 46:A:548:A:N1     | 2.24                     | 0.52              |
| 46:A:229:A:O2'    | 46:A:231:A:N1     | 2.36                     | 0.52              |
| 1:O:15:LEU:O      | 1:O:18:THR:HG23   | 2.10                     | 0.52              |
| 51:a:1379:G:C2    | 51:a:1380:G:C8    | 2.98                     | 0.52              |
| 46:A:1072:A:OP2   | 46:A:1180:C:O2'   | 2.18                     | 0.52              |
| 46:A:1363:G:C2    | 46:A:1367:G:N1    | 2.78                     | 0.52              |
| 46:A:656:A:H2     | 46:A:662:G:H22    | 1.57                     | 0.51              |
| 46:A:1322:G:O2'   | 46:A:1324:G:N7    | 2.31                     | 0.51              |
| 51:a:1072:U:H2'   | 51:a:1073:C:C6    | 2.45                     | 0.51              |
| 15:L:69:ILE:HD13  | 46:A:2435:C:C6    | 2.46                     | 0.51              |
| 35:j:70:HIS:HD1   | 51:a:1161:A:P     | 2.33                     | 0.51              |
| 46:A:1073:A:C2    | 46:A:2517:A:H5'   | 2.46                     | 0.51              |
| 51:a:421:G:N7     | 52:d:28:LYS:NZ    | 2.58                     | 0.51              |
| 46:A:1327:U:H5    | 46:A:1365:U:O2    | 1.94                     | 0.51              |
| 8:C:63:ARG:NH2    | 46:A:1616:G:OP2   | 2.44                     | 0.51              |
| 8:C:180:GLU:OE1   | 46:A:1828:G:O2'   | 2.24                     | 0.51              |
| 46:A:1485:A:H2    | 46:A:1600:G:H21   | 1.59                     | 0.50              |
| 14:K:63:VAL:HG12  | 14:K:106:LEU:HD11 | 1.93                     | 0.50              |
| 46:A:1755:C:O2'   | 46:A:2883:C:N3    | 2.43                     | 0.50              |
| 46:A:2360:G:O2'   | 46:A:2365:A:N1    | 2.41                     | 0.50              |
| 26:X:23:ASN:ND2   | 46:A:2108:U:O2'   | 2.44                     | 0.50              |
| 51:a:1084:G:O2'   | 51:a:1111:A:N1    | 2.41                     | 0.50              |
| 46:A:1028:C:O2    | 46:A:1028:C:O5'   | 2.29                     | 0.50              |
| 17:N:66:ILE:HD11  | 17:N:83:LEU:HD22  | 1.93                     | 0.50              |
| 1:O:11:VAL:HG22   | 46:A:17:G:H5''    | 1.93                     | 0.50              |
| 41:p:6:ARG:HB2    | 51:a:384:G:H5''   | 1.93                     | 0.50              |
| 46:A:2817:C:O2'   | 46:A:2834:A:N3    | 2.39                     | 0.50              |
| 9:D:59:LYS:NZ     | 46:A:2856:G:OP1   | 2.44                     | 0.50              |
| 35:j:100:ILE:HG22 | 35:j:102:LEU:HG   | 1.94                     | 0.50              |
| 17:N:21:THR:HG23  | 17:N:44:VAL:HG22  | 1.93                     | 0.49              |
| 46:A:1245:G:C5'   | 46:A:1245:G:N3    | 2.75                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:A:1363:G:N1   | 46:A:1367:G:C6   | 2.81                     | 0.49              |
| 34:i:130:ARG:NH2 | 45:v:33:U:OP2    | 2.45                     | 0.49              |
| 51:a:1378:C:H2'  | 51:a:1379:G:C8   | 2.48                     | 0.49              |
| 46:A:2651:C:O2'  | 46:A:2850:G:N7   | 2.46                     | 0.49              |
| 46:A:2877:G:H2'  | 46:A:2878:U:O4'  | 2.13                     | 0.48              |
| 21:R:76:TYR:OH   | 46:A:608:C:OP1   | 2.29                     | 0.48              |
| 51:a:224:U:H2'   | 51:a:225:A:C8    | 2.49                     | 0.48              |
| 24:U:46:LYS:HG2  | 46:A:530:A:H5''  | 1.96                     | 0.48              |
| 46:A:2421:A:C8   | 46:A:2458:G:C2   | 3.02                     | 0.48              |
| 46:A:2818:C:H2'  | 46:A:2819:A:C8   | 2.49                     | 0.48              |
| 17:N:108:ARG:NH2 | 46:A:1366:C:O2'  | 2.47                     | 0.48              |
| 46:A:150:A:H61   | 46:A:179:A:H2    | 1.59                     | 0.47              |
| 46:A:1713:A:O2'  | 46:A:1719:G:N7   | 2.38                     | 0.47              |
| 46:A:2035:C:O2'  | 46:A:2848:A:N3   | 2.48                     | 0.47              |
| 47:b:96:TRP:CZ2  | 47:b:100:THR:HB  | 2.49                     | 0.47              |
| 46:A:482:C:O2'   | 46:A:483:C:P     | 2.72                     | 0.47              |
| 22:S:90:MET:HB3  | 49:5:99:TYR:HA   | 1.96                     | 0.47              |
| 46:A:1411:U:HO2' | 46:A:2241:A:H8   | 1.62                     | 0.47              |
| 46:A:2366:G:C2   | 46:A:2367:G:C8   | 3.02                     | 0.47              |
| 46:A:2656:G:O2'  | 46:A:2810:A:N1   | 2.44                     | 0.47              |
| 51:a:1355:A:C8   | 51:a:1357:U:C2   | 3.02                     | 0.47              |
| 8:C:210:ARG:NE   | 46:A:1614:A:OP1  | 2.48                     | 0.47              |
| 46:A:2349:A:C2   | 46:A:2362:A:C8   | 3.02                     | 0.47              |
| 22:S:42:ALA:HB2  | 46:A:2039:G:H5'' | 1.97                     | 0.46              |
| 51:a:1106:C:H2'  | 51:a:1107:C:O4'  | 2.14                     | 0.46              |
| 46:A:1756:U:C4   | 46:A:1757:G:C5   | 3.04                     | 0.46              |
| 46:A:614:G:H2'   | 46:A:2059:A:N7   | 2.30                     | 0.46              |
| 46:A:1941:A:H2   | 46:A:1946:U:H3   | 1.63                     | 0.46              |
| 51:a:1062:U:O4   | 51:a:1209:C:C2   | 2.69                     | 0.46              |
| 46:A:761:U:O2'   | 46:A:763:A:N7    | 2.44                     | 0.46              |
| 46:A:957:A:H2'   | 46:A:958:A:C8    | 2.50                     | 0.46              |
| 25:W:54:TYR:OH   | 46:A:2361:C:OP1  | 2.27                     | 0.46              |
| 8:C:243:ARG:NH2  | 46:A:2268:G:OP2  | 2.49                     | 0.46              |
| 16:M:101:LYS:NZ  | 46:A:954:U:O3'   | 2.49                     | 0.46              |
| 17:N:66:ILE:CD1  | 17:N:83:LEU:HD22 | 2.45                     | 0.46              |
| 51:a:1434:A:H2'  | 51:a:1435:A:O4'  | 2.16                     | 0.46              |
| 46:A:1363:G:C2   | 46:A:1367:G:C6   | 3.03                     | 0.46              |
| 46:A:1755:C:C4   | 46:A:1756:U:C4   | 3.03                     | 0.46              |
| 46:A:1941:A:N7   | 51:a:1505:U:H1'  | 2.31                     | 0.46              |
| 46:A:1385:G:C6   | 46:A:1386:G:N7   | 2.85                     | 0.45              |
| 51:a:1411:C:O2   | 51:a:1510:A:N1   | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:A:796:A:N1    | 46:A:800:G:O2'   | 2.39                     | 0.45              |
| 51:a:1510:A:H5'' | 51:a:1518:G:H5'' | 1.99                     | 0.45              |
| 23:T:58:ASN:HD21 | 23:T:77:ARG:HH11 | 1.61                     | 0.45              |
| 51:a:777:A:N3    | 51:a:1522:U:O2'  | 2.47                     | 0.45              |
| 46:A:903:G:H2'   | 46:A:904:A:C8    | 2.52                     | 0.45              |
| 46:A:2508:U:OP1  | 46:A:2566:U:O2'  | 2.31                     | 0.45              |
| 51:a:1045:G:H3'  | 51:a:1046:G:H5'' | 1.99                     | 0.45              |
| 46:A:732:A:H1'   | 46:A:735:U:O4    | 2.17                     | 0.44              |
| 51:a:1187:G:N2   | 51:a:1189:A:H3'  | 2.32                     | 0.44              |
| 46:A:908:A:C2    | 46:A:964:A:C4    | 3.06                     | 0.44              |
| 46:A:1424:A:C4   | 46:A:1425:C:C5   | 3.05                     | 0.44              |
| 46:A:1066:A:C2   | 46:A:1187:U:C2   | 3.06                     | 0.44              |
| 46:A:1573:C:N4   | 46:A:1574:G:C6   | 2.86                     | 0.44              |
| 5:4:33:LYS:NZ    | 46:A:2772:U:OP1  | 2.49                     | 0.44              |
| 46:A:1363:G:C6   | 46:A:1367:G:C6   | 3.05                     | 0.44              |
| 51:a:1139:C:H2'  | 51:a:1148:G:N7   | 2.33                     | 0.44              |
| 46:A:58:G:N3     | 46:A:73:A:H2     | 2.16                     | 0.44              |
| 8:C:145:GLU:HB2  | 8:C:188:CYS:HB3  | 2.00                     | 0.44              |
| 13:J:111:PRO:O   | 13:J:116:GLY:HA3 | 2.17                     | 0.44              |
| 51:a:1354:U:C2   | 51:a:1386:A:C2   | 3.05                     | 0.44              |
| 7:B:40:C:O2      | 11:F:90:THR:N    | 2.45                     | 0.44              |
| 46:A:210:A:H2'   | 46:A:211:C:O4'   | 2.18                     | 0.44              |
| 46:A:2884:G:C6   | 46:A:2885:A:N6   | 2.86                     | 0.44              |
| 51:a:24:G:O2'    | 51:a:923:A:N1    | 2.49                     | 0.44              |
| 51:a:963:G:C6    | 51:a:1238:A:C6   | 3.05                     | 0.44              |
| 17:N:4:ARG:NH1   | 17:N:39:GLU:OE1  | 2.46                     | 0.43              |
| 51:a:98:U:H1'    | 51:a:99:A:C2     | 2.53                     | 0.43              |
| 4:3:31:HIS:HE1   | 46:A:2421:A:OP2  | 2.01                     | 0.43              |
| 46:A:674:G:H4'   | 46:A:697:G:O2'   | 2.17                     | 0.43              |
| 46:A:2438:G:C6   | 46:A:2439:G:C5   | 3.06                     | 0.43              |
| 46:A:2439:G:C6   | 46:A:2440:A:C4   | 3.05                     | 0.43              |
| 9:D:17:ALA:HB2   | 9:D:23:ILE:CD1   | 2.48                     | 0.43              |
| 46:A:486:A:H2'   | 46:A:487:G:O4'   | 2.18                     | 0.43              |
| 46:A:1359:G:N1   | 46:A:1368:U:H5'' | 2.34                     | 0.43              |
| 51:a:1379:G:N3   | 51:a:1380:G:C8   | 2.86                     | 0.43              |
| 51:a:1440:C:H2'  | 51:a:1441:G:O4'  | 2.19                     | 0.43              |
| 35:j:50:THR:HG23 | 35:j:64:GLN:HG2  | 2.01                     | 0.43              |
| 46:A:200:A:N6    | 46:A:2459:A:H2'  | 2.34                     | 0.43              |
| 46:A:1480:A:H2'  | 46:A:1481:G:O4'  | 2.19                     | 0.43              |
| 8:C:140:VAL:HG13 | 8:C:161:SER:HB2  | 2.01                     | 0.43              |
| 46:A:494:A:O2'   | 46:A:520:G:N7    | 2.50                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:E:131:LEU:HD21 | 10:E:142:ILE:HD12 | 2.01                     | 0.43              |
| 46:A:876:A:N7     | 46:A:2276:A:O2'   | 2.49                     | 0.43              |
| 46:A:2540:U:O4    | 46:A:2604:C:N3    | 2.51                     | 0.43              |
| 25:W:74:THR:O     | 25:W:89:VAL:HA    | 2.18                     | 0.43              |
| 46:A:2322:C:N4    | 46:A:2323:C:N4    | 2.66                     | 0.43              |
| 51:a:1366:A:H2'   | 51:a:1367:U:C6    | 2.54                     | 0.43              |
| 46:A:364:A:H4'    | 46:A:366:A:C8     | 2.54                     | 0.43              |
| 2:1:7:LEU:HB2     | 2:1:17:TYR:HB2    | 2.01                     | 0.42              |
| 30:e:52:LYS:HE3   | 51:a:1091:G:OP2   | 2.19                     | 0.42              |
| 46:A:2875:A:OP2   | 46:A:2891:G:N1    | 2.35                     | 0.42              |
| 46:A:1527:C:H3'   | 46:A:1528:U:H5''  | 2.01                     | 0.42              |
| 51:a:968:A:N6     | 51:a:1230:G:O2'   | 2.52                     | 0.42              |
| 51:a:1295:C:H2'   | 51:a:1296:A:H4'   | 2.00                     | 0.42              |
| 46:A:1514:C:N4    | 46:A:1515:C:N4    | 2.67                     | 0.42              |
| 51:a:723:G:H2'    | 51:a:724:A:C8     | 2.54                     | 0.42              |
| 51:a:798:U:O2'    | 51:a:800:G:N7     | 2.50                     | 0.42              |
| 8:C:243:ARG:HH22  | 46:A:2268:G:P     | 2.42                     | 0.42              |
| 46:A:1308:A:H2'   | 46:A:1309:G:O4'   | 2.18                     | 0.42              |
| 46:A:1371:G:N3    | 46:A:1371:G:H5'   | 2.34                     | 0.42              |
| 46:A:1426:A:C6    | 46:A:1427:G:C5    | 3.08                     | 0.42              |
| 16:M:54:MET:HE2   | 16:M:121:ALA:CB   | 2.50                     | 0.42              |
| 9:D:149:VAL:HG11  | 46:A:2601:A:N7    | 2.34                     | 0.42              |
| 42:q:68:PRO:HG3   | 51:a:242:C:H4'    | 2.01                     | 0.42              |
| 46:A:681:C:O2'    | 46:A:685:U:OP1    | 2.29                     | 0.42              |
| 46:A:2027:A:O2'   | 46:A:2753:U:O2'   | 2.35                     | 0.42              |
| 46:A:2439:G:C2    | 46:A:2440:A:H1'   | 2.54                     | 0.42              |
| 51:a:527:C:H2'    | 51:a:539:G:C8     | 2.54                     | 0.42              |
| 12:G:8:LEU:HD13   | 12:G:50:VAL:HG13  | 2.02                     | 0.42              |
| 14:K:24:VAL:HG13  | 14:K:33:ALA:HB2   | 2.01                     | 0.42              |
| 46:A:268:A:N1     | 46:A:474:U:O2'    | 2.46                     | 0.42              |
| 46:A:617:G:O2'    | 46:A:618:A:H3'    | 2.20                     | 0.42              |
| 46:A:1424:A:C2    | 46:A:1425:C:C2    | 3.08                     | 0.42              |
| 9:D:126:HIS:CD2   | 9:D:159:LEU:HB3   | 2.55                     | 0.42              |
| 28:Z:13:ILE:HD11  | 46:A:1035:G:C8    | 2.55                     | 0.42              |
| 46:A:689:A:N1     | 46:A:2398:A:O2'   | 2.52                     | 0.42              |
| 46:A:704:U:H2'    | 46:A:705:A:C8     | 2.55                     | 0.42              |
| 46:A:2362:A:H5'   | 46:A:2364:A:H1'   | 2.01                     | 0.42              |
| 46:A:2408:G:H2'   | 46:A:2409:U:C6    | 2.55                     | 0.42              |
| 5:4:11:CYS:SG     | 5:4:27:CYS:SG     | 3.18                     | 0.41              |
| 35:j:56:HIS:O     | 35:j:57:LYS:HG2   | 2.20                     | 0.41              |
| 46:A:248:G:O2'    | 46:A:431:A:N1     | 2.51                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 46:A:655:C:H42   | 46:A:663:A:H61    | 1.68                     | 0.41              |
| 46:A:2716:U:H2'  | 46:A:2717:G:O4'   | 2.19                     | 0.41              |
| 51:a:172:U:O4'   | 51:a:211:A:C5     | 2.73                     | 0.41              |
| 3:2:12:ARG:HG2   | 3:2:44:ALA:HB1    | 2.03                     | 0.41              |
| 46:A:250:G:H4'   | 46:A:433:G:C5     | 2.55                     | 0.41              |
| 46:A:340:U:H2'   | 46:A:341:G:O4'    | 2.19                     | 0.41              |
| 46:A:854:U:O2'   | 46:A:2089:A:N1    | 2.52                     | 0.41              |
| 51:a:180:G:C2    | 51:a:209:A:C4     | 3.08                     | 0.41              |
| 51:a:381:A:O2'   | 51:a:459:A:N7     | 2.53                     | 0.41              |
| 6:6:32:ARG:CG    | 6:6:32:ARG:HH11   | 2.32                     | 0.41              |
| 46:A:183:A:H5'   | 46:A:184:G:H5''   | 2.02                     | 0.41              |
| 46:A:1723:A:H2'  | 46:A:1724:A:O4'   | 2.20                     | 0.41              |
| 46:A:656:A:H2    | 46:A:662:G:N2     | 2.17                     | 0.41              |
| 46:A:1366:C:N4   | 46:A:1367:G:N1    | 2.68                     | 0.41              |
| 35:j:7:ARG:O     | 35:j:101:LYS:N    | 2.54                     | 0.41              |
| 46:A:1779:G:C6   | 46:A:1780:C:C4    | 3.08                     | 0.41              |
| 46:A:2752:C:N4   | 46:A:2753:U:C4    | 2.89                     | 0.41              |
| 51:a:996:A:H2'   | 51:a:997:G:C8     | 2.56                     | 0.41              |
| 17:N:41:ARG:NH1  | 46:A:2906:U:O2    | 2.53                     | 0.41              |
| 46:A:252:C:OP2   | 46:A:2423:C:O2'   | 2.33                     | 0.41              |
| 26:X:12:THR:HG21 | 46:A:1404:A:OP1   | 2.21                     | 0.41              |
| 35:j:6:ILE:HB    | 35:j:76:ILE:HB    | 2.03                     | 0.41              |
| 46:A:2785:U:H5   | 46:A:2787:A:N7    | 2.18                     | 0.41              |
| 51:a:332:G:N2    | 51:a:334:G:H3'    | 2.36                     | 0.41              |
| 1:0:18:THR:HG22  | 46:A:15:G:H4'     | 2.02                     | 0.41              |
| 9:D:149:VAL:HG23 | 46:A:2604:C:H5'   | 2.02                     | 0.41              |
| 10:E:51:VAL:HG21 | 10:E:91:GLY:HA3   | 2.02                     | 0.41              |
| 14:K:66:LYS:HA   | 14:K:79:PHE:O     | 2.20                     | 0.41              |
| 46:A:1825:U:H2'  | 46:A:1826:C:C6    | 2.55                     | 0.41              |
| 46:A:2327:A:H2'  | 46:A:2328:G:O4'   | 2.21                     | 0.41              |
| 51:a:803:A:C5    | 51:a:804:C:C4     | 3.08                     | 0.41              |
| 51:a:1107:C:H2'  | 51:a:1108:C:C5    | 2.55                     | 0.41              |
| 8:C:207:LYS:HB2  | 46:A:776:G:C6     | 2.56                     | 0.41              |
| 16:M:104:PHE:HE1 | 16:M:125:LEU:HD11 | 1.85                     | 0.41              |
| 20:Q:49:ASP:OD2  | 46:A:580:U:O2'    | 2.21                     | 0.41              |
| 46:A:1439:U:C4   | 46:A:1440:G:N7    | 2.89                     | 0.41              |
| 46:A:2055:U:H2'  | 46:A:2056:G:O4'   | 2.21                     | 0.41              |
| 51:a:1113:C:H2'  | 51:a:1114:G:O4'   | 2.21                     | 0.41              |
| 8:C:43:ARG:HA    | 8:C:48:LYS:O      | 2.21                     | 0.40              |
| 35:j:7:ARG:HA    | 35:j:75:ASP:HA    | 2.03                     | 0.40              |
| 44:t:32:ILE:HG23 | 44:t:79:LEU:HD21  | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 46:A:382:G:C5    | 46:A:383:U:C5    | 3.09                     | 0.40              |
| 8:C:155:VAL:HG21 | 8:C:162:ALA:HB2  | 2.03                     | 0.40              |
| 9:D:79:PHE:CG    | 9:D:199:LEU:HD13 | 2.56                     | 0.40              |
| 11:F:66:VAL:N    | 11:F:88:LYS:O    | 2.52                     | 0.40              |
| 46:A:1426:A:H2'  | 46:A:1427:G:O4'  | 2.20                     | 0.40              |
| 46:A:1659:A:OP2  | 49:5:90:TYR:OH   | 2.30                     | 0.40              |
| 46:A:1830:G:H4'  | 46:A:2232:G:C2   | 2.56                     | 0.40              |
| 46:A:2785:U:C5   | 46:A:2787:A:N7   | 2.88                     | 0.40              |
| 13:J:36:ILE:HD11 | 13:J:141:TYR:CE2 | 2.56                     | 0.40              |
| 46:A:790:A:H2'   | 46:A:791:C:O4'   | 2.21                     | 0.40              |
| 46:A:2465:G:O2'  | 46:A:2627:A:N1   | 2.50                     | 0.40              |
| 51:a:876:C:C4    | 51:a:877:G:H1'   | 2.56                     | 0.40              |
| 46:A:58:G:N3     | 46:A:73:A:C2     | 2.89                     | 0.40              |
| 46:A:566:G:C5    | 46:A:567:U:C4    | 3.09                     | 0.40              |
| 46:A:1322:G:N2   | 46:A:1324:G:H3'  | 2.35                     | 0.40              |
| 51:a:1234:A:N3   | 51:a:1234:A:H2'  | 2.36                     | 0.40              |
| 46:A:662:G:H8    | 46:A:662:G:O5'   | 2.05                     | 0.40              |
| 46:A:803:C:H2'   | 46:A:804:G:O4'   | 2.21                     | 0.40              |
| 47:b:15:HIS:HB3  | 47:b:43:LEU:HD21 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed    | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 1   | 0     | 53/59 (90%) | 48 (91%)  | 5 (9%)  | 0        | 100         | 100 |
| 2   | 1     | 46/49 (94%) | 42 (91%)  | 4 (9%)  | 0        | 100         | 100 |
| 3   | 2     | 42/44 (96%) | 41 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 4   | 3     | 62/66 (94%) | 62 (100%) | 0       | 0        | 100         | 100 |
| 5   | 4     | 35/37 (95%) | 35 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6   | 6     | 44/66 (67%)   | 37 (84%)  | 7 (16%)  | 0        | 100         | 100 |
| 8   | C     | 271/277 (98%) | 261 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 9   | D     | 205/209 (98%) | 199 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 10  | E     | 204/207 (99%) | 199 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 11  | F     | 176/179 (98%) | 159 (90%) | 17 (10%) | 0        | 100         | 100 |
| 12  | G     | 173/179 (97%) | 156 (90%) | 17 (10%) | 0        | 100         | 100 |
| 13  | J     | 141/145 (97%) | 137 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 14  | K     | 120/122 (98%) | 111 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 15  | L     | 144/146 (99%) | 139 (96%) | 4 (3%)   | 1 (1%)   | 18          | 23  |
| 16  | M     | 133/144 (92%) | 125 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 17  | N     | 117/120 (98%) | 108 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 18  | O     | 118/120 (98%) | 109 (92%) | 6 (5%)   | 3 (2%)   | 4           | 3   |
| 19  | P     | 112/115 (97%) | 111 (99%) | 0        | 1 (1%)   | 14          | 17  |
| 20  | Q     | 116/119 (98%) | 113 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 21  | R     | 100/102 (98%) | 99 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 22  | S     | 108/113 (96%) | 107 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 23  | T     | 89/95 (94%)   | 85 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 24  | U     | 100/103 (97%) | 92 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 25  | W     | 80/94 (85%)   | 75 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 26  | X     | 59/62 (95%)   | 58 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 27  | Y     | 64/66 (97%)   | 63 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 28  | Z     | 56/59 (95%)   | 52 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 29  | c     | 202/218 (93%) | 184 (91%) | 17 (8%)  | 1 (0%)   | 24          | 31  |
| 30  | e     | 162/166 (98%) | 159 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 31  | f     | 91/95 (96%)   | 89 (98%)  | 1 (1%)   | 1 (1%)   | 11          | 13  |
| 32  | g     | 149/156 (96%) | 139 (93%) | 9 (6%)   | 1 (1%)   | 18          | 23  |
| 33  | h     | 128/132 (97%) | 125 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 34  | i     | 126/130 (97%) | 115 (91%) | 10 (8%)  | 1 (1%)   | 16          | 20  |
| 35  | j     | 96/102 (94%)  | 87 (91%)  | 8 (8%)   | 1 (1%)   | 12          | 15  |
| 36  | k     | 113/131 (86%) | 105 (93%) | 6 (5%)   | 2 (2%)   | 6           | 6   |
| 37  | l     | 132/138 (96%) | 127 (96%) | 5 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 38  | m     | 115/121 (95%)   | 107 (93%)  | 7 (6%)   | 1 (1%)   | 14          | 17  |
| 39  | n     | 58/61 (95%)     | 55 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 40  | o     | 85/89 (96%)     | 81 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 41  | p     | 85/90 (94%)     | 82 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 42  | q     | 82/87 (94%)     | 78 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 43  | r     | 63/79 (80%)     | 62 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 44  | t     | 84/88 (96%)     | 81 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 47  | b     | 191/246 (78%)   | 181 (95%)  | 9 (5%)   | 1 (0%)   | 24          | 31  |
| 48  | s     | 81/92 (88%)     | 73 (90%)   | 7 (9%)   | 1 (1%)   | 10          | 12  |
| 49  | 5     | 36/38 (95%)     | 32 (89%)   | 4 (11%)  | 0        | 100         | 100 |
| 52  | d     | 197/200 (98%)   | 185 (94%)  | 11 (6%)  | 1 (0%)   | 24          | 31  |
| All | All   | 5244/5556 (94%) | 4970 (95%) | 258 (5%) | 16 (0%)  | 37          | 46  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | O     | 2   | ILE  |
| 31  | f     | 88  | HIS  |
| 36  | k     | 121 | ASN  |
| 38  | m     | 36  | GLU  |
| 52  | d     | 67  | GLN  |
| 32  | g     | 130 | ASN  |
| 15  | L     | 29  | LYS  |
| 36  | k     | 123 | CYS  |
| 48  | s     | 65  | ASP  |
| 18  | O     | 62  | ASP  |
| 18  | O     | 67  | SER  |
| 19  | P     | 28  | VAL  |
| 47  | b     | 98  | GLY  |
| 29  | c     | 25  | GLY  |
| 35  | j     | 39  | PRO  |
| 34  | i     | 26  | GLY  |

### 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     | 49/53 (92%)    | 49 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 39/39 (100%)   | 39 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 54/56 (96%)    | 53 (98%)   | 1 (2%)   | 50          | 69  |
| 5   | 4     | 35/35 (100%)   | 35 (100%)  | 0        | 100         | 100 |
| 6   | 6     | 39/55 (71%)    | 38 (97%)   | 1 (3%)   | 40          | 59  |
| 8   | C     | 221/225 (98%)  | 219 (99%)  | 2 (1%)   | 70          | 84  |
| 9   | D     | 168/170 (99%)  | 166 (99%)  | 2 (1%)   | 63          | 79  |
| 10  | E     | 169/170 (99%)  | 166 (98%)  | 3 (2%)   | 51          | 70  |
| 11  | F     | 153/154 (99%)  | 151 (99%)  | 2 (1%)   | 61          | 77  |
| 12  | G     | 148/151 (98%)  | 147 (99%)  | 1 (1%)   | 76          | 87  |
| 13  | J     | 121/123 (98%)  | 121 (100%) | 0        | 100         | 100 |
| 14  | K     | 101/101 (100%) | 97 (96%)   | 4 (4%)   | 28          | 42  |
| 15  | L     | 110/110 (100%) | 107 (97%)  | 3 (3%)   | 39          | 58  |
| 16  | M     | 109/116 (94%)  | 108 (99%)  | 1 (1%)   | 70          | 84  |
| 17  | N     | 99/100 (99%)   | 98 (99%)   | 1 (1%)   | 68          | 82  |
| 18  | O     | 93/93 (100%)   | 91 (98%)   | 2 (2%)   | 45          | 65  |
| 19  | P     | 99/100 (99%)   | 98 (99%)   | 1 (1%)   | 68          | 82  |
| 20  | Q     | 97/98 (99%)    | 96 (99%)   | 1 (1%)   | 68          | 82  |
| 21  | R     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 22  | S     | 91/93 (98%)    | 88 (97%)   | 3 (3%)   | 33          | 50  |
| 23  | T     | 82/85 (96%)    | 81 (99%)   | 1 (1%)   | 63          | 79  |
| 24  | U     | 86/87 (99%)    | 85 (99%)   | 1 (1%)   | 63          | 79  |
| 25  | W     | 63/74 (85%)    | 62 (98%)   | 1 (2%)   | 55          | 73  |
| 26  | X     | 49/50 (98%)    | 49 (100%)  | 0        | 100         | 100 |
| 27  | Y     | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 28  | Z     | 52/53 (98%)    | 51 (98%)   | 1 (2%)   | 50          | 69  |
| 29  | c     | 167/178 (94%)  | 163 (98%)  | 4 (2%)   | 43          | 62  |
| 30  | e     | 128/130 (98%)  | 127 (99%)  | 1 (1%)   | 73          | 86  |
| 31  | f     | 82/84 (98%)    | 79 (96%)   | 3 (4%)   | 30          | 45  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 32  | g     | 127/132 (96%)   | 126 (99%)  | 1 (1%)   | 73          | 86  |
| 33  | h     | 110/112 (98%)   | 108 (98%)  | 2 (2%)   | 51          | 70  |
| 34  | i     | 101/102 (99%)   | 101 (100%) | 0        | 100         | 100 |
| 35  | j     | 89/92 (97%)     | 88 (99%)   | 1 (1%)   | 65          | 81  |
| 36  | k     | 87/100 (87%)    | 86 (99%)   | 1 (1%)   | 65          | 81  |
| 37  | l     | 112/115 (97%)   | 111 (99%)  | 1 (1%)   | 70          | 84  |
| 38  | m     | 100/104 (96%)   | 99 (99%)   | 1 (1%)   | 68          | 82  |
| 39  | n     | 53/54 (98%)     | 53 (100%)  | 0        | 100         | 100 |
| 40  | o     | 82/83 (99%)     | 82 (100%)  | 0        | 100         | 100 |
| 41  | p     | 74/76 (97%)     | 74 (100%)  | 0        | 100         | 100 |
| 42  | q     | 77/80 (96%)     | 77 (100%)  | 0        | 100         | 100 |
| 43  | r     | 56/64 (88%)     | 56 (100%)  | 0        | 100         | 100 |
| 44  | t     | 69/70 (99%)     | 66 (96%)   | 3 (4%)   | 26          | 39  |
| 47  | b     | 167/212 (79%)   | 164 (98%)  | 3 (2%)   | 51          | 70  |
| 48  | s     | 73/81 (90%)     | 72 (99%)   | 1 (1%)   | 59          | 76  |
| 49  | 5     | 38/38 (100%)    | 36 (95%)   | 2 (5%)   | 20          | 30  |
| 52  | d     | 172/173 (99%)   | 169 (98%)  | 3 (2%)   | 53          | 72  |
| All | All   | 4478/4659 (96%) | 4419 (99%) | 59 (1%)  | 59          | 77  |

All (59) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 31  | HIS  |
| 6   | 6     | 32  | ARG  |
| 8   | C     | 51  | VAL  |
| 8   | C     | 182 | ARG  |
| 9   | D     | 61  | SER  |
| 9   | D     | 191 | ASN  |
| 10  | E     | 32  | VAL  |
| 10  | E     | 49  | HIS  |
| 10  | E     | 126 | LEU  |
| 11  | F     | 89  | VAL  |
| 11  | F     | 167 | ARG  |
| 12  | G     | 19  | LEU  |
| 14  | K     | 32  | THR  |
| 14  | K     | 34  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | K     | 42  | THR  |
| 14  | K     | 78  | SER  |
| 15  | L     | 1   | MET  |
| 15  | L     | 69  | ILE  |
| 15  | L     | 104 | LYS  |
| 16  | M     | 129 | THR  |
| 17  | N     | 12  | GLN  |
| 18  | O     | 62  | ASP  |
| 18  | O     | 63  | LEU  |
| 19  | P     | 93  | ARG  |
| 20  | Q     | 9   | VAL  |
| 22  | S     | 29  | VAL  |
| 22  | S     | 82  | LEU  |
| 22  | S     | 92  | ARG  |
| 23  | T     | 91  | GLU  |
| 24  | U     | 34  | LEU  |
| 25  | W     | 78  | GLU  |
| 28  | Z     | 58  | GLU  |
| 29  | c     | 27  | ASP  |
| 29  | c     | 35  | ASP  |
| 29  | c     | 37  | LYS  |
| 29  | c     | 53  | LYS  |
| 30  | e     | 151 | GLU  |
| 31  | f     | 72  | VAL  |
| 31  | f     | 87  | ARG  |
| 31  | f     | 88  | HIS  |
| 32  | g     | 17  | ILE  |
| 33  | h     | 56  | LYS  |
| 33  | h     | 57  | GLN  |
| 35  | j     | 74  | ILE  |
| 36  | k     | 128 | ARG  |
| 37  | l     | 10  | LYS  |
| 38  | m     | 97  | VAL  |
| 44  | t     | 6   | SER  |
| 44  | t     | 13  | THR  |
| 44  | t     | 48  | LYS  |
| 47  | b     | 33  | THR  |
| 47  | b     | 75  | GLN  |
| 47  | b     | 92  | VAL  |
| 48  | s     | 28  | LYS  |
| 49  | 5     | 94  | ARG  |
| 49  | 5     | 100 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | d     | 41  | ARG  |
| 52  | d     | 63  | VAL  |
| 52  | d     | 71  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 40  | HIS  |
| 1   | 0     | 50  | ASN  |
| 2   | 1     | 26  | ASN  |
| 4   | 3     | 26  | HIS  |
| 4   | 3     | 31  | HIS  |
| 4   | 3     | 35  | ASN  |
| 4   | 3     | 60  | GLN  |
| 8   | C     | 86  | ASN  |
| 8   | C     | 153 | GLN  |
| 8   | C     | 163 | GLN  |
| 9   | D     | 14  | GLN  |
| 9   | D     | 95  | GLN  |
| 9   | D     | 172 | GLN  |
| 10  | E     | 9   | GLN  |
| 10  | E     | 49  | HIS  |
| 11  | F     | 37  | ASN  |
| 12  | G     | 102 | ASN  |
| 13  | J     | 118 | GLN  |
| 14  | K     | 4   | GLN  |
| 15  | L     | 17  | ASN  |
| 17  | N     | 12  | GLN  |
| 18  | O     | 32  | ASN  |
| 20  | Q     | 52  | GLN  |
| 22  | S     | 28  | GLN  |
| 22  | S     | 73  | GLN  |
| 23  | T     | 58  | ASN  |
| 24  | U     | 51  | ASN  |
| 24  | U     | 53  | GLN  |
| 26  | X     | 23  | ASN  |
| 27  | Y     | 27  | ASN  |
| 27  | Y     | 31  | GLN  |
| 29  | c     | 135 | GLN  |
| 29  | c     | 146 | GLN  |
| 31  | f     | 61  | GLN  |
| 31  | f     | 64  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | g     | 86  | GLN  |
| 33  | h     | 18  | ASN  |
| 33  | h     | 57  | GLN  |
| 34  | i     | 5   | GLN  |
| 35  | j     | 82  | GLN  |
| 36  | k     | 42  | ASN  |
| 38  | m     | 105 | ASN  |
| 38  | m     | 118 | ASN  |
| 40  | o     | 72  | ASN  |
| 43  | r     | 21  | ASN  |
| 44  | t     | 41  | ASN  |
| 47  | b     | 8   | GLN  |
| 47  | b     | 77  | GLN  |
| 48  | s     | 43  | GLN  |
| 52  | d     | 115 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 45  | v     | 75/76 (98%)     | 20 (26%)          | 0               |
| 46  | A     | 2716/2928 (92%) | 418 (15%)         | 91 (3%)         |
| 50  | 7     | 5/6 (83%)       | 2 (40%)           | 0               |
| 51  | a     | 1504/1554 (96%) | 251 (16%)         | 0               |
| 7   | B     | 111/112 (99%)   | 24 (21%)          | 7 (6%)          |
| All | All   | 4411/4676 (94%) | 715 (16%)         | 98 (2%)         |

All (715) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | B     | 10  | G    |
| 7   | B     | 12  | U    |
| 7   | B     | 23  | U    |
| 7   | B     | 32  | U    |
| 7   | B     | 33  | U    |
| 7   | B     | 38  | U    |
| 7   | B     | 40  | C    |
| 7   | B     | 43  | A    |
| 7   | B     | 48  | G    |
| 7   | B     | 49  | G    |
| 7   | B     | 50  | A    |
| 7   | B     | 51  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | B     | 53  | U    |
| 7   | B     | 54  | U    |
| 7   | B     | 58  | C    |
| 7   | B     | 61  | U    |
| 7   | B     | 63  | C    |
| 7   | B     | 64  | A    |
| 7   | B     | 87  | U    |
| 7   | B     | 88  | C    |
| 7   | B     | 97  | A    |
| 7   | B     | 107 | G    |
| 7   | B     | 108 | C    |
| 7   | B     | 110 | G    |
| 45  | v     | 6   | G    |
| 45  | v     | 7   | G    |
| 45  | v     | 9   | A    |
| 45  | v     | 10  | G    |
| 45  | v     | 14  | A    |
| 45  | v     | 17  | U    |
| 45  | v     | 18  | G    |
| 45  | v     | 19  | G    |
| 45  | v     | 20  | U    |
| 45  | v     | 21  | A    |
| 45  | v     | 46  | G    |
| 45  | v     | 47  | U    |
| 45  | v     | 48  | C    |
| 45  | v     | 51  | C    |
| 45  | v     | 58  | A    |
| 45  | v     | 61  | C    |
| 45  | v     | 65  | C    |
| 45  | v     | 69  | A    |
| 45  | v     | 70  | G    |
| 45  | v     | 76  | A    |
| 46  | A     | 12  | A    |
| 46  | A     | 13  | A    |
| 46  | A     | 34  | U    |
| 46  | A     | 46  | C    |
| 46  | A     | 60  | G    |
| 46  | A     | 63  | G    |
| 46  | A     | 71  | A    |
| 46  | A     | 74  | U    |
| 46  | A     | 75  | G    |
| 46  | A     | 89  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | A     | 90  | A    |
| 46  | A     | 93  | C    |
| 46  | A     | 96  | G    |
| 46  | A     | 117 | A    |
| 46  | A     | 118 | A    |
| 46  | A     | 119 | U    |
| 46  | A     | 150 | A    |
| 46  | A     | 164 | U    |
| 46  | A     | 166 | A    |
| 46  | A     | 175 | G    |
| 46  | A     | 176 | A    |
| 46  | A     | 177 | G    |
| 46  | A     | 183 | A    |
| 46  | A     | 184 | G    |
| 46  | A     | 199 | A    |
| 46  | A     | 202 | A    |
| 46  | A     | 203 | U    |
| 46  | A     | 216 | A    |
| 46  | A     | 219 | A    |
| 46  | A     | 224 | A    |
| 46  | A     | 225 | A    |
| 46  | A     | 226 | A    |
| 46  | A     | 229 | A    |
| 46  | A     | 236 | A    |
| 46  | A     | 248 | G    |
| 46  | A     | 251 | G    |
| 46  | A     | 258 | A    |
| 46  | A     | 272 | C    |
| 46  | A     | 275 | A    |
| 46  | A     | 299 | U    |
| 46  | A     | 300 | G    |
| 46  | A     | 301 | U    |
| 46  | A     | 302 | A    |
| 46  | A     | 307 | A    |
| 46  | A     | 309 | U    |
| 46  | A     | 310 | C    |
| 46  | A     | 346 | G    |
| 46  | A     | 350 | U    |
| 46  | A     | 355 | A    |
| 46  | A     | 361 | G    |
| 46  | A     | 373 | A    |
| 46  | A     | 374 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | A     | 389 | A    |
| 46  | A     | 390 | A    |
| 46  | A     | 407 | A    |
| 46  | A     | 411 | G    |
| 46  | A     | 412 | A    |
| 46  | A     | 418 | A    |
| 46  | A     | 419 | G    |
| 46  | A     | 430 | C    |
| 46  | A     | 433 | G    |
| 46  | A     | 458 | G    |
| 46  | A     | 459 | A    |
| 46  | A     | 467 | C    |
| 46  | A     | 471 | G    |
| 46  | A     | 482 | C    |
| 46  | A     | 483 | C    |
| 46  | A     | 491 | C    |
| 46  | A     | 498 | U    |
| 46  | A     | 503 | C    |
| 46  | A     | 504 | A    |
| 46  | A     | 528 | G    |
| 46  | A     | 551 | A    |
| 46  | A     | 554 | U    |
| 46  | A     | 568 | G    |
| 46  | A     | 576 | G    |
| 46  | A     | 577 | U    |
| 46  | A     | 578 | A    |
| 46  | A     | 579 | G    |
| 46  | A     | 592 | A    |
| 46  | A     | 595 | G    |
| 46  | A     | 599 | G    |
| 46  | A     | 600 | A    |
| 46  | A     | 607 | G    |
| 46  | A     | 615 | U    |
| 46  | A     | 616 | A    |
| 46  | A     | 617 | G    |
| 46  | A     | 619 | A    |
| 46  | A     | 631 | G    |
| 46  | A     | 647 | A    |
| 46  | A     | 657 | G    |
| 46  | A     | 658 | A    |
| 46  | A     | 659 | A    |
| 46  | A     | 673 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 680  | G    |
| 46  | A     | 683  | A    |
| 46  | A     | 691  | U    |
| 46  | A     | 692  | A    |
| 46  | A     | 700  | U    |
| 46  | A     | 701  | G    |
| 46  | A     | 702  | A    |
| 46  | A     | 732  | A    |
| 46  | A     | 733  | U    |
| 46  | A     | 777  | C    |
| 46  | A     | 793  | U    |
| 46  | A     | 794  | U    |
| 46  | A     | 811  | A    |
| 46  | A     | 812  | G    |
| 46  | A     | 822  | G    |
| 46  | A     | 829  | A    |
| 46  | A     | 831  | U    |
| 46  | A     | 832  | G    |
| 46  | A     | 837  | U    |
| 46  | A     | 838  | C    |
| 46  | A     | 839  | G    |
| 46  | A     | 852  | G    |
| 46  | A     | 859  | C    |
| 46  | A     | 866  | A    |
| 46  | A     | 874  | U    |
| 46  | A     | 875  | U    |
| 46  | A     | 892  | U    |
| 46  | A     | 906  | G    |
| 46  | A     | 913  | A    |
| 46  | A     | 930  | C    |
| 46  | A     | 954  | U    |
| 46  | A     | 957  | A    |
| 46  | A     | 959  | C    |
| 46  | A     | 964  | A    |
| 46  | A     | 973  | G    |
| 46  | A     | 987  | A    |
| 46  | A     | 991  | A    |
| 46  | A     | 992  | G    |
| 46  | A     | 1007 | G    |
| 46  | A     | 1015 | G    |
| 46  | A     | 1020 | A    |
| 46  | A     | 1029 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 1038 | C    |
| 46  | A     | 1042 | A    |
| 46  | A     | 1058 | U    |
| 46  | A     | 1059 | A    |
| 46  | A     | 1068 | G    |
| 46  | A     | 1072 | A    |
| 46  | A     | 1073 | A    |
| 46  | A     | 1079 | U    |
| 46  | A     | 1084 | A    |
| 46  | A     | 1092 | A    |
| 46  | A     | 1093 | G    |
| 46  | A     | 1098 | C    |
| 46  | A     | 1153 | G    |
| 46  | A     | 1158 | G    |
| 46  | A     | 1160 | G    |
| 46  | A     | 1174 | A    |
| 46  | A     | 1178 | U    |
| 46  | A     | 1179 | A    |
| 46  | A     | 1180 | C    |
| 46  | A     | 1181 | C    |
| 46  | A     | 1182 | G    |
| 46  | A     | 1185 | G    |
| 46  | A     | 1188 | A    |
| 46  | A     | 1189 | A    |
| 46  | A     | 1190 | A    |
| 46  | A     | 1203 | G    |
| 46  | A     | 1244 | A    |
| 46  | A     | 1245 | G    |
| 46  | A     | 1247 | G    |
| 46  | A     | 1250 | G    |
| 46  | A     | 1251 | U    |
| 46  | A     | 1278 | G    |
| 46  | A     | 1290 | G    |
| 46  | A     | 1293 | A    |
| 46  | A     | 1296 | G    |
| 46  | A     | 1311 | G    |
| 46  | A     | 1312 | A    |
| 46  | A     | 1315 | G    |
| 46  | A     | 1328 | C    |
| 46  | A     | 1339 | A    |
| 46  | A     | 1340 | A    |
| 46  | A     | 1341 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 1342 | G    |
| 46  | A     | 1346 | A    |
| 46  | A     | 1360 | A    |
| 46  | A     | 1364 | C    |
| 46  | A     | 1371 | G    |
| 46  | A     | 1372 | C    |
| 46  | A     | 1375 | A    |
| 46  | A     | 1376 | G    |
| 46  | A     | 1388 | A    |
| 46  | A     | 1389 | C    |
| 46  | A     | 1391 | U    |
| 46  | A     | 1404 | A    |
| 46  | A     | 1414 | G    |
| 46  | A     | 1418 | U    |
| 46  | A     | 1423 | A    |
| 46  | A     | 1433 | U    |
| 46  | A     | 1435 | U    |
| 46  | A     | 1450 | C    |
| 46  | A     | 1465 | A    |
| 46  | A     | 1473 | A    |
| 46  | A     | 1474 | C    |
| 46  | A     | 1489 | U    |
| 46  | A     | 1490 | A    |
| 46  | A     | 1498 | U    |
| 46  | A     | 1499 | A    |
| 46  | A     | 1500 | U    |
| 46  | A     | 1501 | U    |
| 46  | A     | 1502 | G    |
| 46  | A     | 1505 | U    |
| 46  | A     | 1506 | A    |
| 46  | A     | 1508 | C    |
| 46  | A     | 1514 | C    |
| 46  | A     | 1516 | A    |
| 46  | A     | 1525 | G    |
| 46  | A     | 1526 | G    |
| 46  | A     | 1527 | C    |
| 46  | A     | 1528 | U    |
| 46  | A     | 1529 | G    |
| 46  | A     | 1531 | G    |
| 46  | A     | 1536 | A    |
| 46  | A     | 1540 | A    |
| 46  | A     | 1542 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 1543 | U    |
| 46  | A     | 1544 | C    |
| 46  | A     | 1556 | A    |
| 46  | A     | 1557 | G    |
| 46  | A     | 1558 | G    |
| 46  | A     | 1559 | C    |
| 46  | A     | 1560 | U    |
| 46  | A     | 1561 | G    |
| 46  | A     | 1563 | G    |
| 46  | A     | 1566 | G    |
| 46  | A     | 1590 | C    |
| 46  | A     | 1595 | U    |
| 46  | A     | 1607 | C    |
| 46  | A     | 1617 | A    |
| 46  | A     | 1626 | U    |
| 46  | A     | 1630 | G    |
| 46  | A     | 1632 | G    |
| 46  | A     | 1653 | A    |
| 46  | A     | 1654 | A    |
| 46  | A     | 1661 | A    |
| 46  | A     | 1691 | A    |
| 46  | A     | 1692 | U    |
| 46  | A     | 1693 | C    |
| 46  | A     | 1708 | U    |
| 46  | A     | 1719 | G    |
| 46  | A     | 1751 | U    |
| 46  | A     | 1752 | G    |
| 46  | A     | 1757 | G    |
| 46  | A     | 1758 | U    |
| 46  | A     | 1759 | U    |
| 46  | A     | 1760 | A    |
| 46  | A     | 1768 | A    |
| 46  | A     | 1770 | C    |
| 46  | A     | 1771 | C    |
| 46  | A     | 1776 | A    |
| 46  | A     | 1777 | G    |
| 46  | A     | 1779 | G    |
| 46  | A     | 1791 | A    |
| 46  | A     | 1792 | G    |
| 46  | A     | 1793 | G    |
| 46  | A     | 1802 | A    |
| 46  | A     | 1805 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 1811 | C    |
| 46  | A     | 1829 | C    |
| 46  | A     | 1830 | G    |
| 46  | A     | 1831 | A    |
| 46  | A     | 1845 | A    |
| 46  | A     | 1858 | A    |
| 46  | A     | 1867 | C    |
| 46  | A     | 1876 | A    |
| 46  | A     | 1877 | A    |
| 46  | A     | 1887 | G    |
| 46  | A     | 1898 | G    |
| 46  | A     | 1899 | U    |
| 46  | A     | 1900 | A    |
| 46  | A     | 1901 | A    |
| 46  | A     | 1902 | G    |
| 46  | A     | 1911 | C    |
| 46  | A     | 1935 | G    |
| 46  | A     | 1936 | G    |
| 46  | A     | 1940 | U    |
| 46  | A     | 1941 | A    |
| 46  | A     | 1942 | A    |
| 46  | A     | 1943 | C    |
| 46  | A     | 1944 | U    |
| 46  | A     | 1945 | A    |
| 46  | A     | 1946 | U    |
| 46  | A     | 1958 | G    |
| 46  | A     | 1959 | G    |
| 46  | A     | 1966 | A    |
| 46  | A     | 1967 | A    |
| 46  | A     | 1984 | U    |
| 46  | A     | 1992 | C    |
| 46  | A     | 1994 | C    |
| 46  | A     | 1996 | C    |
| 46  | A     | 1999 | A    |
| 46  | A     | 2000 | A    |
| 46  | A     | 2001 | G    |
| 46  | A     | 2020 | U    |
| 46  | A     | 2022 | U    |
| 46  | A     | 2025 | C    |
| 46  | A     | 2026 | A    |
| 46  | A     | 2052 | A    |
| 46  | A     | 2060 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 2061 | G    |
| 46  | A     | 2062 | A    |
| 46  | A     | 2065 | C    |
| 46  | A     | 2072 | C    |
| 46  | A     | 2084 | C    |
| 46  | A     | 2085 | G    |
| 46  | A     | 2089 | A    |
| 46  | A     | 2090 | G    |
| 46  | A     | 2091 | A    |
| 46  | A     | 2098 | G    |
| 46  | A     | 2099 | G    |
| 46  | A     | 2122 | G    |
| 46  | A     | 2124 | A    |
| 46  | A     | 2128 | U    |
| 46  | A     | 2129 | G    |
| 46  | A     | 2131 | U    |
| 46  | A     | 2219 | G    |
| 46  | A     | 2227 | A    |
| 46  | A     | 2232 | G    |
| 46  | A     | 2233 | C    |
| 46  | A     | 2240 | U    |
| 46  | A     | 2241 | A    |
| 46  | A     | 2254 | A    |
| 46  | A     | 2267 | G    |
| 46  | A     | 2268 | G    |
| 46  | A     | 2302 | A    |
| 46  | A     | 2312 | C    |
| 46  | A     | 2315 | A    |
| 46  | A     | 2316 | A    |
| 46  | A     | 2334 | U    |
| 46  | A     | 2335 | U    |
| 46  | A     | 2337 | G    |
| 46  | A     | 2338 | A    |
| 46  | A     | 2341 | U    |
| 46  | A     | 2342 | C    |
| 46  | A     | 2348 | C    |
| 46  | A     | 2349 | A    |
| 46  | A     | 2350 | G    |
| 46  | A     | 2351 | A    |
| 46  | A     | 2354 | G    |
| 46  | A     | 2356 | A    |
| 46  | A     | 2360 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 2363 | C    |
| 46  | A     | 2364 | A    |
| 46  | A     | 2376 | C    |
| 46  | A     | 2379 | C    |
| 46  | A     | 2408 | G    |
| 46  | A     | 2412 | G    |
| 46  | A     | 2414 | C    |
| 46  | A     | 2431 | U    |
| 46  | A     | 2432 | C    |
| 46  | A     | 2435 | C    |
| 46  | A     | 2451 | C    |
| 46  | A     | 2452 | U    |
| 46  | A     | 2453 | C    |
| 46  | A     | 2454 | A    |
| 46  | A     | 2457 | G    |
| 46  | A     | 2458 | G    |
| 46  | A     | 2459 | A    |
| 46  | A     | 2464 | A    |
| 46  | A     | 2470 | C    |
| 46  | A     | 2477 | A    |
| 46  | A     | 2498 | A    |
| 46  | A     | 2505 | A    |
| 46  | A     | 2513 | G    |
| 46  | A     | 2531 | G    |
| 46  | A     | 2534 | G    |
| 46  | A     | 2547 | A    |
| 46  | A     | 2558 | G    |
| 46  | A     | 2559 | U    |
| 46  | A     | 2564 | G    |
| 46  | A     | 2583 | U    |
| 46  | A     | 2595 | A    |
| 46  | A     | 2596 | G    |
| 46  | A     | 2602 | C    |
| 46  | A     | 2631 | A    |
| 46  | A     | 2632 | G    |
| 46  | A     | 2637 | G    |
| 46  | A     | 2638 | U    |
| 46  | A     | 2642 | U    |
| 46  | A     | 2692 | G    |
| 46  | A     | 2714 | G    |
| 46  | A     | 2718 | PSU  |
| 46  | A     | 2720 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 2743 | G    |
| 46  | A     | 2755 | U    |
| 46  | A     | 2763 | C    |
| 46  | A     | 2764 | G    |
| 46  | A     | 2765 | G    |
| 46  | A     | 2773 | G    |
| 46  | A     | 2777 | A    |
| 46  | A     | 2780 | G    |
| 46  | A     | 2786 | A    |
| 46  | A     | 2794 | A    |
| 46  | A     | 2795 | G    |
| 46  | A     | 2806 | G    |
| 46  | A     | 2807 | A    |
| 46  | A     | 2818 | C    |
| 46  | A     | 2820 | U    |
| 46  | A     | 2822 | C    |
| 46  | A     | 2823 | C    |
| 46  | A     | 2824 | G    |
| 46  | A     | 2828 | G    |
| 46  | A     | 2833 | U    |
| 46  | A     | 2845 | A    |
| 46  | A     | 2892 | G    |
| 46  | A     | 2893 | A    |
| 46  | A     | 2897 | G    |
| 46  | A     | 2898 | A    |
| 46  | A     | 2899 | C    |
| 46  | A     | 2900 | A    |
| 46  | A     | 2904 | A    |
| 46  | A     | 2905 | C    |
| 46  | A     | 2918 | G    |
| 50  | 7     | 404  | U    |
| 50  | 7     | 405  | G    |
| 51  | a     | 9    | G    |
| 51  | a     | 11   | G    |
| 51  | a     | 24   | G    |
| 51  | a     | 34   | A    |
| 51  | a     | 41   | G    |
| 51  | a     | 46   | G    |
| 51  | a     | 49   | C    |
| 51  | a     | 50   | C    |
| 51  | a     | 53   | A    |
| 51  | a     | 74   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | a     | 75  | G    |
| 51  | a     | 76  | A    |
| 51  | a     | 99  | A    |
| 51  | a     | 119 | C    |
| 51  | a     | 128 | A    |
| 51  | a     | 137 | G    |
| 51  | a     | 143 | C    |
| 51  | a     | 148 | A    |
| 51  | a     | 153 | U    |
| 51  | a     | 158 | G    |
| 51  | a     | 162 | C    |
| 51  | a     | 172 | U    |
| 51  | a     | 181 | G    |
| 51  | a     | 182 | U    |
| 51  | a     | 188 | G    |
| 51  | a     | 189 | A    |
| 51  | a     | 194 | C    |
| 51  | a     | 195 | A    |
| 51  | a     | 197 | G    |
| 51  | a     | 209 | A    |
| 51  | a     | 219 | U    |
| 51  | a     | 220 | C    |
| 51  | a     | 221 | G    |
| 51  | a     | 222 | G    |
| 51  | a     | 234 | A    |
| 51  | a     | 253 | U    |
| 51  | a     | 255 | G    |
| 51  | a     | 259 | G    |
| 51  | a     | 261 | U    |
| 51  | a     | 274 | G    |
| 51  | a     | 275 | C    |
| 51  | a     | 284 | G    |
| 51  | a     | 288 | C    |
| 51  | a     | 297 | G    |
| 51  | a     | 313 | G    |
| 51  | a     | 314 | A    |
| 51  | a     | 325 | U    |
| 51  | a     | 329 | A    |
| 51  | a     | 336 | C    |
| 51  | a     | 337 | A    |
| 51  | a     | 338 | C    |
| 51  | a     | 340 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | a     | 355 | G    |
| 51  | a     | 360 | C    |
| 51  | a     | 362 | G    |
| 51  | a     | 373 | U    |
| 51  | a     | 375 | U    |
| 51  | a     | 380 | C    |
| 51  | a     | 385 | G    |
| 51  | a     | 388 | G    |
| 51  | a     | 389 | A    |
| 51  | a     | 400 | G    |
| 51  | a     | 401 | A    |
| 51  | a     | 414 | G    |
| 51  | a     | 419 | A    |
| 51  | a     | 420 | U    |
| 51  | a     | 422 | A    |
| 51  | a     | 429 | U    |
| 51  | a     | 430 | C    |
| 51  | a     | 431 | G    |
| 51  | a     | 432 | G    |
| 51  | a     | 435 | C    |
| 51  | a     | 437 | U    |
| 51  | a     | 439 | A    |
| 51  | a     | 447 | U    |
| 51  | a     | 461 | C    |
| 51  | a     | 465 | U    |
| 51  | a     | 468 | C    |
| 51  | a     | 475 | A    |
| 51  | a     | 476 | U    |
| 51  | a     | 493 | G    |
| 51  | a     | 494 | G    |
| 51  | a     | 506 | A    |
| 51  | a     | 510 | C    |
| 51  | a     | 514 | G    |
| 51  | a     | 520 | C    |
| 51  | a     | 527 | C    |
| 51  | a     | 530 | G    |
| 51  | a     | 531 | C    |
| 51  | a     | 532 | A    |
| 51  | a     | 536 | G    |
| 51  | a     | 541 | A    |
| 51  | a     | 542 | A    |
| 51  | a     | 545 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | a     | 556 | A    |
| 51  | a     | 568 | A    |
| 51  | a     | 571 | U    |
| 51  | a     | 581 | A    |
| 51  | a     | 582 | A    |
| 51  | a     | 585 | G    |
| 51  | a     | 586 | G    |
| 51  | a     | 627 | C    |
| 51  | a     | 642 | U    |
| 51  | a     | 643 | C    |
| 51  | a     | 662 | U    |
| 51  | a     | 663 | G    |
| 51  | a     | 665 | G    |
| 51  | a     | 674 | A    |
| 51  | a     | 697 | G    |
| 51  | a     | 732 | U    |
| 51  | a     | 733 | G    |
| 51  | a     | 740 | G    |
| 51  | a     | 743 | A    |
| 51  | a     | 757 | A    |
| 51  | a     | 758 | A    |
| 51  | a     | 764 | G    |
| 51  | a     | 786 | A    |
| 51  | a     | 787 | G    |
| 51  | a     | 802 | U    |
| 51  | a     | 803 | A    |
| 51  | a     | 824 | A    |
| 51  | a     | 826 | C    |
| 51  | a     | 849 | G    |
| 51  | a     | 855 | G    |
| 51  | a     | 856 | C    |
| 51  | a     | 924 | A    |
| 51  | a     | 932 | G    |
| 51  | a     | 936 | G    |
| 51  | a     | 944 | C    |
| 51  | a     | 945 | A    |
| 51  | a     | 958 | C    |
| 51  | a     | 964 | G    |
| 51  | a     | 965 | U    |
| 51  | a     | 966 | U    |
| 51  | a     | 967 | U    |
| 51  | a     | 968 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | a     | 970  | U    |
| 51  | a     | 971  | U    |
| 51  | a     | 975  | A    |
| 51  | a     | 978  | A    |
| 51  | a     | 979  | A    |
| 51  | a     | 985  | A    |
| 51  | a     | 986  | G    |
| 51  | a     | 987  | A    |
| 51  | a     | 1002 | U    |
| 51  | a     | 1003 | G    |
| 51  | a     | 1004 | A    |
| 51  | a     | 1007 | U    |
| 51  | a     | 1008 | C    |
| 51  | a     | 1012 | U    |
| 51  | a     | 1013 | G    |
| 51  | a     | 1014 | A    |
| 51  | a     | 1019 | C    |
| 51  | a     | 1020 | C    |
| 51  | a     | 1028 | A    |
| 51  | a     | 1033 | G    |
| 51  | a     | 1034 | U    |
| 51  | a     | 1035 | C    |
| 51  | a     | 1039 | U    |
| 51  | a     | 1044 | G    |
| 51  | a     | 1045 | G    |
| 51  | a     | 1046 | G    |
| 51  | a     | 1049 | G    |
| 51  | a     | 1050 | A    |
| 51  | a     | 1051 | G    |
| 51  | a     | 1056 | A    |
| 51  | a     | 1063 | G    |
| 51  | a     | 1066 | U    |
| 51  | a     | 1067 | G    |
| 51  | a     | 1074 | G    |
| 51  | a     | 1075 | U    |
| 51  | a     | 1076 | C    |
| 51  | a     | 1095 | U    |
| 51  | a     | 1099 | G    |
| 51  | a     | 1104 | G    |
| 51  | a     | 1105 | U    |
| 51  | a     | 1106 | C    |
| 51  | a     | 1111 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | a     | 1114 | G    |
| 51  | a     | 1135 | U    |
| 51  | a     | 1139 | C    |
| 51  | a     | 1140 | A    |
| 51  | a     | 1142 | C    |
| 51  | a     | 1144 | U    |
| 51  | a     | 1145 | U    |
| 51  | a     | 1148 | G    |
| 51  | a     | 1149 | U    |
| 51  | a     | 1150 | U    |
| 51  | a     | 1166 | A    |
| 51  | a     | 1169 | G    |
| 51  | a     | 1176 | A    |
| 51  | a     | 1178 | A    |
| 51  | a     | 1180 | A    |
| 51  | a     | 1193 | G    |
| 51  | a     | 1205 | A    |
| 51  | a     | 1206 | A    |
| 51  | a     | 1220 | U    |
| 51  | a     | 1221 | U    |
| 51  | a     | 1222 | A    |
| 51  | a     | 1234 | A    |
| 51  | a     | 1235 | C    |
| 51  | a     | 1236 | A    |
| 51  | a     | 1237 | C    |
| 51  | a     | 1247 | A    |
| 51  | a     | 1265 | C    |
| 51  | a     | 1266 | A    |
| 51  | a     | 1267 | G    |
| 51  | a     | 1269 | G    |
| 51  | a     | 1287 | C    |
| 51  | a     | 1289 | A    |
| 51  | a     | 1299 | U    |
| 51  | a     | 1302 | G    |
| 51  | a     | 1309 | G    |
| 51  | a     | 1311 | U    |
| 51  | a     | 1312 | C    |
| 51  | a     | 1314 | G    |
| 51  | a     | 1321 | G    |
| 51  | a     | 1328 | A    |
| 51  | a     | 1329 | C    |
| 51  | a     | 1344 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | a     | 1345 | U    |
| 51  | a     | 1347 | G    |
| 51  | a     | 1355 | A    |
| 51  | a     | 1362 | G    |
| 51  | a     | 1373 | U    |
| 51  | a     | 1379 | G    |
| 51  | a     | 1388 | G    |
| 51  | a     | 1407 | A    |
| 51  | a     | 1415 | U    |
| 51  | a     | 1428 | G    |
| 51  | a     | 1432 | G    |
| 51  | a     | 1435 | A    |
| 51  | a     | 1449 | U    |
| 51  | a     | 1452 | G    |
| 51  | a     | 1455 | A    |
| 51  | a     | 1460 | U    |
| 51  | a     | 1464 | G    |
| 51  | a     | 1497 | G    |
| 51  | a     | 1502 | A    |
| 51  | a     | 1503 | A    |
| 51  | a     | 1504 | G    |
| 51  | a     | 1507 | G    |
| 51  | a     | 1509 | A    |
| 51  | a     | 1513 | A    |
| 51  | a     | 1515 | G    |
| 51  | a     | 1516 | U    |
| 51  | a     | 1527 | G    |
| 51  | a     | 1529 | A    |
| 51  | a     | 1530 | G    |
| 51  | a     | 1539 | G    |
| 51  | a     | 1540 | G    |

All (98) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | B     | 12  | U    |
| 7   | B     | 32  | U    |
| 7   | B     | 37  | A    |
| 7   | B     | 48  | G    |
| 7   | B     | 49  | G    |
| 7   | B     | 63  | C    |
| 7   | B     | 64  | A    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 12   | A    |
| 46  | A     | 60   | G    |
| 46  | A     | 75   | G    |
| 46  | A     | 88   | G    |
| 46  | A     | 92   | G    |
| 46  | A     | 176  | A    |
| 46  | A     | 181  | G    |
| 46  | A     | 202  | A    |
| 46  | A     | 252  | C    |
| 46  | A     | 299  | U    |
| 46  | A     | 300  | G    |
| 46  | A     | 337  | A    |
| 46  | A     | 389  | A    |
| 46  | A     | 411  | G    |
| 46  | A     | 458  | G    |
| 46  | A     | 482  | C    |
| 46  | A     | 549  | A    |
| 46  | A     | 599  | G    |
| 46  | A     | 615  | U    |
| 46  | A     | 631  | G    |
| 46  | A     | 691  | U    |
| 46  | A     | 701  | G    |
| 46  | A     | 732  | A    |
| 46  | A     | 742  | G    |
| 46  | A     | 793  | U    |
| 46  | A     | 811  | A    |
| 46  | A     | 831  | U    |
| 46  | A     | 837  | U    |
| 46  | A     | 848  | G    |
| 46  | A     | 855  | G    |
| 46  | A     | 874  | U    |
| 46  | A     | 905  | G    |
| 46  | A     | 986  | G    |
| 46  | A     | 990  | C    |
| 46  | A     | 1025 | A    |
| 46  | A     | 1030 | G    |
| 46  | A     | 1091 | U    |
| 46  | A     | 1092 | A    |
| 46  | A     | 1179 | A    |
| 46  | A     | 1187 | U    |
| 46  | A     | 1188 | A    |
| 46  | A     | 1244 | A    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 1246 | G    |
| 46  | A     | 1250 | G    |
| 46  | A     | 1266 | A    |
| 46  | A     | 1317 | G    |
| 46  | A     | 1325 | A    |
| 46  | A     | 1339 | A    |
| 46  | A     | 1344 | C    |
| 46  | A     | 1371 | G    |
| 46  | A     | 1382 | G    |
| 46  | A     | 1485 | A    |
| 46  | A     | 1498 | U    |
| 46  | A     | 1505 | U    |
| 46  | A     | 1525 | G    |
| 46  | A     | 1527 | C    |
| 46  | A     | 1530 | G    |
| 46  | A     | 1535 | U    |
| 46  | A     | 1543 | U    |
| 46  | A     | 1558 | G    |
| 46  | A     | 1565 | U    |
| 46  | A     | 1631 | A    |
| 46  | A     | 1653 | A    |
| 46  | A     | 1663 | A    |
| 46  | A     | 1691 | A    |
| 46  | A     | 1751 | U    |
| 46  | A     | 1757 | G    |
| 46  | A     | 1791 | A    |
| 46  | A     | 1887 | G    |
| 46  | A     | 1941 | A    |
| 46  | A     | 1942 | A    |
| 46  | A     | 2026 | A    |
| 46  | A     | 2064 | G    |
| 46  | A     | 2080 | A    |
| 46  | A     | 2127 | U    |
| 46  | A     | 2315 | A    |
| 46  | A     | 2337 | G    |
| 46  | A     | 2348 | C    |
| 46  | A     | 2349 | A    |
| 46  | A     | 2375 | A    |
| 46  | A     | 2451 | C    |
| 46  | A     | 2459 | A    |
| 46  | A     | 2497 | A    |
| 46  | A     | 2558 | G    |

*Continued on next page...*



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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | A     | 2631 | A    |
| 46  | A     | 2785 | U    |
| 46  | A     | 2805 | A    |
| 46  | A     | 2823 | C    |
| 46  | A     | 2892 | G    |
| 46  | A     | 2898 | A    |
| 46  | A     | 2904 | A    |

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

2 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 | $\# Z  > 2$ |
| 46  | PSU  | A     | 2718 | 46    | 18,21,22     | 0.90 | 1 (5%)      | 21,30,33    | 0.86 | 0           |
| 46  | OMG  | A     | 2280 | 45,46 | 23,26,27     | 0.41 | 0           | 32,38,41    | 0.65 | 1 (3%)      |

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   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 46  | PSU  | A     | 2718 | 46    | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | OMG  | A     | 2280 | 45,46 | -       | 0/9/27/28 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 46  | A     | 2718 | PSU  | C6-C5 | 3.10 | 1.38        | 1.35     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|------|------------------------|---------------------|
| 46  | A     | 2280 | OMG  | O3'-C3'-C2' | 2.07 | 116.99                 | 111.19              |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

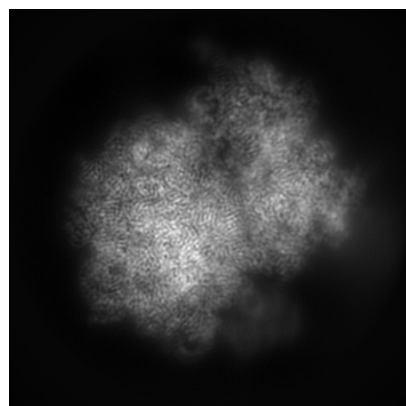
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50856. These allow visual inspection of the internal detail of the map and identification of artifacts.

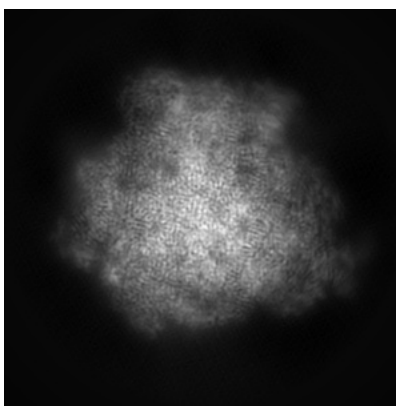
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

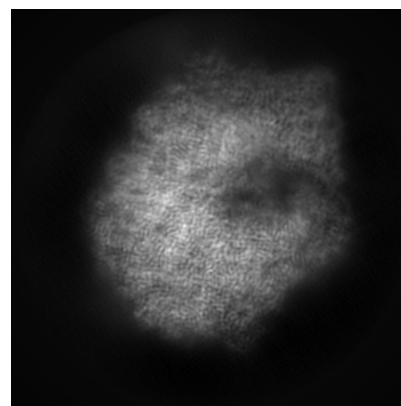
#### 6.1.1 Primary map



X

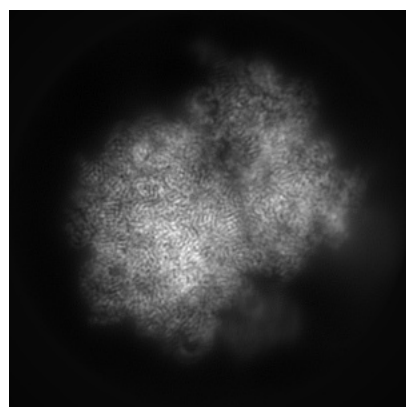


Y

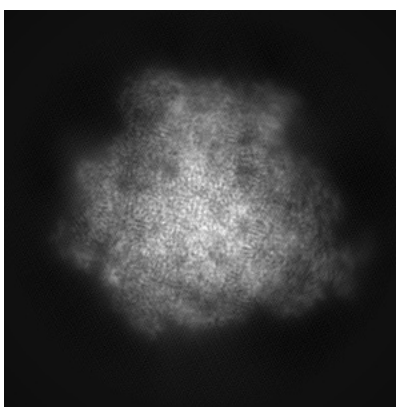


Z

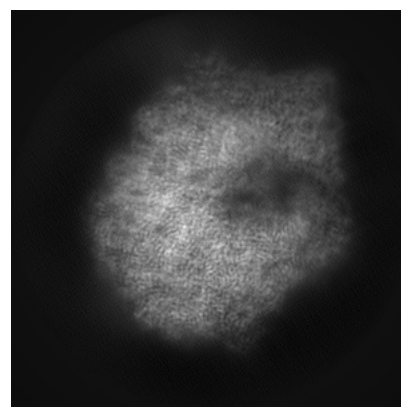
#### 6.1.2 Raw map



X



Y

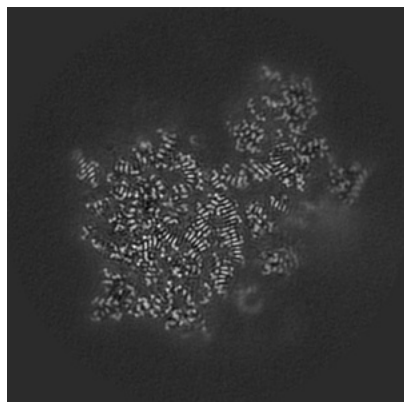


Z

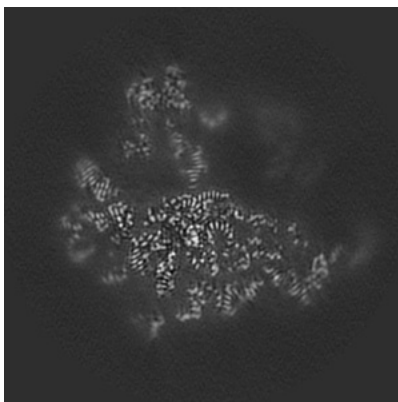
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

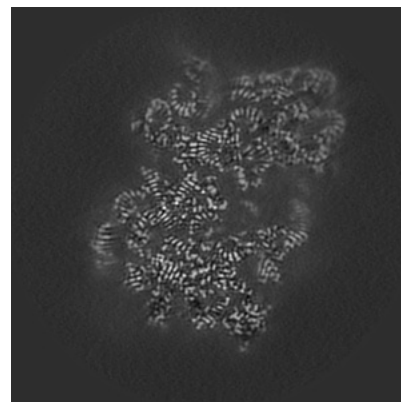
### 6.2.1 Primary map



X Index: 192

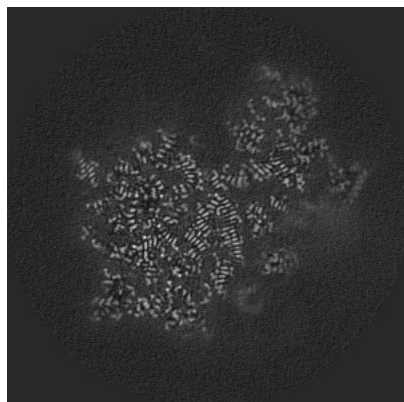


Y Index: 192

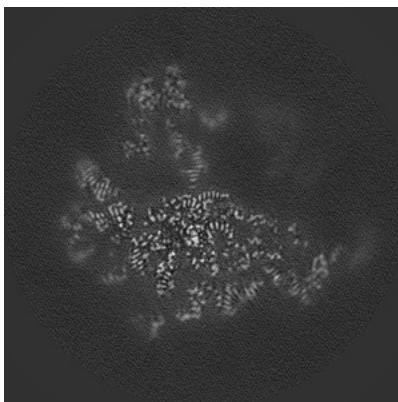


Z Index: 192

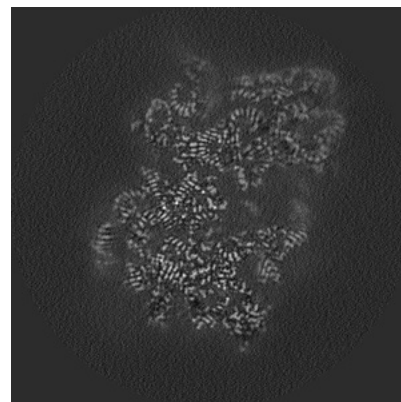
### 6.2.2 Raw map



X Index: 192



Y Index: 192

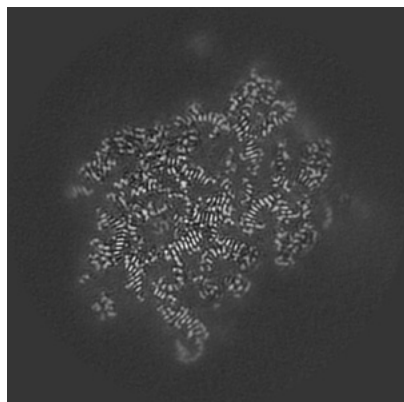


Z Index: 192

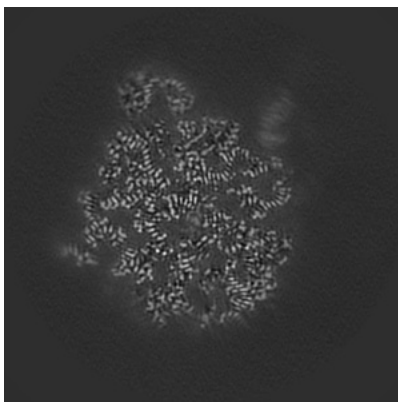
The images above show central slices of the map in three orthogonal directions.

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

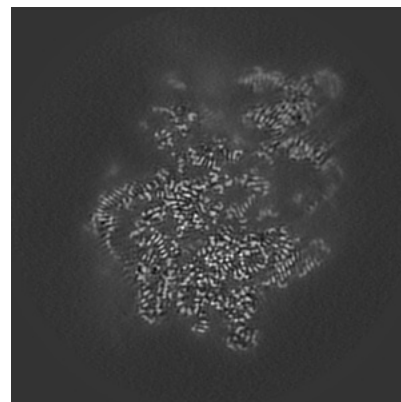
### 6.3.1 Primary map



X Index: 164

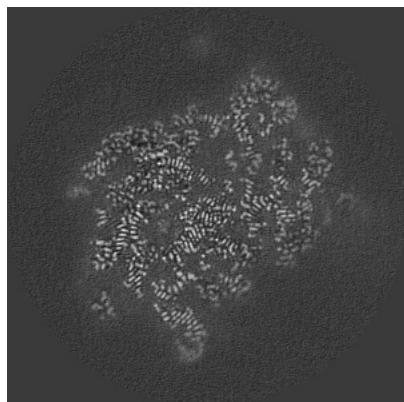


Y Index: 156

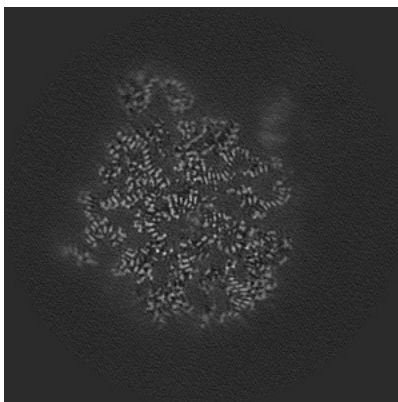


Z Index: 178

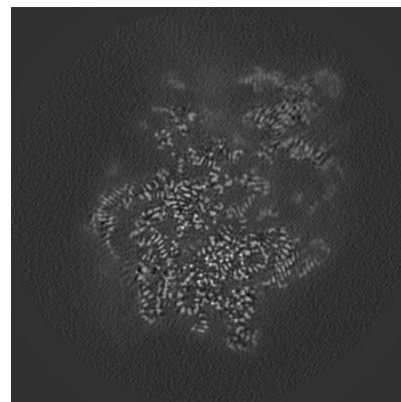
### 6.3.2 Raw map



X Index: 166



Y Index: 156



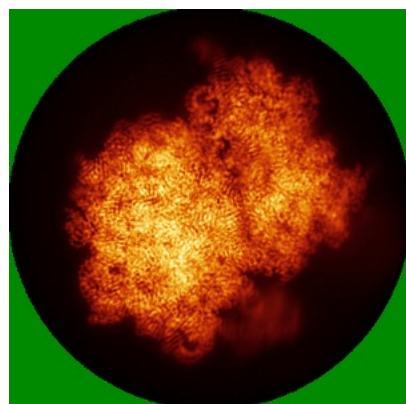
Z Index: 178

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

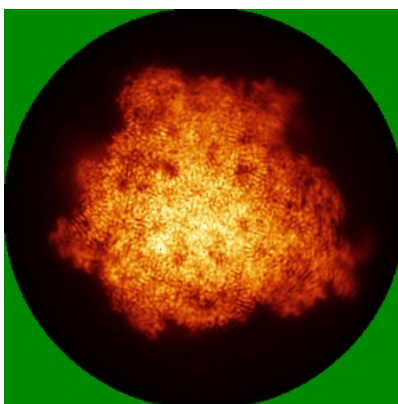


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

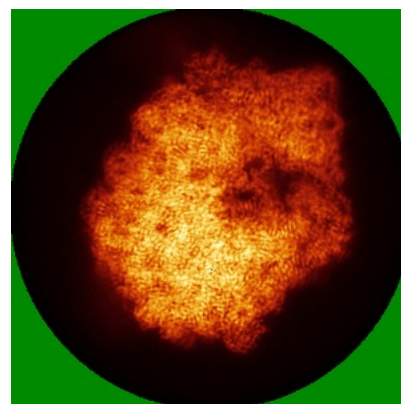
### 6.4.1 Primary map



X

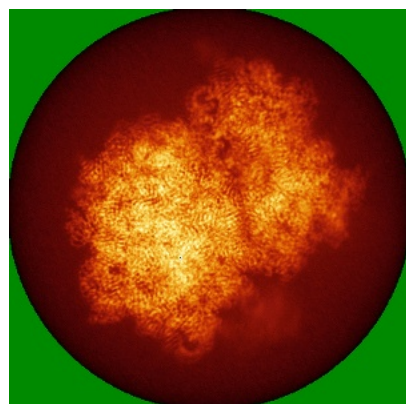


Y

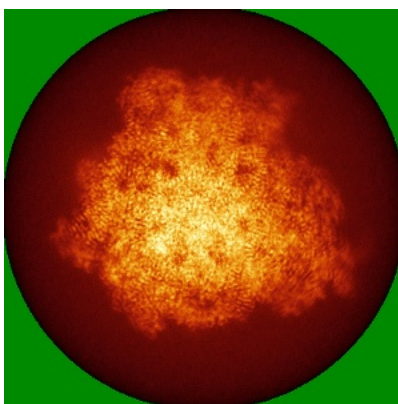


Z

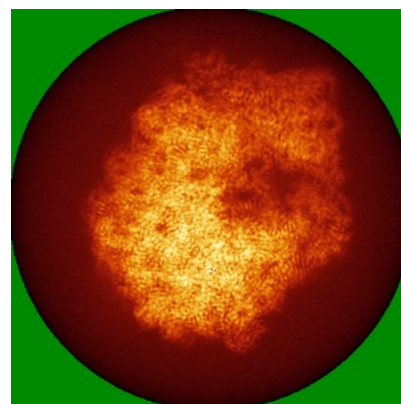
### 6.4.2 Raw map



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](#)

This section was not generated.

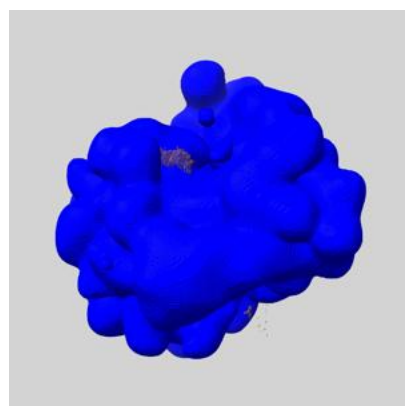
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

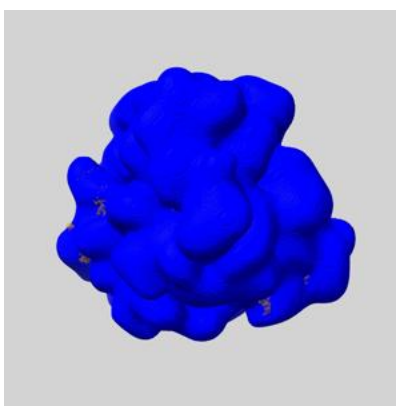
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

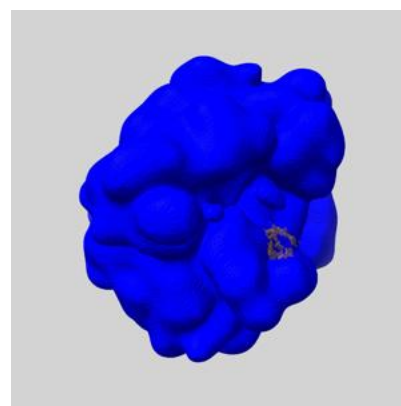
### 6.6.1 emd\_50856\_msk\_1.map [i](#)



X



Y

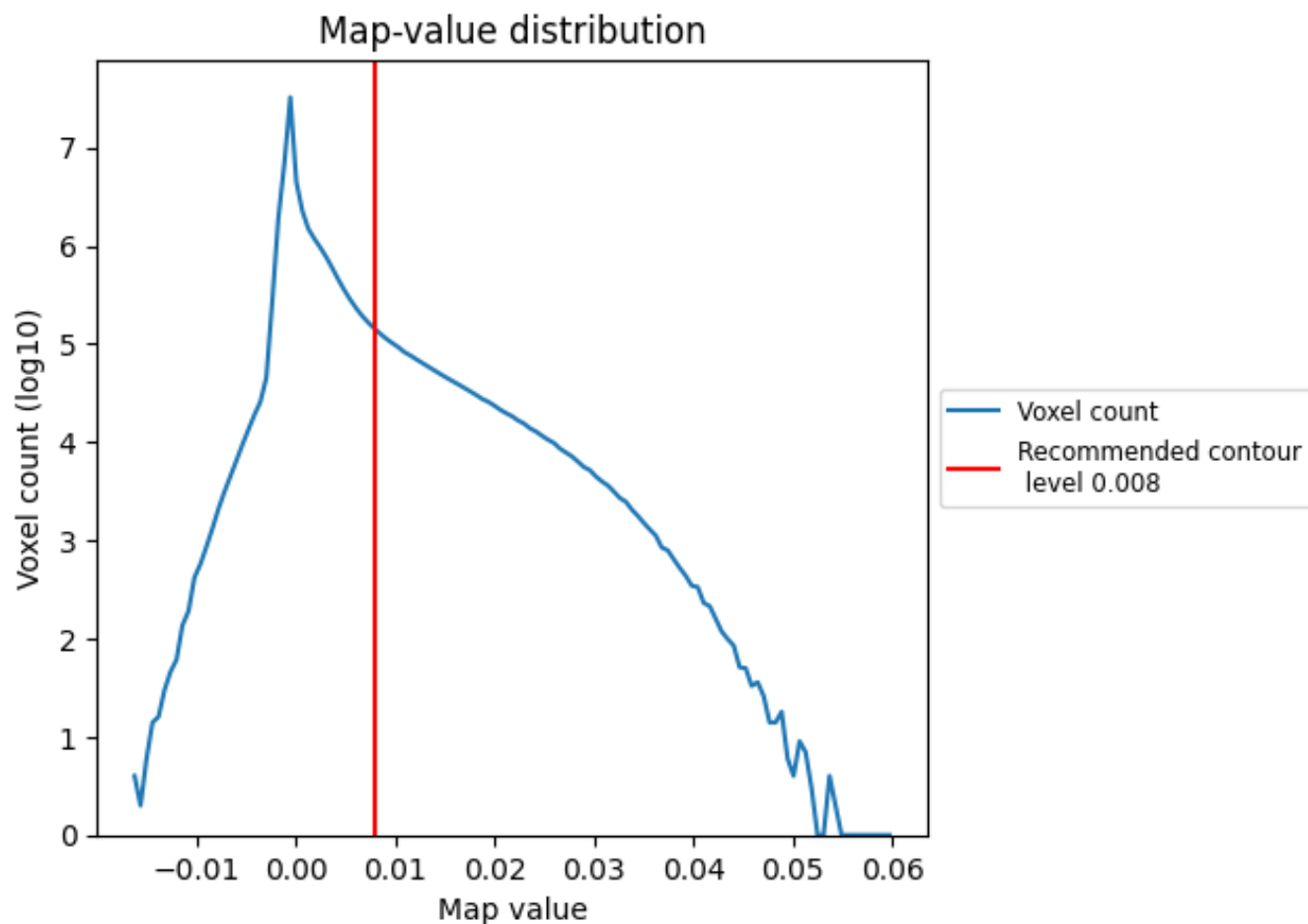


Z

## 7 Map analysis [i](#)

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

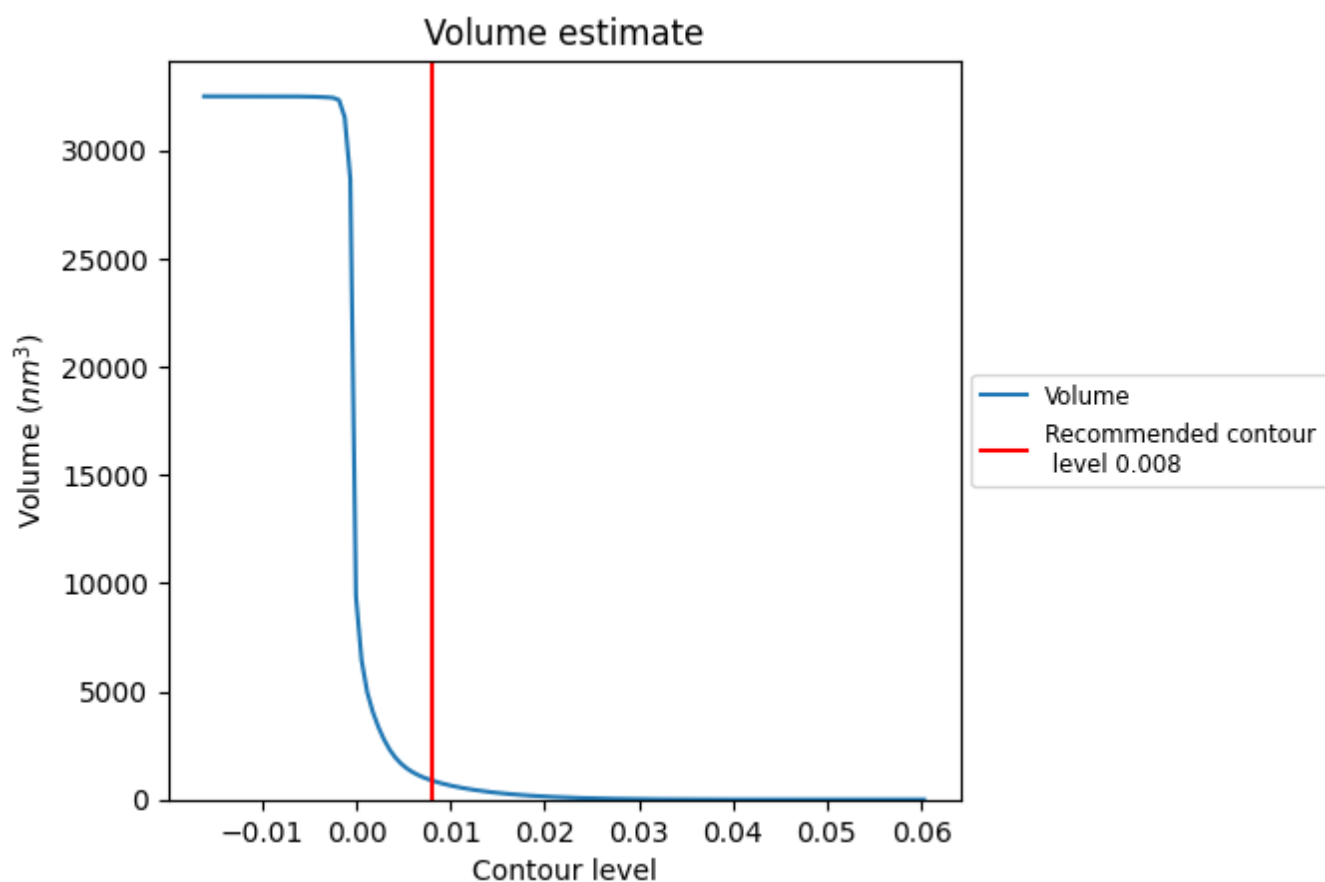
### 7.1 Map-value distribution [i](#)



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.



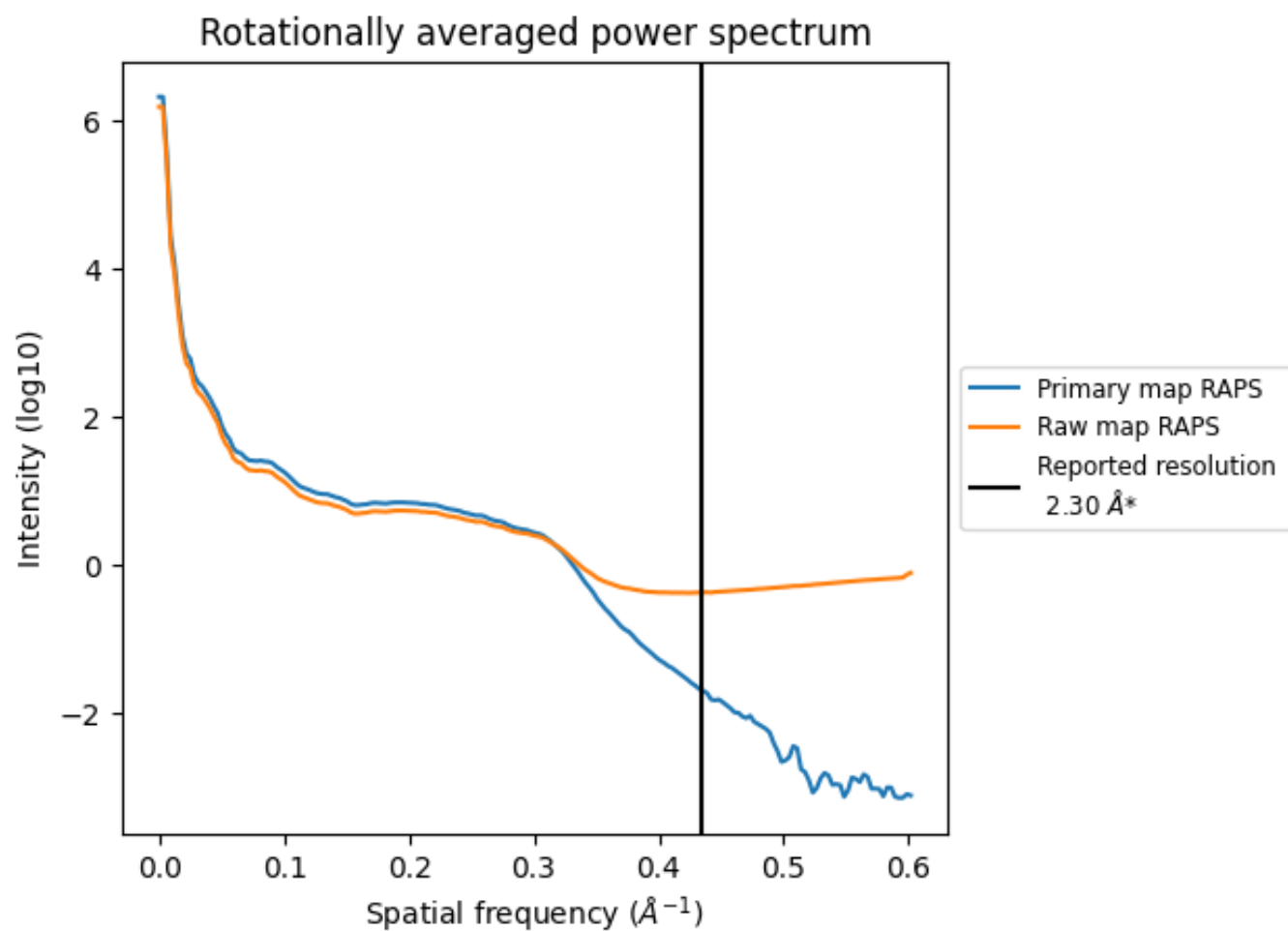
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 887 nm<sup>3</sup>; this corresponds to an approximate mass of 802 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 ⓘ

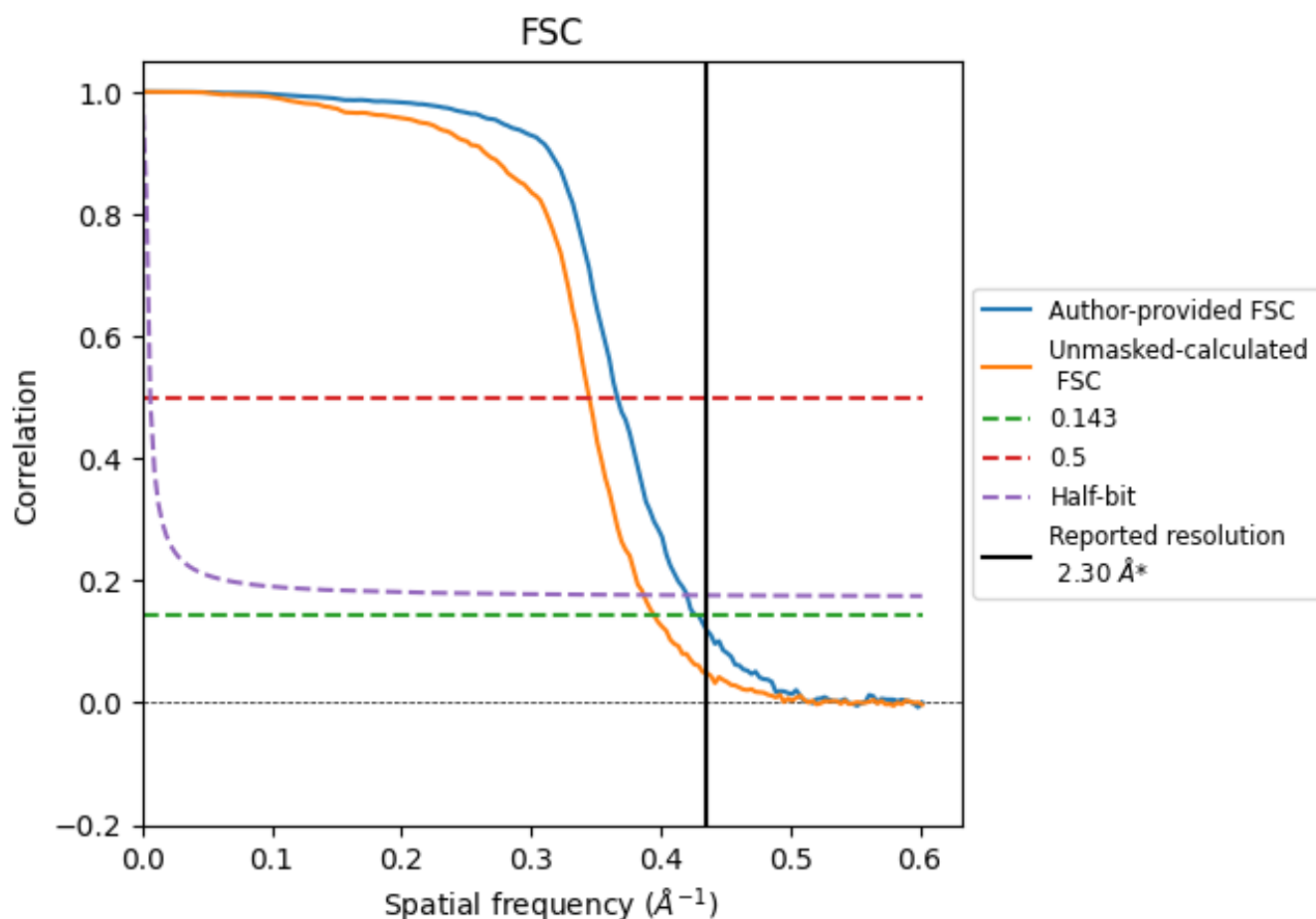


\*Reported resolution corresponds to spatial frequency of  $0.435 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.30                               | -    | -        |
| Author-provided FSC curve | 2.33                               | 2.73 | 2.38     |
| Unmasked-calculated*      | 2.53                               | 2.90 | 2.58     |

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

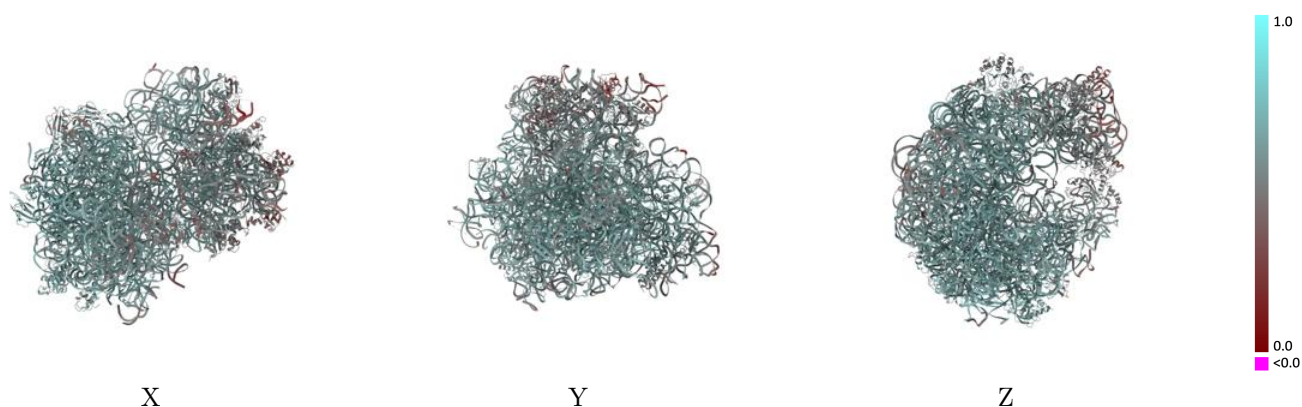
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50856 and PDB model 9FY2. Per-residue inclusion information can be found in section 3 on page 14.

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

This section was not generated.

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

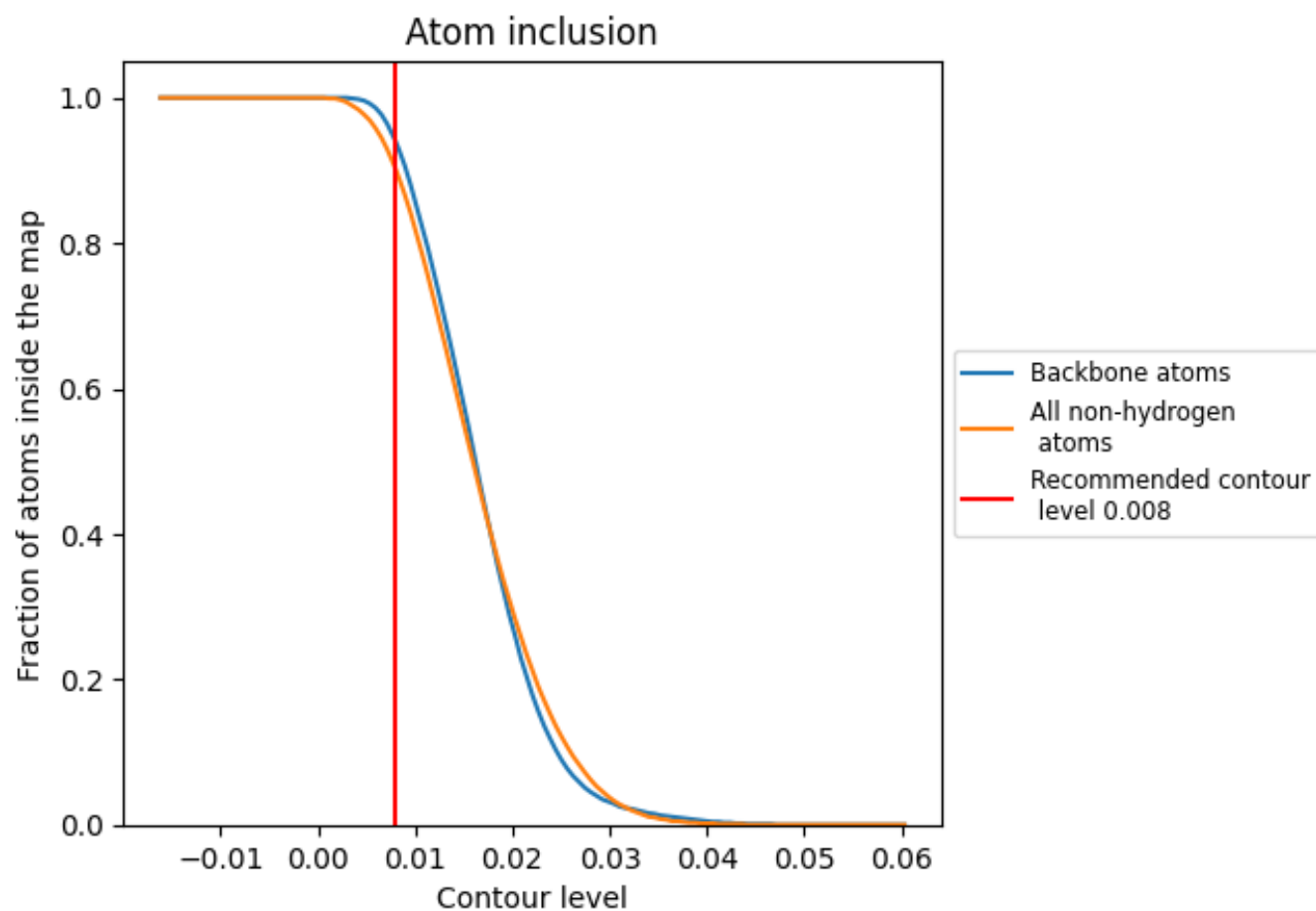


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





































The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9020   |  0.6000   |
| 0     |  0.8930   |  0.6150   |
| 1     |  0.8050   |  0.5810   |
| 2     |  0.9770   |  0.6700   |
| 3     |  0.9520   |  0.6510   |
| 4     |  0.9000   |  0.6210   |
| 5     |  0.7620   |  0.5910   |
| 6     |  0.4500   |  0.4170   |
| 7     |  0.9110   |  0.5770   |
| A     |  0.9710   |  0.6320   |
| B     |  0.9270   |  0.5660   |
| C     |  0.9380   |  0.6500   |
| D     |  0.8930   |  0.6390   |
| E     |  0.8400   |  0.6210   |
| F     |  0.6150  |  0.4830  |
| G     |  0.6110 |  0.5230 |
| J     |  0.9150 |  0.6400 |
| K     |  0.9060 |  0.6400 |
| L     |  0.8450 |  0.6170 |
| M     |  0.9020 |  0.6140 |
| N     |  0.8870 |  0.5990 |
| O     |  0.7010 |  0.5240 |
| P     |  0.8610 |  0.6090 |
| Q     |  0.9140 |  0.6510 |
| R     |  0.8420 |  0.6290 |
| S     |  0.8960 |  0.6310 |
| T     |  0.8240 |  0.5790 |
| U     |  0.7540 |  0.5800 |
| W     |  0.9140 |  0.6210 |
| X     |  0.8170 |  0.5990 |
| Y     |  0.7270 |  0.5480 |
| Z     |  0.8590 |  0.6120 |
| a     |  0.9280 |  0.5790 |
| b     |  0.6150 |  0.5310 |
| c     |  0.6650 |  0.5090 |



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| Chain | Atom inclusion  | Q-score   |
|-------|---|---|
| d     |  0.6880  |  0.5510  |
| e     |  0.8230  |  0.5990  |
| f     |  0.7310  |  0.5760  |
| g     |  0.6170  |  0.4740  |
| h     |  0.8550  |  0.6060  |
| i     |  0.5810  |  0.4540  |
| j     |  0.4940  |  0.4220  |
| k     |  0.7360  |  0.5530  |
| l     |  0.8480  |  0.6070  |
| m     |  0.6710  |  0.4830  |
| n     |  0.8170  |  0.5450  |
| o     |  0.8330  |  0.5960  |
| p     |  0.8120  |  0.5780  |
| q     |  0.7880  |  0.5700  |
| r     |  0.7980  |  0.5930  |
| s     |  0.6290  |  0.4700  |
| t     |  0.7090  |  0.5260  |
| v     |  0.9250 |  0.5730 |