



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:49 PM UTC

PDB ID : 9HCH / pdb\_00009hch  
EMDB ID : EMD-52049  
Title : Mouse mitoribosome large subunit assembly intermediate bound to NSUN4, METRF4, GTPBP7 and the MALSU1-L0R8F8-mt-ACP complex, State C1 (SAMC knock-out)  
Authors : Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenber, A.  
Deposited on : 2024-11-10  
Resolution : 2.85 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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

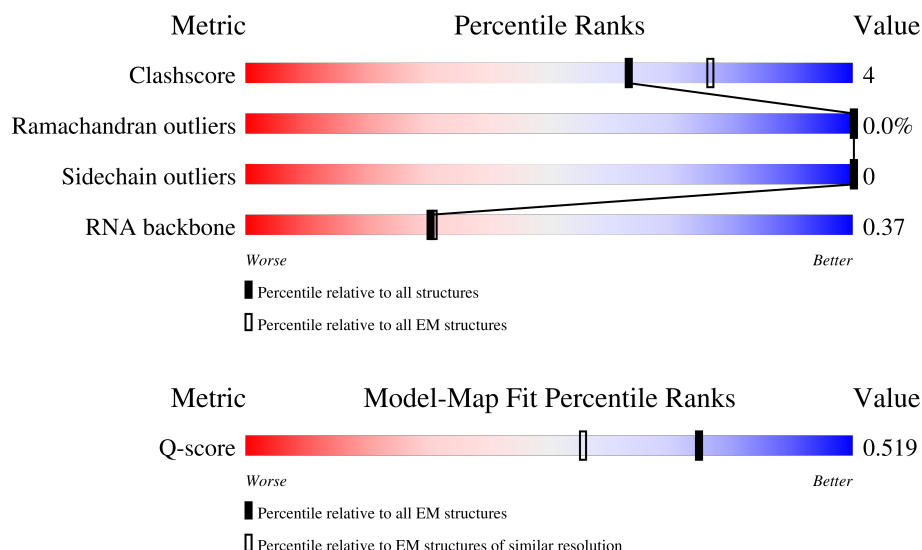
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.85 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                       | 11965 ( 2.35 - 3.35 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1584   |                  |
| 2   | B     | 68     |                  |
| 3   | D     | 246    |                  |

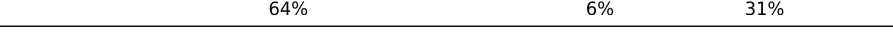
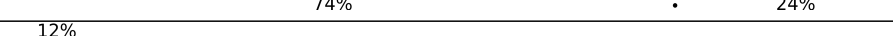
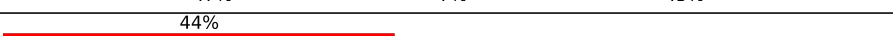
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | E     | 348    |                  |
| 5   | F     | 294    |                  |
| 6   | H     | 265    |                  |
| 7   | I     | 262    |                  |
| 8   | J     | 192    |                  |
| 9   | K     | 178    |                  |
| 10  | L     | 145    |                  |
| 11  | M     | 295    |                  |
| 12  | N     | 251    |                  |
| 13  | O     | 176    |                  |
| 14  | P     | 180    |                  |
| 15  | Q     | 292    |                  |
| 16  | R     | 149    |                  |
| 17  | S     | 209    |                  |
| 18  | T     | 206    |                  |
| 19  | U     | 146    |                  |
| 20  | V     | 216    |                  |
| 21  | W     | 148    |                  |
| 22  | X     | 294    |                  |
| 23  | Y     | 252    |                  |
| 24  | Z     | 160    |                  |
| 25  | x     | 356    |                  |
| 26  | 0     | 187    |                  |
| 27  | 1     | 65     |                  |
| 28  | 2     | 92     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | 3     | 188    |    |
| 30  | 4     | 101    |    |
| 31  | 6     | 380    |    |
| 32  | 7     | 336    |    |
| 33  | b     | 159    |    |
| 34  | c     | 303    |    |
| 35  | d     | 306    |    |
| 36  | e     | 283    |    |
| 37  | f     | 211    |    |
| 38  | g     | 166    |    |
| 39  | h     | 159    |    |
| 40  | i     | 128    |   |
| 41  | j     | 121    |  |
| 42  | o     | 102    |  |
| 43  | p     | 206    |  |
| 44  | q     | 222    |  |
| 45  | r     | 196    |  |
| 46  | s     | 442    |  |
| 47  | u     | 228    |  |
| 48  | v     | 70     |  |
| 49  | w     | 156    |  |
| 50  | 5     | 423    |  |
| 51  | 8     | 206    |  |
| 52  | 9     | 135    |  |
| 53  | a     | 142    |  |

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| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 54  | m     | 127    | <div><div><div></div><div></div><div></div></div><div>35%30%6%65%</div></div>  |
| 55  | l     | 135    | <div><div><div></div><div></div><div></div></div><div>35%38%7%56%</div></div>  |
| 56  | z     | 326    | <div><div><div></div><div></div><div></div></div><div>30%76%19%5%</div></div>  |
| 57  | y     | 346    | <div><div><div></div><div></div><div></div></div><div>13%65%32%</div></div>    |
| 58  | k     | 118    | <div><div><div></div><div></div><div></div></div><div>36%56%16%28%</div></div> |

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 198705 atoms, of which 91907 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA (1584-MER).

| Mol | Chain | Residues | Atoms |       |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|------|------|---------|-------|
| 1   | A     | 1441     | Total | C     | H     | N    | O    | P    | 0       | 0     |
|     |       |          | 46100 | 13756 | 15471 | 5518 | 9914 | 1441 |         |       |

- Molecule 2 is a RNA chain called tRNA-Phe (68-MER).

| Mol | Chain | Residues | Atoms |     |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 2   | B     | 62       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 1993  | 595 | 667 | 244 | 425 | 62 |         |       |

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 3   | D     | 227      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3598  | 1105 | 1830 | 349 | 305 | 9 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 4   | E     | 308      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4901  | 1577 | 2442 | 432 | 442 | 8 |         |       |

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 5   | F     | 250      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4030  | 1286 | 2025 | 364 | 349 | 6 |         |       |

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

| Mol | Chain | Residues | Atoms |     |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|
| 6   | H     | 95       | Total | C   | H   | N   | O   | 0       | 0     |
|     |       |          | 1593  | 492 | 814 | 150 | 137 |         |       |

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 7   | I     | 161      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2700  | 851 | 1393 | 235 | 214 | 7 |         |       |

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 8   | J     | 175      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2720  | 846 | 1394 | 234 | 243 | 3 |         |       |

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 9   | K     | 177      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2893  | 927 | 1444 | 262 | 253 | 7 |         |       |

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 10  | L     | 115      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1837  | 560 | 944 | 174 | 155 | 4 |         |       |

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 11  | M     | 287      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4692  | 1475 | 2377 | 428 | 406 | 6 |         |       |

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 12  | N     | 198      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3264  | 1051 | 1639 | 289 | 275 | 10 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 13  | O     | 153      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2541  | 795 | 1282 | 240 | 219 | 5 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 14  | P     | 141      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2302  | 725 | 1148 | 221 | 203 | 5 |         |       |

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 15  | Q     | 217      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3612  | 1150 | 1822 | 309 | 322 | 9 |         |       |

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 16  | R     | 140      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2385  | 738 | 1224 | 233 | 187 | 3 |         |       |

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 17  | S     | 159      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2673  | 840 | 1372 | 233 | 226 | 2 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 18  | T     | 166      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2771  | 871 | 1402 | 256 | 234 | 8 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 19  | U     | 127      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2109  | 675 | 1057 | 196 | 178 | 3 |         |       |

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 20  | V     | 201      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3295  | 1043 | 1643 | 305 | 298 | 6 |         |       |

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 21  | W     | 100      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1602  | 515 | 808 | 141 | 135 | 3 |         |       |

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 22  | X     | 242      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4072  | 1304 | 2051 | 358 | 355 | 4 |         |       |

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 23  | Y     | 176      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3076  | 973 | 1553 | 290 | 255 | 5 |         |       |

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 24  | Z     | 121      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2026  | 632 | 1039 | 182 | 170 | 3 |         |       |

- Molecule 25 is a protein called 5-cytosine rRNA methyltransferase NSUN4.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 25  | x     | 325      | Total | C    | H    | N   | O   | S  | 1       | 0     |
|     |       |          | 5110  | 1626 | 2546 | 448 | 473 | 17 |         |       |

- Molecule 26 is a protein called Large ribosomal subunit protein bL32m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 26  | 0     | 108      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1789  | 546 | 908 | 174 | 155 | 6 |         |       |

- Molecule 27 is a protein called Large ribosomal subunit protein bL33m.

| Mol | Chain | Residues | Atoms |     |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|--|---------|-------|
| 27  | 1     | 52       | Total | C   | H   | N  | O  |  | 0       | 0     |
|     |       |          | 900   | 278 | 472 | 80 | 70 |  |         |       |

- Molecule 28 is a protein called Large ribosomal subunit protein bL34m.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 28  | 2     | 46       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 787   | 235 | 407 | 86 | 58 | 1 |         |       |

- Molecule 29 is a protein called Large ribosomal subunit protein bL35m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 29  | 3     | 95       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 528 | 872 | 164 | 127 | 4 |         |       |

- Molecule 30 is a protein called Large ribosomal subunit protein bL36m.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 30  | 4     | 37       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 676   | 206 | 354 | 68 | 45 | 3 |         |       |

- Molecule 31 is a protein called Large ribosomal subunit protein mL38.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 31  | 6     | 315      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5248  | 1726 | 2559 | 487 | 470 | 6 |         |       |

- Molecule 32 is a protein called Large ribosomal subunit protein mL39.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 32  | 7     | 292      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4757  | 1517 | 2378 | 409 | 438 | 15 |         |       |

- Molecule 33 is a protein called Large ribosomal subunit protein mL43.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 33  | b     | 148      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2376  | 731 | 1195 | 234 | 214 | 2 |         |       |

- Molecule 34 is a protein called Large ribosomal subunit protein mL44.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 34  | c     | 281      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4535  | 1450 | 2273 | 392 | 412 | 8 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein mL45.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 35  | d     | 211      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3471  | 1119 | 1728 | 309 | 304 | 11 |         |       |

- Molecule 36 is a protein called Large ribosomal subunit protein mL46.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 36  | e     | 193      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3174  | 1013 | 1598 | 278 | 279 | 6 |         |       |

- Molecule 37 is a protein called Large ribosomal subunit protein mL48.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 37  | f     | 104      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1674  | 533 | 836 | 141 | 160 | 4 |         |       |

- Molecule 38 is a protein called Large ribosomal subunit protein mL49.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 38  | g     | 132      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2184  | 709 | 1094 | 187 | 192 | 2 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein mL50.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 39  | h     | 110      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1739  | 552 | 867 | 156 | 160 | 4 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein mL51.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 40  | i     | 97       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1685  | 540 | 854 | 161 | 128 | 2 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein mL52.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 41  | j     | 93       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1512  | 467 | 768 | 145 | 130 | 2 |         |       |

- Molecule 42 is a protein called Large ribosomal subunit protein mL63.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 42  | o     | 78       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1263  | 402 | 623 | 118 | 116 | 4 |         |       |

- Molecule 43 is a protein called Large ribosomal subunit protein mL62.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 43  | p     | 144      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2374  | 735 | 1198 | 218 | 219 | 4 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein mL64.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 44  | q     | 135      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2253  | 703 | 1123 | 223 | 199 | 5 |         |       |

- Molecule 45 is a protein called Large ribosomal subunit protein mL66.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 45  | r     | 157      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2604  | 812 | 1329 | 242 | 210 | 11 |         |       |

- Molecule 46 is a protein called Large ribosomal subunit protein mL65.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 46  | s     | 377      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6103  | 1938 | 3058 | 555 | 540 | 12 |         |       |

- Molecule 47 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 47  | u     | 125      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2041  | 659 | 1012 | 170 | 191 | 9 |         |       |

- Molecule 48 is a protein called Predicted gene, 55359.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 48  | v     | 69       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1189  | 374 | 603 | 112 | 99 | 1 |         |       |

- Molecule 49 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 49  | w     | 79       | Total | C   | H   | N  | O   | S | 0       | 0     |
|     |       |          | 1277  | 410 | 640 | 95 | 127 | 5 |         |       |

- Molecule 50 is a protein called Large ribosomal subunit protein mL37.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 50  | 5     | 394      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 6468  | 2081 | 3243 | 564 | 571 | 9 |         |       |

- Molecule 51 is a protein called Large ribosomal subunit protein mL40.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 51  | 8     | 70       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 368 | 574 | 102 | 117 | 2 |         |       |

- Molecule 52 is a protein called Large ribosomal subunit protein mL41.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 52  | 9     | 122      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1973  | 635 | 990 | 167 | 179 | 2 |         |       |

- Molecule 53 is a protein called Large ribosomal subunit protein mL42.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 53  | a     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1703  | 542 | 843 | 156 | 159 | 3 |         |       |

- Molecule 54 is a protein called Large ribosomal subunit protein mL55.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 54  | m     | 45       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 769   | 233 | 395 | 77 | 61 | 3 |         |       |

- Molecule 55 is a protein called Large ribosomal subunit protein mL54.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 55  | 1     | 60       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1007  | 315 | 505 | 94 | 91 | 2 |         |       |

- Molecule 56 is a protein called Mitochondrial ribosome-associated GTPase 1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 56  | z     | 311      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 5001  | 1562 | 2546 | 444 | 433 | 16 |         |       |

- Molecule 57 is a protein called Transcription termination factor 4, mitochondrial.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 57  | y     | 237      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3938  | 1238 | 1995 | 345 | 351 | 9 |         |       |

- Molecule 58 is a protein called Large ribosomal subunit protein mL53.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 58  | k     | 85       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1331  | 413 | 667 | 121 | 125 | 5 |         |       |

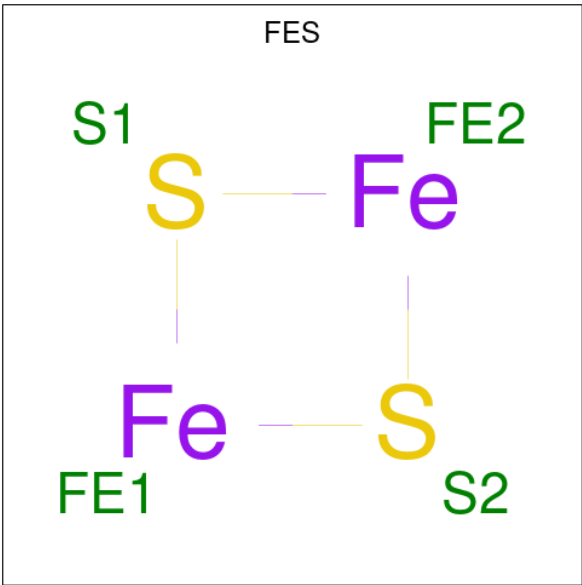
- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 59  | A     | 96       | Total | Mg | 0       |
|     |       |          | 96    | 96 |         |
| 59  | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 59  | M     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 59  | O     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

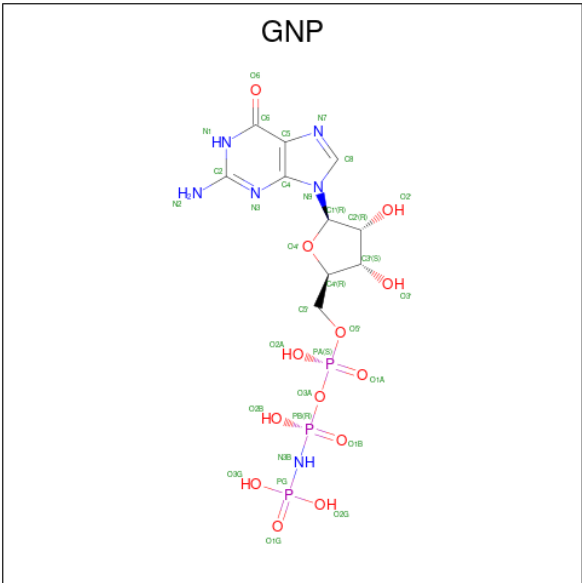
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 60  | 0     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 60  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 61  | r     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 62 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 62  | z     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 45    | 10 | 13 | 6 | 13 | 3 |         |

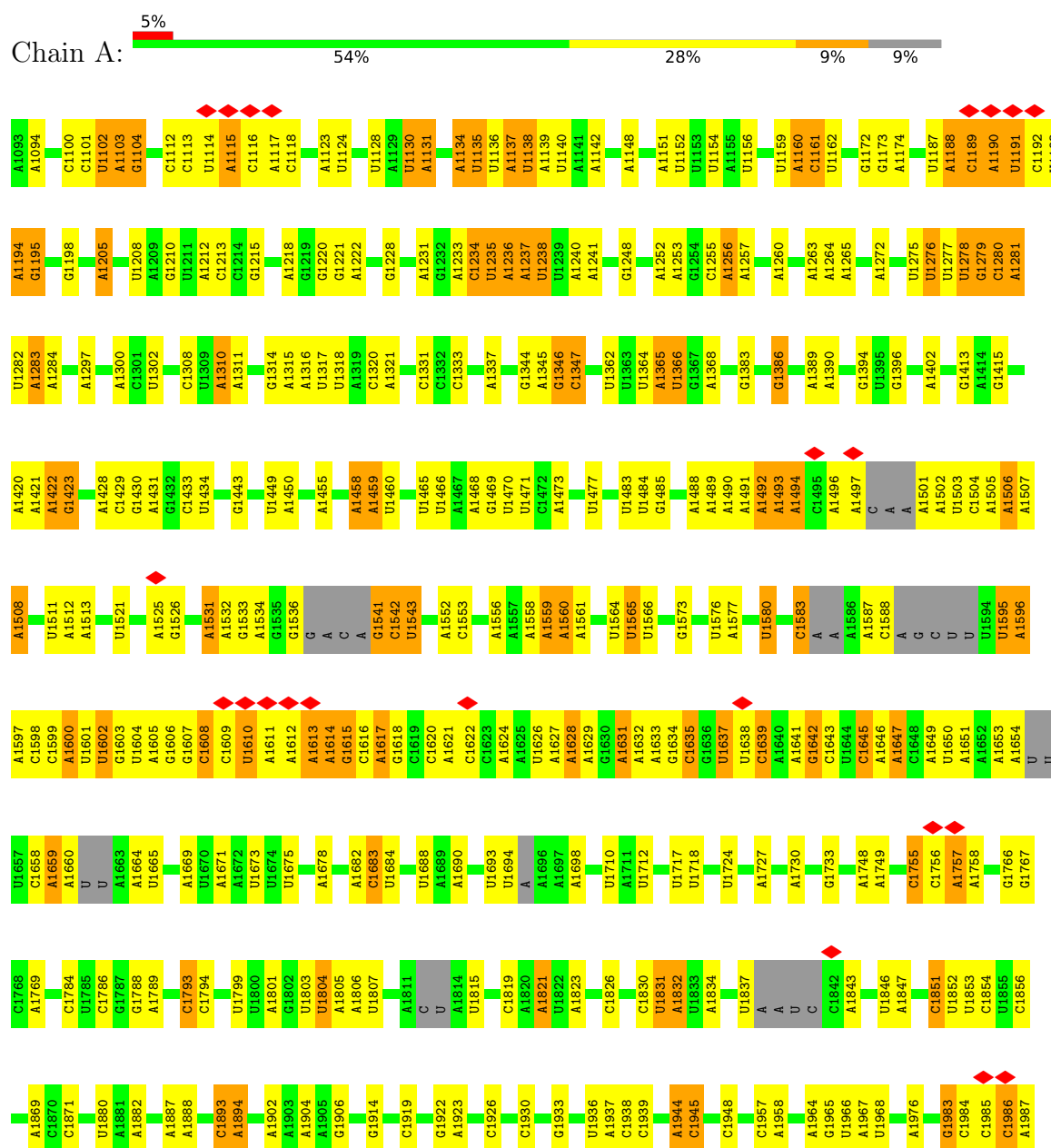
- Molecule 63 is water.

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 63  | A     | 1        | Total<br>1 | O<br>1 | 0       |

### 3 Residue-property plots

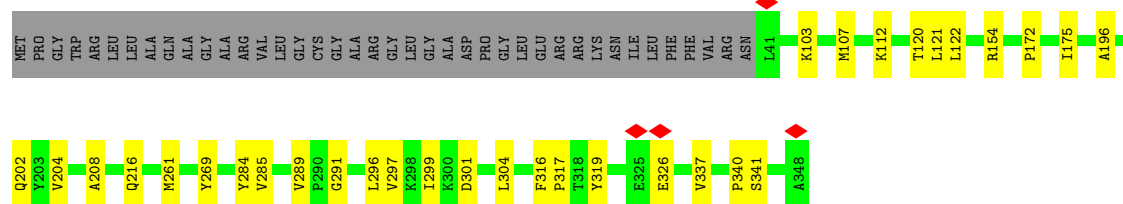
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S rRNA (1584-MER)



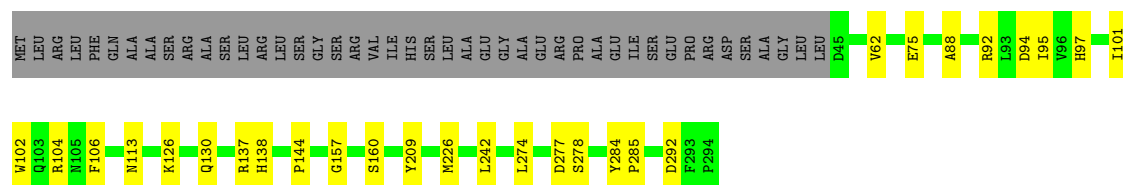


Chain E: 



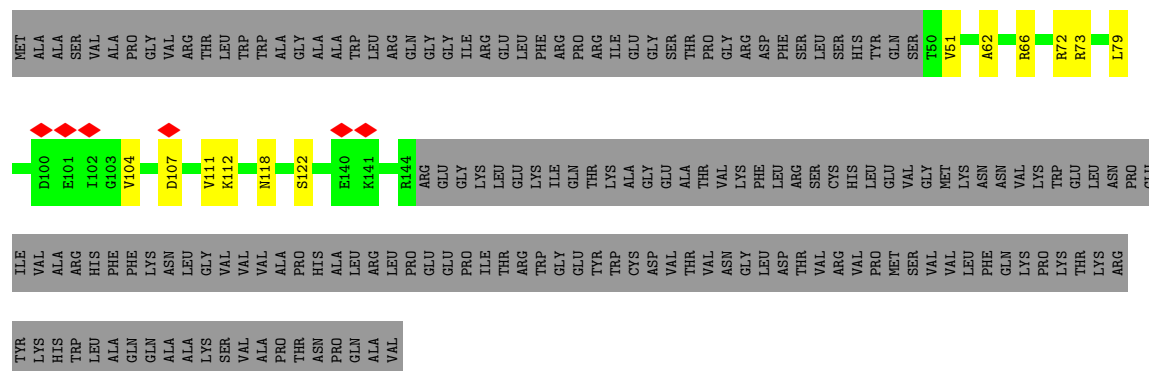
- Molecule 5: Large ribosomal subunit protein uL4m

Chain F: 



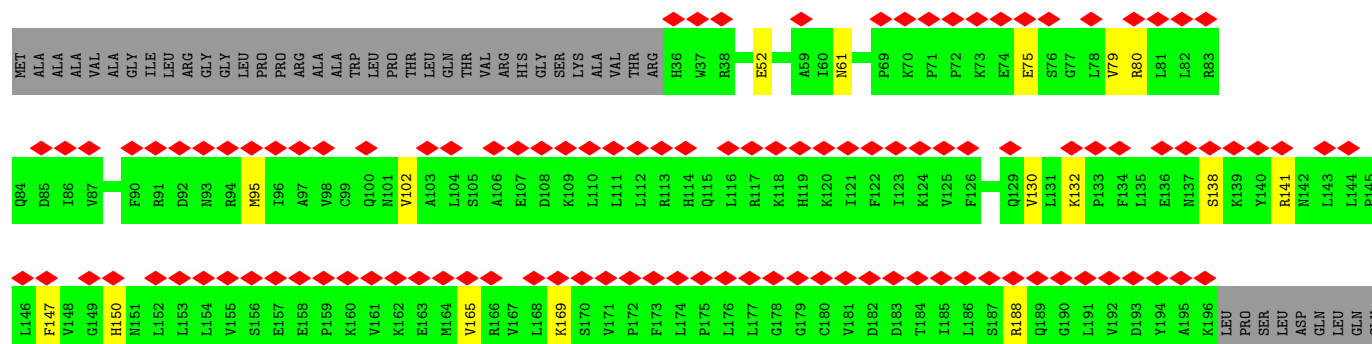
- Molecule 6: Large ribosomal subunit protein bL9m

Chain H: 



- Molecule 7: Large ribosomal subunit protein uL10m

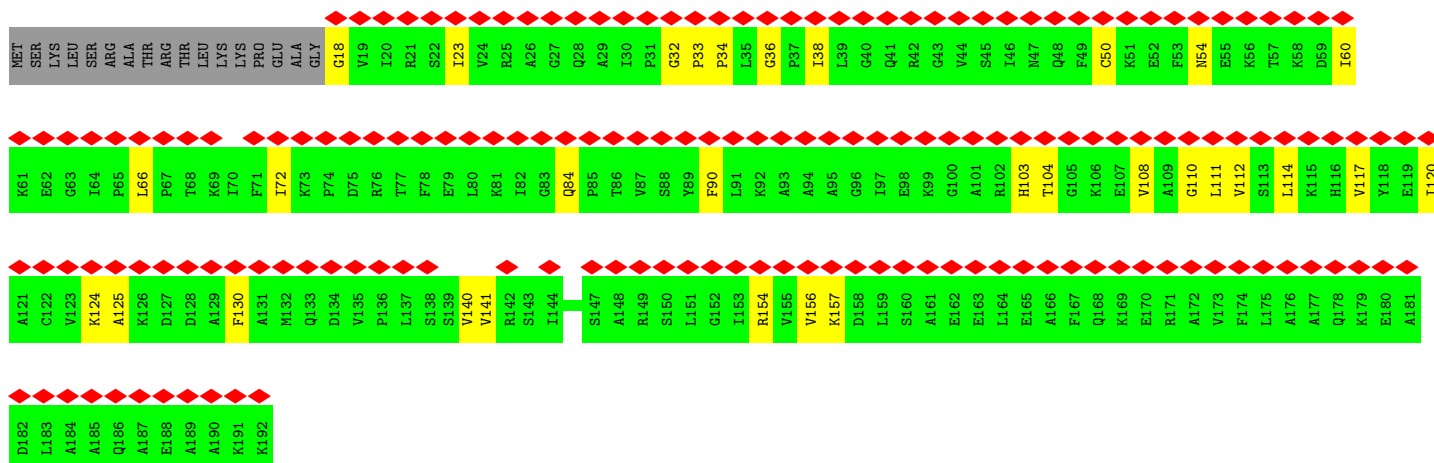
Chain I: 



GLN LEU VAL GLY GLY THR HIS LEU MET MET ALA ALA THR GLN ARG ARG TYR LEU LEU GLN HIS GLN PRO VAL VAL GLN LEU THR SER LEU LEU ASP GLN TVR VAL LYS LYS GLU GLN ASN GLU GLY ASP CYS THR SER THR ALA ASN GLU LYS LYS LEU HIS PRO PRO ASP PRO ALA ASP ALA

• Molecule 8: Large ribosomal subunit protein uL11m

Chain J: 88% 75% 16% 9%



• Molecule 9: Large ribosomal subunit protein uL13m

Chain K: 88% 11%



• Molecule 10: Large ribosomal subunit protein uL14m

Chain L: 70% 10% 21%



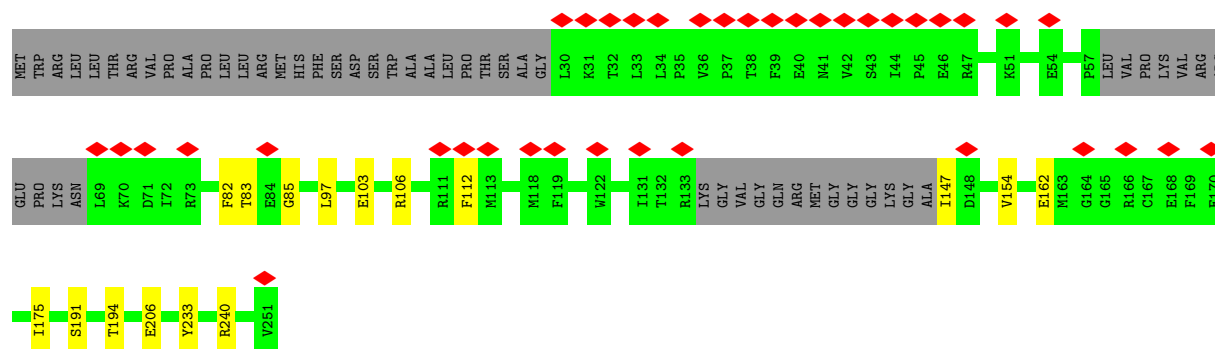
• Molecule 11: Large ribosomal subunit protein uL15m

Chain M: 91% 6%

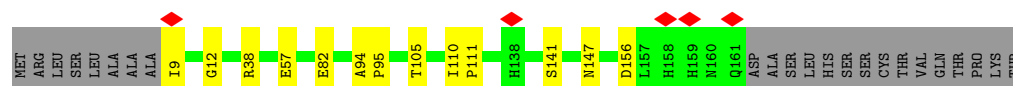
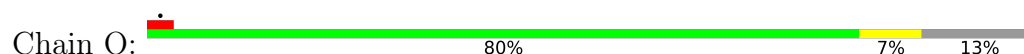


• Molecule 12: Large ribosomal subunit protein uL16m

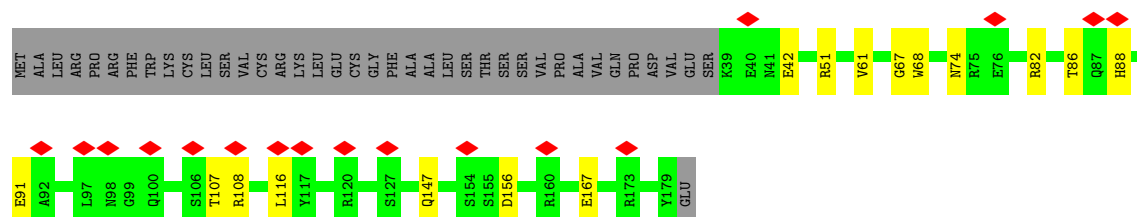
Chain N: 15% 73% 6% 21%



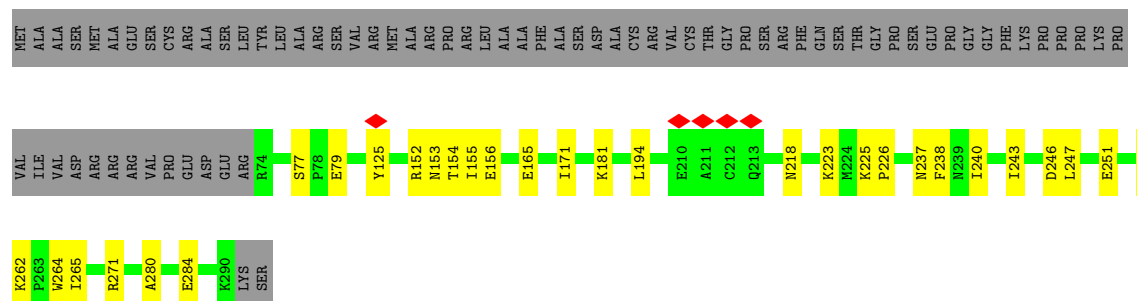
- Molecule 13: Large ribosomal subunit protein bL17m



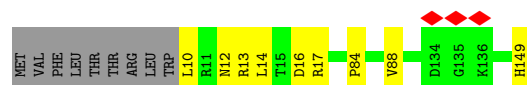
- Molecule 14: Large ribosomal subunit protein uL18m



- Molecule 15: Large ribosomal subunit protein bL19m

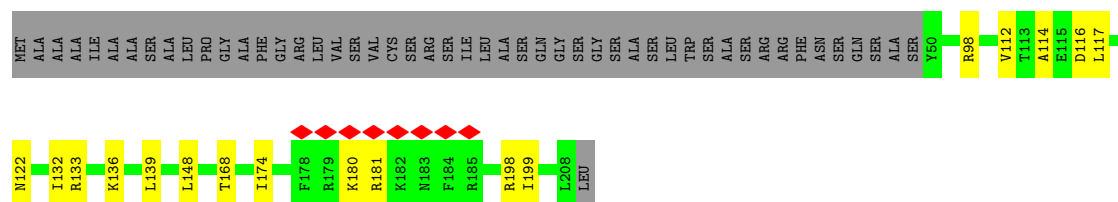


- Molecule 16: Large ribosomal subunit protein bL20m



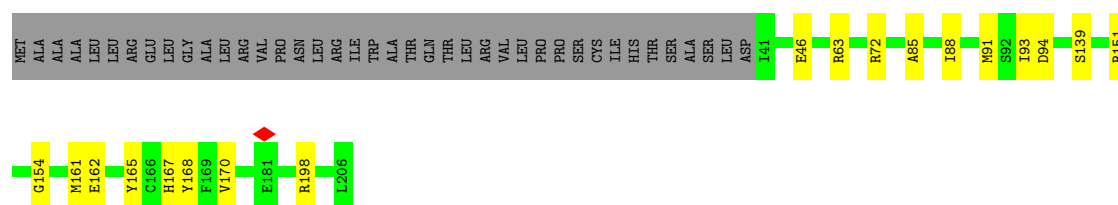
- Molecule 17: Large ribosomal subunit protein bL21m

Chain S: 



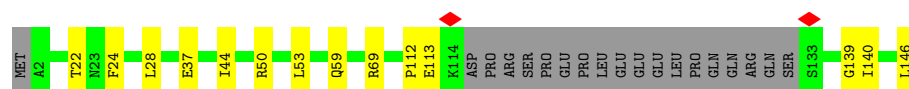
- Molecule 18: Large ribosomal subunit protein uL22m

Chain T: 



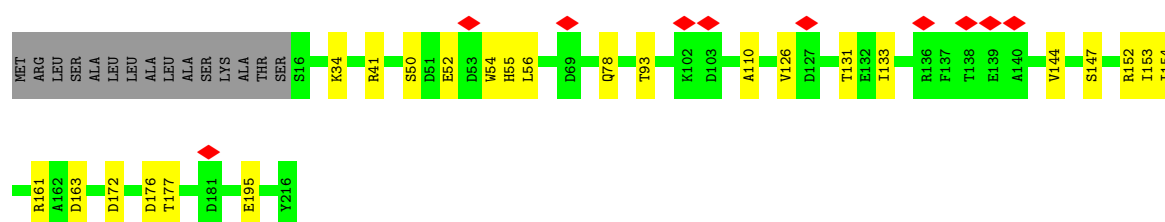
- Molecule 19: Large ribosomal subunit protein uL23m

Chain U: 



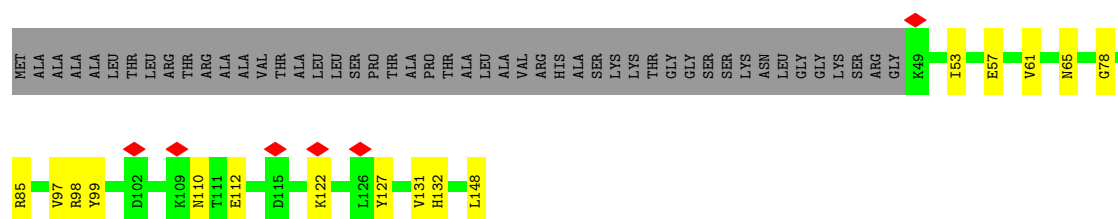
- Molecule 20: Large ribosomal subunit protein uL24m

Chain V: 



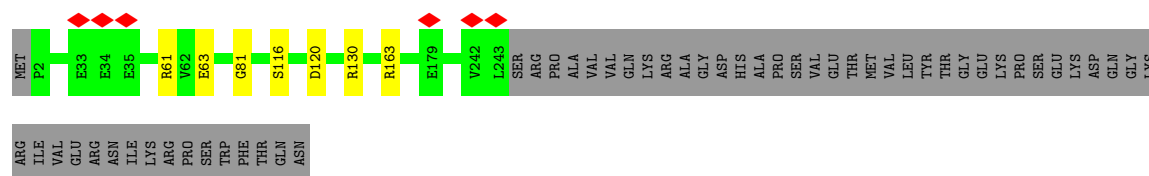
- Molecule 21: Large ribosomal subunit protein bL27m

Chain W: 



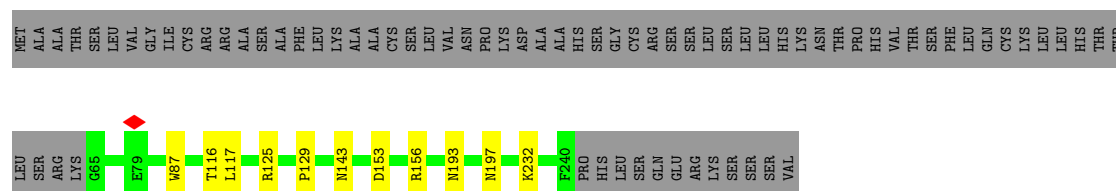
- Molecule 22: Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m

Chain X:  80% 18%



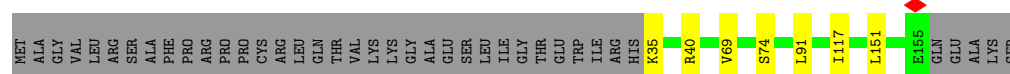
- Molecule 23: Large ribosomal subunit protein uL29m

Chain Y:  65% 30%



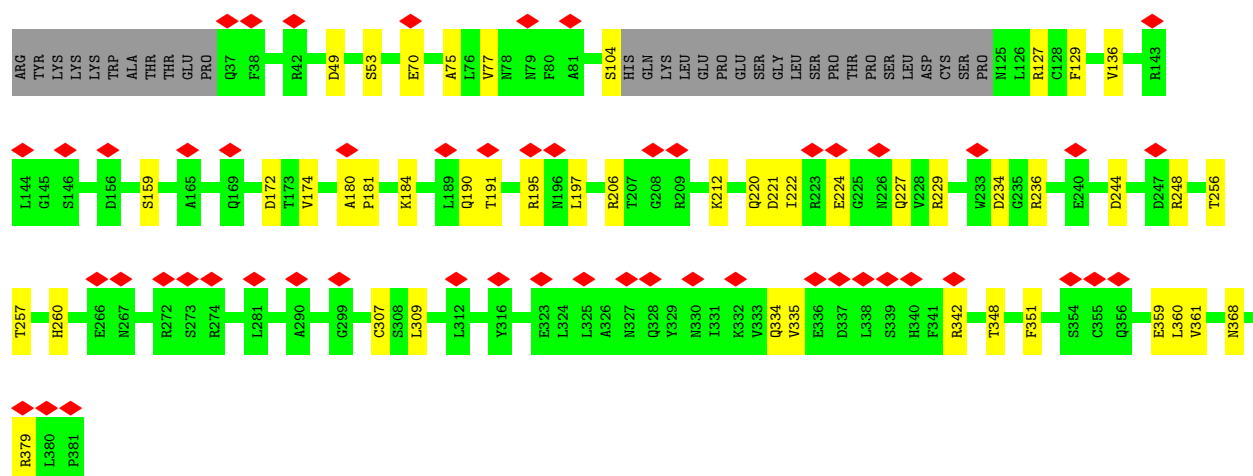
- Molecule 24: Large ribosomal subunit protein uL30m

Chain Z:  71% 24%



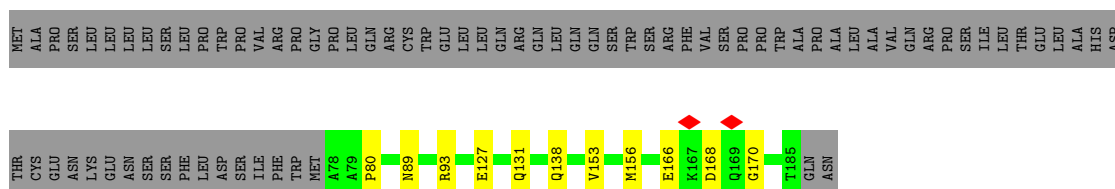
- Molecule 25: 5-cytosine rRNA methyltransferase NSUN4

Chain x:  15% 78% 13% 9%

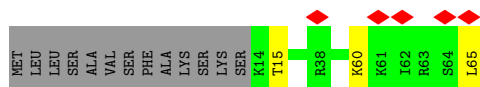
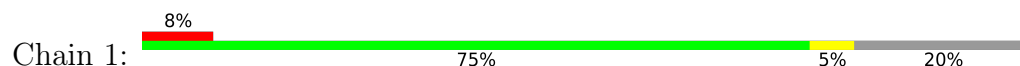


- Molecule 26: Large ribosomal subunit protein bL32m

Chain 0:  52% 6% 42%



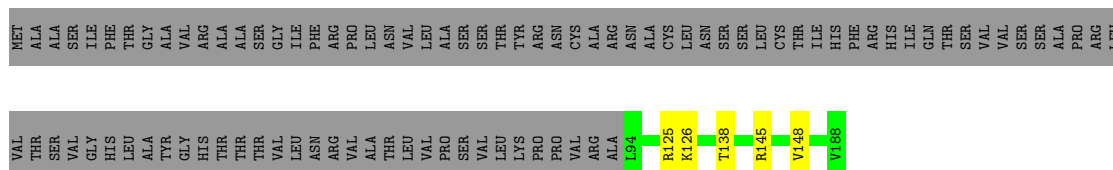
- Molecule 27: Large ribosomal subunit protein bL33m



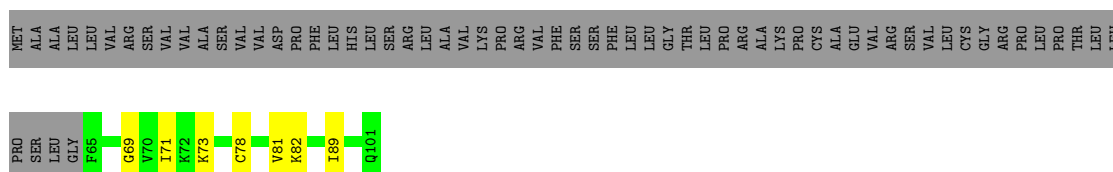
- Molecule 28: Large ribosomal subunit protein bL34m



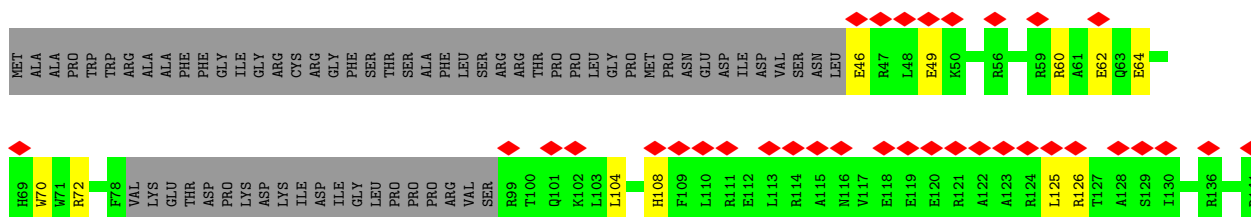
- Molecule 29: Large ribosomal subunit protein bL35m

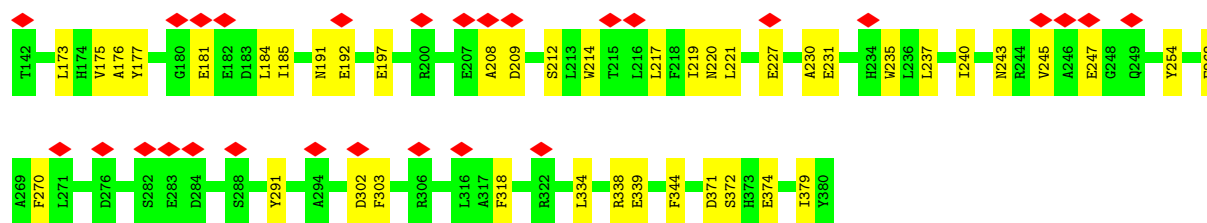


- Molecule 30: Large ribosomal subunit protein bL36m



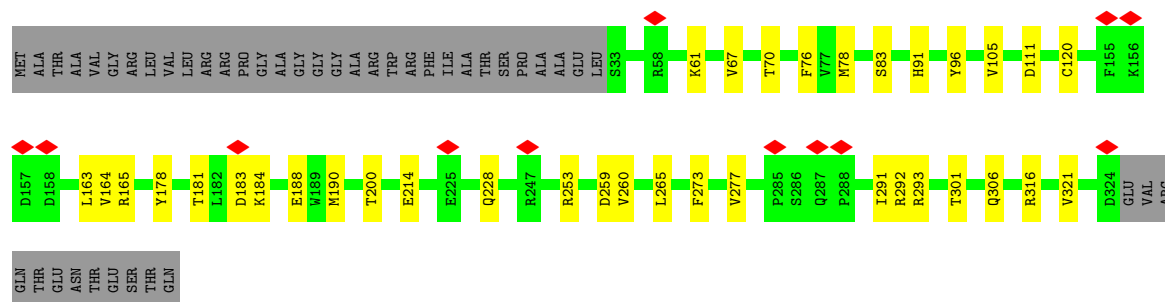
- Molecule 31: Large ribosomal subunit protein mL38





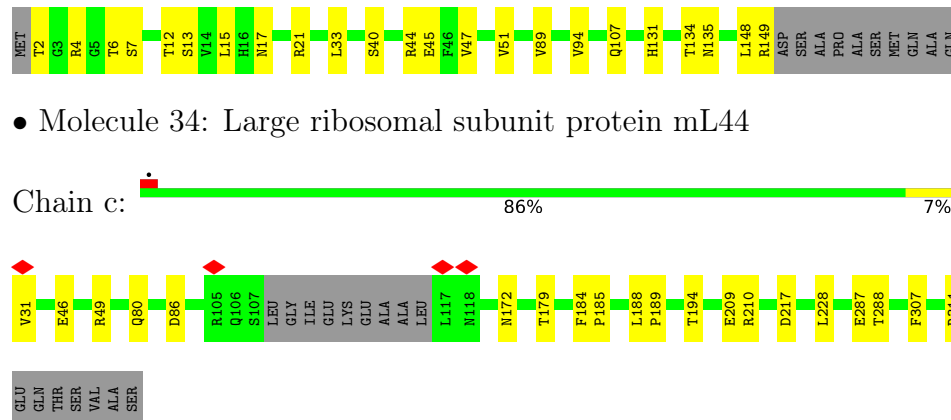
- Molecule 32: Large ribosomal subunit protein mL39

Chain 7: 76% 11% 13%



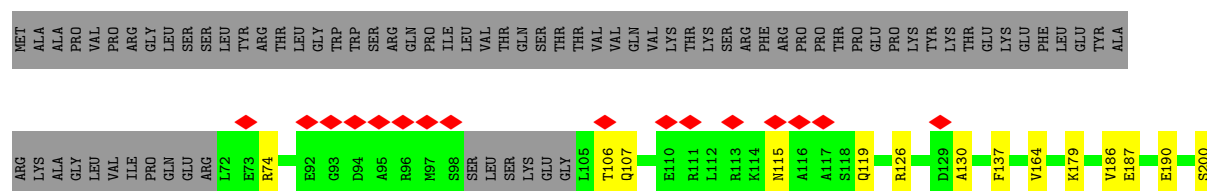
- Molecule 33: Large ribosomal subunit protein mL43

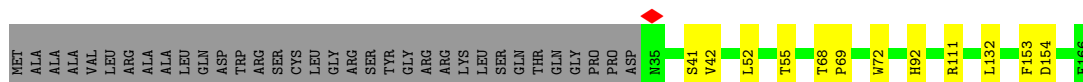
Chain b: 79% 14% 7%

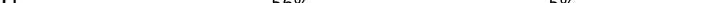


- Molecule 35: Large ribosomal subunit protein mL45

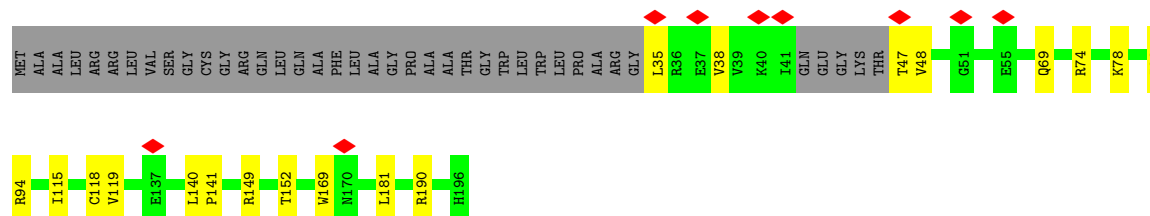
Chain d: 7% 59% 10% 31%



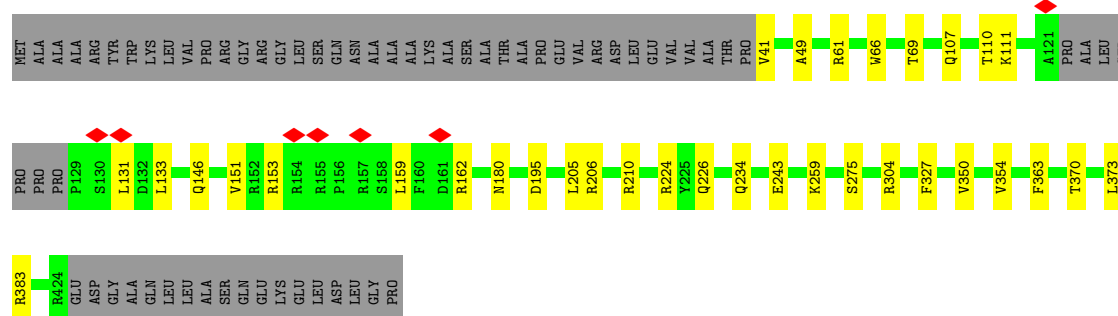
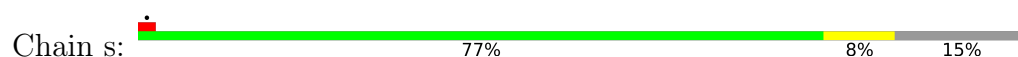


- Chain q: 

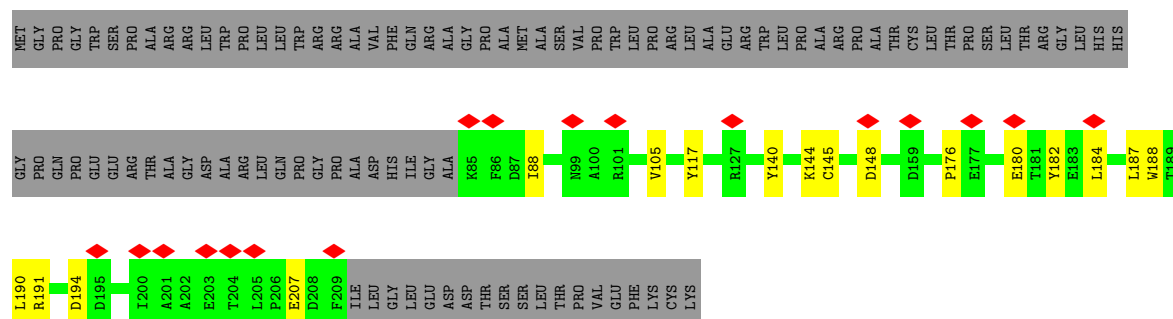
- Molecule 45: Large ribosomal subunit protein mL66



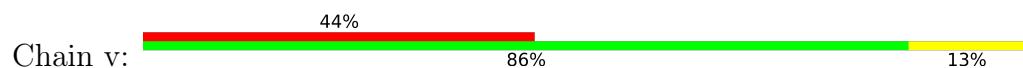
- Molecule 46: Large ribosomal subunit protein mL65

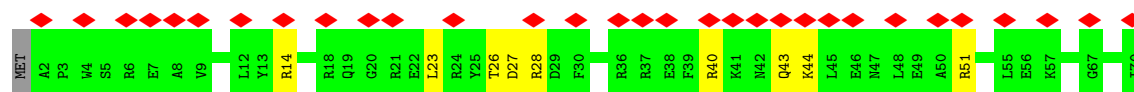


- Molecule 47: Mitochondrial assembly of ribosomal large subunit protein 1

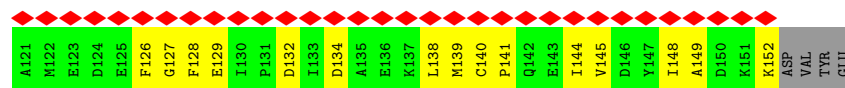
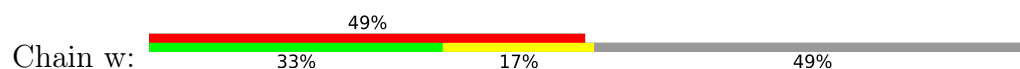


- Molecule 48: Predicted gene, 55359

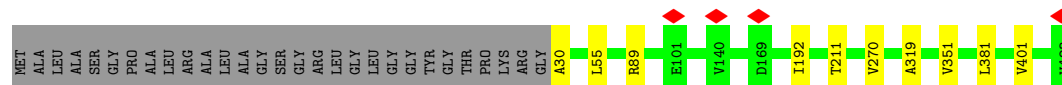
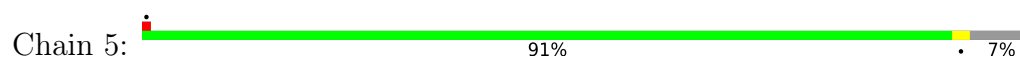




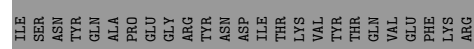
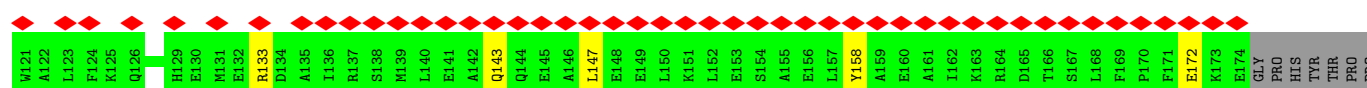
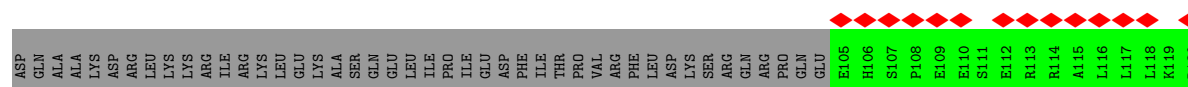
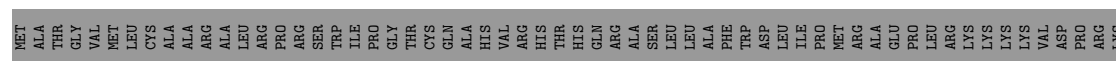
- Molecule 49: Acyl carrier protein, mitochondrial



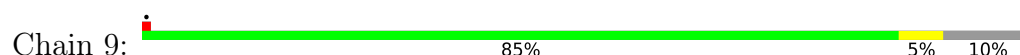
- Molecule 50: Large ribosomal subunit protein mL37



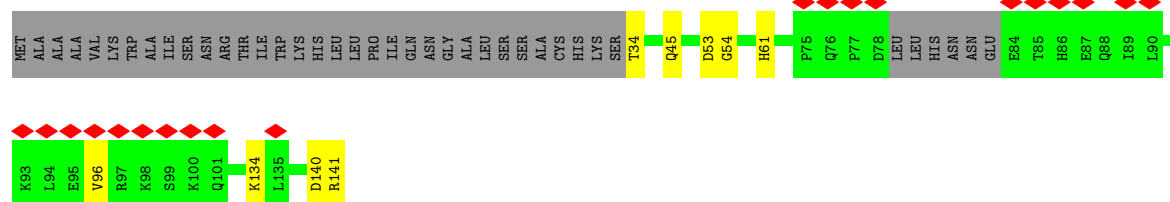
- Molecule 51: Large ribosomal subunit protein mL40



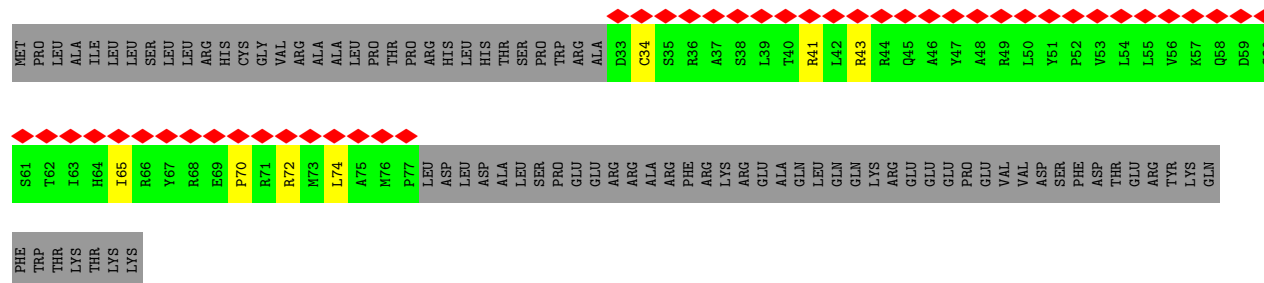
- Molecule 52: Large ribosomal subunit protein mL41



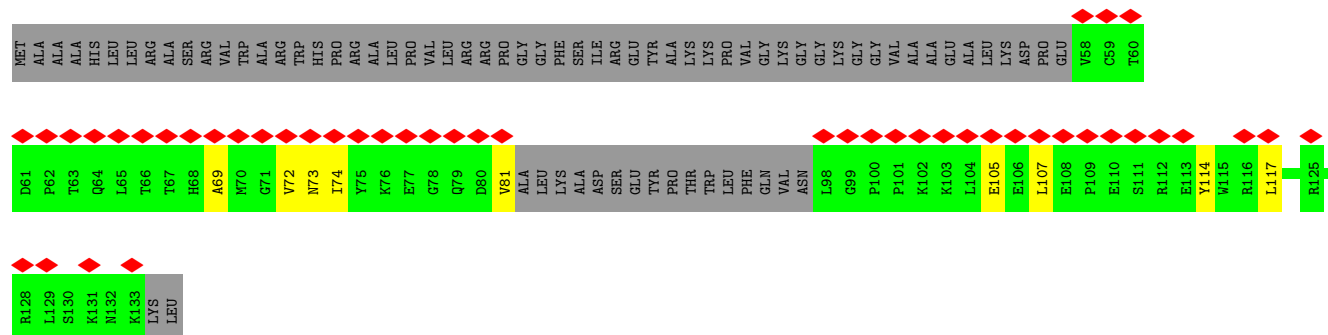
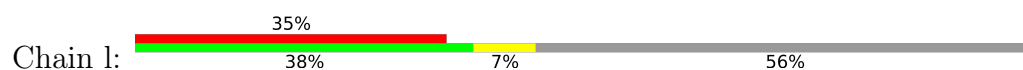
- Molecule 53: Large ribosomal subunit protein mL42



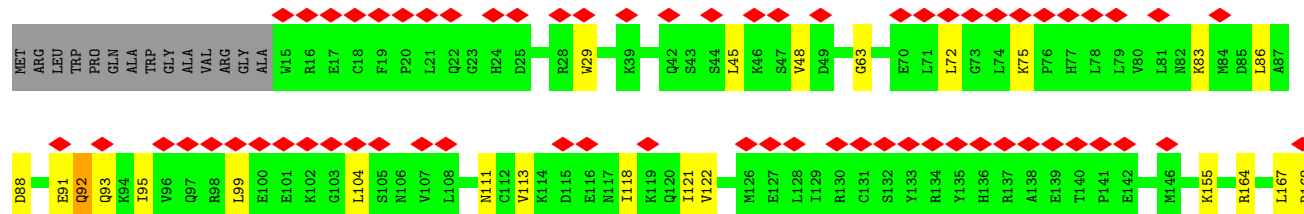
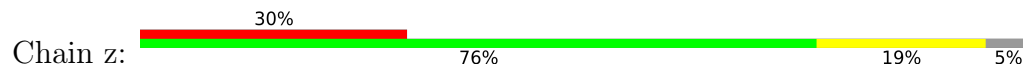
• Molecule 54: Large ribosomal subunit protein mL55

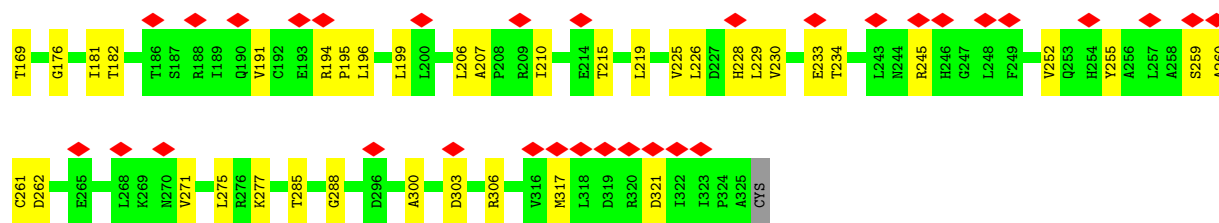


• Molecule 55: Large ribosomal subunit protein mL54

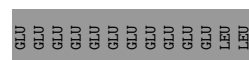
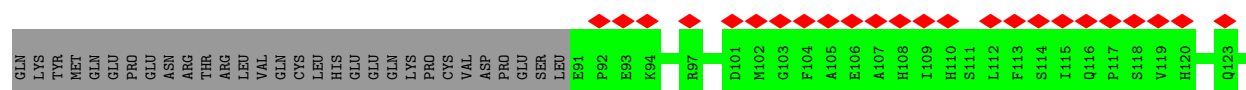
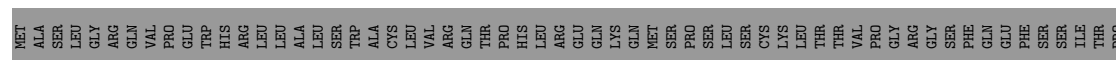


• Molecule 56: Mitochondrial ribosome-associated GTPase 1

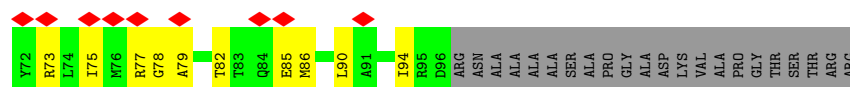
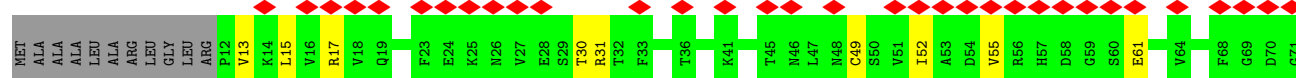




- Molecule 57: Transcription termination factor 4, mitochondrial



- Molecule 58: Large ribosomal subunit protein mL53



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 55461                                   | 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 ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 400                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.070                                   | Depositor |
| Minimum map value                    | -0.022                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.009                                   | Depositor |
| Map size (Å)                         | 457.2925, 457.2925, 457.2925            | wwPDB     |
| Map dimensions                       | 540, 540, 540                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.846838, 0.846838, 0.846838            | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PSU, GNP, FES

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.16         | 0/34254     | 0.29        | 0/53277     |
| 2   | B     | 0.14         | 0/1483      | 0.29        | 0/2299      |
| 3   | D     | 0.12         | 0/1802      | 0.28        | 0/2424      |
| 4   | E     | 0.13         | 0/2535      | 0.28        | 0/3443      |
| 5   | F     | 0.14         | 0/2061      | 0.29        | 0/2805      |
| 6   | H     | 0.10         | 0/793       | 0.25        | 0/1066      |
| 7   | I     | 0.09         | 0/1339      | 0.25        | 0/1813      |
| 8   | J     | 0.09         | 0/1346      | 0.29        | 0/1809      |
| 9   | K     | 0.12         | 0/1491      | 0.25        | 0/2022      |
| 10  | L     | 0.12         | 0/908       | 0.28        | 0/1224      |
| 11  | M     | 0.12         | 0/2369      | 0.26        | 0/3197      |
| 12  | N     | 0.08         | 0/1670      | 0.22        | 0/2252      |
| 13  | O     | 0.13         | 0/1285      | 0.30        | 0/1732      |
| 14  | P     | 0.08         | 0/1181      | 0.23        | 0/1600      |
| 15  | Q     | 0.12         | 0/1832      | 0.27        | 0/2471      |
| 16  | R     | 0.14         | 0/1182      | 0.26        | 0/1585      |
| 17  | S     | 0.13         | 0/1328      | 0.29        | 0/1798      |
| 18  | T     | 0.15         | 0/1402      | 0.29        | 0/1885      |
| 19  | U     | 0.13         | 0/1080      | 0.27        | 0/1464      |
| 20  | V     | 0.12         | 0/1695      | 0.26        | 0/2295      |
| 21  | W     | 0.11         | 0/816       | 0.27        | 0/1105      |
| 22  | X     | 0.11         | 0/2075      | 0.24        | 0/2806      |
| 23  | Y     | 0.12         | 0/1561      | 0.22        | 0/2093      |
| 24  | Z     | 0.11         | 0/1013      | 0.27        | 0/1368      |
| 25  | x     | 0.09         | 0/2620      | 0.24        | 0/3549      |
| 26  | 0     | 0.13         | 0/896       | 0.28        | 0/1200      |
| 27  | 1     | 0.08         | 0/434       | 0.24        | 0/578       |
| 28  | 2     | 0.14         | 0/387       | 0.27        | 0/514       |
| 29  | 3     | 0.14         | 0/843       | 0.28        | 0/1122      |
| 30  | 4     | 0.10         | 0/328       | 0.26        | 0/430       |
| 31  | 6     | 0.10         | 0/2783      | 0.26        | 0/3781      |
| 32  | 7     | 0.10         | 0/2436      | 0.23        | 0/3300      |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 33  | b     | 0.13         | 0/1203   | 0.30        | 0/1625   |
| 34  | c     | 0.11         | 0/2313   | 0.24        | 0/3128   |
| 35  | d     | 0.10         | 0/1792   | 0.26        | 0/2429   |
| 36  | e     | 0.09         | 0/1608   | 0.26        | 0/2165   |
| 37  | f     | 0.09         | 0/851    | 0.27        | 0/1149   |
| 38  | g     | 0.13         | 0/1126   | 0.28        | 0/1533   |
| 39  | h     | 0.10         | 0/894    | 0.24        | 0/1216   |
| 40  | i     | 0.15         | 0/855    | 0.28        | 0/1147   |
| 41  | j     | 0.10         | 0/759    | 0.26        | 0/1019   |
| 42  | o     | 0.10         | 0/655    | 0.23        | 0/880    |
| 43  | p     | 0.09         | 0/1195   | 0.24        | 0/1603   |
| 44  | q     | 0.10         | 0/1161   | 0.23        | 0/1571   |
| 45  | r     | 0.12         | 0/1309   | 0.28        | 0/1767   |
| 46  | s     | 0.12         | 0/3118   | 0.26        | 0/4232   |
| 47  | u     | 0.08         | 0/1053   | 0.22        | 0/1425   |
| 48  | v     | 0.08         | 0/596    | 0.22        | 0/795    |
| 49  | w     | 0.13         | 0/646    | 0.32        | 0/869    |
| 50  | 5     | 0.11         | 0/3317   | 0.25        | 0/4519   |
| 51  | 8     | 0.07         | 0/598    | 0.21        | 0/799    |
| 52  | 9     | 0.12         | 0/1009   | 0.25        | 0/1358   |
| 53  | a     | 0.13         | 0/884    | 0.28        | 0/1197   |
| 54  | m     | 0.10         | 0/380    | 0.26        | 0/510    |
| 55  | l     | 0.07         | 0/512    | 0.22        | 0/689    |
| 56  | z     | 0.10         | 0/2500   | 0.27        | 0/3380   |
| 57  | y     | 0.07         | 0/1980   | 0.20        | 0/2667   |
| 58  | k     | 0.08         | 0/674    | 0.24        | 0/910    |
| All | All   | 0.13         | 0/112216 | 0.27        | 0/158889 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 30629 | 15471    | 15492    | 210     | 0            |
| 2   | B     | 1326  | 667      | 670      | 23      | 0            |
| 3   | D     | 1768  | 1830     | 1830     | 15      | 0            |
| 4   | E     | 2459  | 2442     | 2441     | 19      | 0            |
| 5   | F     | 2005  | 2025     | 2024     | 19      | 0            |
| 6   | H     | 779   | 814      | 814      | 7       | 0            |
| 7   | I     | 1307  | 1393     | 1393     | 11      | 0            |
| 8   | J     | 1326  | 1394     | 1394     | 18      | 0            |
| 9   | K     | 1449  | 1444     | 1444     | 13      | 0            |
| 10  | L     | 893   | 944      | 944      | 12      | 0            |
| 11  | M     | 2315  | 2377     | 2377     | 14      | 0            |
| 12  | N     | 1625  | 1639     | 1639     | 10      | 0            |
| 13  | O     | 1259  | 1282     | 1282     | 8       | 0            |
| 14  | P     | 1154  | 1148     | 1148     | 15      | 0            |
| 15  | Q     | 1790  | 1822     | 1822     | 19      | 0            |
| 16  | R     | 1161  | 1224     | 1224     | 6       | 0            |
| 17  | S     | 1301  | 1372     | 1372     | 16      | 0            |
| 18  | T     | 1369  | 1402     | 1402     | 13      | 0            |
| 19  | U     | 1052  | 1057     | 1057     | 12      | 0            |
| 20  | V     | 1652  | 1643     | 1643     | 20      | 0            |
| 21  | W     | 794   | 808      | 808      | 15      | 0            |
| 22  | X     | 2021  | 2051     | 2051     | 4       | 0            |
| 23  | Y     | 1523  | 1553     | 1553     | 10      | 0            |
| 24  | Z     | 987   | 1039     | 1039     | 7       | 0            |
| 25  | x     | 2564  | 2546     | 2546     | 30      | 0            |
| 26  | 0     | 881   | 908      | 908      | 7       | 0            |
| 27  | 1     | 428   | 472      | 472      | 2       | 0            |
| 28  | 2     | 380   | 407      | 407      | 3       | 0            |
| 29  | 3     | 823   | 872      | 872      | 3       | 0            |
| 30  | 4     | 322   | 354      | 354      | 6       | 0            |
| 31  | 6     | 2689  | 2559     | 2559     | 42      | 0            |
| 32  | 7     | 2379  | 2378     | 2378     | 23      | 0            |
| 33  | b     | 1181  | 1195     | 1195     | 18      | 0            |
| 34  | c     | 2262  | 2273     | 2273     | 15      | 0            |
| 35  | d     | 1743  | 1728     | 1728     | 21      | 0            |
| 36  | e     | 1576  | 1598     | 1598     | 27      | 0            |
| 37  | f     | 838   | 836      | 836      | 24      | 0            |
| 38  | g     | 1090  | 1094     | 1094     | 12      | 0            |
| 39  | h     | 872   | 867      | 867      | 7       | 0            |
| 40  | i     | 831   | 854      | 854      | 7       | 0            |
| 41  | j     | 744   | 768      | 768      | 6       | 0            |
| 42  | o     | 640   | 623      | 623      | 2       | 0            |
| 43  | p     | 1176  | 1198     | 1198     | 9       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44  | q     | 1130   | 1123     | 1123     | 7       | 0            |
| 45  | r     | 1275   | 1329     | 1329     | 15      | 0            |
| 46  | s     | 3045   | 3058     | 3057     | 25      | 0            |
| 47  | u     | 1029   | 1012     | 1012     | 12      | 0            |
| 48  | v     | 586    | 603      | 603      | 5       | 0            |
| 49  | w     | 637    | 640      | 640      | 24      | 0            |
| 50  | 5     | 3225   | 3243     | 3243     | 8       | 0            |
| 51  | 8     | 589    | 574      | 574      | 4       | 0            |
| 52  | 9     | 983    | 990      | 990      | 5       | 0            |
| 53  | a     | 860    | 843      | 843      | 6       | 0            |
| 54  | m     | 374    | 395      | 395      | 8       | 0            |
| 55  | l     | 502    | 505      | 505      | 7       | 0            |
| 56  | z     | 2455   | 2546     | 2546     | 48      | 0            |
| 57  | y     | 1943   | 1995     | 1995     | 7       | 0            |
| 58  | k     | 664    | 667      | 667      | 13      | 0            |
| 59  | A     | 96     | 0        | 0        | 0       | 0            |
| 59  | E     | 1      | 0        | 0        | 0       | 0            |
| 59  | M     | 1      | 0        | 0        | 0       | 0            |
| 59  | O     | 1      | 0        | 0        | 0       | 0            |
| 60  | 0     | 1      | 0        | 0        | 0       | 0            |
| 60  | 4     | 1      | 0        | 0        | 0       | 0            |
| 61  | r     | 4      | 0        | 0        | 0       | 0            |
| 62  | z     | 32     | 13       | 13       | 3       | 0            |
| 63  | A     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 106798 | 91907    | 91928    | 820     | 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 4.

All (820) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1965:G:OP1  | 3:D:136:ARG:NH2  | 2.09                     | 0.85              |
| 1:A:2080:G:O2'  | 1:A:2082:G:OP2   | 1.95                     | 0.84              |
| 3:D:139:ASP:OD1 | 3:D:249:SER:OG   | 1.95                     | 0.83              |
| 47:u:140:TYR:OH | 47:u:148:ASP:OD2 | 1.96                     | 0.83              |
| 4:E:107:MET:HE3 | 4:E:121:LEU:HD11 | 1.62                     | 0.82              |
| 1:A:2275:A:O2'  | 1:A:2276:U:OP1   | 1.97                     | 0.82              |
| 14:P:82:ARG:NH2 | 31:6:62:GLU:OE1  | 2.13                     | 0.81              |
| 46:s:66:TRP:O   | 46:s:69:THR:OG1  | 2.00                     | 0.80              |
| 1:A:2076:A:O2'  | 1:A:2077:A:OP2   | 1.98                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2286:G:O2'    | 25:x:212:LYS:NZ   | 2.15                     | 0.79              |
| 17:S:139:LEU:HD13 | 17:S:148:LEU:HD23 | 1.62                     | 0.78              |
| 1:A:2326:A:OP1    | 21:W:85:ARG:NH2   | 2.16                     | 0.78              |
| 1:A:1531:A:HO2'   | 24:Z:35:LYS:N     | 1.82                     | 0.77              |
| 1:A:1308:C:OP2    | 38:g:111:ARG:NH2  | 2.19                     | 0.76              |
| 1:A:2505:G:O2'    | 1:A:2508:C:OP2    | 2.04                     | 0.75              |
| 12:N:206:GLU:OE2  | 12:N:240:ARG:NH2  | 2.19                     | 0.75              |
| 32:7:190:MET:SD   | 32:7:292:ARG:NH2  | 2.59                     | 0.75              |
| 31:6:374:GLU:OE2  | 43:p:145:ARG:NH2  | 2.19                     | 0.75              |
| 20:V:177:THR:HG23 | 52:9:71:TYR:O     | 1.87                     | 0.74              |
| 49:w:80:LYS:HG2   | 49:w:145:VAL:HG11 | 1.69                     | 0.74              |
| 1:A:2254:G:O6     | 1:A:2428:C:N4     | 2.20                     | 0.74              |
| 56:z:72:LEU:HD12  | 56:z:72:LEU:O     | 1.88                     | 0.74              |
| 15:Q:155:ILE:HG22 | 15:Q:156:GLU:OE1  | 1.88                     | 0.74              |
| 3:D:296:TYR:OH    | 57:y:269:GLU:OE2  | 2.05                     | 0.73              |
| 1:A:1620:C:O2'    | 8:J:104:THR:OG1   | 1.99                     | 0.73              |
| 56:z:63:GLY:HA3   | 56:z:219:LEU:HD11 | 1.71                     | 0.73              |
| 19:U:139:GLY:O    | 35:d:179:LYS:NZ   | 2.22                     | 0.73              |
| 20:V:177:THR:HG22 | 52:9:69:LYS:H     | 1.54                     | 0.72              |
| 1:A:2072:G:O2'    | 1:A:2073:G:OP1    | 2.07                     | 0.72              |
| 17:S:116:ASP:OD1  | 17:S:117:LEU:N    | 2.22                     | 0.72              |
| 1:A:1598:C:N4     | 1:A:1645:C:OP1    | 2.23                     | 0.72              |
| 31:6:247:GLU:OE1  | 31:6:247:GLU:N    | 2.23                     | 0.72              |
| 21:W:127:TYR:OH   | 31:6:64:GLU:OE2   | 2.09                     | 0.71              |
| 16:R:10:LEU:HD13  | 16:R:13:ARG:HD3   | 1.73                     | 0.70              |
| 18:T:198:ARG:NH2  | 34:c:287:GLU:OE1  | 2.24                     | 0.70              |
| 1:A:1265:A:OP1    | 33:b:4:ARG:NH2    | 2.25                     | 0.70              |
| 2:B:65:A:OP1      | 36:e:265:LYS:NZ   | 2.19                     | 0.70              |
| 12:N:85:GLY:N     | 12:N:162:GLU:OE2  | 2.25                     | 0.70              |
| 10:L:101:ASP:OD2  | 15:Q:152:ARG:NH2  | 2.25                     | 0.69              |
| 45:r:48:VAL:HG22  | 58:k:75:ILE:HB    | 1.74                     | 0.69              |
| 46:s:206:ARG:HD2  | 46:s:373:LEU:HD12 | 1.74                     | 0.69              |
| 32:7:183:ASP:OD1  | 32:7:184:LYS:N    | 2.25                     | 0.69              |
| 55:l:107:LEU:HD11 | 55:l:117:LEU:HD12 | 1.74                     | 0.69              |
| 48:v:23:LEU:O     | 48:v:28:ARG:NE    | 2.24                     | 0.69              |
| 35:d:226:ASP:OD1  | 35:d:232:MET:HE2  | 1.91                     | 0.69              |
| 56:z:45:LEU:O     | 56:z:75:LYS:NZ    | 2.25                     | 0.69              |
| 56:z:226:LEU:O    | 56:z:229:LEU:HD23 | 1.93                     | 0.69              |
| 7:I:61:ASN:OD1    | 45:r:78:LYS:NZ    | 2.27                     | 0.68              |
| 45:r:93:ILE:HD11  | 45:r:119:VAL:HG21 | 1.76                     | 0.68              |
| 34:c:46:GLU:OE1   | 34:c:49:ARG:NH1   | 2.26                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:e:263:GLN:N    | 36:e:263:GLN:OE1  | 2.27                     | 0.67              |
| 2:B:22:A:OP2      | 2:B:45:A:N6       | 2.27                     | 0.67              |
| 7:I:75:GLU:O      | 7:I:80:ARG:NH2    | 2.28                     | 0.67              |
| 14:P:68:TRP:N     | 21:W:78:GLY:O     | 2.27                     | 0.67              |
| 1:A:1620:C:O2'    | 8:J:103:HIS:O     | 2.12                     | 0.67              |
| 1:A:1102:U:O2'    | 1:A:1103:A:OP2    | 2.09                     | 0.67              |
| 47:u:88:ILE:HD11  | 47:u:105:VAL:HG11 | 1.77                     | 0.66              |
| 32:7:228:GLN:OE1  | 32:7:228:GLN:N    | 2.27                     | 0.66              |
| 57:y:162:ARG:NH2  | 57:y:189:MET:O    | 2.27                     | 0.66              |
| 31:6:46:GLU:N     | 31:6:46:GLU:OE1   | 2.29                     | 0.66              |
| 32:7:61:LYS:NZ    | 35:d:278:LYS:O    | 2.29                     | 0.65              |
| 1:A:1984:C:H5     | 1:A:2068:G:H21    | 1.44                     | 0.65              |
| 9:K:26:GLN:NE2    | 9:K:147:GLN:OE1   | 2.30                     | 0.65              |
| 12:N:82:PHE:O     | 12:N:83:THR:OG1   | 2.11                     | 0.65              |
| 1:A:1846:U:O2'    | 50:5:270:VAL:O    | 2.15                     | 0.65              |
| 20:V:54:TRP:NE1   | 20:V:56:LEU:O     | 2.30                     | 0.65              |
| 1:A:1205:A:N6     | 1:A:1208:U:OP2    | 2.29                     | 0.65              |
| 3:D:125:GLU:HB3   | 3:D:143:VAL:HG22  | 1.78                     | 0.65              |
| 5:F:126:LYS:NZ    | 5:F:130:GLN:OE1   | 2.28                     | 0.65              |
| 6:H:104:VAL:N     | 6:H:107:ASP:OD2   | 2.29                     | 0.64              |
| 4:E:121:LEU:HD22  | 4:E:284:TYR:CE1   | 2.32                     | 0.64              |
| 5:F:209:TYR:O     | 39:h:57:ARG:NH1   | 2.30                     | 0.64              |
| 49:w:76:LEU:HD22  | 49:w:149:ALA:HB1  | 1.78                     | 0.64              |
| 48:v:43:GLN:O     | 48:v:51:ARG:NH2   | 2.30                     | 0.64              |
| 6:H:62:ALA:O      | 6:H:66:ARG:NH1    | 2.30                     | 0.64              |
| 8:J:84:GLN:NE2    | 8:J:124:LYS:O     | 2.31                     | 0.64              |
| 1:A:1804:U:O2     | 19:U:69:ARG:NH1   | 2.31                     | 0.64              |
| 1:A:2342:U:O2'    | 1:A:2343:A:OP1    | 2.14                     | 0.64              |
| 5:F:126:LYS:NZ    | 5:F:138:HIS:O     | 2.31                     | 0.63              |
| 20:V:177:THR:HG21 | 23:Y:87:TRP:CZ2   | 2.34                     | 0.63              |
| 44:q:44:ASN:O     | 44:q:47:THR:HG22  | 1.98                     | 0.63              |
| 1:A:1493:A:O2'    | 21:W:57:GLU:OE1   | 2.12                     | 0.63              |
| 35:d:244:GLU:N    | 35:d:244:GLU:OE1  | 2.31                     | 0.63              |
| 7:I:52:GLU:N      | 7:I:52:GLU:OE1    | 2.32                     | 0.63              |
| 7:I:138:SER:O     | 7:I:141:ARG:NH1   | 2.31                     | 0.63              |
| 23:Y:87:TRP:O     | 23:Y:143:ASN:ND2  | 2.32                     | 0.63              |
| 47:u:188:TRP:O    | 47:u:191:ARG:NH1  | 2.31                     | 0.63              |
| 36:e:264:PRO:O    | 36:e:268:ALA:N    | 2.29                     | 0.63              |
| 35:d:106:THR:OG1  | 35:d:107:GLN:N    | 2.31                     | 0.62              |
| 37:f:160:GLY:O    | 37:f:161:LEU:HD22 | 2.00                     | 0.62              |
| 25:x:221:ASP:OD1  | 25:x:222:ILE:N    | 2.32                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1983:G:O2'    | 1:A:2068:G:N2     | 2.27                     | 0.62              |
| 1:A:2057:G:O2'    | 1:A:2058:G:OP1    | 2.18                     | 0.62              |
| 31:6:70:TRP:O     | 31:6:72:ARG:NH2   | 2.33                     | 0.62              |
| 56:z:245:ARG:NH2  | 56:z:321:ASP:OD2  | 2.32                     | 0.62              |
| 58:k:17:ARG:HG2   | 58:k:52:ILE:HD11  | 1.82                     | 0.62              |
| 1:A:1237:A:O2'    | 1:A:1238:U:OP1    | 2.14                     | 0.62              |
| 1:A:1786:C:OP1    | 18:T:165:TYR:OH   | 2.18                     | 0.62              |
| 14:P:86:THR:OG1   | 14:P:88:HIS:O     | 2.18                     | 0.61              |
| 23:Y:117:LEU:HD21 | 23:Y:129:PRO:HD2  | 1.82                     | 0.61              |
| 20:V:93:THR:HG21  | 20:V:110:ALA:HB1  | 1.82                     | 0.61              |
| 46:s:159:LEU:HD23 | 46:s:159:LEU:O    | 2.00                     | 0.61              |
| 1:A:1893:C:O2'    | 1:A:1894:A:OP2    | 2.17                     | 0.61              |
| 41:j:112:THR:HG22 | 41:j:112:THR:O    | 1.99                     | 0.61              |
| 1:A:1280:C:N3     | 1:A:1281:A:N6     | 2.47                     | 0.60              |
| 1:A:2617:A:O2'    | 1:A:2618:A:OP2    | 2.19                     | 0.60              |
| 43:p:172:ASP:OD1  | 43:p:173:ALA:N    | 2.34                     | 0.60              |
| 1:A:2625:A:O3'    | 45:r:94:ARG:NH1   | 2.34                     | 0.60              |
| 21:W:148:LEU:O    | 31:6:339:GLU:N    | 2.34                     | 0.60              |
| 56:z:63:GLY:CA    | 56:z:219:LEU:HD11 | 2.31                     | 0.60              |
| 20:V:78:GLN:OE1   | 35:d:74:ARG:NH1   | 2.34                     | 0.60              |
| 1:A:2402:U:O4     | 1:A:2458:G:N2     | 2.33                     | 0.60              |
| 14:P:51:ARG:NH2   | 31:6:221:LEU:O    | 2.35                     | 0.60              |
| 34:c:209:GLU:OE1  | 34:c:209:GLU:N    | 2.34                     | 0.60              |
| 32:7:163:LEU:HD22 | 32:7:178:TYR:HE2  | 1.65                     | 0.60              |
| 50:5:401:VAL:O    | 50:5:401:VAL:HG13 | 2.01                     | 0.60              |
| 1:A:1628:A:O2'    | 1:A:1647:A:N3     | 2.34                     | 0.60              |
| 35:d:126:ARG:O    | 35:d:130:ALA:N    | 2.35                     | 0.60              |
| 20:V:93:THR:CG2   | 20:V:110:ALA:HB1  | 2.32                     | 0.59              |
| 8:J:125:ALA:HB2   | 8:J:140:VAL:HG21  | 1.83                     | 0.59              |
| 58:k:13:VAL:HG23  | 58:k:49:CYS:HB3   | 1.82                     | 0.59              |
| 35:d:115:ASN:O    | 35:d:119:GLN:N    | 2.35                     | 0.59              |
| 15:Q:237:ASN:OD1  | 15:Q:238:PHE:N    | 2.36                     | 0.59              |
| 7:I:132:LYS:NZ    | 7:I:147:PHE:O     | 2.32                     | 0.59              |
| 20:V:161:ARG:NH2  | 20:V:163:ASP:OD2  | 2.36                     | 0.59              |
| 25:x:221:ASP:OD2  | 44:q:155:ARG:NH1  | 2.35                     | 0.59              |
| 53:a:34:THR:HG22  | 53:a:34:THR:O     | 2.02                     | 0.59              |
| 49:w:126:PHE:CE2  | 49:w:148:ILE:HD13 | 2.38                     | 0.59              |
| 22:X:61:ARG:NH2   | 22:X:63:GLU:OE2   | 2.35                     | 0.59              |
| 2:B:9:A:OP1       | 2:B:45:A:O2'      | 2.19                     | 0.59              |
| 31:6:219:ILE:HG21 | 31:6:231:GLU:HG3  | 1.85                     | 0.59              |
| 25:x:180:ALA:HB3  | 25:x:181:PRO:CD   | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:z:196:LEU:HD23 | 56:z:196:LEU:O    | 2.02                     | 0.59              |
| 37:f:178:PRO:O    | 37:f:179:GLU:HB3  | 2.03                     | 0.58              |
| 56:z:191:VAL:HG21 | 56:z:199:LEU:HG   | 1.86                     | 0.58              |
| 18:T:88:ILE:HA    | 18:T:91:MET:HE2   | 1.84                     | 0.58              |
| 36:e:158:LEU:HD21 | 36:e:262:LEU:HD11 | 1.84                     | 0.58              |
| 47:u:207:GLU:N    | 47:u:207:GLU:OE1  | 2.36                     | 0.58              |
| 10:L:70:GLY:O     | 10:L:134:TYR:OH   | 2.13                     | 0.58              |
| 32:7:76:PHE:HB3   | 32:7:78:MET:HE3   | 1.86                     | 0.58              |
| 55:l:69:ALA:N     | 55:l:81:VAL:O     | 2.33                     | 0.58              |
| 14:P:74:ASN:O     | 14:P:147:GLN:NE2  | 2.35                     | 0.58              |
| 39:h:136:GLN:N    | 39:h:136:GLN:OE1  | 2.34                     | 0.57              |
| 2:B:57:U:H2'      | 2:B:58:C:O4'      | 2.05                     | 0.57              |
| 1:A:1215:G:N2     | 1:A:1218:A:OP2    | 2.36                     | 0.57              |
| 25:x:309:LEU:CD1  | 25:x:360:LEU:HD21 | 2.34                     | 0.57              |
| 1:A:1263:A:OP1    | 53:a:134:LYS:NZ   | 2.37                     | 0.57              |
| 34:c:80:GLN:O     | 34:c:210:ARG:NH2  | 2.38                     | 0.57              |
| 56:z:91:GLU:O     | 56:z:93:GLN:N     | 2.38                     | 0.57              |
| 37:f:97:TYR:CZ    | 54:m:65:ILE:HG22  | 2.40                     | 0.57              |
| 1:A:1115:A:H4'    | 1:A:1115:A:OP2    | 2.05                     | 0.56              |
| 19:U:59:GLN:NE2   | 52:9:58:PHE:O     | 2.38                     | 0.56              |
| 1:A:2334:G:N2     | 1:A:2358:G:O4'    | 2.38                     | 0.56              |
| 5:F:75:GLU:OE2    | 39:h:57:ARG:NH2   | 2.37                     | 0.56              |
| 29:3:125:ARG:NH1  | 29:3:145:ARG:O    | 2.39                     | 0.56              |
| 33:b:89:VAL:HG12  | 33:b:89:VAL:O     | 2.05                     | 0.56              |
| 48:v:14:ARG:NH1   | 49:w:132:ASP:OD2  | 2.39                     | 0.56              |
| 21:W:112:GLU:OE1  | 21:W:112:GLU:N    | 2.33                     | 0.56              |
| 40:i:77:PRO:HD2   | 40:i:80:LEU:HD11  | 1.87                     | 0.56              |
| 44:q:111:GLU:OE1  | 44:q:114:ARG:NH2  | 2.37                     | 0.56              |
| 6:H:118:ASN:O     | 6:H:122:SER:OG    | 2.24                     | 0.56              |
| 39:h:115:ASN:HA   | 39:h:118:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:1564:U:O2'    | 1:A:1577:A:N3     | 2.38                     | 0.56              |
| 56:z:194:ARG:HB2  | 56:z:195:PRO:HD3  | 1.88                     | 0.56              |
| 12:N:97:LEU:HD12  | 12:N:154:VAL:HG21 | 1.88                     | 0.56              |
| 56:z:167:LEU:HG   | 56:z:169:THR:HG23 | 1.88                     | 0.56              |
| 36:e:46:SER:OG    | 36:e:228:LYS:O    | 2.22                     | 0.55              |
| 1:A:1854:C:OP2    | 46:s:304:ARG:NH1  | 2.40                     | 0.55              |
| 14:P:61:VAL:HG12  | 14:P:61:VAL:O     | 2.07                     | 0.55              |
| 1:A:1383:G:O2'    | 1:A:1386:G:O2'    | 2.20                     | 0.55              |
| 5:F:277:ASP:O     | 5:F:278:SER:OG    | 2.17                     | 0.55              |
| 32:7:293:ARG:NH1  | 32:7:321:VAL:O    | 2.39                     | 0.55              |
| 41:j:62:GLN:OE1   | 41:j:65:ARG:NH1   | 2.38                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1104:G:OP2    | 23:Y:232:LYS:NZ   | 2.39                     | 0.55              |
| 31:6:181:GLU:N    | 31:6:181:GLU:OE1  | 2.39                     | 0.55              |
| 49:w:80:LYS:CG    | 49:w:145:VAL:HG11 | 2.37                     | 0.55              |
| 11:M:283:LYS:NZ   | 38:g:41:SER:OG    | 2.40                     | 0.55              |
| 1:A:1237:A:HO2'   | 1:A:1238:U:P      | 2.31                     | 0.54              |
| 49:w:138:LEU:HD12 | 49:w:139:MET:N    | 2.22                     | 0.54              |
| 1:A:2524:G:N2     | 1:A:2527:A:OP2    | 2.31                     | 0.54              |
| 25:x:190:GLN:O    | 25:x:191:THR:OG1  | 2.24                     | 0.54              |
| 56:z:259:SER:O    | 56:z:260:ALA:HB3  | 2.06                     | 0.54              |
| 5:F:113:ASN:OD1   | 5:F:157:GLY:N     | 2.35                     | 0.54              |
| 17:S:136:LYS:NZ   | 41:j:47:ASP:OD1   | 2.25                     | 0.54              |
| 20:V:177:THR:HG21 | 23:Y:87:TRP:HZ2   | 1.72                     | 0.54              |
| 30:4:71:ILE:CG2   | 30:4:89:ILE:HD12  | 2.38                     | 0.54              |
| 25:x:75:ALA:O     | 25:x:129:PHE:N    | 2.37                     | 0.54              |
| 8:J:18:GLY:N      | 8:J:72:ILE:O      | 2.39                     | 0.54              |
| 55:l:107:LEU:HD13 | 55:l:114:TYR:HA   | 1.90                     | 0.54              |
| 1:A:1234:C:H3'    | 1:A:1235:U:C5'    | 2.38                     | 0.54              |
| 31:6:212:SER:O    | 31:6:214:TRP:NE1  | 2.41                     | 0.54              |
| 32:7:163:LEU:HD22 | 32:7:178:TYR:CE2  | 2.42                     | 0.54              |
| 1:A:1389:A:OP2    | 18:T:154:GLY:O    | 2.26                     | 0.54              |
| 1:A:2057:G:O2'    | 1:A:2058:G:P      | 2.66                     | 0.54              |
| 33:b:131:HIS:CE1  | 33:b:134:THR:HG23 | 2.43                     | 0.54              |
| 56:z:275:LEU:O    | 56:z:277:LYS:NZ   | 2.33                     | 0.54              |
| 1:A:1583:C:OP2    | 45:r:190:ARG:NH2  | 2.41                     | 0.53              |
| 13:O:57:GLU:OE2   | 13:O:105:THR:OG1  | 2.25                     | 0.53              |
| 1:A:1154:U:OP1    | 6:H:73:ARG:NH1    | 2.40                     | 0.53              |
| 17:S:112:VAL:HG13 | 17:S:199:ILE:HG13 | 1.89                     | 0.53              |
| 37:f:92:ILE:CD1   | 37:f:158:ILE:HD12 | 2.38                     | 0.53              |
| 1:A:1646:A:H2'    | 1:A:1647:A:H5''   | 1.90                     | 0.53              |
| 1:A:1815:U:O3'    | 50:5:89:ARG:NH1   | 2.41                     | 0.53              |
| 8:J:117:VAL:HG12  | 8:J:141:VAL:HG23  | 1.90                     | 0.53              |
| 4:E:269:TYR:HB3   | 4:E:304:LEU:HD11  | 1.91                     | 0.53              |
| 7:I:150:HIS:O     | 58:k:31:ARG:NH2   | 2.42                     | 0.53              |
| 26:O:127:GLU:OE2  | 26:O:131:GLN:NE2  | 2.41                     | 0.53              |
| 32:7:200:THR:HG22 | 32:7:277:VAL:H    | 1.73                     | 0.53              |
| 56:z:271:VAL:HG13 | 56:z:300:ALA:HB1  | 1.89                     | 0.53              |
| 36:e:45:LEU:HD23  | 36:e:228:LYS:HE2  | 1.91                     | 0.53              |
| 54:m:70:PRO:O     | 54:m:72:ARG:NH1   | 2.42                     | 0.53              |
| 49:w:81:ASP:O     | 49:w:85:TYR:N     | 2.41                     | 0.52              |
| 1:A:1188:A:O2'    | 1:A:1189:C:OP2    | 2.23                     | 0.52              |
| 2:B:48:G:N2       | 2:B:59:C:O2       | 2.41                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:x:172:ASP:O    | 25:x:195:ARG:N    | 2.42                     | 0.52              |
| 31:6:104:LEU:O    | 31:6:108:HIS:ND1  | 2.42                     | 0.52              |
| 1:A:1755:C:OP1    | 26:0:138:GLN:NE2  | 2.42                     | 0.52              |
| 21:W:99:TYR:CD2   | 21:W:131:VAL:HG22 | 2.44                     | 0.52              |
| 1:A:1595:U:O2'    | 1:A:1596:A:O5'    | 2.24                     | 0.52              |
| 15:Q:153:ASN:OD1  | 15:Q:154:THR:N    | 2.42                     | 0.52              |
| 25:x:220:GLN:O    | 25:x:224:GLU:N    | 2.36                     | 0.52              |
| 5:F:92:ARG:HG2    | 5:F:95:ILE:HD12   | 1.90                     | 0.52              |
| 1:A:1283:A:O4'    | 1:A:2130:A:N6     | 2.42                     | 0.52              |
| 33:b:33:LEU:HD11  | 33:b:47:VAL:HG21  | 1.91                     | 0.52              |
| 37:f:97:TYR:CE2   | 54:m:65:ILE:HG22  | 2.45                     | 0.52              |
| 1:A:1431:A:OP2    | 1:A:2171:A:O2'    | 2.28                     | 0.52              |
| 1:A:1789:A:N1     | 18:T:151:ARG:HD3  | 2.25                     | 0.52              |
| 4:E:216:GLN:HG3   | 4:E:261:MET:HE2   | 1.92                     | 0.52              |
| 10:L:129:ARG:NH2  | 15:Q:125:TYR:O    | 2.43                     | 0.52              |
| 55:l:74:ILE:HG22  | 55:l:74:ILE:O     | 2.10                     | 0.52              |
| 1:A:1390:A:OP2    | 1:A:1938:C:N4     | 2.42                     | 0.52              |
| 14:P:167:GLU:O    | 43:p:187:ARG:NH1  | 2.42                     | 0.52              |
| 38:g:68:THR:HG22  | 38:g:69:PRO:HD2   | 1.92                     | 0.52              |
| 39:h:81:SER:O     | 39:h:82:SER:OG    | 2.14                     | 0.52              |
| 17:S:139:LEU:HD13 | 17:S:148:LEU:CD2  | 2.36                     | 0.51              |
| 1:A:1134:A:N7     | 23:Y:197:ASN:ND2  | 2.58                     | 0.51              |
| 1:A:2395:U:O4     | 1:A:2396:A:N6     | 2.42                     | 0.51              |
| 16:R:14:LEU:HD23  | 16:R:16:ASP:H     | 1.76                     | 0.51              |
| 47:u:88:ILE:HD12  | 47:u:117:TYR:CD2  | 2.46                     | 0.51              |
| 31:6:302:ASP:OD1  | 31:6:303:PHE:N    | 2.43                     | 0.51              |
| 1:A:1188:A:H61    | 44:q:33:ARG:HA    | 1.75                     | 0.51              |
| 10:L:96:MET:HE1   | 15:Q:171:ILE:HD11 | 1.92                     | 0.51              |
| 15:Q:251:GLU:OE1  | 15:Q:251:GLU:N    | 2.38                     | 0.51              |
| 31:6:176:ALA:HB3  | 31:6:184:LEU:HD12 | 1.92                     | 0.51              |
| 34:c:31:VAL:HG13  | 34:c:31:VAL:O     | 2.10                     | 0.51              |
| 45:r:93:ILE:HG22  | 45:r:94:ARG:O     | 2.10                     | 0.51              |
| 53:a:96:VAL:O     | 53:a:96:VAL:HG13  | 2.09                     | 0.51              |
| 29:3:126:LYS:HD3  | 29:3:148:VAL:HG21 | 1.92                     | 0.51              |
| 45:r:47:THR:N     | 58:k:73:ARG:O     | 2.43                     | 0.51              |
| 56:z:99:LEU:HG    | 56:z:104:LEU:HD12 | 1.92                     | 0.51              |
| 46:s:131:LEU:HD11 | 46:s:133:LEU:HD23 | 1.92                     | 0.51              |
| 1:A:1156:U:O3'    | 40:i:95:LYS:NZ    | 2.44                     | 0.51              |
| 2:B:32:U:N3       | 54:m:43:ARG:O     | 2.44                     | 0.51              |
| 1:A:2116:U:O2'    | 26:0:80:PRO:O     | 2.28                     | 0.51              |
| 36:e:190:LEU:HD22 | 36:e:198:MET:HE1  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1799:U:O2     | 23:Y:125:ARG:NH2  | 2.45                     | 0.50              |
| 1:A:1990:G:H3'    | 1:A:1991:A:H4'    | 1.93                     | 0.50              |
| 4:E:208:ALA:HB2   | 4:E:297:VAL:HG12  | 1.94                     | 0.50              |
| 21:W:61:VAL:HG21  | 21:W:97:VAL:CG2   | 2.41                     | 0.50              |
| 49:w:134:ASP:OD1  | 49:w:134:ASP:N    | 2.44                     | 0.50              |
| 1:A:2614:C:O2     | 9:K:97:ARG:NH2    | 2.42                     | 0.50              |
| 2:B:4:A:H2'       | 2:B:5:A:C8        | 2.47                     | 0.50              |
| 36:e:58:THR:HG22  | 54:m:34:CYS:SG    | 2.51                     | 0.50              |
| 1:A:1160:A:O2'    | 1:A:1161:C:P      | 2.70                     | 0.50              |
| 56:z:261:CYS:SG   | 56:z:262:ASP:N    | 2.84                     | 0.50              |
| 17:S:168:THR:HG22 | 33:b:107:GLN:HG2  | 1.92                     | 0.50              |
| 21:W:61:VAL:HG13  | 21:W:65:ASN:HB2   | 1.92                     | 0.50              |
| 46:s:354:VAL:HG12 | 46:s:363:PHE:CD2  | 2.47                     | 0.50              |
| 1:A:1832:A:H4'    | 1:A:1832:A:OP1    | 2.12                     | 0.50              |
| 3:D:203:ARG:O     | 50:5:30:ALA:N     | 2.45                     | 0.50              |
| 33:b:12:THR:HG22  | 33:b:13:SER:N     | 2.27                     | 0.50              |
| 57:y:169:LEU:O    | 57:y:213:THR:HG22 | 2.12                     | 0.50              |
| 1:A:1137:A:O2'    | 1:A:1138:U:OP1    | 2.27                     | 0.50              |
| 1:A:2656:C:H2'    | 1:A:2656:C:O2     | 2.12                     | 0.50              |
| 23:Y:153:ASP:OD1  | 23:Y:156:ARG:NH2  | 2.41                     | 0.50              |
| 46:s:354:VAL:HG12 | 46:s:363:PHE:HD2  | 1.76                     | 0.50              |
| 8:J:33:PRO:N      | 8:J:34:PRO:HD2    | 2.27                     | 0.50              |
| 26:0:166:GLU:OE1  | 26:0:166:GLU:N    | 2.37                     | 0.50              |
| 36:e:262:LEU:HD23 | 36:e:267:LEU:HB3  | 1.94                     | 0.50              |
| 12:N:147:ILE:O    | 12:N:147:ILE:HG23 | 2.11                     | 0.49              |
| 15:Q:181:LYS:O    | 15:Q:218:ASN:N    | 2.40                     | 0.49              |
| 25:x:136:VAL:HG12 | 25:x:136:VAL:O    | 2.13                     | 0.49              |
| 37:f:126:MET:SD   | 37:f:155:VAL:HG23 | 2.52                     | 0.49              |
| 53:a:53:ASP:OD1   | 53:a:54:GLY:N     | 2.45                     | 0.49              |
| 14:P:42:GLU:OE2   | 31:6:338:ARG:NH1  | 2.45                     | 0.49              |
| 58:k:86:MET:O     | 58:k:90:LEU:HD23  | 2.12                     | 0.49              |
| 17:S:112:VAL:CG1  | 17:S:199:ILE:HG21 | 2.42                     | 0.49              |
| 20:V:133:ILE:HG21 | 20:V:154:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:1458:A:H4'    | 1:A:1459:A:OP1    | 2.11                     | 0.49              |
| 1:A:1688:U:O2'    | 17:S:122:ASN:ND2  | 2.46                     | 0.49              |
| 4:E:202:GLN:NE2   | 4:E:301:ASP:OD1   | 2.45                     | 0.49              |
| 49:w:105:MET:HG2  | 49:w:139:MET:CE   | 2.43                     | 0.49              |
| 30:4:71:ILE:HG22  | 30:4:89:ILE:HD12  | 1.94                     | 0.49              |
| 37:f:160:GLY:C    | 37:f:161:LEU:HD22 | 2.37                     | 0.49              |
| 31:6:371:ASP:OD1  | 31:6:372:SER:N    | 2.44                     | 0.49              |
| 46:s:205:LEU:CD2  | 46:s:224:ARG:HG2  | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1469:G:O2'    | 11:M:55:GLU:OE1   | 2.31                     | 0.49              |
| 10:L:58:ILE:HD11  | 10:L:76:ALA:HB2   | 1.95                     | 0.49              |
| 18:T:85:ALA:O     | 18:T:139:SER:OG   | 2.30                     | 0.49              |
| 3:D:226:ILE:HD11  | 57:y:133:LEU:HD22 | 1.95                     | 0.49              |
| 20:V:50:SER:OG    | 20:V:52:GLU:OE1   | 2.31                     | 0.49              |
| 36:e:48:ALA:N     | 36:e:230:PHE:O    | 2.46                     | 0.49              |
| 45:r:115:ILE:O    | 45:r:119:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:1236:A:H2'    | 1:A:1237:A:O4'    | 2.12                     | 0.49              |
| 1:A:1345:A:OP1    | 28:2:63:LYS:NZ    | 2.41                     | 0.49              |
| 17:S:98:ARG:NH2   | 17:S:114:ALA:O    | 2.45                     | 0.48              |
| 33:b:89:VAL:O     | 33:b:89:VAL:CG1   | 2.60                     | 0.48              |
| 38:g:132:LEU:HD21 | 38:g:153:PHE:HZ   | 1.77                     | 0.48              |
| 49:w:141:PRO:O    | 49:w:145:VAL:HG23 | 2.13                     | 0.48              |
| 19:U:146:LEU:HD11 | 35:d:240:LYS:HB2  | 1.94                     | 0.48              |
| 35:d:190:GLU:OE2  | 35:d:215:ARG:NH1  | 2.45                     | 0.48              |
| 53:a:45:GLN:O     | 53:a:61:HIS:HA    | 2.14                     | 0.48              |
| 49:w:79:ILE:HG22  | 49:w:145:VAL:HG22 | 1.95                     | 0.48              |
| 56:z:191:VAL:HG21 | 56:z:199:LEU:CG   | 2.42                     | 0.48              |
| 1:A:1134:A:H1'    | 1:A:1135:U:H5'    | 1.96                     | 0.48              |
| 1:A:2600:A:O2'    | 13:O:12:GLY:O     | 2.29                     | 0.48              |
| 38:g:132:LEU:HD21 | 38:g:153:PHE:CZ   | 2.49                     | 0.48              |
| 2:B:43:A:H2'      | 2:B:44:G:O4'      | 2.14                     | 0.48              |
| 25:x:244:ASP:OD1  | 25:x:379:ARG:NH1  | 2.46                     | 0.48              |
| 56:z:181:ILE:HD11 | 62:z:401:GNP:O1A  | 2.14                     | 0.48              |
| 1:A:2341:A:O2'    | 27:1:60:LYS:NZ    | 2.47                     | 0.48              |
| 8:J:32:GLY:O      | 8:J:36:GLY:N      | 2.42                     | 0.48              |
| 20:V:126:VAL:HB   | 20:V:152:ARG:NH1  | 2.29                     | 0.48              |
| 25:x:348:THR:O    | 25:x:348:THR:HG22 | 2.14                     | 0.48              |
| 1:A:1821:A:C2     | 3:D:129:VAL:HG11  | 2.49                     | 0.48              |
| 5:F:97:HIS:CE1    | 5:F:101:ILE:HD12  | 2.49                     | 0.48              |
| 8:J:90:PHE:CE2    | 8:J:120:ILE:HG21  | 2.49                     | 0.48              |
| 11:M:190:ILE:HD11 | 38:g:52:LEU:HD22  | 1.96                     | 0.48              |
| 17:S:180:LYS:O    | 17:S:181:ARG:HG2  | 2.13                     | 0.48              |
| 1:A:1235:U:H1'    | 1:A:1236:A:OP2    | 2.14                     | 0.48              |
| 33:b:6:THR:HG22   | 33:b:7:SER:N      | 2.28                     | 0.48              |
| 46:s:226:GLN:NE2  | 46:s:275:SER:OG   | 2.46                     | 0.48              |
| 55:l:69:ALA:HB1   | 55:l:72:VAL:HG13  | 1.95                     | 0.48              |
| 9:K:174:ASP:O     | 45:r:35:LEU:N     | 2.47                     | 0.47              |
| 35:d:213:THR:HG22 | 35:d:247:VAL:HG22 | 1.95                     | 0.47              |
| 1:A:2071:C:O2'    | 56:z:168:ARG:O    | 2.32                     | 0.47              |
| 34:c:307:PHE:O    | 34:c:307:PHE:CD2  | 2.67                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:f:90:LEU:HD23  | 37:f:185:VAL:CG1  | 2.44                     | 0.47              |
| 26:0:153:VAL:HG21 | 26:0:170:GLY:O    | 2.14                     | 0.47              |
| 31:6:60:ARG:O     | 31:6:60:ARG:NH1   | 2.47                     | 0.47              |
| 51:8:172:GLU:OE1  | 51:8:172:GLU:N    | 2.46                     | 0.47              |
| 1:A:1317:U:OP1    | 11:M:132:LYS:NZ   | 2.42                     | 0.47              |
| 1:A:1607:G:N1     | 1:A:1608:C:O2     | 2.47                     | 0.47              |
| 1:A:2283:A:H2'    | 1:A:2284:A:O4'    | 2.14                     | 0.47              |
| 21:W:98:ARG:N     | 21:W:132:HIS:O    | 2.41                     | 0.47              |
| 31:6:175:VAL:HG11 | 31:6:270:PHE:CE2  | 2.48                     | 0.47              |
| 45:r:69:GLN:O     | 45:r:74:ARG:NH2   | 2.46                     | 0.47              |
| 57:y:202:ARG:HG2  | 57:y:212:ILE:HD11 | 1.97                     | 0.47              |
| 10:L:142:GLN:HG3  | 47:u:187:LEU:HD21 | 1.96                     | 0.47              |
| 13:O:38:ARG:NE    | 13:O:82:GLU:OE1   | 2.44                     | 0.47              |
| 16:R:149:HIS:O    | 24:Z:151:LEU:N    | 2.46                     | 0.47              |
| 32:7:67:VAL:O     | 32:7:67:VAL:HG22  | 2.14                     | 0.47              |
| 1:A:1210:G:O2'    | 1:A:1221:G:O6     | 2.25                     | 0.47              |
| 1:A:1458:A:H1'    | 1:A:1459:A:C8     | 2.49                     | 0.47              |
| 25:x:257:THR:HG23 | 25:x:257:THR:O    | 2.15                     | 0.47              |
| 25:x:342:ARG:NE   | 25:x:359:GLU:OE1  | 2.40                     | 0.47              |
| 38:g:154:ASP:OD1  | 38:g:154:ASP:N    | 2.48                     | 0.47              |
| 46:s:151:VAL:HG12 | 46:s:153:ARG:HG3  | 1.96                     | 0.47              |
| 1:A:1278:U:H2'    | 1:A:1279:G:H5''   | 1.96                     | 0.47              |
| 1:A:1712:U:OP2    | 40:i:46:ARG:NH1   | 2.41                     | 0.47              |
| 19:U:112:PRO:O    | 19:U:113:GLU:HB2  | 2.14                     | 0.47              |
| 20:V:55:HIS:HB2   | 20:V:133:ILE:HD11 | 1.97                     | 0.47              |
| 25:x:180:ALA:CB   | 25:x:181:PRO:CD   | 2.93                     | 0.47              |
| 25:x:334:GLN:NE2  | 25:x:335:VAL:O    | 2.48                     | 0.47              |
| 31:6:173:LEU:HD21 | 31:6:175:VAL:HG23 | 1.97                     | 0.47              |
| 46:s:41:VAL:HG22  | 46:s:41:VAL:O     | 2.15                     | 0.47              |
| 1:A:1142:A:OP2    | 6:H:72:ARG:NH1    | 2.47                     | 0.47              |
| 5:F:62:VAL:HG21   | 5:F:88:ALA:HB2    | 1.96                     | 0.47              |
| 5:F:226:MET:SD    | 5:F:242:LEU:HD21  | 2.54                     | 0.47              |
| 8:J:114:LEU:HG    | 8:J:157:LYS:O     | 2.15                     | 0.47              |
| 31:6:191:ASN:OD1  | 31:6:192:GLU:N    | 2.48                     | 0.47              |
| 32:7:259:ASP:OD1  | 32:7:260:VAL:N    | 2.47                     | 0.47              |
| 33:b:21:ARG:NE    | 34:c:217:ASP:OD2  | 2.40                     | 0.47              |
| 1:A:1190:A:H4'    | 1:A:1191:U:H2'    | 1.96                     | 0.47              |
| 1:A:2070:A:H3'    | 1:A:2071:C:H5''   | 1.97                     | 0.47              |
| 1:A:2122:U:O2'    | 1:A:2546:U:H5'    | 2.15                     | 0.47              |
| 31:6:208:ALA:O    | 31:6:209:ASP:CB   | 2.62                     | 0.47              |
| 1:A:1507:A:H3'    | 1:A:1508:A:H5''   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1613:A:H4'    | 1:A:1614:A:OP1    | 2.15                     | 0.47              |
| 1:A:2253:G:N2     | 1:A:2430:C:O4'    | 2.48                     | 0.47              |
| 1:A:1501:A:OP1    | 24:Z:40:ARG:NH1   | 2.47                     | 0.46              |
| 7:I:95:MET:SD     | 7:I:95:MET:N      | 2.84                     | 0.46              |
| 20:V:144:VAL:HG21 | 20:V:153:ILE:HD12 | 1.96                     | 0.46              |
| 21:W:110:ASN:OD1  | 21:W:110:ASN:O    | 2.33                     | 0.46              |
| 24:Z:69:VAL:HG23  | 24:Z:91:LEU:HD21  | 1.97                     | 0.46              |
| 33:b:45:GLU:HB2   | 33:b:94:VAL:HG22  | 1.96                     | 0.46              |
| 46:s:107:GLN:O    | 46:s:111:LYS:N    | 2.48                     | 0.46              |
| 47:u:182:TYR:HB3  | 47:u:184:LEU:HD12 | 1.97                     | 0.46              |
| 1:A:1819:C:OP2    | 3:D:71:LYS:NZ     | 2.47                     | 0.46              |
| 1:A:2161:G:O2'    | 1:A:2162:A:H5'    | 2.15                     | 0.46              |
| 2:B:14:A:N1       | 2:B:21:A:O2'      | 2.45                     | 0.46              |
| 5:F:284:TYR:HB2   | 5:F:285:PRO:HD2   | 1.97                     | 0.46              |
| 56:z:86:LEU:HD23  | 56:z:86:LEU:H     | 1.80                     | 0.46              |
| 1:A:1542:C:H2'    | 1:A:1543:U:H5'    | 1.98                     | 0.46              |
| 1:A:1710:U:O2'    | 5:F:104:ARG:NH2   | 2.48                     | 0.46              |
| 1:A:1757:A:O2'    | 46:s:210:ARG:NH1  | 2.48                     | 0.46              |
| 4:E:316:PHE:HB3   | 4:E:317:PRO:HD3   | 1.98                     | 0.46              |
| 20:V:195:GLU:OE1  | 20:V:195:GLU:N    | 2.46                     | 0.46              |
| 25:x:70:GLU:O     | 25:x:368:ASN:ND2  | 2.48                     | 0.46              |
| 36:e:154:ASN:C    | 36:e:155:LEU:HD12 | 2.40                     | 0.46              |
| 56:z:215:THR:O    | 56:z:219:LEU:HD13 | 2.15                     | 0.46              |
| 2:B:4:A:H2        | 2:B:63:A:H61      | 1.63                     | 0.46              |
| 7:I:102:VAL:HG22  | 7:I:102:VAL:O     | 2.16                     | 0.46              |
| 10:L:38:VAL:HG21  | 10:L:105:VAL:HG13 | 1.97                     | 0.46              |
| 36:e:53:ARG:HH11  | 36:e:155:LEU:HD13 | 1.80                     | 0.46              |
| 47:u:144:LYS:O    | 47:u:145:CYS:SG   | 2.72                     | 0.46              |
| 56:z:91:GLU:O     | 56:z:92:GLN:C     | 2.59                     | 0.46              |
| 1:A:2598:A:N1     | 15:Q:261:ASN:O    | 2.49                     | 0.46              |
| 46:s:205:LEU:HB2  | 46:s:374:THR:HG22 | 1.97                     | 0.46              |
| 1:A:1172:G:OP2    | 1:A:1174:A:N6     | 2.49                     | 0.46              |
| 1:A:2501:A:H5'    | 1:A:2503:G:O3'    | 2.16                     | 0.46              |
| 7:I:188:ARG:NH2   | 58:k:55:VAL:O     | 2.48                     | 0.46              |
| 35:d:164:VAL:HG12 | 35:d:261:MET:HB3  | 1.96                     | 0.46              |
| 36:e:203:LEU:HD13 | 37:f:170:LEU:HD21 | 1.98                     | 0.46              |
| 37:f:167:GLU:OE1  | 51:8:143:GLN:NE2  | 2.48                     | 0.46              |
| 56:z:29:TRP:HE1   | 56:z:225:VAL:HG13 | 1.80                     | 0.46              |
| 1:A:2629:A:N3     | 1:A:2629:A:H2'    | 2.31                     | 0.46              |
| 38:g:72:TRP:NE1   | 38:g:92:HIS:O     | 2.42                     | 0.46              |
| 40:i:80:LEU:HD12  | 40:i:80:LEU:O     | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:z:118:ILE:O    | 56:z:121:ILE:HG22 | 2.15                     | 0.46              |
| 41:j:112:THR:O    | 41:j:112:THR:CG2  | 2.63                     | 0.46              |
| 49:w:128:PHE:O    | 49:w:129:GLU:HB2  | 2.15                     | 0.46              |
| 1:A:1966:U:H2'    | 3:D:209:ARG:HG3   | 1.98                     | 0.45              |
| 1:A:1986:C:H4'    | 1:A:1986:C:OP1    | 2.16                     | 0.45              |
| 11:M:155:VAL:O    | 11:M:175:THR:HA   | 2.16                     | 0.45              |
| 1:A:1831:U:H4'    | 1:A:1831:U:OP1    | 2.16                     | 0.45              |
| 22:X:116:SER:O    | 22:X:120:ASP:N    | 2.49                     | 0.45              |
| 49:w:81:ASP:OD1   | 49:w:82:ARG:N     | 2.50                     | 0.45              |
| 56:z:83:LYS:HB3   | 56:z:86:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:2075:U:OP2    | 1:A:2076:A:O2'    | 2.34                     | 0.45              |
| 12:N:103:GLU:OE1  | 12:N:106:ARG:NH2  | 2.48                     | 0.45              |
| 31:6:177:TYR:N    | 31:6:185:ILE:O    | 2.44                     | 0.45              |
| 31:6:217:LEU:HD21 | 31:6:219:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:1188:A:H1'    | 1:A:1189:C:C5'    | 2.46                     | 0.45              |
| 2:B:27:A:OP1      | 37:f:115:ARG:NE   | 2.49                     | 0.45              |
| 10:L:118:ARG:NH2  | 47:u:194:ASP:OD2  | 2.48                     | 0.45              |
| 30:4:81:VAL:HG12  | 30:4:82:LYS:N     | 2.31                     | 0.45              |
| 37:f:126:MET:HE2  | 37:f:153:GLU:CB   | 2.47                     | 0.45              |
| 56:z:121:ILE:HG23 | 56:z:122:VAL:N    | 2.31                     | 0.45              |
| 5:F:102:TRP:O     | 5:F:106:PHE:HD1   | 1.99                     | 0.45              |
| 10:L:77:ILE:HG23  | 10:L:77:ILE:O     | 2.16                     | 0.45              |
| 15:Q:265:ILE:HG12 | 15:Q:271:ARG:NH1  | 2.32                     | 0.45              |
| 17:S:181:ARG:O    | 17:S:181:ARG:CG   | 2.64                     | 0.45              |
| 25:x:256:THR:O    | 25:x:256:THR:HG22 | 2.16                     | 0.45              |
| 36:e:199:GLU:OE1  | 36:e:238:THR:OG1  | 2.34                     | 0.45              |
| 1:A:1188:A:H1'    | 1:A:1189:C:OP2    | 2.17                     | 0.45              |
| 1:A:2293:A:OP1    | 29:3:138:THR:OG1  | 2.31                     | 0.45              |
| 4:E:154:ARG:O     | 32:7:306:GLN:NE2  | 2.49                     | 0.45              |
| 12:N:112:PHE:CD1  | 12:N:175:ILE:HG21 | 2.52                     | 0.45              |
| 36:e:174:VAL:HG12 | 36:e:175:GLU:N    | 2.32                     | 0.45              |
| 1:A:1102:U:O2'    | 1:A:1103:A:P      | 2.75                     | 0.45              |
| 1:A:1228:G:O6     | 20:V:41:ARG:NH1   | 2.43                     | 0.45              |
| 2:B:64:A:H2'      | 2:B:65:A:C8       | 2.52                     | 0.45              |
| 12:N:112:PHE:CE1  | 12:N:175:ILE:HG21 | 2.50                     | 0.45              |
| 35:d:186:VAL:HG12 | 35:d:187:GLU:N    | 2.32                     | 0.45              |
| 55:l:105:GLU:OE1  | 55:l:105:GLU:N    | 2.44                     | 0.45              |
| 15:Q:240:ILE:HG21 | 15:Q:243:ILE:HD12 | 1.98                     | 0.45              |
| 31:6:185:ILE:HG12 | 43:p:189:ARG:HG3  | 1.99                     | 0.45              |
| 36:e:194:SER:O    | 36:e:246:LYS:NZ   | 2.39                     | 0.45              |
| 45:r:149:ARG:HD3  | 45:r:152:THR:HG21 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:S:181:ARG:O    | 17:S:181:ARG:HG3  | 2.17                     | 0.45              |
| 32:7:70:THR:HG23  | 32:7:96:TYR:OH    | 2.16                     | 0.45              |
| 2:B:8:U:O3'       | 2:B:45:A:H1'      | 2.17                     | 0.45              |
| 3:D:111:ARG:NH2   | 3:D:180:GLY:O     | 2.41                     | 0.45              |
| 31:6:214:TRP:N    | 31:6:240:ILE:O    | 2.47                     | 0.45              |
| 37:f:95:THR:HG23  | 37:f:182:ARG:HB3  | 1.98                     | 0.45              |
| 56:z:303:ASP:OD1  | 56:z:306:ARG:NH1  | 2.50                     | 0.45              |
| 1:A:1256:A:O2'    | 1:A:2121:C:H5     | 2.00                     | 0.44              |
| 14:P:116:LEU:C    | 14:P:116:LEU:HD12 | 2.43                     | 0.44              |
| 35:d:200:SER:OG   | 35:d:208:MET:SD   | 2.74                     | 0.44              |
| 49:w:138:LEU:HD12 | 49:w:140:CYS:H    | 1.82                     | 0.44              |
| 56:z:271:VAL:CG1  | 56:z:300:ALA:HB1  | 2.47                     | 0.44              |
| 1:A:1237:A:O2'    | 1:A:1238:U:P      | 2.74                     | 0.44              |
| 1:A:1560:A:N6     | 1:A:1561:A:H62    | 2.15                     | 0.44              |
| 3:D:159:LYS:N     | 3:D:162:ASP:OD2   | 2.45                     | 0.44              |
| 34:c:228:LEU:HB2  | 34:c:307:PHE:CD2  | 2.52                     | 0.44              |
| 39:h:114:PRO:O    | 39:h:118:LEU:HD12 | 2.17                     | 0.44              |
| 1:A:1612:A:H2'    | 1:A:1613:A:O4'    | 2.16                     | 0.44              |
| 1:A:2062:U:H3'    | 1:A:2063:A:H5''   | 1.99                     | 0.44              |
| 3:D:143:VAL:HG21  | 3:D:164:ILE:HD11  | 1.98                     | 0.44              |
| 12:N:191:SER:N    | 12:N:194:THR:OG1  | 2.51                     | 0.44              |
| 36:e:52:GLN:O     | 36:e:236:LEU:N    | 2.45                     | 0.44              |
| 38:g:68:THR:CG2   | 38:g:69:PRO:HD2   | 2.47                     | 0.44              |
| 45:r:140:LEU:HD12 | 45:r:141:PRO:O    | 2.17                     | 0.44              |
| 1:A:1488:A:H2'    | 1:A:1489:A:O4'    | 2.18                     | 0.44              |
| 39:h:130:PHE:O    | 39:h:133:VAL:HG22 | 2.18                     | 0.44              |
| 51:8:147:LEU:HD23 | 51:8:158:TYR:HE1  | 1.83                     | 0.44              |
| 58:k:90:LEU:O     | 58:k:94:ILE:HG12  | 2.18                     | 0.44              |
| 1:A:1635:C:N4     | 1:A:1642:G:H22    | 2.14                     | 0.44              |
| 1:A:2177:A:N3     | 1:A:2362:A:O2'    | 2.40                     | 0.44              |
| 1:A:2617:A:O2'    | 1:A:2618:A:C8     | 2.70                     | 0.44              |
| 25:x:257:THR:HA   | 25:x:307:CYS:SG   | 2.57                     | 0.44              |
| 32:7:78:MET:HB3   | 32:7:83:SER:OG    | 2.18                     | 0.44              |
| 46:s:49:ALA:O     | 46:s:61:ARG:NH1   | 2.43                     | 0.44              |
| 49:w:74:LEU:HD13  | 49:w:152:LYS:HB3  | 1.99                     | 0.44              |
| 57:y:227:PRO:O    | 57:y:228:ASN:HB2  | 2.18                     | 0.44              |
| 1:A:1137:A:HO2'   | 1:A:1138:U:P      | 2.40                     | 0.44              |
| 1:A:2617:A:N6     | 1:A:2643:U:O4'    | 2.50                     | 0.44              |
| 25:x:234:ASP:OD1  | 25:x:236:ARG:N    | 2.50                     | 0.44              |
| 26:0:156:MET:HE1  | 26:0:168:ASP:OD1  | 2.18                     | 0.44              |
| 46:s:110:THR:HG23 | 46:s:327:PHE:CD1  | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:w:74:LEU:HD12  | 49:w:79:ILE:HD11  | 1.99                     | 0.44              |
| 1:A:1894:A:OP1    | 13:O:9:ILE:N      | 2.50                     | 0.44              |
| 2:B:63:A:H2'      | 2:B:64:A:C1'      | 2.48                     | 0.44              |
| 10:L:96:MET:HE2   | 15:Q:165:GLU:H    | 1.82                     | 0.44              |
| 11:M:61:ARG:O     | 40:i:128:ARG:NH2  | 2.46                     | 0.44              |
| 19:U:28:LEU:O     | 23:Y:116:THR:HG23 | 2.18                     | 0.44              |
| 19:U:146:LEU:HD23 | 35:d:222:LEU:HB3  | 1.99                     | 0.44              |
| 31:6:220:ASN:O    | 31:6:231:GLU:HB2  | 2.18                     | 0.44              |
| 1:A:2373:G:OP1    | 5:F:137:ARG:NH1   | 2.41                     | 0.44              |
| 4:E:121:LEU:HD22  | 4:E:284:TYR:CD1   | 2.53                     | 0.44              |
| 5:F:160:SER:HB3   | 40:i:80:LEU:HD13  | 1.99                     | 0.44              |
| 18:T:168:TYR:CE2  | 18:T:170:VAL:HG13 | 2.53                     | 0.44              |
| 31:6:235:TRP:HB3  | 31:6:254:TYR:HA   | 2.00                     | 0.44              |
| 1:A:2073:G:P      | 56:z:164:ARG:HE   | 2.41                     | 0.44              |
| 1:A:2113:A:OP1    | 18:T:162:GLU:N    | 2.49                     | 0.44              |
| 1:A:2281:C:H2'    | 1:A:2282:G:O4'    | 2.18                     | 0.44              |
| 2:B:3:U:H3'       | 2:B:4:A:H8        | 1.83                     | 0.44              |
| 8:J:23:ILE:O      | 8:J:23:ILE:HG23   | 2.17                     | 0.44              |
| 16:R:14:LEU:HD22  | 16:R:17:ARG:HB2   | 1.99                     | 0.44              |
| 37:f:125:ALA:HB2  | 37:f:154:ARG:NE   | 2.32                     | 0.44              |
| 1:A:2575:C:H4'    | 1:A:2575:C:OP1    | 2.18                     | 0.43              |
| 4:E:154:ARG:HG2   | 4:E:172:PRO:HG3   | 1.99                     | 0.43              |
| 8:J:110:GLY:O     | 8:J:111:LEU:HD12  | 2.18                     | 0.43              |
| 32:7:111:ASP:OD1  | 32:7:265:LEU:N    | 2.43                     | 0.43              |
| 33:b:47:VAL:O     | 33:b:51:VAL:HG12  | 2.17                     | 0.43              |
| 35:d:235:GLN:HB2  | 35:d:240:LYS:HZ1  | 1.83                     | 0.43              |
| 37:f:92:ILE:HD13  | 37:f:158:ILE:HD12 | 2.00                     | 0.43              |
| 1:A:1493:A:O2'    | 21:W:99:TYR:HB2   | 2.17                     | 0.43              |
| 9:K:101:VAL:O     | 9:K:101:VAL:HG12  | 2.18                     | 0.43              |
| 11:M:190:ILE:HD11 | 38:g:52:LEU:CD2   | 2.48                     | 0.43              |
| 14:P:107:THR:HG22 | 14:P:107:THR:O    | 2.17                     | 0.43              |
| 19:U:37:GLU:OE2   | 46:s:259:LYS:NZ   | 2.37                     | 0.43              |
| 25:x:159:SER:O    | 25:x:184:LYS:NZ   | 2.40                     | 0.43              |
| 37:f:198:LYS:HB2  | 37:f:203:LEU:HD11 | 2.00                     | 0.43              |
| 46:s:146:GLN:O    | 46:s:151:VAL:HG23 | 2.18                     | 0.43              |
| 54:m:65:ILE:HD11  | 54:m:74:LEU:HD12  | 2.01                     | 0.43              |
| 1:A:1610:U:H1'    | 1:A:1617:A:H61    | 1.82                     | 0.43              |
| 4:E:120:THR:HG21  | 4:E:289:VAL:HG23  | 2.01                     | 0.43              |
| 8:J:50:CYS:O      | 8:J:54:ASN:N      | 2.44                     | 0.43              |
| 9:K:67:PHE:HD2    | 9:K:72:TRP:CE2    | 2.36                     | 0.43              |
| 15:Q:246:ASP:OD1  | 15:Q:247:LEU:N    | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:x:257:THR:OG1  | 25:x:260:HIS:HB3  | 2.18                     | 0.43              |
| 37:f:92:ILE:HD11  | 37:f:158:ILE:HD12 | 2.00                     | 0.43              |
| 1:A:1556:A:H2'    | 1:A:1559:A:H61    | 1.82                     | 0.43              |
| 1:A:2389:C:H2'    | 1:A:2390:C:O4'    | 2.18                     | 0.43              |
| 14:P:156:ASP:OD1  | 14:P:156:ASP:N    | 2.51                     | 0.43              |
| 15:Q:194:LEU:HD23 | 15:Q:223:LYS:O    | 2.19                     | 0.43              |
| 34:c:184:PHE:HA   | 34:c:185:PRO:C    | 2.43                     | 0.43              |
| 36:e:121:MET:O    | 36:e:124:GLN:NE2  | 2.49                     | 0.43              |
| 38:g:42:VAL:HG12  | 38:g:42:VAL:O     | 2.18                     | 0.43              |
| 48:v:40:ARG:O     | 48:v:44:LYS:HG2   | 2.18                     | 0.43              |
| 56:z:48:VAL:O     | 56:z:75:LYS:NZ    | 2.41                     | 0.43              |
| 1:A:2654:A:C3'    | 1:A:2655:C:H5'    | 2.48                     | 0.43              |
| 11:M:237:MET:O    | 43:p:155:ARG:NH2  | 2.51                     | 0.43              |
| 25:x:104:SER:O    | 25:x:104:SER:OG   | 2.37                     | 0.43              |
| 31:6:197:GLU:OE2  | 43:p:185:ARG:NH2  | 2.52                     | 0.43              |
| 36:e:181:THR:HG23 | 36:e:184:GLY:H    | 1.83                     | 0.43              |
| 49:w:97:LYS:NZ    | 49:w:107:ASP:OD2  | 2.27                     | 0.43              |
| 56:z:176:GLY:N    | 56:z:181:ILE:HD13 | 2.33                     | 0.43              |
| 56:z:255:TYR:CD1  | 56:z:271:VAL:HG23 | 2.52                     | 0.43              |
| 1:A:1188:A:H1'    | 1:A:1189:C:P      | 2.59                     | 0.43              |
| 17:S:198:ARG:NH2  | 33:b:13:SER:OG    | 2.52                     | 0.43              |
| 18:T:93:ILE:HG23  | 18:T:94:ASP:N     | 2.33                     | 0.43              |
| 23:Y:193:ASN:O    | 23:Y:197:ASN:ND2  | 2.51                     | 0.43              |
| 45:r:118:CYS:SG   | 45:r:181:LEU:HD11 | 2.58                     | 0.43              |
| 1:A:1561:A:N3     | 1:A:1561:A:H2'    | 2.34                     | 0.43              |
| 1:A:1580:U:C2     | 45:r:169:TRP:CD1  | 3.07                     | 0.43              |
| 4:E:103:LYS:NZ    | 4:E:291:GLY:O     | 2.49                     | 0.43              |
| 13:O:141:SER:O    | 13:O:147:ASN:ND2  | 2.52                     | 0.43              |
| 26:0:89:ASN:O     | 26:0:93:ARG:HG2   | 2.18                     | 0.43              |
| 30:4:71:ILE:HG22  | 30:4:89:ILE:CD1   | 2.48                     | 0.43              |
| 33:b:15:LEU:HD11  | 34:c:172:ASN:HB2  | 2.00                     | 0.43              |
| 34:c:86:ASP:N     | 34:c:86:ASP:OD1   | 2.50                     | 0.43              |
| 47:u:187:LEU:C    | 47:u:187:LEU:HD23 | 2.44                     | 0.43              |
| 56:z:210:ILE:O    | 56:z:210:ILE:HG22 | 2.19                     | 0.43              |
| 1:A:1489:A:O2'    | 1:A:1506:A:N1     | 2.51                     | 0.43              |
| 1:A:1615:G:H2'    | 1:A:1616:C:O4'    | 2.19                     | 0.43              |
| 13:O:94:ALA:HB3   | 13:O:95:PRO:HD3   | 2.00                     | 0.43              |
| 36:e:155:LEU:HD23 | 36:e:252:TRP:HB3  | 2.00                     | 0.43              |
| 40:i:57:TYR:OH    | 44:q:28:PRO:O     | 2.29                     | 0.43              |
| 49:w:105:MET:HG2  | 49:w:139:MET:HE1  | 2.01                     | 0.43              |
| 56:z:225:VAL:HG11 | 56:z:230:VAL:HG21 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2063:A:OP1    | 1:A:2063:A:O4'    | 2.37                     | 0.43              |
| 4:E:326:GLU:O     | 4:E:326:GLU:HG2   | 2.18                     | 0.43              |
| 9:K:17:MET:HE3    | 9:K:142:VAL:HG11  | 2.00                     | 0.43              |
| 9:K:136:ASP:OD1   | 9:K:137:ILE:N     | 2.52                     | 0.43              |
| 31:6:177:TYR:O    | 31:6:185:ILE:N    | 2.44                     | 0.43              |
| 1:A:2337:C:H2'    | 1:A:2338:C:O4'    | 2.19                     | 0.43              |
| 7:I:165:VAL:O     | 7:I:169:LYS:N     | 2.41                     | 0.43              |
| 36:e:190:LEU:HD13 | 36:e:200:ALA:HB3  | 2.01                     | 0.43              |
| 1:A:1194:A:HO2'   | 1:A:1195:G:P      | 2.42                     | 0.42              |
| 1:A:1231:A:OP2    | 20:V:34:LYS:NZ    | 2.51                     | 0.42              |
| 1:A:1365:A:H4'    | 1:A:1366:U:O4'    | 2.19                     | 0.42              |
| 1:A:1621:A:H61    | 1:A:1631:A:C2'    | 2.32                     | 0.42              |
| 3:D:112:PHE:CZ    | 3:D:168:ASN:HB2   | 2.54                     | 0.42              |
| 4:E:340:PRO:O     | 4:E:341:SER:OG    | 2.32                     | 0.42              |
| 7:I:79:VAL:HG22   | 7:I:130:VAL:HG11  | 2.01                     | 0.42              |
| 50:5:351:VAL:HG22 | 50:5:381:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:1492:A:H1'    | 1:A:1493:A:O4'    | 2.19                     | 0.42              |
| 1:A:1492:A:H4'    | 1:A:1493:A:OP1    | 2.18                     | 0.42              |
| 1:A:1542:C:C2'    | 1:A:1543:U:H5'    | 2.49                     | 0.42              |
| 1:A:2302:U:O2'    | 1:A:2303:A:P      | 2.77                     | 0.42              |
| 5:F:292:ASP:OD1   | 38:g:55:THR:HG22  | 2.19                     | 0.42              |
| 8:J:34:PRO:O      | 8:J:38:ILE:HD12   | 2.19                     | 0.42              |
| 11:M:103:LEU:CD2  | 11:M:108:ARG:HE   | 2.32                     | 0.42              |
| 25:x:77:VAL:HG22  | 25:x:127:ARG:HG3  | 2.01                     | 0.42              |
| 25:x:197:LEU:N    | 25:x:227:GLN:O    | 2.52                     | 0.42              |
| 32:7:188:GLU:OE1  | 32:7:188:GLU:N    | 2.52                     | 0.42              |
| 34:c:287:GLU:HG3  | 34:c:288:THR:HG23 | 2.01                     | 0.42              |
| 36:e:237:LEU:O    | 36:e:238:THR:HG23 | 2.19                     | 0.42              |
| 1:A:1137:A:O2'    | 1:A:1138:U:P      | 2.77                     | 0.42              |
| 1:A:1683:C:O2     | 1:A:1683:C:C2'    | 2.67                     | 0.42              |
| 31:6:125:LEU:O    | 31:6:126:ARG:HG2  | 2.19                     | 0.42              |
| 31:6:227:GLU:OE1  | 31:6:230:ALA:N    | 2.44                     | 0.42              |
| 33:b:17:ASN:O     | 33:b:21:ARG:O     | 2.37                     | 0.42              |
| 43:p:75:ASP:OD1   | 43:p:76:ARG:N     | 2.53                     | 0.42              |
| 49:w:83:VAL:HA    | 49:w:86:VAL:HG22  | 2.01                     | 0.42              |
| 56:z:181:ILE:N    | 62:z:401:GNP:O3G  | 2.52                     | 0.42              |
| 56:z:226:LEU:O    | 56:z:228:HIS:N    | 2.52                     | 0.42              |
| 1:A:1533:G:OP1    | 12:N:233:TYR:OH   | 2.27                     | 0.42              |
| 28:2:78:VAL:HG22  | 28:2:81:ARG:HH22  | 1.85                     | 0.42              |
| 30:4:73:LYS:NZ    | 30:4:78:CYS:O     | 2.53                     | 0.42              |
| 32:7:164:VAL:HG13 | 32:7:165:ARG:N    | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:e:49:LEU:HB3   | 36:e:189:ILE:HG21 | 2.01                     | 0.42              |
| 46:s:110:THR:O    | 46:s:110:THR:HG22 | 2.18                     | 0.42              |
| 46:s:370:THR:CG2  | 46:s:383:ARG:HB2  | 2.50                     | 0.42              |
| 1:A:1346:G:H4'    | 1:A:1347:C:OP2    | 2.20                     | 0.42              |
| 1:A:2485:C:H2'    | 1:A:2486:A:C8     | 2.54                     | 0.42              |
| 4:E:122:LEU:HD12  | 4:E:285:VAL:HG21  | 2.01                     | 0.42              |
| 19:U:140:ILE:HD11 | 35:d:232:MET:SD   | 2.60                     | 0.42              |
| 32:7:78:MET:HE1   | 32:7:91:HIS:CD2   | 2.54                     | 0.42              |
| 46:s:243:GLU:HA   | 46:s:350:VAL:HG21 | 2.01                     | 0.42              |
| 1:A:1310:A:C5     | 31:6:379:ILE:HG21 | 2.54                     | 0.42              |
| 1:A:1420:A:N1     | 3:D:275:LEU:HD12  | 2.34                     | 0.42              |
| 1:A:1455:A:O2'    | 1:A:1477:U:H5''   | 2.19                     | 0.42              |
| 1:A:2302:U:HO2'   | 1:A:2303:A:P      | 2.42                     | 0.42              |
| 2:B:7:G:H5''      | 2:B:8:U:OP1       | 2.19                     | 0.42              |
| 9:K:60:ILE:HG21   | 9:K:133:ILE:HD11  | 2.02                     | 0.42              |
| 13:O:156:ASP:OD2  | 32:7:316:ARG:NH2  | 2.53                     | 0.42              |
| 15:Q:280:ALA:O    | 15:Q:284:GLU:OE1  | 2.38                     | 0.42              |
| 53:a:140:ASP:O    | 53:a:141:ARG:O    | 2.38                     | 0.42              |
| 2:B:9:A:H4'       | 2:B:10:G:OP1      | 2.19                     | 0.42              |
| 2:B:15:A:O2'      | 2:B:17:A:N6       | 2.48                     | 0.42              |
| 8:J:60:ILE:HG21   | 8:J:66:LEU:HD11   | 2.01                     | 0.42              |
| 15:Q:225:LYS:HB2  | 15:Q:226:PRO:CD   | 2.50                     | 0.42              |
| 18:T:72:ARG:O     | 18:T:167:HIS:CD2  | 2.72                     | 0.42              |
| 24:Z:117:ILE:O    | 42:o:45:ASN:ND2   | 2.50                     | 0.42              |
| 25:x:49:ASP:O     | 25:x:53:SER:OG    | 2.37                     | 0.42              |
| 34:c:188:LEU:N    | 34:c:189:PRO:HD2  | 2.34                     | 0.42              |
| 35:d:186:VAL:HG12 | 35:d:187:GLU:H    | 1.84                     | 0.42              |
| 36:e:258:LEU:HD12 | 36:e:262:LEU:HD13 | 2.01                     | 0.42              |
| 56:z:111:ASN:OD1  | 56:z:113:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:1189:C:H4'    | 1:A:1190:A:OP1    | 2.20                     | 0.42              |
| 1:A:1494:A:O2'    | 21:W:53:ILE:HD11  | 2.20                     | 0.42              |
| 5:F:94:ASP:OD1    | 5:F:94:ASP:N      | 2.52                     | 0.42              |
| 9:K:154:ARG:NH1   | 9:K:156:ASP:OD1   | 2.53                     | 0.42              |
| 18:T:46:GLU:OE1   | 18:T:46:GLU:N     | 2.42                     | 0.42              |
| 25:x:351:PHE:CE1  | 25:x:361:VAL:HG22 | 2.55                     | 0.42              |
| 27:1:15:THR:O     | 27:1:65:LEU:N     | 2.48                     | 0.42              |
| 31:6:217:LEU:HD21 | 31:6:219:ILE:CD1  | 2.49                     | 0.42              |
| 32:7:105:VAL:HG13 | 32:7:120:CYS:SG   | 2.60                     | 0.42              |
| 33:b:148:LEU:O    | 33:b:149:ARG:CB   | 2.67                     | 0.42              |
| 37:f:175:SER:O    | 54:m:34:CYS:HA    | 2.20                     | 0.42              |
| 58:k:78:GLY:O     | 58:k:79:ALA:C     | 2.63                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1610:U:H1'   | 1:A:1617:A:N6    | 2.35                     | 0.42              |
| 1:A:2062:U:C3'   | 1:A:2063:A:H5''  | 2.50                     | 0.42              |
| 2:B:51:A:C6      | 2:B:52:U:O4      | 2.73                     | 0.42              |
| 5:F:274:LEU:O    | 5:F:277:ASP:OD1  | 2.37                     | 0.42              |
| 9:K:90:VAL:HG22  | 9:K:94:GLN:HB2   | 2.02                     | 0.42              |
| 25:x:174:VAL:HA  | 25:x:248:ARG:O   | 2.19                     | 0.42              |
| 1:A:1607:G:N3    | 1:A:1607:G:H2'   | 2.35                     | 0.42              |
| 8:J:112:VAL:O    | 8:J:156:VAL:O    | 2.38                     | 0.42              |
| 31:6:208:ALA:N   | 31:6:243:ASN:OD1 | 2.43                     | 0.42              |
| 33:b:40:SER:OG   | 33:b:44:ARG:NH1  | 2.53                     | 0.42              |
| 36:e:57:ILE:HG21 | 36:e:134:ARG:HA  | 2.02                     | 0.42              |
| 56:z:233:GLU:HG2 | 56:z:234:THR:N   | 2.34                     | 0.42              |
| 1:A:1610:U:C6    | 1:A:1610:U:OP2   | 2.73                     | 0.41              |
| 9:K:171:THR:O    | 9:K:171:THR:HG23 | 2.19                     | 0.41              |
| 19:U:44:ILE:HG21 | 19:U:53:LEU:HD12 | 2.02                     | 0.41              |
| 22:X:163:ARG:HE  | 50:5:55:LEU:HD11 | 1.85                     | 0.41              |
| 25:x:180:ALA:HB1 | 25:x:206:ARG:HB3 | 2.01                     | 0.41              |
| 43:p:102:ARG:NE  | 43:p:132:GLU:OE2 | 2.50                     | 0.41              |
| 49:w:79:ILE:HG21 | 49:w:148:ILE:HB  | 2.02                     | 0.41              |
| 56:z:155:LYS:NZ  | 62:z:401:GNP:O2G | 2.52                     | 0.41              |
| 58:k:61:GLU:OE2  | 58:k:77:ARG:NH1  | 2.53                     | 0.41              |
| 1:A:1130:U:O2'   | 1:A:1131:A:O5'   | 2.36                     | 0.41              |
| 1:A:1220:G:N7    | 28:2:87:ARG:NH2  | 2.59                     | 0.41              |
| 1:A:1724:U:O2    | 16:R:12:ASN:ND2  | 2.53                     | 0.41              |
| 1:A:1906:G:O2'   | 10:L:36:THR:HG22 | 2.20                     | 0.41              |
| 14:P:91:GLU:OE2  | 14:P:108:ARG:NH2 | 2.45                     | 0.41              |
| 1:A:1576:U:OP2   | 41:j:22:ALA:N    | 2.54                     | 0.41              |
| 1:A:1600:A:N6    | 1:A:1645:C:OP2   | 2.53                     | 0.41              |
| 1:A:2251:U:H4'   | 1:A:2251:U:OP1   | 2.20                     | 0.41              |
| 1:A:2302:U:C2'   | 1:A:2303:A:O5'   | 2.68                     | 0.41              |
| 2:B:30:A:OP1     | 54:m:41:ARG:NE   | 2.53                     | 0.41              |
| 8:J:108:VAL:HG21 | 8:J:154:ARG:HB2  | 2.02                     | 0.41              |
| 11:M:167:GLU:OE2 | 11:M:219:ARG:NH2 | 2.52                     | 0.41              |
| 14:P:61:VAL:HG11 | 31:6:344:PHE:CE2 | 2.55                     | 0.41              |
| 37:f:95:THR:HG23 | 37:f:95:THR:O    | 2.21                     | 0.41              |
| 42:o:29:PHE:CZ   | 42:o:33:GLU:OE2  | 2.73                     | 0.41              |
| 43:p:97:SER:O    | 43:p:146:ASN:ND2 | 2.53                     | 0.41              |
| 44:q:153:ARG:O   | 44:q:157:GLN:N   | 2.46                     | 0.41              |
| 1:A:1275:U:H5''  | 11:M:46:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:1541:G:H2'   | 1:A:1542:C:O4'   | 2.20                     | 0.41              |
| 1:A:1659:A:OP2   | 1:A:1659:A:N3    | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1831:U:OP1    | 1:A:1831:U:C4'    | 2.68                     | 0.41              |
| 1:A:2075:U:H3'    | 1:A:2076:A:H2'    | 2.02                     | 0.41              |
| 1:A:2616:U:C6     | 1:A:2616:U:OP2    | 2.73                     | 0.41              |
| 4:E:112:LYS:NZ    | 4:E:337:VAL:O     | 2.53                     | 0.41              |
| 15:Q:77:SER:OG    | 15:Q:79:GLU:OE1   | 2.37                     | 0.41              |
| 17:S:132:ILE:HG22 | 17:S:133:ARG:N    | 2.35                     | 0.41              |
| 11:M:115:ILE:HG13 | 11:M:151:ILE:HD11 | 2.02                     | 0.41              |
| 14:P:67:GLY:HA3   | 21:W:78:GLY:O     | 2.20                     | 0.41              |
| 20:V:172:ASP:HB2  | 20:V:176:ASP:HB2  | 2.02                     | 0.41              |
| 37:f:107:GLN:HG3  | 37:f:108:TYR:N    | 2.35                     | 0.41              |
| 50:5:211:THR:HG21 | 50:5:319:ALA:O    | 2.21                     | 0.41              |
| 1:A:1856:C:OP2    | 19:U:50:ARG:NE    | 2.52                     | 0.41              |
| 1:A:2073:G:O5'    | 56:z:164:ARG:NE   | 2.54                     | 0.41              |
| 1:A:2074:C:H2'    | 1:A:2075:U:O5'    | 2.20                     | 0.41              |
| 1:A:2564:G:H1'    | 1:A:2565:U:OP2    | 2.21                     | 0.41              |
| 11:M:232:ARG:HH21 | 11:M:243:LEU:HD21 | 1.86                     | 0.41              |
| 18:T:63:ARG:O     | 35:d:230:ARG:HD3  | 2.21                     | 0.41              |
| 20:V:133:ILE:HG22 | 20:V:147:SER:HA   | 2.03                     | 0.41              |
| 35:d:267:PRO:HG2  | 35:d:270:ALA:HB2  | 2.03                     | 0.41              |
| 36:e:52:GLN:N     | 36:e:234:ALA:O    | 2.52                     | 0.41              |
| 49:w:80:LYS:HA    | 49:w:145:VAL:HG21 | 2.02                     | 0.41              |
| 1:A:1275:U:H2'    | 1:A:1276:U:O4'    | 2.21                     | 0.41              |
| 1:A:1637:U:H2'    | 1:A:1639:C:OP2    | 2.20                     | 0.41              |
| 2:B:9:A:OP2       | 2:B:9:A:H3'       | 2.21                     | 0.41              |
| 2:B:13:U:O2'      | 2:B:14:A:P        | 2.79                     | 0.41              |
| 6:H:111:VAL:HG12  | 6:H:112:LYS:N     | 2.35                     | 0.41              |
| 14:P:91:GLU:OE2   | 14:P:108:ARG:NE   | 2.47                     | 0.41              |
| 56:z:181:ILE:HG13 | 56:z:182:THR:N    | 2.35                     | 0.41              |
| 56:z:225:VAL:HG11 | 56:z:230:VAL:CG2  | 2.50                     | 0.41              |
| 56:z:259:SER:O    | 56:z:260:ALA:CB   | 2.68                     | 0.41              |
| 1:A:1712:U:H4'    | 11:M:23:LEU:HD12  | 2.03                     | 0.41              |
| 1:A:2394:U:OP1    | 30:4:69:GLY:N     | 2.52                     | 0.41              |
| 22:X:81:GLY:O     | 22:X:130:ARG:NE   | 2.49                     | 0.41              |
| 37:f:89:VAL:HG23  | 37:f:89:VAL:O     | 2.21                     | 0.41              |
| 47:u:190:LEU:N    | 47:u:190:LEU:HD12 | 2.36                     | 0.41              |
| 49:w:127:GLY:C    | 49:w:128:PHE:CD1  | 2.99                     | 0.41              |
| 49:w:138:LEU:HD22 | 49:w:144:ILE:HD13 | 2.01                     | 0.41              |
| 56:z:252:VAL:HG11 | 56:z:260:ALA:HB2  | 2.03                     | 0.41              |
| 58:k:30:THR:HG23  | 58:k:31:ARG:N     | 2.35                     | 0.41              |
| 1:A:1422:A:C5'    | 1:A:1423:G:OP1    | 2.69                     | 0.41              |
| 1:A:1821:A:O2'    | 3:D:131:ARG:NH1   | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1851:C:O2     | 46:s:162:ARG:NH1  | 2.47                     | 0.41              |
| 4:E:204:VAL:HG21  | 4:E:299:ILE:CG1   | 2.51                     | 0.41              |
| 9:K:67:PHE:HB3    | 9:K:71:LYS:HB2    | 2.02                     | 0.41              |
| 13:O:110:ILE:CG2  | 13:O:111:PRO:HD2  | 2.51                     | 0.41              |
| 15:Q:262:LYS:HA   | 15:Q:264:TRP:CZ3  | 2.55                     | 0.41              |
| 17:S:98:ARG:HG3   | 34:c:311:ARG:O    | 2.20                     | 0.41              |
| 18:T:151:ARG:HE   | 18:T:161:MET:HE2  | 1.86                     | 0.41              |
| 19:U:22:THR:HG22  | 19:U:24:PHE:H     | 1.85                     | 0.41              |
| 21:W:122:LYS:N    | 31:6:49:GLU:O     | 2.42                     | 0.41              |
| 24:Z:151:LEU:HD21 | 41:j:44:GLU:OE1   | 2.20                     | 0.41              |
| 31:6:268:PHE:O    | 31:6:318:PHE:HA   | 2.21                     | 0.41              |
| 46:s:180:ASN:OD1  | 50:5:192:ILE:HD12 | 2.21                     | 0.41              |
| 52:9:101:ASP:O    | 52:9:105:GLY:N    | 2.54                     | 0.41              |
| 52:9:134:PRO:O    | 52:9:135:ARG:C    | 2.64                     | 0.41              |
| 55:l:72:VAL:HG23  | 55:l:73:ASN:N     | 2.35                     | 0.41              |
| 57:y:302:LEU:O    | 57:y:307:CYS:N    | 2.54                     | 0.41              |
| 58:k:15:LEU:HD21  | 58:k:17:ARG:HE    | 1.86                     | 0.41              |
| 1:A:1433:C:H2'    | 1:A:1434:U:C6     | 2.56                     | 0.41              |
| 1:A:1506:A:H2'    | 1:A:1507:A:O4'    | 2.21                     | 0.41              |
| 1:A:1639:C:OP2    | 1:A:1639:C:C6     | 2.73                     | 0.41              |
| 1:A:1944:A:O2'    | 1:A:1945:C:OP1    | 2.36                     | 0.41              |
| 1:A:2072:G:O2'    | 1:A:2073:G:P      | 2.78                     | 0.41              |
| 1:A:2175:U:O2'    | 1:A:2176:A:H2'    | 2.21                     | 0.41              |
| 1:A:2617:A:O2'    | 1:A:2618:A:P      | 2.79                     | 0.41              |
| 2:B:26:A:O2'      | 51:8:133:ARG:NH2  | 2.53                     | 0.41              |
| 31:6:237:LEU:HD13 | 31:6:240:ILE:HD11 | 2.02                     | 0.41              |
| 32:7:181:THR:HG22 | 32:7:291:ILE:HG12 | 2.03                     | 0.41              |
| 32:7:273:PHE:HB2  | 32:7:301:THR:HG22 | 2.02                     | 0.41              |
| 37:f:91:ASN:N     | 37:f:186:ARG:O    | 2.52                     | 0.41              |
| 49:w:139:MET:HE3  | 49:w:139:MET:HA   | 2.03                     | 0.41              |
| 56:z:206:LEU:O    | 56:z:207:ALA:HB2  | 2.21                     | 0.41              |
| 1:A:1103:A:H2'    | 1:A:1104:G:O4'    | 2.21                     | 0.40              |
| 1:A:1333:C:H5''   | 5:F:144:PRO:HD2   | 2.03                     | 0.40              |
| 1:A:1793:C:H2'    | 1:A:1794:C:O4'    | 2.21                     | 0.40              |
| 1:A:2076:A:HO2'   | 1:A:2077:A:P      | 2.32                     | 0.40              |
| 20:V:131:THR:O    | 20:V:131:THR:HG23 | 2.21                     | 0.40              |
| 31:6:212:SER:O    | 31:6:214:TRP:CD1  | 2.73                     | 0.40              |
| 33:b:134:THR:O    | 33:b:135:ASN:HB2  | 2.22                     | 0.40              |
| 56:z:88:ASP:O     | 56:z:317:MET:HE3  | 2.20                     | 0.40              |
| 1:A:1113:C:H2'    | 1:A:1114:U:O4'    | 2.21                     | 0.40              |
| 1:A:1565:U:H5'    | 24:Z:74:SER:HB2   | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1602:U:O3'    | 8:J:130:PHE:HB2   | 2.21                     | 0.40              |
| 1:A:1985:C:H3'    | 1:A:1986:C:H5''   | 2.02                     | 0.40              |
| 1:A:2630:A:N3     | 1:A:2630:A:H3'    | 2.36                     | 0.40              |
| 4:E:175:ILE:HG22  | 4:E:296:LEU:HD23  | 2.04                     | 0.40              |
| 9:K:177:ARG:NH2   | 45:r:38:VAL:HG23  | 2.37                     | 0.40              |
| 10:L:95:ARG:O     | 10:L:96:MET:HB2   | 2.21                     | 0.40              |
| 16:R:84:PRO:O     | 16:R:88:VAL:HG22  | 2.22                     | 0.40              |
| 31:6:240:ILE:HD12 | 31:6:245:VAL:HA   | 2.04                     | 0.40              |
| 32:7:214:GLU:OE1  | 32:7:253:ARG:NE   | 2.50                     | 0.40              |
| 48:v:26:THR:HG22  | 48:v:27:ASP:N     | 2.36                     | 0.40              |
| 56:z:285:THR:HG22 | 56:z:288:GLY:O    | 2.21                     | 0.40              |
| 1:A:2599:A:C8     | 15:Q:271:ARG:HG2  | 2.55                     | 0.40              |
| 25:x:229:ARG:NH1  | 37:f:198:LYS:O    | 2.54                     | 0.40              |
| 31:6:291:TYR:CE1  | 31:6:334:LEU:HD12 | 2.56                     | 0.40              |
| 34:c:179:THR:HG23 | 34:c:194:THR:HG21 | 2.04                     | 0.40              |
| 46:s:195:ASP:HB2  | 46:s:234:GLN:HG2  | 2.04                     | 0.40              |
| 47:u:176:PRO:O    | 47:u:180:GLU:OE1  | 2.40                     | 0.40              |
| 56:z:95:ILE:HD11  | 56:z:317:MET:SD   | 2.61                     | 0.40              |
| 1:A:1212:A:H2'    | 1:A:1213:C:O4'    | 2.22                     | 0.40              |
| 1:A:1422:A:H5'    | 1:A:1423:G:OP1    | 2.22                     | 0.40              |
| 1:A:2267:A:N1     | 1:A:2276:U:O4     | 2.55                     | 0.40              |
| 4:E:196:ALA:HB3   | 4:E:319:TYR:CD2   | 2.57                     | 0.40              |
| 17:S:174:ILE:HD12 | 33:b:2:THR:HB     | 2.04                     | 0.40              |
| 31:6:334:LEU:H    | 31:6:334:LEU:HD23 | 1.86                     | 0.40              |
| 36:e:163:LEU:N    | 36:e:166:GLN:O    | 2.47                     | 0.40              |
| 44:q:149:ASP:HA   | 44:q:152:ARG:HG3  | 2.04                     | 0.40              |
| 58:k:82:THR:HG23  | 58:k:85:GLU:H     | 1.87                     | 0.40              |
| 1:A:1985:C:H3'    | 1:A:1986:C:C5'    | 2.52                     | 0.40              |
| 6:H:51:VAL:HG13   | 6:H:79:LEU:CD1    | 2.51                     | 0.40              |
| 35:d:137:PHE:CE2  | 35:d:212:VAL:HG11 | 2.57                     | 0.40              |
| 37:f:178:PRO:O    | 37:f:179:GLU:CB   | 2.68                     | 0.40              |
| 46:s:370:THR:HG22 | 46:s:383:ARG:HB2  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

entries.

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 3   | D     | 223/246 (91%) | 221 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 4   | E     | 306/348 (88%) | 293 (96%)  | 13 (4%) | 0        | 100         | 100 |
| 5   | F     | 248/294 (84%) | 245 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 6   | H     | 93/265 (35%)  | 93 (100%)  | 0       | 0        | 100         | 100 |
| 7   | I     | 159/262 (61%) | 156 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 8   | J     | 173/192 (90%) | 167 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 9   | K     | 175/178 (98%) | 175 (100%) | 0       | 0        | 100         | 100 |
| 10  | L     | 113/145 (78%) | 111 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 11  | M     | 285/295 (97%) | 281 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 12  | N     | 192/251 (76%) | 190 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 13  | O     | 151/176 (86%) | 149 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 14  | P     | 139/180 (77%) | 137 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 15  | Q     | 215/292 (74%) | 212 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 16  | R     | 138/149 (93%) | 137 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 17  | S     | 157/209 (75%) | 151 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 18  | T     | 164/206 (80%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 19  | U     | 123/146 (84%) | 122 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 20  | V     | 199/216 (92%) | 196 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 21  | W     | 98/148 (66%)  | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 22  | X     | 240/294 (82%) | 236 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 23  | Y     | 174/252 (69%) | 174 (100%) | 0       | 0        | 100         | 100 |
| 24  | Z     | 119/160 (74%) | 118 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 25  | x     | 322/356 (90%) | 310 (96%)  | 12 (4%) | 0        | 100         | 100 |
| 26  | 0     | 106/187 (57%) | 106 (100%) | 0       | 0        | 100         | 100 |
| 27  | 1     | 50/65 (77%)   | 50 (100%)  | 0       | 0        | 100         | 100 |
| 28  | 2     | 44/92 (48%)   | 43 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 29  | 3     | 93/188 (50%)  | 92 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 30  | 4     | 35/101 (35%)  | 35 (100%)  | 0       | 0        | 100         | 100 |
| 31  | 6     | 311/380 (82%) | 295 (95%)  | 16 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 32  | 7     | 290/336 (86%)    | 280 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 33  | b     | 146/159 (92%)    | 142 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 34  | c     | 277/303 (91%)    | 273 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 35  | d     | 205/306 (67%)    | 199 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 36  | e     | 187/283 (66%)    | 178 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 37  | f     | 98/211 (46%)     | 96 (98%)   | 1 (1%)   | 1 (1%)   | 12          | 25  |
| 38  | g     | 130/166 (78%)    | 128 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 39  | h     | 108/159 (68%)    | 105 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 40  | i     | 95/128 (74%)     | 94 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 41  | j     | 91/121 (75%)     | 88 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 42  | o     | 76/102 (74%)     | 76 (100%)  | 0        | 0        | 100         | 100 |
| 43  | p     | 140/206 (68%)    | 135 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 44  | q     | 133/222 (60%)    | 133 (100%) | 0        | 0        | 100         | 100 |
| 45  | r     | 153/196 (78%)    | 146 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 46  | s     | 373/442 (84%)    | 365 (98%)  | 8 (2%)   | 0        | 100         | 100 |
| 47  | u     | 123/228 (54%)    | 120 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 48  | v     | 67/70 (96%)      | 67 (100%)  | 0        | 0        | 100         | 100 |
| 49  | w     | 77/156 (49%)     | 71 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 50  | 5     | 392/423 (93%)    | 388 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 51  | 8     | 68/206 (33%)     | 67 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 52  | 9     | 120/135 (89%)    | 118 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 53  | a     | 99/142 (70%)     | 96 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 54  | m     | 43/127 (34%)     | 41 (95%)   | 2 (5%)   | 0        | 100         | 100 |
| 55  | l     | 56/135 (42%)     | 56 (100%)  | 0        | 0        | 100         | 100 |
| 56  | z     | 309/326 (95%)    | 293 (95%)  | 15 (5%)  | 1 (0%)   | 36          | 54  |
| 57  | y     | 235/346 (68%)    | 232 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 58  | k     | 83/118 (70%)     | 78 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| All | All   | 9019/12025 (75%) | 8818 (98%) | 199 (2%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | z     | 92  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | f     | 179 | GLU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 3   | D     | 186/197 (94%) | 186 (100%) | 0        | 100         | 100 |
| 4   | E     | 270/298 (91%) | 270 (100%) | 0        | 100         | 100 |
| 5   | F     | 216/250 (86%) | 216 (100%) | 0        | 100         | 100 |
| 6   | H     | 86/228 (38%)  | 86 (100%)  | 0        | 100         | 100 |
| 7   | I     | 149/230 (65%) | 149 (100%) | 0        | 100         | 100 |
| 8   | J     | 138/152 (91%) | 138 (100%) | 0        | 100         | 100 |
| 9   | K     | 157/158 (99%) | 157 (100%) | 0        | 100         | 100 |
| 10  | L     | 99/122 (81%)  | 99 (100%)  | 0        | 100         | 100 |
| 11  | M     | 248/252 (98%) | 248 (100%) | 0        | 100         | 100 |
| 12  | N     | 175/216 (81%) | 175 (100%) | 0        | 100         | 100 |
| 13  | O     | 133/152 (88%) | 133 (100%) | 0        | 100         | 100 |
| 14  | P     | 123/157 (78%) | 123 (100%) | 0        | 100         | 100 |
| 15  | Q     | 197/258 (76%) | 197 (100%) | 0        | 100         | 100 |
| 16  | R     | 119/128 (93%) | 119 (100%) | 0        | 100         | 100 |
| 17  | S     | 145/180 (81%) | 145 (100%) | 0        | 100         | 100 |
| 18  | T     | 147/180 (82%) | 147 (100%) | 0        | 100         | 100 |
| 19  | U     | 114/133 (86%) | 114 (100%) | 0        | 100         | 100 |
| 20  | V     | 179/190 (94%) | 179 (100%) | 0        | 100         | 100 |
| 21  | W     | 84/116 (72%)  | 84 (100%)  | 0        | 100         | 100 |
| 22  | X     | 219/265 (83%) | 219 (100%) | 0        | 100         | 100 |
| 23  | Y     | 162/228 (71%) | 162 (100%) | 0        | 100         | 100 |
| 24  | Z     | 114/146 (78%) | 114 (100%) | 0        | 100         | 100 |
| 25  | x     | 283/311 (91%) | 283 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 26  | 0     | 97/170 (57%)  | 97 (100%)  | 0        | 100         | 100 |
| 27  | 1     | 49/60 (82%)   | 49 (100%)  | 0        | 100         | 100 |
| 28  | 2     | 40/77 (52%)   | 40 (100%)  | 0        | 100         | 100 |
| 29  | 3     | 88/165 (53%)  | 88 (100%)  | 0        | 100         | 100 |
| 30  | 4     | 35/90 (39%)   | 35 (100%)  | 0        | 100         | 100 |
| 31  | 6     | 280/335 (84%) | 280 (100%) | 0        | 100         | 100 |
| 32  | 7     | 269/301 (89%) | 269 (100%) | 0        | 100         | 100 |
| 33  | b     | 130/138 (94%) | 130 (100%) | 0        | 100         | 100 |
| 34  | c     | 245/262 (94%) | 245 (100%) | 0        | 100         | 100 |
| 35  | d     | 189/272 (70%) | 189 (100%) | 0        | 100         | 100 |
| 36  | e     | 166/238 (70%) | 166 (100%) | 0        | 100         | 100 |
| 37  | f     | 93/185 (50%)  | 93 (100%)  | 0        | 100         | 100 |
| 38  | g     | 122/148 (82%) | 122 (100%) | 0        | 100         | 100 |
| 39  | h     | 100/143 (70%) | 100 (100%) | 0        | 100         | 100 |
| 40  | i     | 87/111 (78%)  | 87 (100%)  | 0        | 100         | 100 |
| 41  | j     | 75/99 (76%)   | 75 (100%)  | 0        | 100         | 100 |
| 42  | o     | 65/85 (76%)   | 65 (100%)  | 0        | 100         | 100 |
| 43  | p     | 129/177 (73%) | 129 (100%) | 0        | 100         | 100 |
| 44  | q     | 117/187 (63%) | 117 (100%) | 0        | 100         | 100 |
| 45  | r     | 142/168 (84%) | 142 (100%) | 0        | 100         | 100 |
| 46  | s     | 329/378 (87%) | 329 (100%) | 0        | 100         | 100 |
| 47  | u     | 115/197 (58%) | 115 (100%) | 0        | 100         | 100 |
| 48  | v     | 60/61 (98%)   | 60 (100%)  | 0        | 100         | 100 |
| 49  | w     | 73/135 (54%)  | 73 (100%)  | 0        | 100         | 100 |
| 50  | 5     | 356/372 (96%) | 356 (100%) | 0        | 100         | 100 |
| 51  | 8     | 62/182 (34%)  | 62 (100%)  | 0        | 100         | 100 |
| 52  | 9     | 104/114 (91%) | 104 (100%) | 0        | 100         | 100 |
| 53  | a     | 97/129 (75%)  | 97 (100%)  | 0        | 100         | 100 |
| 54  | m     | 40/114 (35%)  | 40 (100%)  | 0        | 100         | 100 |
| 55  | l     | 56/112 (50%)  | 56 (100%)  | 0        | 100         | 100 |
| 56  | z     | 270/280 (96%) | 270 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 57  | y     | 220/322 (68%)    | 220 (100%)  | 0        | 100         | 100 |
| 58  | k     | 76/95 (80%)      | 76 (100%)   | 0        | 100         | 100 |
| All | All   | 8119/10449 (78%) | 8119 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 234 | GLN  |
| 4   | E     | 281 | ASN  |
| 4   | E     | 294 | ASN  |
| 5   | F     | 97  | HIS  |
| 8   | J     | 48  | GLN  |
| 9   | K     | 74  | GLN  |
| 10  | L     | 104 | ASN  |
| 11  | M     | 31  | ASN  |
| 11  | M     | 113 | GLN  |
| 11  | M     | 218 | ASN  |
| 13  | O     | 100 | GLN  |
| 14  | P     | 88  | HIS  |
| 15  | Q     | 88  | ASN  |
| 15  | Q     | 172 | GLN  |
| 18  | T     | 127 | ASN  |
| 24  | Z     | 67  | HIS  |
| 25  | x     | 328 | GLN  |
| 25  | x     | 340 | HIS  |
| 26  | 0     | 117 | GLN  |
| 31  | 6     | 174 | HIS  |
| 31  | 6     | 239 | ASN  |
| 31  | 6     | 275 | GLN  |
| 32  | 7     | 252 | HIS  |
| 32  | 7     | 302 | HIS  |
| 33  | b     | 16  | HIS  |
| 34  | c     | 139 | GLN  |
| 34  | c     | 168 | HIS  |
| 35  | d     | 119 | GLN  |
| 36  | e     | 73  | GLN  |
| 37  | f     | 174 | GLN  |
| 37  | f     | 176 | ASN  |
| 40  | i     | 59  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | i     | 65  | ASN  |
| 41  | j     | 94  | GLN  |
| 45  | r     | 167 | HIS  |
| 46  | s     | 71  | HIS  |
| 46  | s     | 107 | GLN  |
| 46  | s     | 226 | GLN  |
| 46  | s     | 228 | ASN  |
| 46  | s     | 337 | GLN  |
| 48  | v     | 54  | GLN  |
| 49  | w     | 103 | HIS  |
| 50  | 5     | 302 | GLN  |
| 50  | 5     | 407 | GLN  |
| 53  | a     | 110 | GLN  |
| 55  | l     | 132 | ASN  |
| 56  | z     | 24  | HIS  |
| 56  | z     | 82  | ASN  |
| 57  | y     | 123 | GLN  |
| 57  | y     | 158 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1421/1584 (89%) | 478 (33%)         | 33 (2%)         |
| 2   | B     | 58/68 (85%)     | 23 (39%)          | 2 (3%)          |
| All | All   | 1479/1652 (89%) | 501 (33%)         | 35 (2%)         |

All (501) RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1094 | A    |
| 1   | A     | 1100 | C    |
| 1   | A     | 1101 | C    |
| 1   | A     | 1102 | U    |
| 1   | A     | 1103 | A    |
| 1   | A     | 1104 | G    |
| 1   | A     | 1112 | C    |
| 1   | A     | 1115 | A    |
| 1   | A     | 1116 | C    |
| 1   | A     | 1117 | A    |
| 1   | A     | 1118 | C    |
| 1   | A     | 1123 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1124 | U    |
| 1   | A     | 1128 | U    |
| 1   | A     | 1131 | A    |
| 1   | A     | 1134 | A    |
| 1   | A     | 1135 | U    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | A    |
| 1   | A     | 1138 | U    |
| 1   | A     | 1139 | A    |
| 1   | A     | 1140 | U    |
| 1   | A     | 1148 | A    |
| 1   | A     | 1151 | A    |
| 1   | A     | 1152 | U    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1160 | A    |
| 1   | A     | 1161 | C    |
| 1   | A     | 1162 | U    |
| 1   | A     | 1173 | G    |
| 1   | A     | 1187 | U    |
| 1   | A     | 1188 | A    |
| 1   | A     | 1189 | C    |
| 1   | A     | 1190 | A    |
| 1   | A     | 1191 | U    |
| 1   | A     | 1192 | C    |
| 1   | A     | 1193 | U    |
| 1   | A     | 1194 | A    |
| 1   | A     | 1195 | G    |
| 1   | A     | 1198 | G    |
| 1   | A     | 1205 | A    |
| 1   | A     | 1222 | A    |
| 1   | A     | 1233 | A    |
| 1   | A     | 1234 | C    |
| 1   | A     | 1235 | U    |
| 1   | A     | 1236 | A    |
| 1   | A     | 1237 | A    |
| 1   | A     | 1238 | U    |
| 1   | A     | 1240 | A    |
| 1   | A     | 1241 | A    |
| 1   | A     | 1248 | G    |
| 1   | A     | 1252 | A    |
| 1   | A     | 1253 | A    |
| 1   | A     | 1255 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | A    |
| 1   | A     | 1260 | A    |
| 1   | A     | 1264 | A    |
| 1   | A     | 1272 | A    |
| 1   | A     | 1276 | U    |
| 1   | A     | 1277 | U    |
| 1   | A     | 1278 | U    |
| 1   | A     | 1279 | G    |
| 1   | A     | 1280 | C    |
| 1   | A     | 1281 | A    |
| 1   | A     | 1282 | U    |
| 1   | A     | 1283 | A    |
| 1   | A     | 1284 | A    |
| 1   | A     | 1297 | A    |
| 1   | A     | 1300 | A    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1310 | A    |
| 1   | A     | 1311 | A    |
| 1   | A     | 1314 | G    |
| 1   | A     | 1315 | A    |
| 1   | A     | 1316 | A    |
| 1   | A     | 1318 | U    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1321 | A    |
| 1   | A     | 1331 | C    |
| 1   | A     | 1337 | A    |
| 1   | A     | 1344 | G    |
| 1   | A     | 1346 | G    |
| 1   | A     | 1347 | C    |
| 1   | A     | 1362 | U    |
| 1   | A     | 1364 | U    |
| 1   | A     | 1365 | A    |
| 1   | A     | 1366 | U    |
| 1   | A     | 1368 | A    |
| 1   | A     | 1386 | G    |
| 1   | A     | 1394 | G    |
| 1   | A     | 1396 | G    |
| 1   | A     | 1402 | A    |
| 1   | A     | 1413 | G    |
| 1   | A     | 1415 | G    |
| 1   | A     | 1421 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1422 | A    |
| 1   | A     | 1423 | G    |
| 1   | A     | 1428 | A    |
| 1   | A     | 1429 | C    |
| 1   | A     | 1430 | G    |
| 1   | A     | 1443 | G    |
| 1   | A     | 1449 | U    |
| 1   | A     | 1450 | A    |
| 1   | A     | 1458 | A    |
| 1   | A     | 1459 | A    |
| 1   | A     | 1460 | U    |
| 1   | A     | 1465 | U    |
| 1   | A     | 1466 | U    |
| 1   | A     | 1468 | A    |
| 1   | A     | 1470 | U    |
| 1   | A     | 1471 | U    |
| 1   | A     | 1473 | A    |
| 1   | A     | 1483 | U    |
| 1   | A     | 1484 | U    |
| 1   | A     | 1485 | G    |
| 1   | A     | 1490 | A    |
| 1   | A     | 1491 | A    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1493 | A    |
| 1   | A     | 1494 | A    |
| 1   | A     | 1496 | A    |
| 1   | A     | 1497 | A    |
| 1   | A     | 1502 | A    |
| 1   | A     | 1503 | U    |
| 1   | A     | 1504 | C    |
| 1   | A     | 1505 | A    |
| 1   | A     | 1506 | A    |
| 1   | A     | 1508 | A    |
| 1   | A     | 1511 | U    |
| 1   | A     | 1512 | A    |
| 1   | A     | 1513 | A    |
| 1   | A     | 1521 | U    |
| 1   | A     | 1525 | A    |
| 1   | A     | 1526 | G    |
| 1   | A     | 1531 | A    |
| 1   | A     | 1532 | A    |
| 1   | A     | 1534 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1536 | G    |
| 1   | A     | 1542 | C    |
| 1   | A     | 1543 | U    |
| 1   | A     | 1552 | A    |
| 1   | A     | 1553 | C    |
| 1   | A     | 1558 | A    |
| 1   | A     | 1559 | A    |
| 1   | A     | 1560 | A    |
| 1   | A     | 1565 | U    |
| 1   | A     | 1566 | U    |
| 1   | A     | 1573 | G    |
| 1   | A     | 1580 | U    |
| 1   | A     | 1583 | C    |
| 1   | A     | 1587 | A    |
| 1   | A     | 1588 | C    |
| 1   | A     | 1595 | U    |
| 1   | A     | 1596 | A    |
| 1   | A     | 1597 | A    |
| 1   | A     | 1599 | C    |
| 1   | A     | 1600 | A    |
| 1   | A     | 1601 | U    |
| 1   | A     | 1602 | U    |
| 1   | A     | 1603 | G    |
| 1   | A     | 1604 | U    |
| 1   | A     | 1605 | A    |
| 1   | A     | 1606 | G    |
| 1   | A     | 1608 | C    |
| 1   | A     | 1609 | C    |
| 1   | A     | 1610 | U    |
| 1   | A     | 1611 | A    |
| 1   | A     | 1613 | A    |
| 1   | A     | 1614 | A    |
| 1   | A     | 1615 | G    |
| 1   | A     | 1617 | A    |
| 1   | A     | 1618 | G    |
| 1   | A     | 1622 | C    |
| 1   | A     | 1624 | A    |
| 1   | A     | 1626 | U    |
| 1   | A     | 1627 | A    |
| 1   | A     | 1628 | A    |
| 1   | A     | 1629 | A    |
| 1   | A     | 1631 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1632 | A    |
| 1   | A     | 1633 | A    |
| 1   | A     | 1634 | G    |
| 1   | A     | 1635 | C    |
| 1   | A     | 1637 | U    |
| 1   | A     | 1638 | U    |
| 1   | A     | 1639 | C    |
| 1   | A     | 1641 | A    |
| 1   | A     | 1642 | G    |
| 1   | A     | 1643 | C    |
| 1   | A     | 1645 | C    |
| 1   | A     | 1647 | A    |
| 1   | A     | 1649 | A    |
| 1   | A     | 1650 | U    |
| 1   | A     | 1651 | A    |
| 1   | A     | 1653 | A    |
| 1   | A     | 1654 | A    |
| 1   | A     | 1658 | C    |
| 1   | A     | 1659 | A    |
| 1   | A     | 1660 | A    |
| 1   | A     | 1664 | A    |
| 1   | A     | 1665 | U    |
| 1   | A     | 1669 | A    |
| 1   | A     | 1671 | A    |
| 1   | A     | 1673 | U    |
| 1   | A     | 1675 | U    |
| 1   | A     | 1678 | A    |
| 1   | A     | 1682 | A    |
| 1   | A     | 1683 | C    |
| 1   | A     | 1684 | U    |
| 1   | A     | 1690 | A    |
| 1   | A     | 1693 | U    |
| 1   | A     | 1694 | U    |
| 1   | A     | 1698 | A    |
| 1   | A     | 1717 | U    |
| 1   | A     | 1718 | U    |
| 1   | A     | 1727 | A    |
| 1   | A     | 1730 | A    |
| 1   | A     | 1733 | G    |
| 1   | A     | 1748 | A    |
| 1   | A     | 1749 | A    |
| 1   | A     | 1755 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1756 | C    |
| 1   | A     | 1757 | A    |
| 1   | A     | 1758 | A    |
| 1   | A     | 1766 | G    |
| 1   | A     | 1767 | G    |
| 1   | A     | 1769 | A    |
| 1   | A     | 1784 | C    |
| 1   | A     | 1788 | G    |
| 1   | A     | 1793 | C    |
| 1   | A     | 1801 | A    |
| 1   | A     | 1804 | U    |
| 1   | A     | 1805 | A    |
| 1   | A     | 1806 | A    |
| 1   | A     | 1807 | U    |
| 1   | A     | 1821 | A    |
| 1   | A     | 1823 | A    |
| 1   | A     | 1826 | C    |
| 1   | A     | 1830 | C    |
| 1   | A     | 1831 | U    |
| 1   | A     | 1832 | A    |
| 1   | A     | 1834 | A    |
| 1   | A     | 1837 | U    |
| 1   | A     | 1843 | A    |
| 1   | A     | 1847 | A    |
| 1   | A     | 1851 | C    |
| 1   | A     | 1852 | U    |
| 1   | A     | 1853 | U    |
| 1   | A     | 1869 | A    |
| 1   | A     | 1871 | C    |
| 1   | A     | 1880 | U    |
| 1   | A     | 1882 | A    |
| 1   | A     | 1887 | A    |
| 1   | A     | 1888 | A    |
| 1   | A     | 1894 | A    |
| 1   | A     | 1902 | A    |
| 1   | A     | 1904 | A    |
| 1   | A     | 1914 | G    |
| 1   | A     | 1919 | C    |
| 1   | A     | 1922 | G    |
| 1   | A     | 1923 | A    |
| 1   | A     | 1926 | C    |
| 1   | A     | 1930 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1933 | G    |
| 1   | A     | 1936 | U    |
| 1   | A     | 1937 | A    |
| 1   | A     | 1939 | C    |
| 1   | A     | 1944 | A    |
| 1   | A     | 1945 | C    |
| 1   | A     | 1948 | C    |
| 1   | A     | 1957 | C    |
| 1   | A     | 1958 | A    |
| 1   | A     | 1964 | A    |
| 1   | A     | 1968 | U    |
| 1   | A     | 1976 | A    |
| 1   | A     | 1983 | G    |
| 1   | A     | 1986 | C    |
| 1   | A     | 1987 | A    |
| 1   | A     | 1988 | G    |
| 1   | A     | 1989 | U    |
| 1   | A     | 1991 | A    |
| 1   | A     | 2041 | A    |
| 1   | A     | 2042 | C    |
| 1   | A     | 2048 | C    |
| 1   | A     | 2050 | U    |
| 1   | A     | 2057 | G    |
| 1   | A     | 2058 | G    |
| 1   | A     | 2059 | G    |
| 1   | A     | 2060 | A    |
| 1   | A     | 2062 | U    |
| 1   | A     | 2063 | A    |
| 1   | A     | 2068 | G    |
| 1   | A     | 2069 | A    |
| 1   | A     | 2071 | C    |
| 1   | A     | 2073 | G    |
| 1   | A     | 2075 | U    |
| 1   | A     | 2076 | A    |
| 1   | A     | 2077 | A    |
| 1   | A     | 2082 | G    |
| 1   | A     | 2083 | G    |
| 1   | A     | 2091 | U    |
| 1   | A     | 2093 | U    |
| 1   | A     | 2097 | U    |
| 1   | A     | 2120 | C    |
| 1   | A     | 2123 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2130 | A    |
| 1   | A     | 2131 | A    |
| 1   | A     | 2132 | G    |
| 1   | A     | 2143 | A    |
| 1   | A     | 2146 | A    |
| 1   | A     | 2156 | G    |
| 1   | A     | 2158 | G    |
| 1   | A     | 2159 | A    |
| 1   | A     | 2161 | G    |
| 1   | A     | 2162 | A    |
| 1   | A     | 2169 | G    |
| 1   | A     | 2170 | G    |
| 1   | A     | 2176 | A    |
| 1   | A     | 2177 | A    |
| 1   | A     | 2180 | U    |
| 1   | A     | 2182 | U    |
| 1   | A     | 2186 | A    |
| 1   | A     | 2187 | C    |
| 1   | A     | 2190 | A    |
| 1   | A     | 2193 | U    |
| 1   | A     | 2194 | A    |
| 1   | A     | 2195 | U    |
| 1   | A     | 2196 | U    |
| 1   | A     | 2197 | U    |
| 1   | A     | 2227 | A    |
| 1   | A     | 2229 | A    |
| 1   | A     | 2230 | G    |
| 1   | A     | 2232 | A    |
| 1   | A     | 2236 | G    |
| 1   | A     | 2239 | U    |
| 1   | A     | 2240 | G    |
| 1   | A     | 2241 | A    |
| 1   | A     | 2248 | G    |
| 1   | A     | 2251 | U    |
| 1   | A     | 2252 | G    |
| 1   | A     | 2253 | G    |
| 1   | A     | 2254 | G    |
| 1   | A     | 2256 | U    |
| 1   | A     | 2257 | G    |
| 1   | A     | 2258 | A    |
| 1   | A     | 2259 | C    |
| 1   | A     | 2275 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2276 | U    |
| 1   | A     | 2277 | C    |
| 1   | A     | 2282 | G    |
| 1   | A     | 2284 | A    |
| 1   | A     | 2285 | U    |
| 1   | A     | 2286 | G    |
| 1   | A     | 2287 | A    |
| 1   | A     | 2289 | U    |
| 1   | A     | 2290 | A    |
| 1   | A     | 2291 | U    |
| 1   | A     | 2292 | A    |
| 1   | A     | 2293 | A    |
| 1   | A     | 2295 | C    |
| 1   | A     | 2297 | A    |
| 1   | A     | 2303 | A    |
| 1   | A     | 2325 | U    |
| 1   | A     | 2326 | A    |
| 1   | A     | 2327 | U    |
| 1   | A     | 2328 | C    |
| 1   | A     | 2329 | U    |
| 1   | A     | 2333 | U    |
| 1   | A     | 2334 | G    |
| 1   | A     | 2339 | A    |
| 1   | A     | 2340 | G    |
| 1   | A     | 2342 | U    |
| 1   | A     | 2343 | A    |
| 1   | A     | 2348 | U    |
| 1   | A     | 2351 | A    |
| 1   | A     | 2352 | U    |
| 1   | A     | 2354 | A    |
| 1   | A     | 2358 | G    |
| 1   | A     | 2359 | A    |
| 1   | A     | 2360 | C    |
| 1   | A     | 2363 | A    |
| 1   | A     | 2367 | A    |
| 1   | A     | 2369 | C    |
| 1   | A     | 2373 | G    |
| 1   | A     | 2375 | G    |
| 1   | A     | 2377 | U    |
| 1   | A     | 2391 | U    |
| 1   | A     | 2394 | U    |
| 1   | A     | 2396 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2397 | A    |
| 1   | A     | 2398 | G    |
| 1   | A     | 2399 | A    |
| 1   | A     | 2402 | U    |
| 1   | A     | 2404 | A    |
| 1   | A     | 2408 | C    |
| 1   | A     | 2410 | A    |
| 1   | A     | 2412 | A    |
| 1   | A     | 2414 | U    |
| 1   | A     | 2415 | U    |
| 1   | A     | 2416 | A    |
| 1   | A     | 2417 | G    |
| 1   | A     | 2418 | G    |
| 1   | A     | 2419 | G    |
| 1   | A     | 2427 | C    |
| 1   | A     | 2428 | C    |
| 1   | A     | 2430 | C    |
| 1   | A     | 2431 | G    |
| 1   | A     | 2437 | G    |
| 1   | A     | 2447 | A    |
| 1   | A     | 2458 | G    |
| 1   | A     | 2462 | A    |
| 1   | A     | 2464 | G    |
| 1   | A     | 2468 | U    |
| 1   | A     | 2475 | U    |
| 1   | A     | 2480 | U    |
| 1   | A     | 2481 | U    |
| 1   | A     | 2482 | G    |
| 1   | A     | 2486 | A    |
| 1   | A     | 2487 | A    |
| 1   | A     | 2493 | A    |
| 1   | A     | 2495 | A    |
| 1   | A     | 2496 | G    |
| 1   | A     | 2501 | A    |
| 1   | A     | 2502 | C    |
| 1   | A     | 2505 | G    |
| 1   | A     | 2515 | C    |
| 1   | A     | 2516 | A    |
| 1   | A     | 2519 | C    |
| 1   | A     | 2520 | C    |
| 1   | A     | 2521 | G    |
| 1   | A     | 2526 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2531 | A    |
| 1   | A     | 2532 | G    |
| 1   | A     | 2533 | G    |
| 1   | A     | 2538 | U    |
| 1   | A     | 2539 | U    |
| 1   | A     | 2542 | U    |
| 1   | A     | 2544 | U    |
| 1   | A     | 2550 | U    |
| 1   | A     | 2552 | C    |
| 1   | A     | 2564 | G    |
| 1   | A     | 2565 | U    |
| 1   | A     | 2570 | A    |
| 1   | A     | 2572 | G    |
| 1   | A     | 2575 | C    |
| 1   | A     | 2576 | A    |
| 1   | A     | 2582 | A    |
| 1   | A     | 2598 | A    |
| 1   | A     | 2600 | A    |
| 1   | A     | 2601 | U    |
| 1   | A     | 2603 | A    |
| 1   | A     | 2605 | C    |
| 1   | A     | 2615 | U    |
| 1   | A     | 2616 | U    |
| 1   | A     | 2617 | A    |
| 1   | A     | 2618 | A    |
| 1   | A     | 2619 | U    |
| 1   | A     | 2621 | U    |
| 1   | A     | 2625 | A    |
| 1   | A     | 2628 | A    |
| 1   | A     | 2629 | A    |
| 1   | A     | 2631 | A    |
| 1   | A     | 2635 | A    |
| 1   | A     | 2636 | A    |
| 1   | A     | 2639 | A    |
| 1   | A     | 2640 | A    |
| 1   | A     | 2647 | U    |
| 1   | A     | 2648 | A    |
| 1   | A     | 2650 | G    |
| 1   | A     | 2654 | A    |
| 1   | A     | 2655 | C    |
| 1   | A     | 2656 | C    |
| 1   | A     | 2659 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2660 | U    |
| 1   | A     | 2665 | U    |
| 1   | A     | 2666 | A    |
| 1   | A     | 2676 | A    |
| 2   | B     | 2    | U    |
| 2   | B     | 3    | U    |
| 2   | B     | 5    | A    |
| 2   | B     | 6    | U    |
| 2   | B     | 7    | G    |
| 2   | B     | 8    | U    |
| 2   | B     | 9    | A    |
| 2   | B     | 14   | A    |
| 2   | B     | 16   | U    |
| 2   | B     | 17   | A    |
| 2   | B     | 21   | A    |
| 2   | B     | 32   | U    |
| 2   | B     | 33   | G    |
| 2   | B     | 44   | G    |
| 2   | B     | 46   | U    |
| 2   | B     | 47   | G    |
| 2   | B     | 48   | G    |
| 2   | B     | 51   | A    |
| 2   | B     | 52   | U    |
| 2   | B     | 53   | U    |
| 2   | B     | 58   | C    |
| 2   | B     | 64   | A    |
| 2   | B     | 66   | C    |

All (35) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1130 | U    |
| 1   | A     | 1134 | A    |
| 1   | A     | 1137 | A    |
| 1   | A     | 1188 | A    |
| 1   | A     | 1189 | C    |
| 1   | A     | 1190 | A    |
| 1   | A     | 1194 | A    |
| 1   | A     | 1235 | U    |
| 1   | A     | 1237 | A    |
| 1   | A     | 1281 | A    |
| 1   | A     | 1422 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1428 | A    |
| 1   | A     | 1458 | A    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1541 | G    |
| 1   | A     | 1613 | A    |
| 1   | A     | 1638 | U    |
| 1   | A     | 1642 | G    |
| 1   | A     | 1683 | C    |
| 1   | A     | 1803 | U    |
| 1   | A     | 1893 | C    |
| 1   | A     | 1944 | A    |
| 1   | A     | 1967 | A    |
| 1   | A     | 2056 | A    |
| 1   | A     | 2057 | G    |
| 1   | A     | 2072 | G    |
| 1   | A     | 2076 | A    |
| 1   | A     | 2275 | A    |
| 1   | A     | 2302 | U    |
| 1   | A     | 2342 | U    |
| 1   | A     | 2414 | U    |
| 1   | A     | 2564 | G    |
| 1   | A     | 2659 | C    |
| 2   | B     | 8    | U    |
| 2   | B     | 52   | U    |

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

1 non-standard protein/DNA/RNA residue is 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 | $\# Z  > 2$ |
| 1   | PSU  | A     | 2509 | 1    | 18,21,22     | 0.46 | 0           | 21,30,33    | 0.58 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | PSU  | A     | 2509 | 1    | -       | 0/7/25/26 | 0/2/2/2 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 103 ligands modelled in this entry, 101 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 62  | GNP  | z     | 401 | -    | 34,34,34     | 1.15 | 5 (14%)     | 47,54,54    | 0.63 | 0           |
| 61  | FES  | r     | 201 | 45,7 | 0,4,4        | -    | -           | -           |      |             |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 62  | GNP  | z     | 401 | -    | -       | 2/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 61  | FES  | r     | 201 | 45,7 | -       | -        | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 62  | z     | 401 | GNP  | PB-O2B | -3.24 | 1.48        | 1.56     |
| 62  | z     | 401 | GNP  | PG-O1G | 3.14  | 1.50        | 1.46     |
| 62  | z     | 401 | GNP  | C6-N1  | -2.91 | 1.33        | 1.38     |
| 62  | z     | 401 | GNP  | PG-O3G | -2.18 | 1.51        | 1.56     |
| 62  | z     | 401 | GNP  | PG-O2G | -2.14 | 1.51        | 1.56     |

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

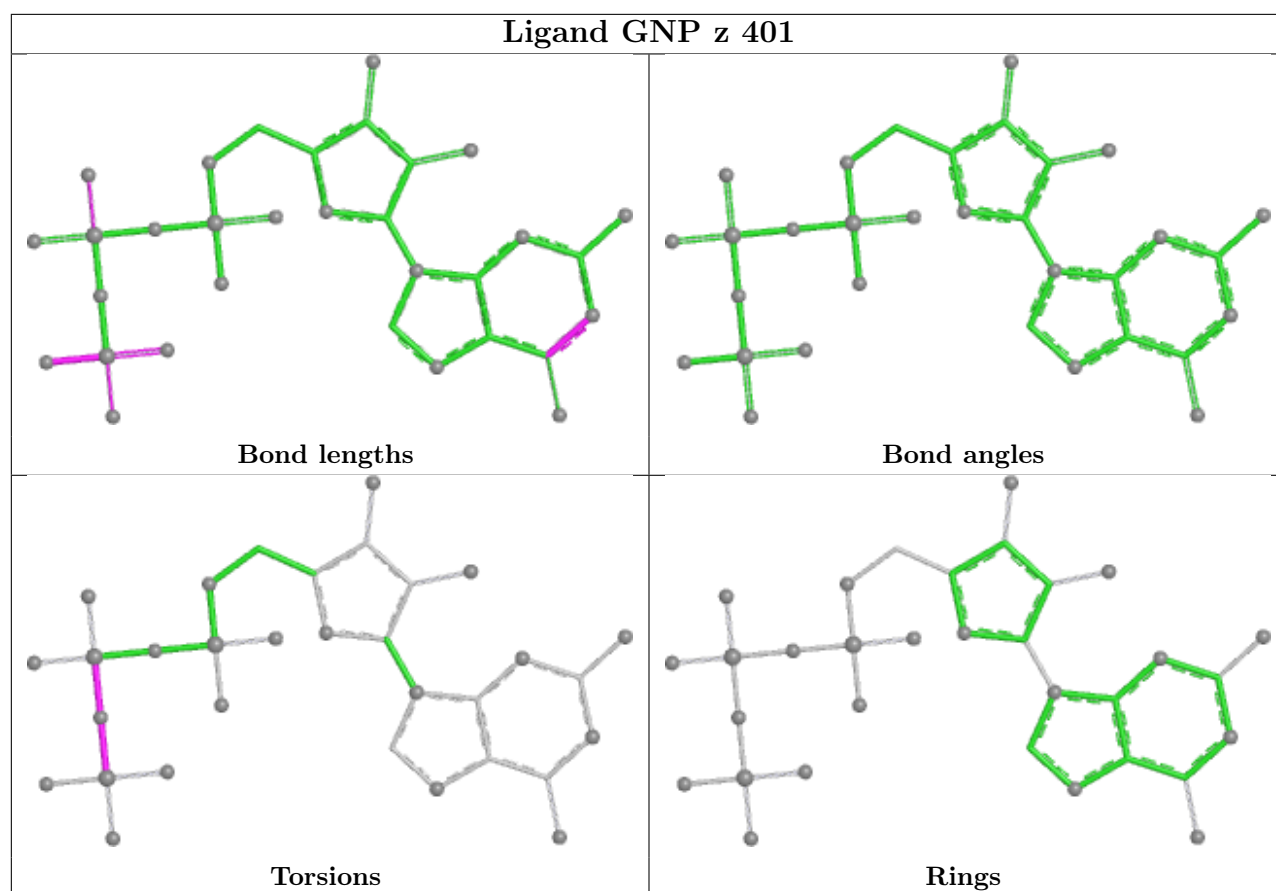
| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 62  | z     | 401 | GNP  | PB-N3B-PG-O1G |
| 62  | z     | 401 | GNP  | PG-N3B-PB-O1B |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 62  | z     | 401 | GNP  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

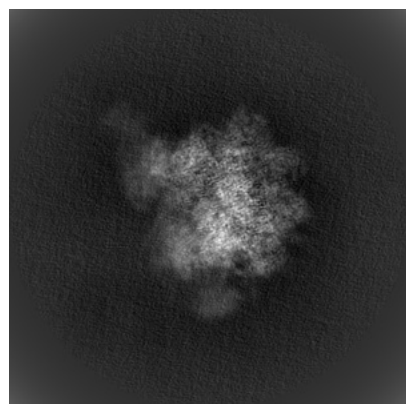
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52049. These allow visual inspection of the internal detail of the map and identification of artifacts.

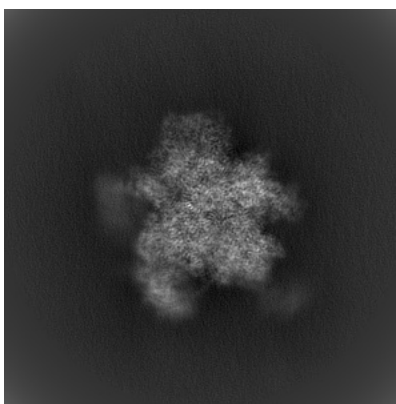
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

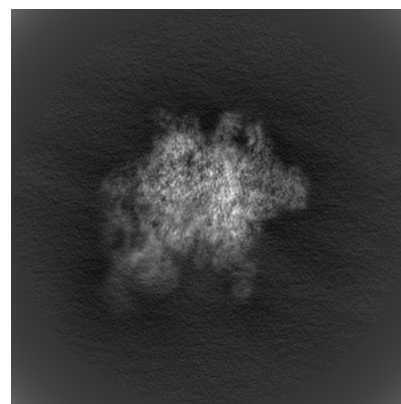
#### 6.1.1 Primary map



X

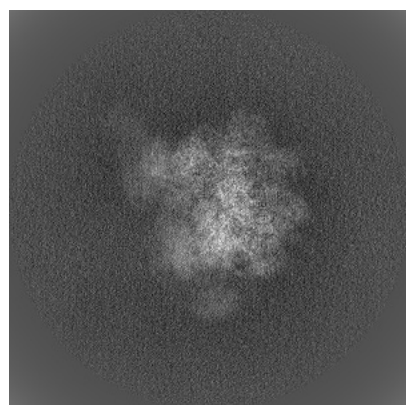


Y

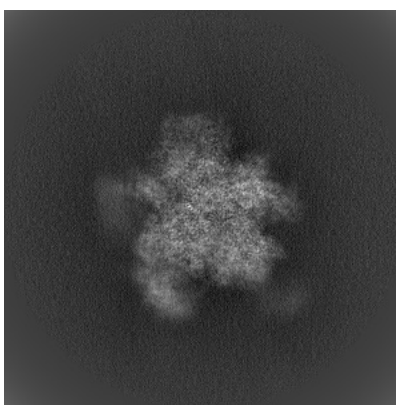


Z

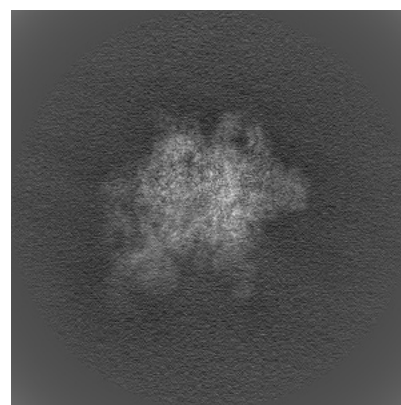
#### 6.1.2 Raw map



X



Y

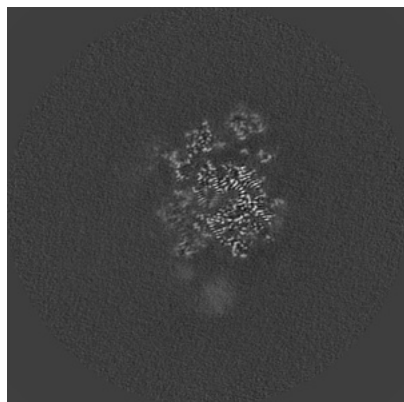


Z

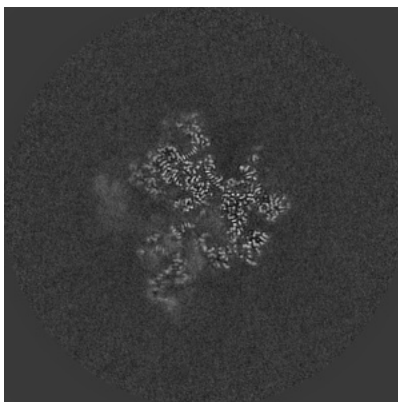
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

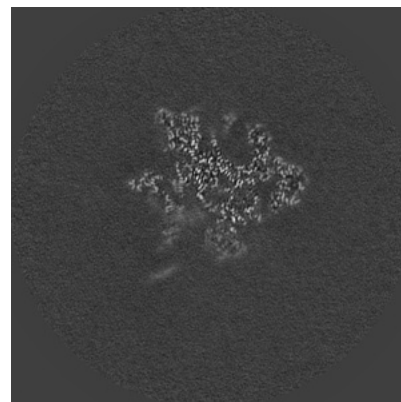
### 6.2.1 Primary map



X Index: 270

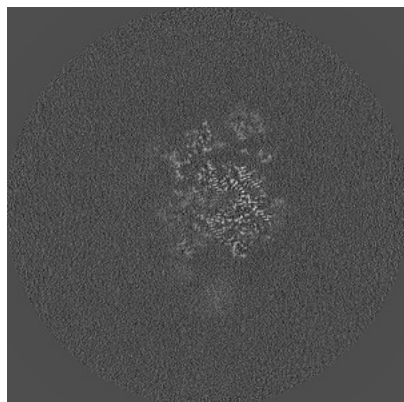


Y Index: 270

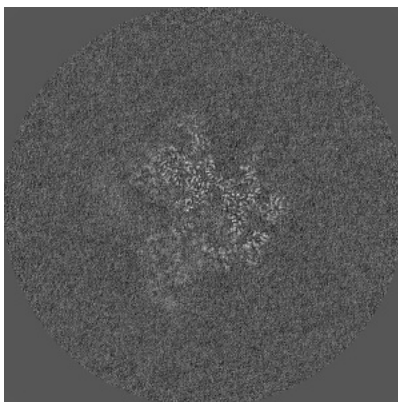


Z Index: 270

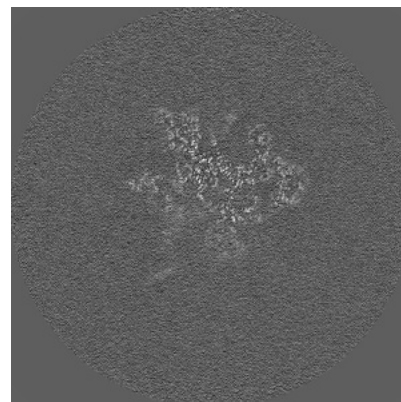
### 6.2.2 Raw map



X Index: 270



Y Index: 270

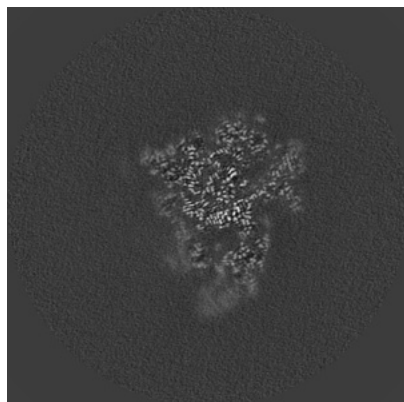


Z Index: 270

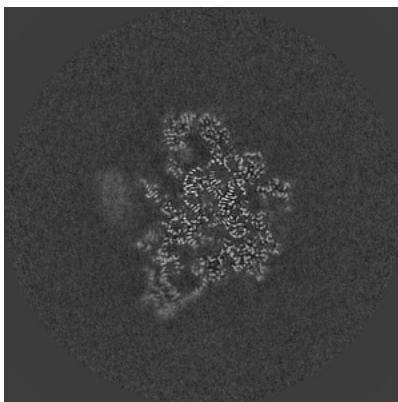
The images above show central slices of the map in three orthogonal directions.

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

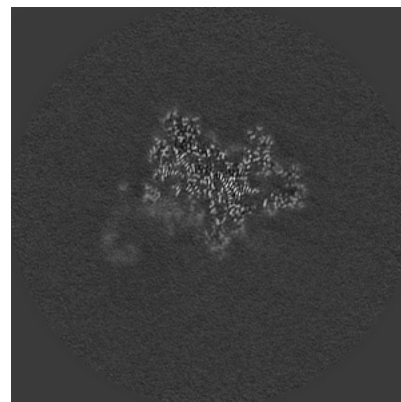
### 6.3.1 Primary map



X Index: 296

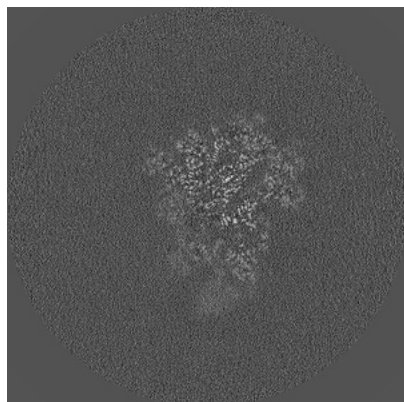


Y Index: 297

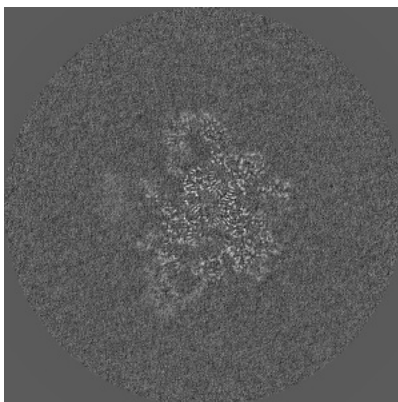


Z Index: 254

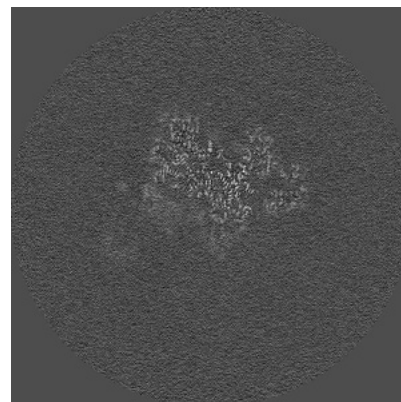
### 6.3.2 Raw map



X Index: 291



Y Index: 297

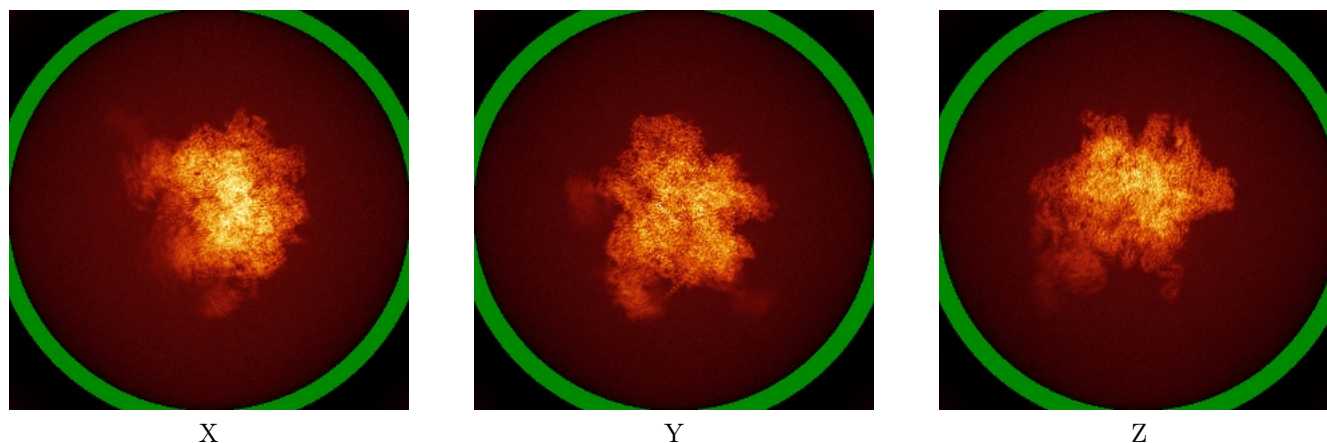


Z Index: 256

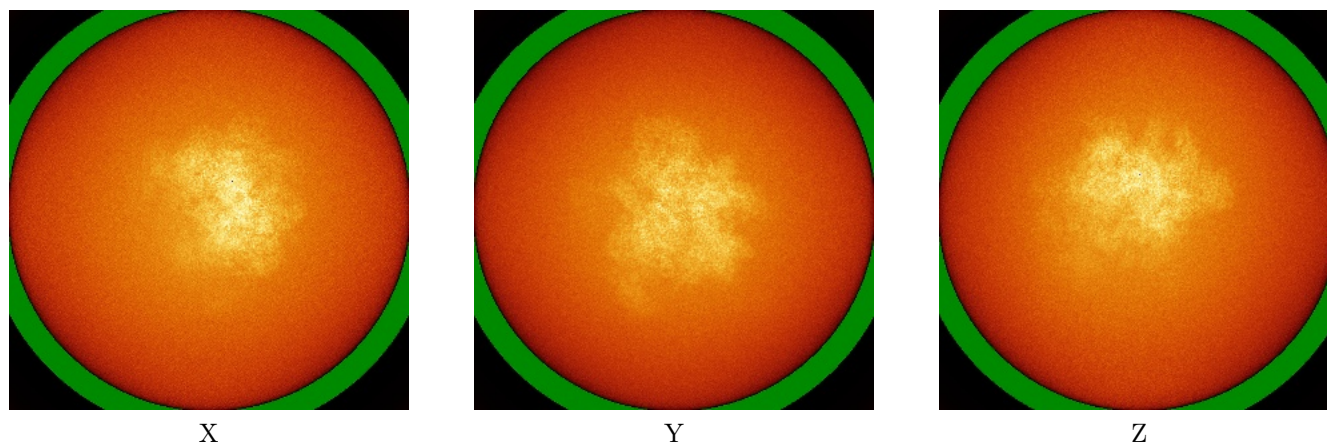
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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.

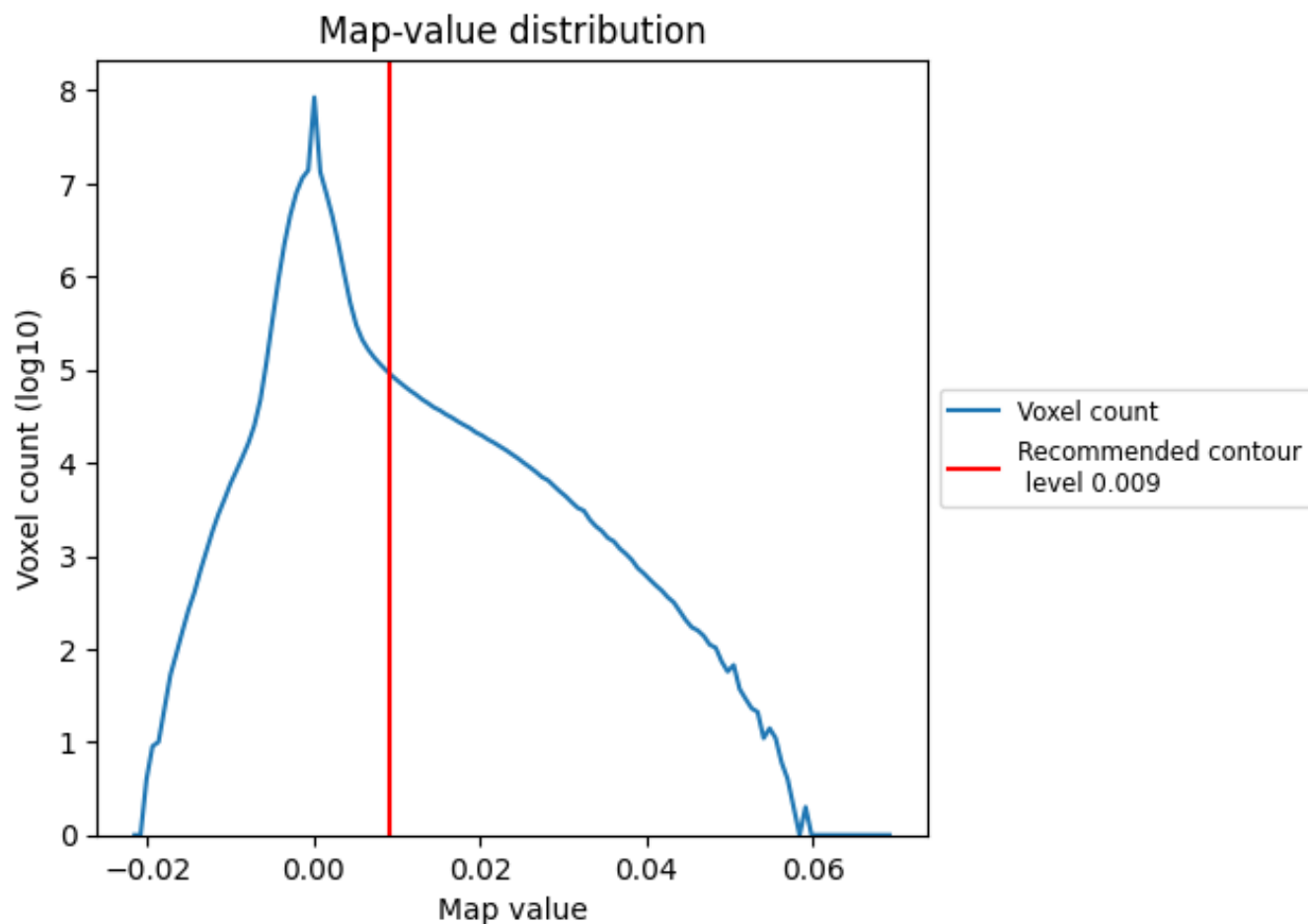
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

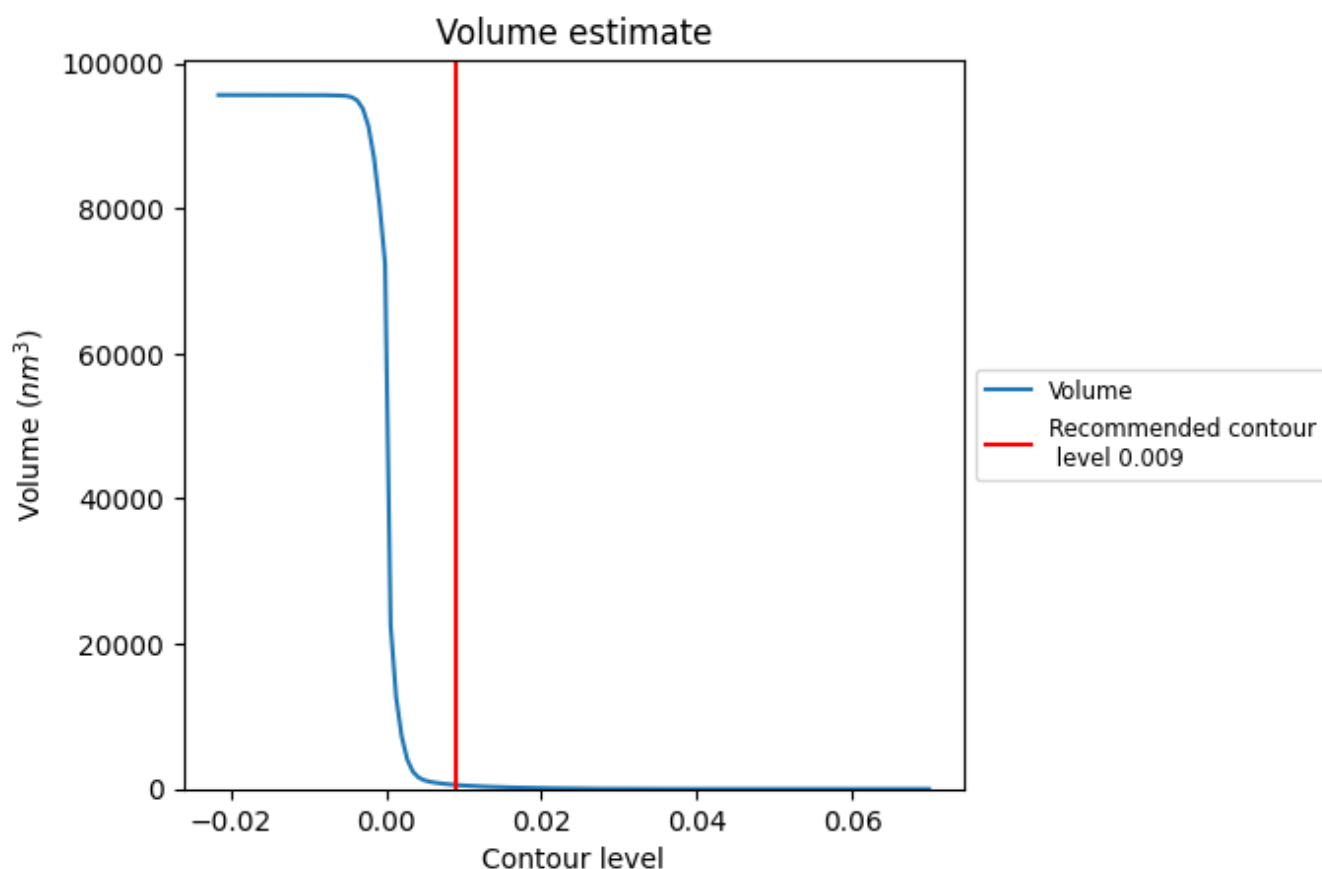
This section contains the results of statistical analysis of the map.

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



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

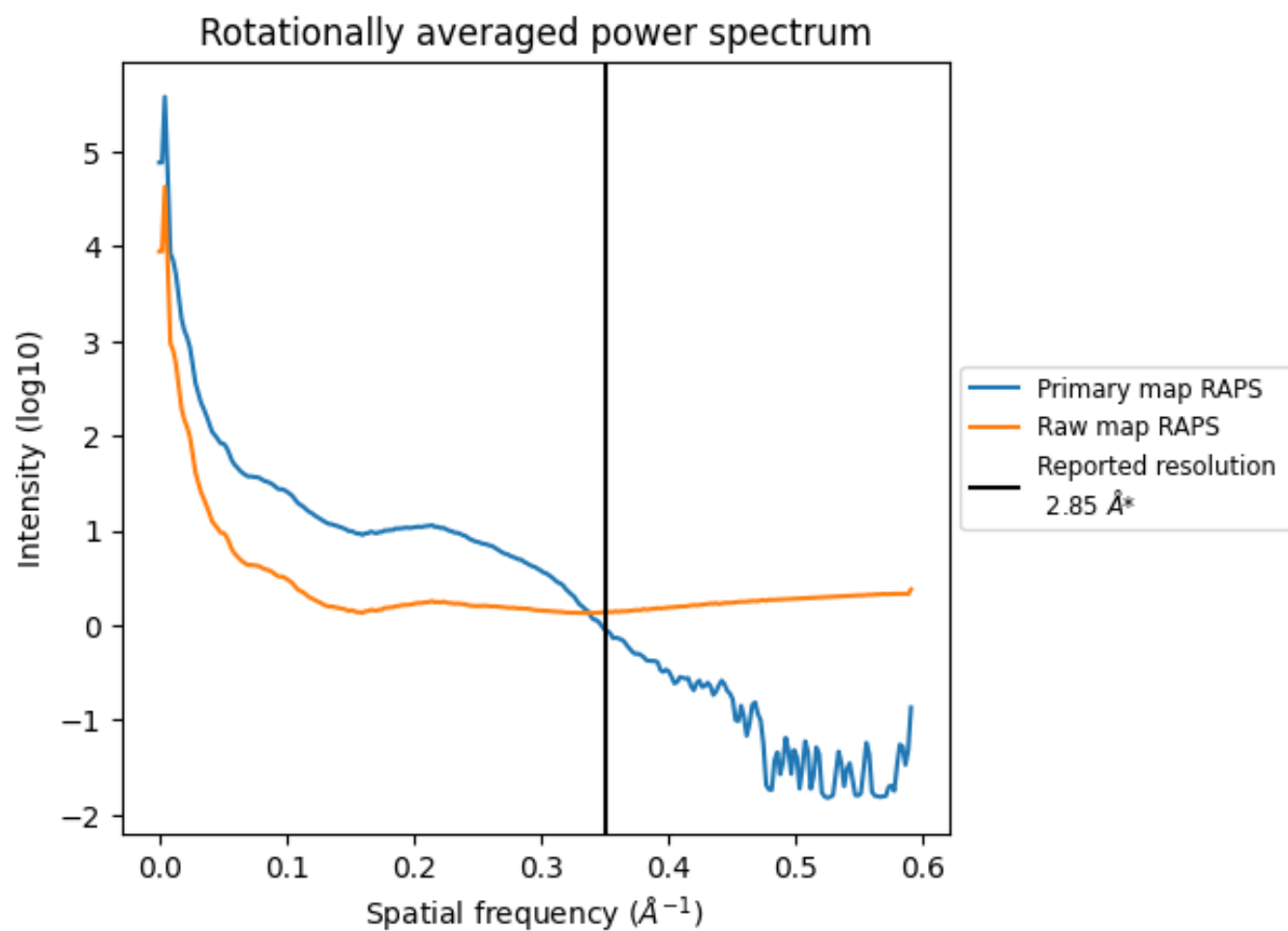
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 555 nm<sup>3</sup>; this corresponds to an approximate mass of 502 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 ⓘ

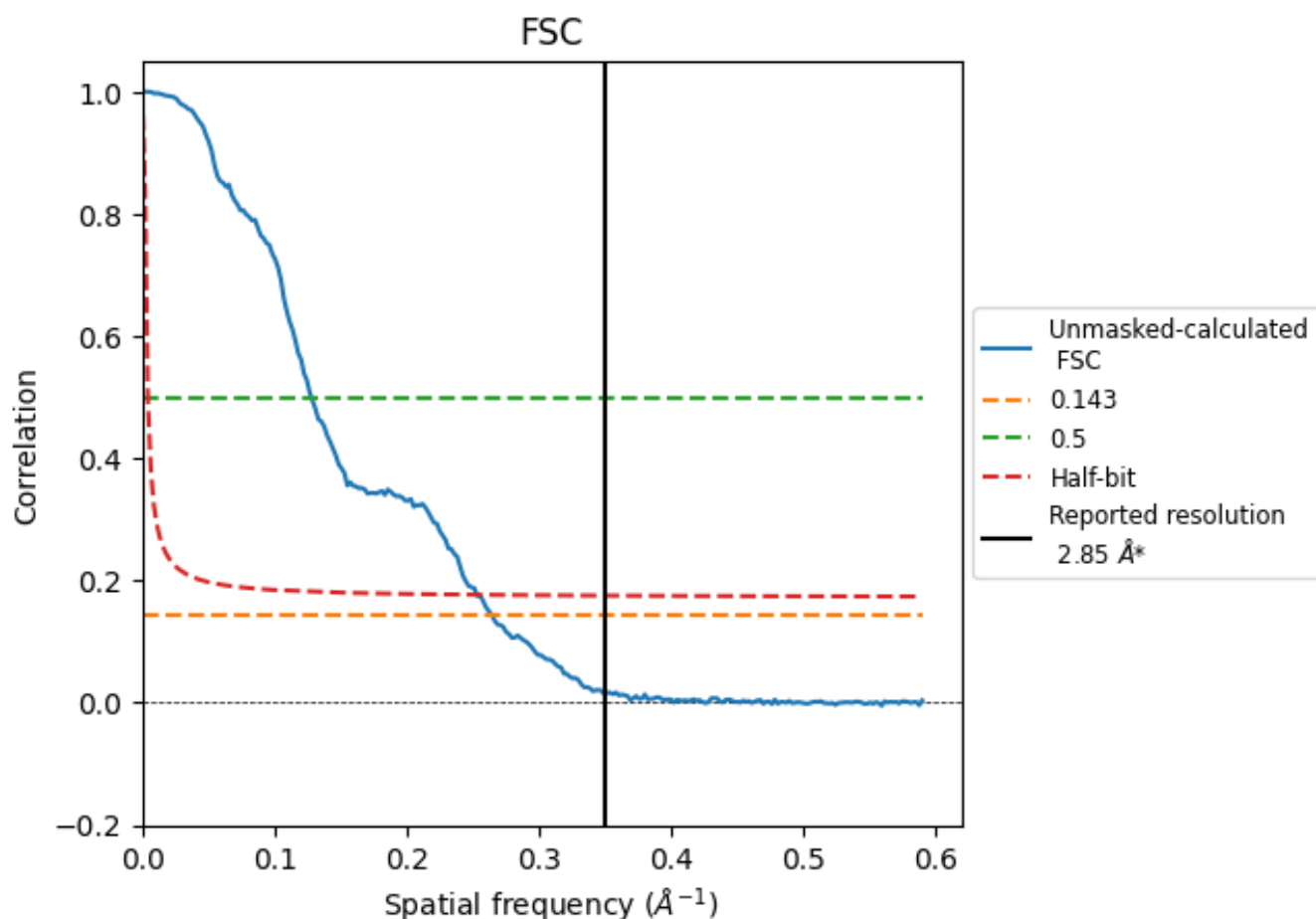


\*Reported resolution corresponds to spatial frequency of 0.351  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

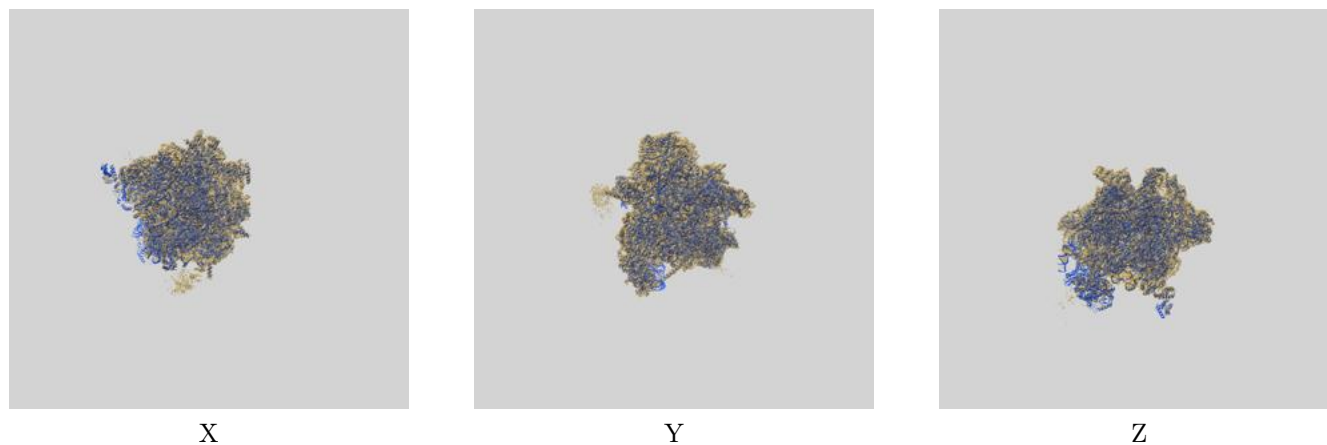
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.85                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.78                               | 7.81 | 3.95     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.85 by more than 10 %

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

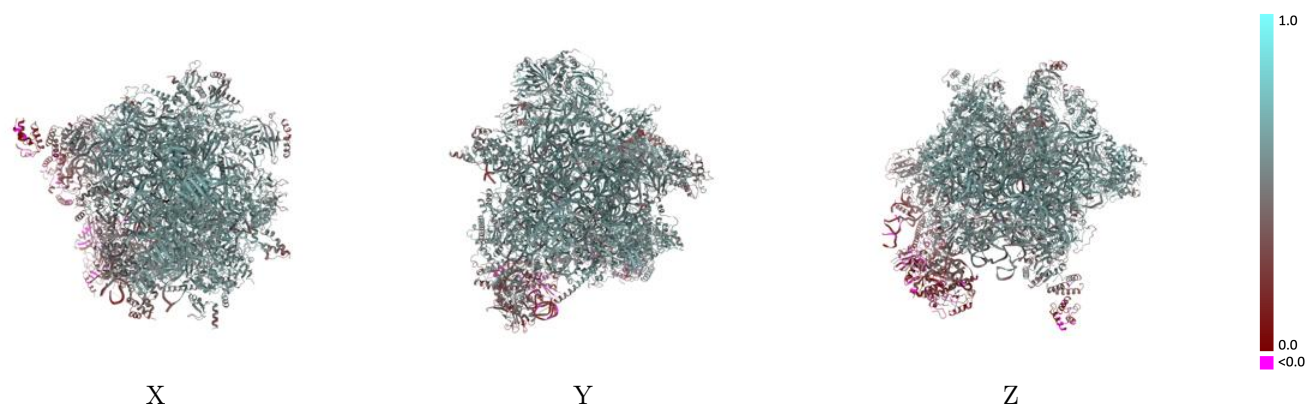
This section contains information regarding the fit between EMDB map EMD-52049 and PDB model 9HCH. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

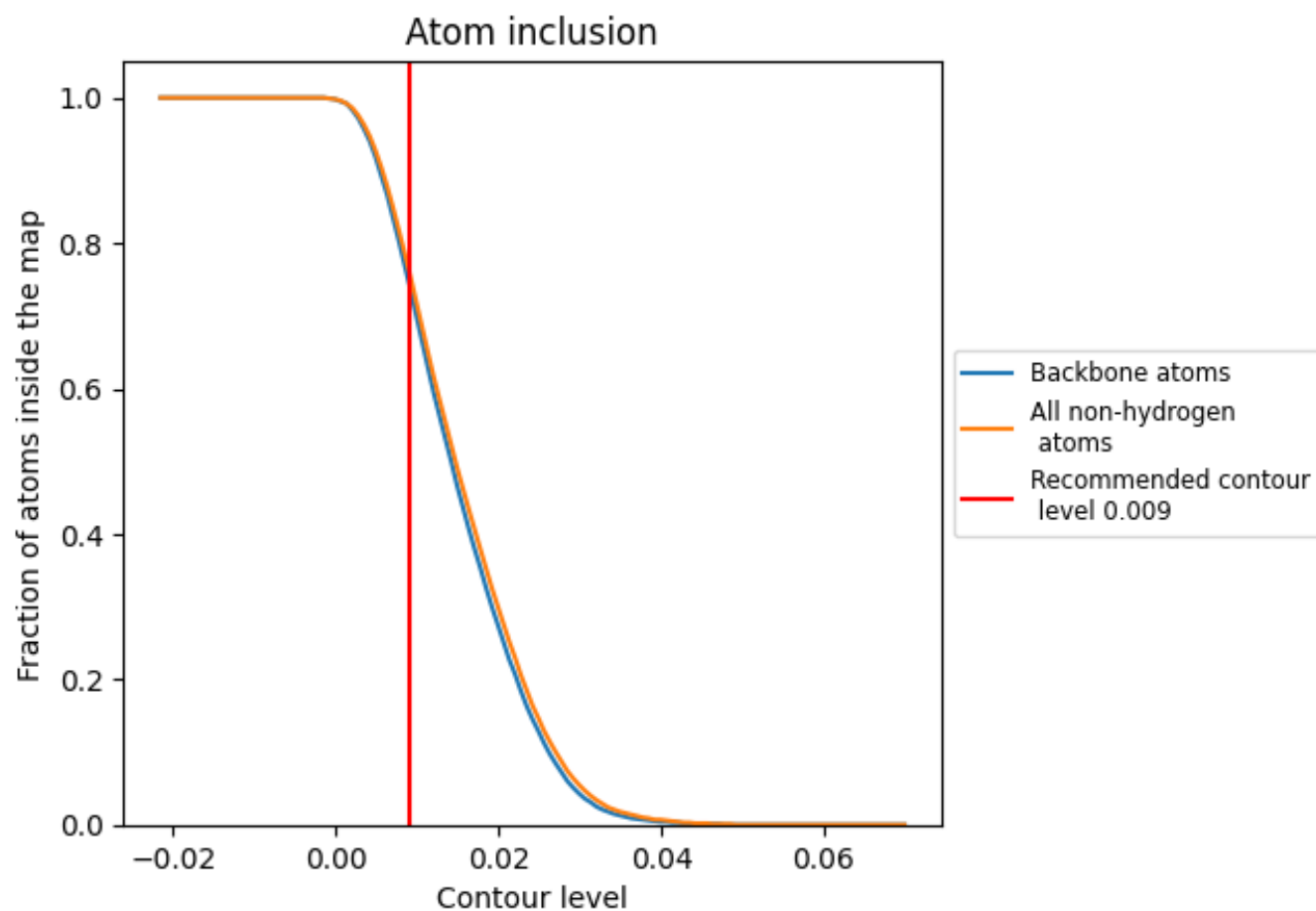


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.009) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7620   |  0.5190   |
| 0     |  0.8480   |  0.5720   |
| 1     |  0.7280   |  0.5280   |
| 2     |  0.9500   |  0.6500   |
| 3     |  0.9310   |  0.6290   |
| 4     |  0.7680   |  0.5470   |
| 5     |  0.8250   |  0.5710   |
| 6     |  0.6240   |  0.4100   |
| 7     |  0.7350   |  0.5160   |
| 8     |  0.1650   |  0.1920   |
| 9     |  0.8080   |  0.5570   |
| A     |  0.8880   |  0.5650   |
| B     |  0.3990   |  0.1710   |
| D     |  0.8340   |  0.5800   |
| E     |  0.8680  |  0.5890  |
| F     |  0.8870 |  0.6040 |
| H     |  0.7670 |  0.5440 |
| I     |  0.3280 |  0.2630 |
| J     |  0.0930 |  0.1730 |
| K     |  0.8870 |  0.6040 |
| L     |  0.7860 |  0.5640 |
| M     |  0.8840 |  0.6020 |
| N     |  0.5860 |  0.4880 |
| O     |  0.8740 |  0.5960 |
| P     |  0.6540 |  0.4370 |
| Q     |  0.8200 |  0.5590 |
| R     |  0.8940 |  0.6170 |
| S     |  0.8090 |  0.5730 |
| T     |  0.8800 |  0.6150 |
| U     |  0.8960 |  0.6150 |
| V     |  0.7770 |  0.5370 |
| W     |  0.7180 |  0.5080 |
| X     |  0.8360 |  0.5730 |
| Y     |  0.8740 |  0.5950 |
| Z     |  0.8310 |  0.5860 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.7110   |  0.5600   |
| b     |  0.8930   |  0.6050   |
| c     |  0.8120   |  0.5580   |
| d     |  0.7010   |  0.4970   |
| e     |  0.0230   |  0.1050   |
| f     |  0.1160   |  0.1880   |
| g     |  0.8660   |  0.5810   |
| h     |  0.7570   |  0.5220   |
| i     |  0.9280   |  0.6390   |
| j     |  0.7820   |  0.5400   |
| k     |  0.3880   |  0.3140   |
| l     |  0.2130   |  0.2380   |
| m     |  0.0400   |  0.1130   |
| o     |  0.8510   |  0.5820   |
| p     |  0.6510   |  0.4550   |
| q     |  0.7360   |  0.4940   |
| r     |  0.7980   |  0.5450   |
| s     |  0.8620  |  0.5900  |
| u     |  0.6290 |  0.4680 |
| v     |  0.4270 |  0.3640 |
| w     |  0.0730 |  0.1440 |
| x     |  0.5980 |  0.4290 |
| y     |  0.5950 |  0.4770 |
| z     |  0.4950 |  0.4590 |