



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 7OF7 / pdb\_00007of7  
EMDB ID : EMD-12872  
Title : Structure of a human mitochondrial ribosome large subunit assembly intermediate in complex with MTERF4-NSUN4 and GTPBP5 (dataset1).  
Authors : Hillen, H.S.; Lavdovskaia, E.; Nadler, F.; Hanitsch, E.; Linden, A.; Bohnsack, K.E.; Urlaub, H.; Richter-Dennerlein, R.  
Deposited on : 2021-05-04  
Resolution : 2.50 Å (reported)  
Based on initial model : 5OOL

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

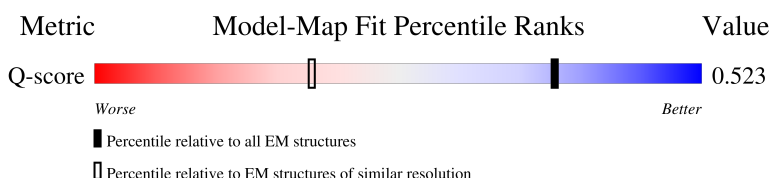
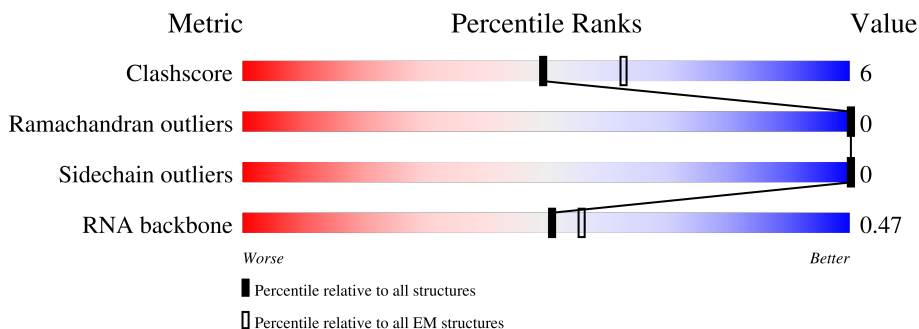
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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.



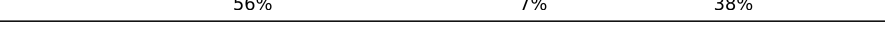
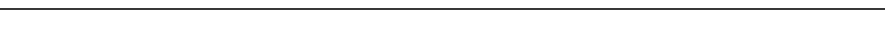
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 7115 ( 2.00 - 3.00 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 108    |                  |
| 2   | 1     | 65     |                  |
| 3   | 2     | 92     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 3     | 188    |    |
| 5   | 4     | 103    |    |
| 6   | 5     | 423    |    |
| 7   | 6     | 380    |    |
| 8   | 7     | 338    |    |
| 9   | 8     | 206    |    |
| 10  | 9     | 137    |    |
| 11  | A     | 1559   |    |
| 12  | B     | 69     |    |
| 13  | C     | 384    |    |
| 14  | D     | 305    |    |
| 15  | E     | 348    |   |
| 16  | F     | 311    |  |
| 17  | G     | 381    |  |
| 18  | H     | 267    |  |
| 19  | I     | 261    |  |
| 20  | J     | 192    |  |
| 21  | K     | 178    |  |
| 22  | L     | 145    |  |
| 23  | M     | 296    |  |
| 24  | N     | 251    |  |
| 25  | O     | 175    |  |
| 26  | P     | 180    |  |
| 27  | Q     | 292    |  |
| 28  | R     | 149    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | S     | 205    |                  |
| 30  | T     | 206    |                  |
| 31  | U     | 153    |                  |
| 32  | V     | 216    |                  |
| 33  | W     | 148    |                  |
| 34  | X     | 256    |                  |
| 35  | Y     | 250    |                  |
| 36  | Z     | 161    |                  |
| 37  | a     | 142    |                  |
| 38  | b     | 215    |                  |
| 39  | c     | 332    |                  |
| 40  | d     | 306    |                  |
| 41  | e     | 279    |                  |
| 42  | f     | 212    |                  |
| 43  | g     | 166    |                  |
| 44  | h     | 158    |                  |
| 45  | i     | 128    |                  |
| 46  | j     | 85     |                  |
| 47  | k     | 112    |                  |
| 48  | m     | 128    |                  |
| 49  | o     | 102    |                  |
| 50  | p     | 206    |                  |
| 51  | q     | 222    |                  |
| 52  | r     | 196    |                  |
| 53  | s     | 439    |                  |

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| Mol | Chain | Length | Quality of chain                             |
|-----|-------|--------|----------------------------------------------|
| 54  | u     | 234    | <div><div></div><div>40%7%53%</div></div>    |
| 55  | v     | 70     | <div><div></div><div>73%26%</div></div>      |
| 56  | w     | 156    | <div><div></div><div>6%37%13%49%</div></div> |
| 57  | x     | 406    | <div><div></div><div>29%7%64%</div></div>    |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 101032 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 0     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 880   | 545 | 172 | 157 | 6 |         |       |

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 433   | 278 | 83 | 70 | 2 |         |       |

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 367   | 227 | 81 | 58 | 1 |         |       |

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 3     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 831   | 539 | 162 | 127 | 3 |         |       |

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 333   | 212 | 71 | 47 | 3 |         |       |

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 5     | 392      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3199  | 2067 | 558 | 563 | 11 |         |       |

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | 6     | 324      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2723  | 1743 | 488 | 484 | 8 |         |       |

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | 7     | 287      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2334  | 1495 | 397 | 425 | 17 |         |       |

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | 8     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 413 | 113 | 123 | 2 |         |       |

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | 9     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 947   | 614 | 163 | 168 | 2 |         |       |

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 11  | A     | 1376     | Total | C     | N    | O    | P    | 0       | 0     |
|     |       |          | 29222 | 13113 | 5273 | 9460 | 1376 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| A     | 3107    | U        | N      | conflict | GB 1025814679 |

- Molecule 12 is a RNA chain called mitochondrial tRNA<sup>Val</sup>.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12  | B     | 56       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1191  | 534 | 214 | 387 | 56 |         |       |

- Molecule 13 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | C     | 338      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2690  | 1715 | 470 | 489 | 16 |         |       |

- Molecule 14 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | D     | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1872  | 1165 | 378 | 320 | 9 |         |       |

- Molecule 15 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | E     | 308      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2427  | 1559 | 423 | 434 | 11 |         |       |

- Molecule 16 is a protein called 39S ribosomal protein L4, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | F     | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2013  | 1294 | 365 | 348 | 6 |         |       |

- Molecule 17 is a protein called Transcription termination factor 4, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | G     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1943  | 1243 | 336 | 352 | 12 |         |       |

- Molecule 18 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18  | H     | 95       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 784   | 498 | 152 | 134 |         |       |

- Molecule 19 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 19  | I     | 158      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1283  | 828 | 235 | 210 | 10 |         |       |

- Molecule 20 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | J     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1061  | 680 | 192 | 187 | 2 |         |       |

- Molecule 21 is a protein called 39S ribosomal protein L13, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | K     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1451  | 934 | 259 | 251 | 7 |         |       |

- Molecule 22 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | L     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 889   | 559 | 171 | 154 | 5 |         |       |

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | M     | 287      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2305  | 1472 | 425 | 402 | 6 |         |       |

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | N     | 205      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1654  | 1056 | 308 | 280 | 10 |         |       |

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | O     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1245  | 784 | 239 | 215 | 7 |         |       |

- Molecule 26 is a protein called 39S ribosomal protein L18, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | P     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1148  | 719 | 221 | 203 | 5 |         |       |

- Molecule 27 is a protein called 39S ribosomal protein L19, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | Q     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1805  | 1159 | 317 | 320 | 9 |         |       |

- Molecule 28 is a protein called 39S ribosomal protein L20, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | R     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 971   | 616 | 200 | 151 | 4 |         |       |

- Molecule 29 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | S     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1251  | 806 | 222 | 219 | 4 |         |       |

- Molecule 30 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | T     | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1368  | 875 | 254 | 232 | 7 |         |       |

- Molecule 31 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | U     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1154  | 734 | 220 | 197 | 3 |         |       |

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | V     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 395   | 255 | 62 | 75 | 3 |         |       |

- Molecule 33 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | W     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 859   | 552 | 162 | 142 | 3 |         |       |

- Molecule 34 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | X     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2035  | 1317 | 351 | 362 | 5 |         |       |

- Molecule 35 is a protein called 39S ribosomal protein L47, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Y     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1517  | 970 | 291 | 252 | 4 |         |       |

- Molecule 36 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Z     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 937   | 598 | 175 | 161 | 3 |         |       |

- Molecule 37 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | a     | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 597   | 378 | 112 | 103 | 4 |         |       |

- Molecule 38 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | b     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1178  | 733 | 229 | 213 | 3 |         |       |

- Molecule 39 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | c     | 275      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2217  | 1415 | 383 | 410 | 9 |         |       |

- Molecule 40 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | d     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1075 | 276 | 293 | 9 |         |       |

- Molecule 41 is a protein called 39S ribosomal protein L46, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | e     | 197      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1599  | 1027 | 277 | 290 | 5 |         |       |

- Molecule 42 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | f     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 549 | 140 | 165 | 3 |         |       |

- Molecule 43 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | g     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1067  | 690 | 185 | 190 | 2 |         |       |

- Molecule 44 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | h     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 548 | 151 | 160 | 3 |         |       |

- Molecule 45 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | i     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 532 | 165 | 126 | 4 |         |       |

- Molecule 46 is a protein called 39S ribosomal protein L52, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | j     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 684   | 423 | 133 | 126 | 2 |         |       |

- Molecule 47 is a protein called 39S ribosomal protein L53, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | k     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 627   | 392 | 116 | 114 | 5 |         |       |

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48  | m     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 234   | 151 | 44 | 37 | 2 |         |       |

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | o     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 495 | 161 | 127 | 3 |         |       |

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | p     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1058  | 661 | 201 | 192 | 4 |         |       |

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | q     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1076  | 671 | 208 | 192 | 5 |         |       |

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | r     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 764 | 232 | 199 | 8 |         |       |

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | s     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3036  | 1946 | 542 | 534 | 14 |         |       |

- Molecule 54 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 54  | u     | 111      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 927   | 595 | 155 | 167 | 10 |         |       |

- Molecule 55 is a protein called MIEF1 upstream open reading frame protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 55  | v     | 69       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 588   | 372 | 116 | 100 |         |       |

- Molecule 56 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 56  | w     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 638   | 410 | 95 | 128 | 5 |         |       |

- Molecule 57 is a protein called Mitochondrial ribosome-associated GTPase 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | x     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1073  | 659 | 205 | 204 | 5 |         |       |

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 58  | 0     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 58  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 58  | r     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

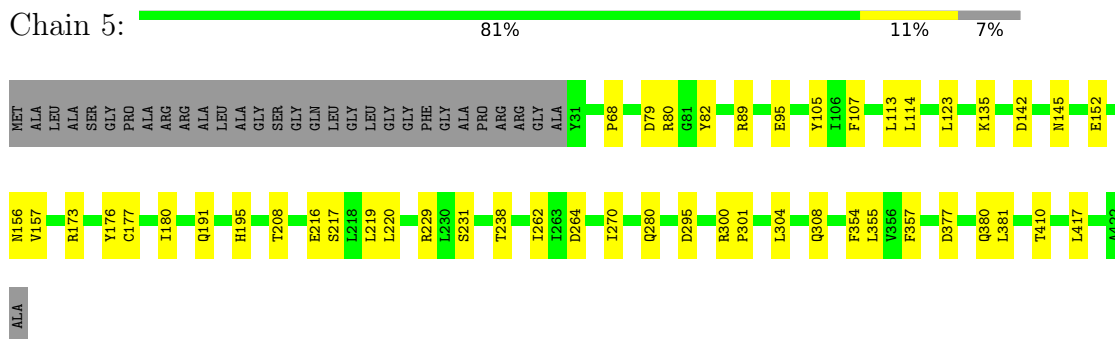
- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 59  | A     | 71       | Total | Mg | 0       |
|     |       |          | 71    | 71 |         |
| 59  | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 59  | W     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 59  | g     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

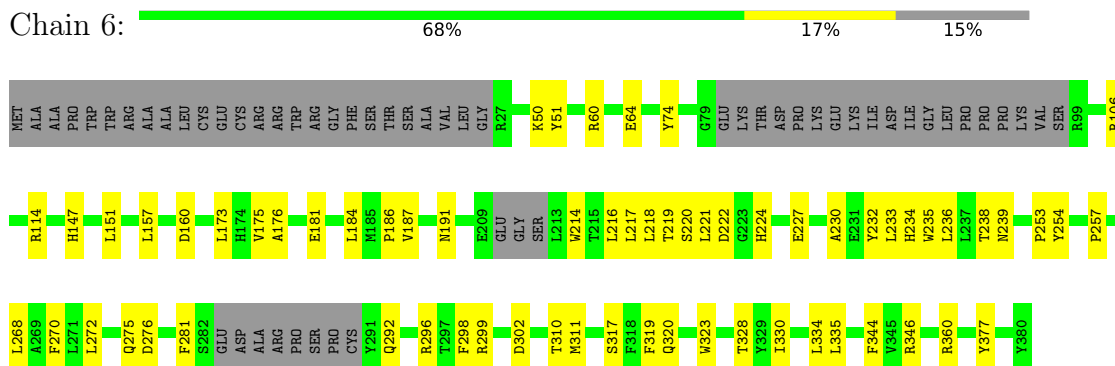




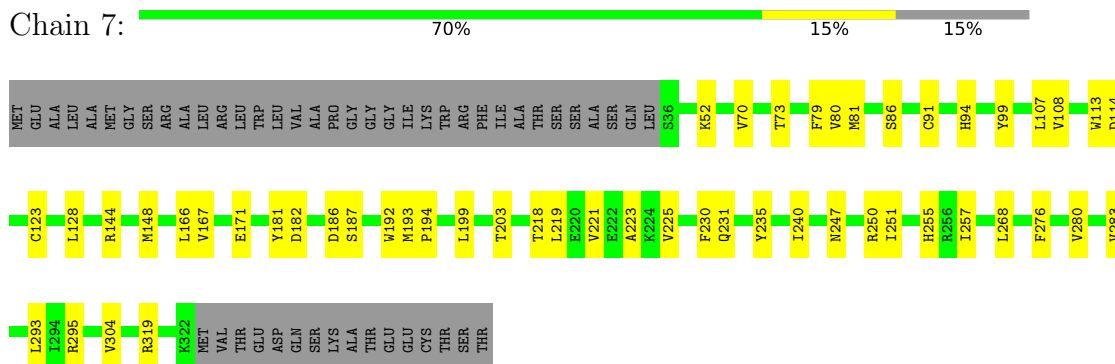
- Molecule 6: 39S ribosomal protein L37, mitochondrial



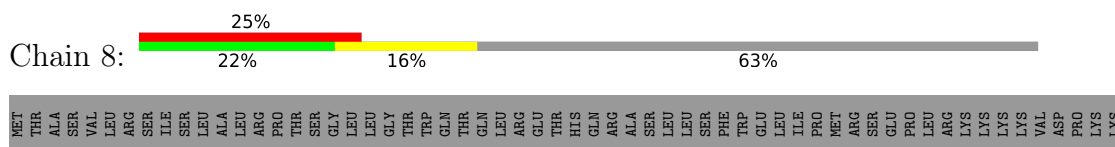
- Molecule 7: 39S ribosomal protein L38, mitochondrial

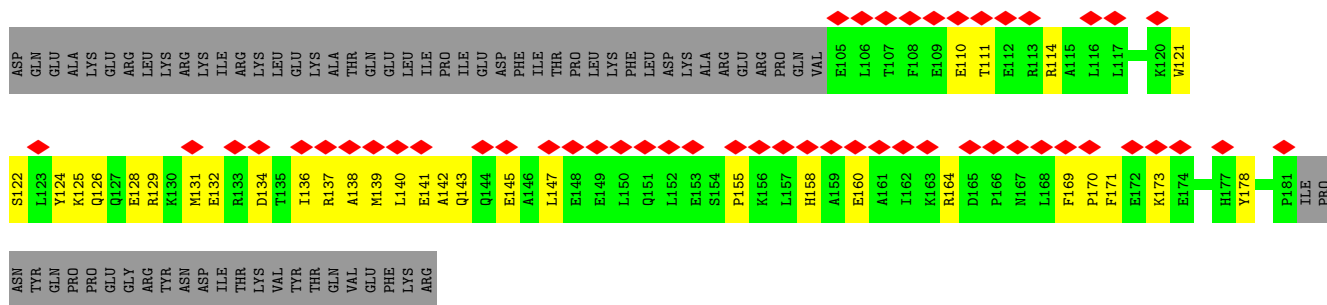


- Molecule 8: 39S ribosomal protein L39, mitochondrial

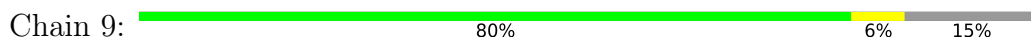


- Molecule 9: 39S ribosomal protein L40, mitochondrial

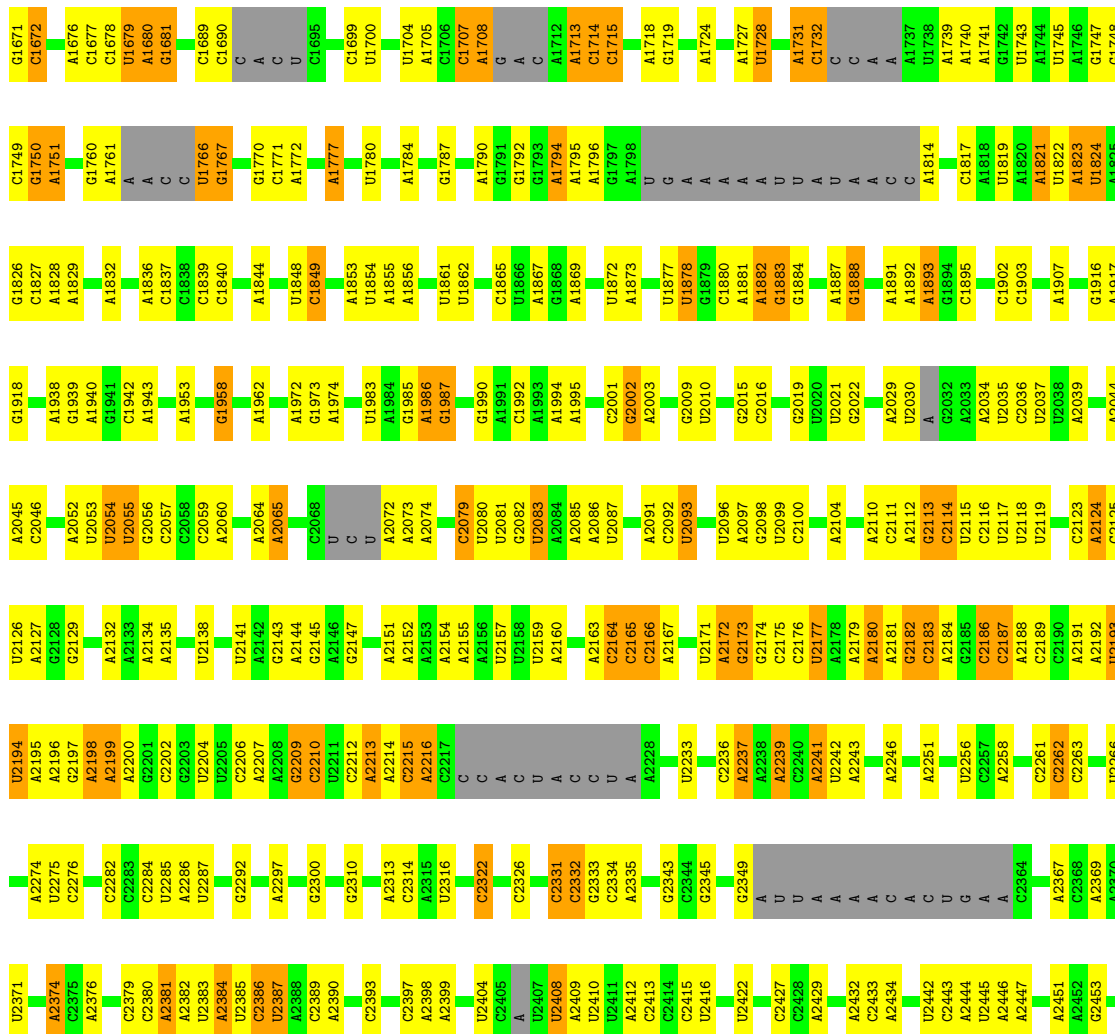




- Molecule 10: 39S ribosomal protein L41, mitochondrial



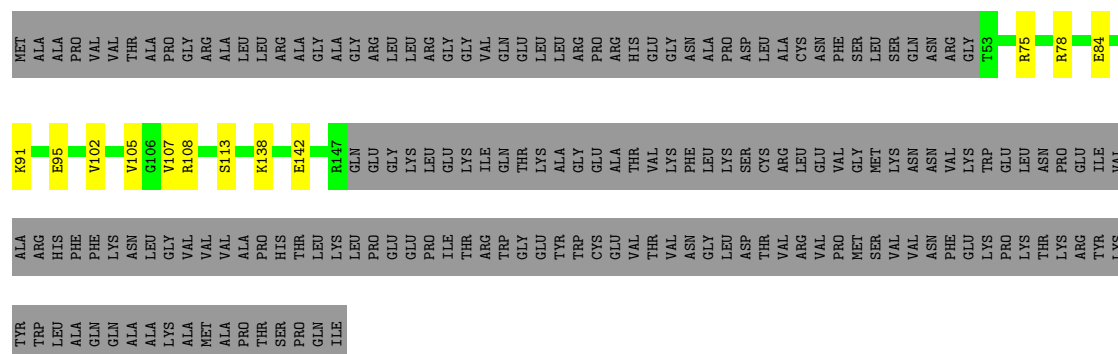
- Molecule 11: 16S ribosomal RNA



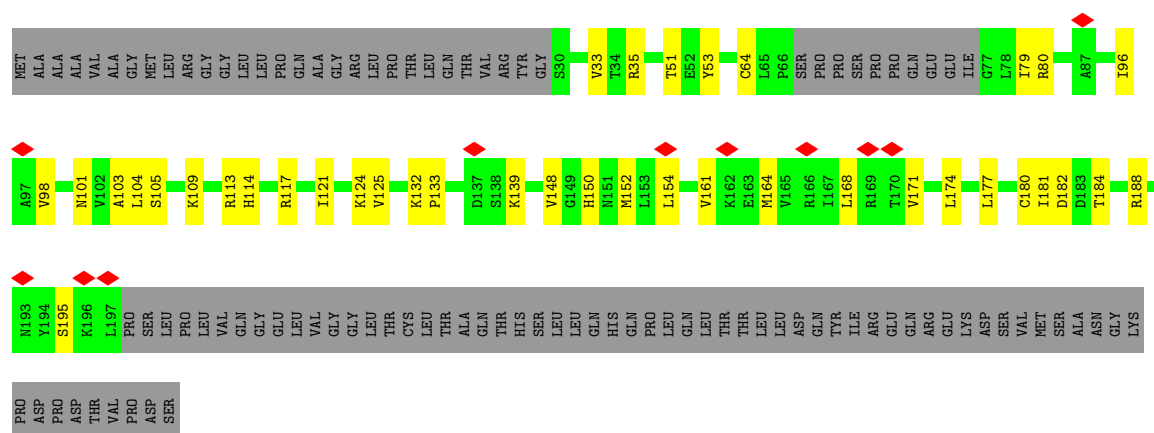




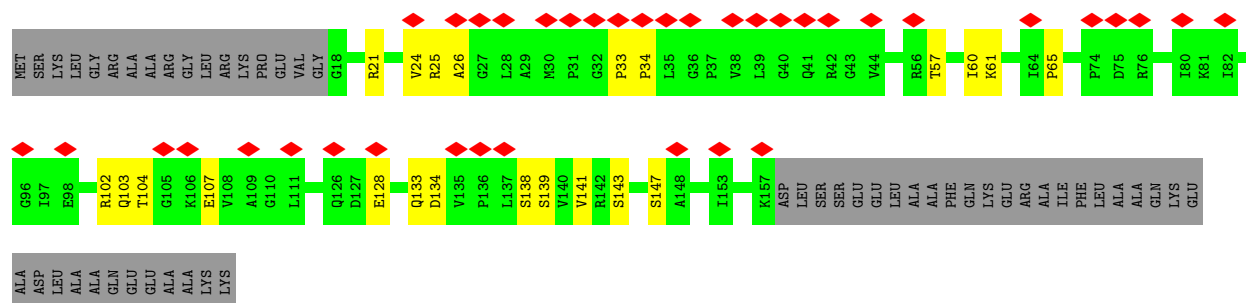
Chain H:  31% 0% 64%



Chain I:  46% 15% 39%



Chain J: 

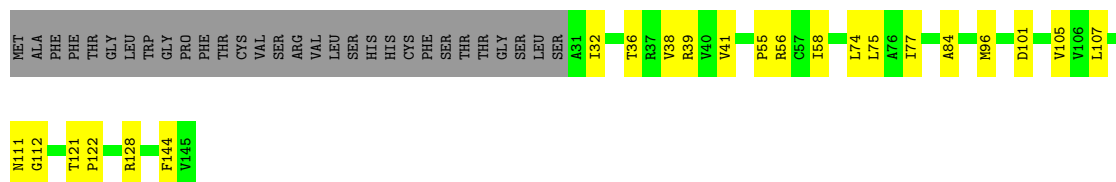


Chain K:  89% 10%



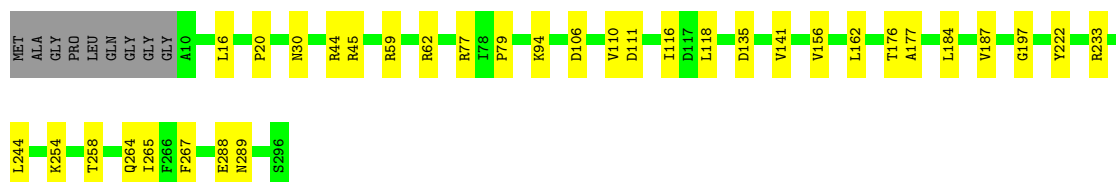
- Molecule 22: 39S ribosomal protein L14, mitochondrial

Chain L: 64% 15% 21%



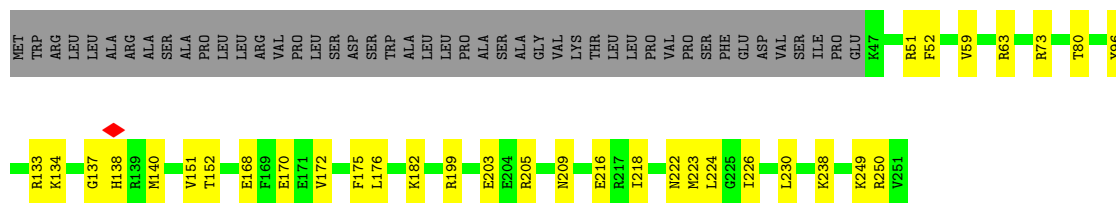
- Molecule 23: 39S ribosomal protein L15, mitochondrial

Chain M: 85% 11% .



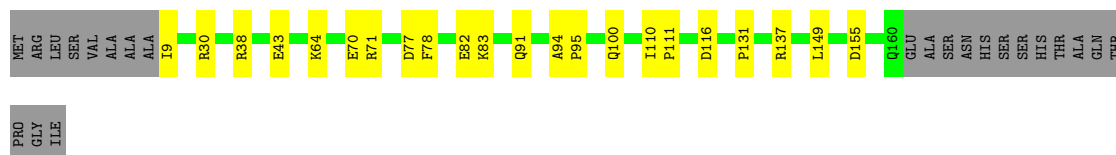
- Molecule 24: 39S ribosomal protein L16, mitochondrial

Chain N: 68% 14% 18%



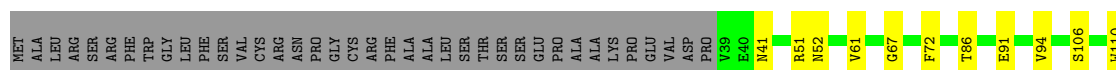
- Molecule 25: 39S ribosomal protein L17, mitochondrial

Chain O: 74% 13% 13%



- Molecule 26: 39S ribosomal protein L18, mitochondrial

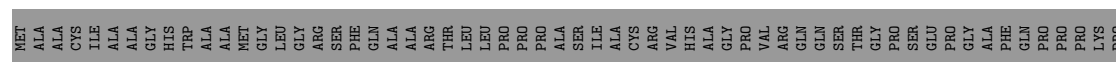
Chain P: 68% 11% 22%





- Molecule 27: 39S ribosomal protein L19, mitochondrial

Chain Q: 67% 7% 26%



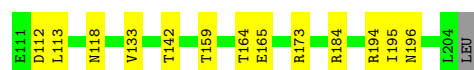
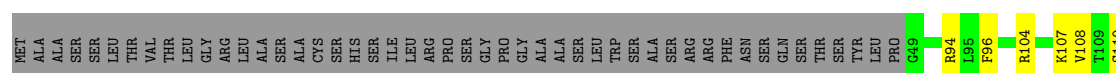
- Molecule 28: 39S ribosomal protein L20, mitochondrial

Chain R: 69% 9% 22%



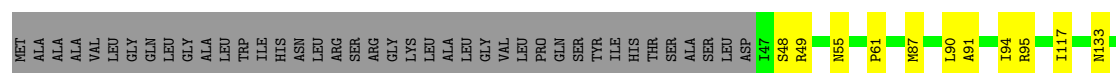
- Molecule 29: 39S ribosomal protein L21, mitochondrial

Chain S: 67% 9% 24%



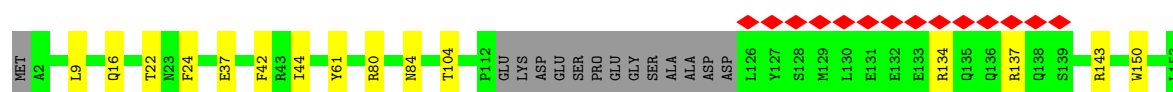
- Molecule 30: 39S ribosomal protein L22, mitochondrial

Chain T: 70% 11% 19%



- Molecule 31: 39S ribosomal protein L23, mitochondrial

Chain U: 9% 81% 10% 9%



- Molecule 32: 39S ribosomal protein L24, mitochondrial

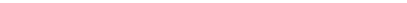
[illegible]

- |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Y99 | T100 | K101 | E102 | V105 | P106 | H107 | I117 | L120 | P121 | K122 | V125 | V131 | H132 | L148 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| MET | ALA  | SER  | VAL  | LEU  | ALA  | LEU  | THR  | ARG  | THR  | ALA  | THR  | LEU  | SER  | PRO  | THR | PRO | ALA | ALA | VAL | ARG | TYR | ALA | SER | SER | LYS | GLY | GLY | SER | SER | K40 | S47 | Y60 | V61 | N65 | I66 | I67 | Q70 | R71 | H72 | G78 | E94 | V97 | P98 |

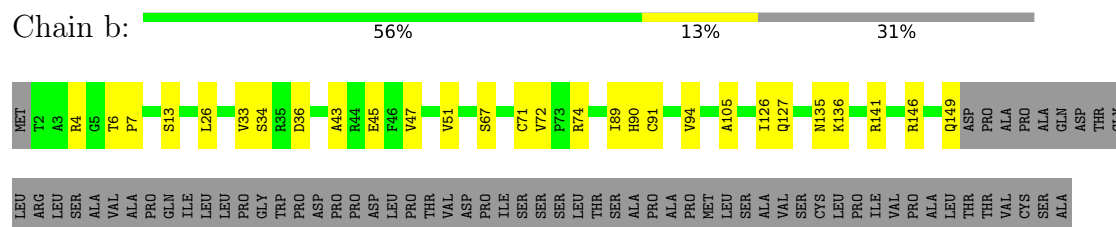
- |     |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | P2 | Y6 | L14 | Q15 | L16 | I20 | R23 | E35 | R44 | R61 | V62 | E63 | W80 | G81 | G82 | K96 | L97 | K102 | Q108 | R112 | V127 | T128 | P129 | R130 | T131 | P178 | E179 | L208 | D222 | S244 | GLJ | PRO | ALA | ALA | VAL | VAL | GLN | LYS | ARG | ALA | ALA | SER | GLY | GLN |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |     |     |     |     |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ARG | LYS | G63 | K80 | R123 | D151 | R154 | R170 | G174 | Q183 | V205 | R218 | F238 | PRO | HIS | LEU | ALA | GLU | ALA | GLN | LYS | SER | SER | GLY | PHE | LEU | SER | LEU | LEU | PRO | LYS | THR | PRO | ASN | VAL | THR | SER | PHE | HIS | GLN | TYR | ARG | LEU | LEU | HIS | THR | THR | LEU | SER |
|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

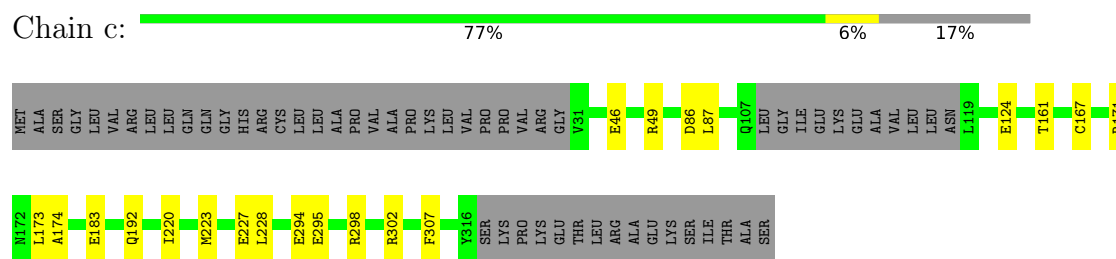
- [illegible]

- Chain a:  45% 5% 50%

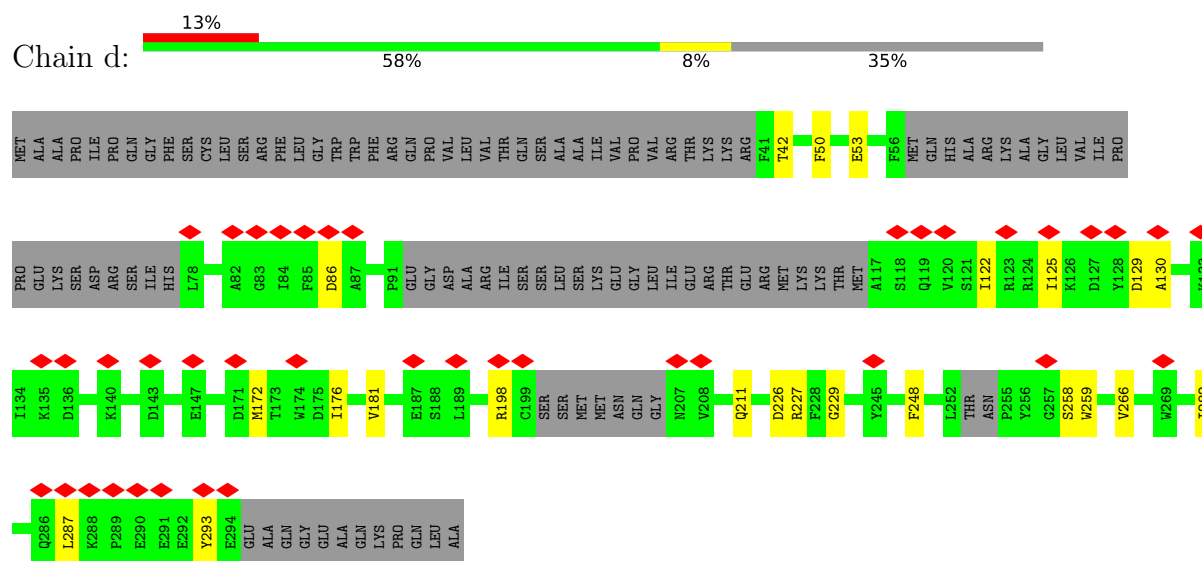
- Molecule 38: 39S ribosomal protein L43, mitochondrial



- Molecule 39: 39S ribosomal protein L44, mitochondrial

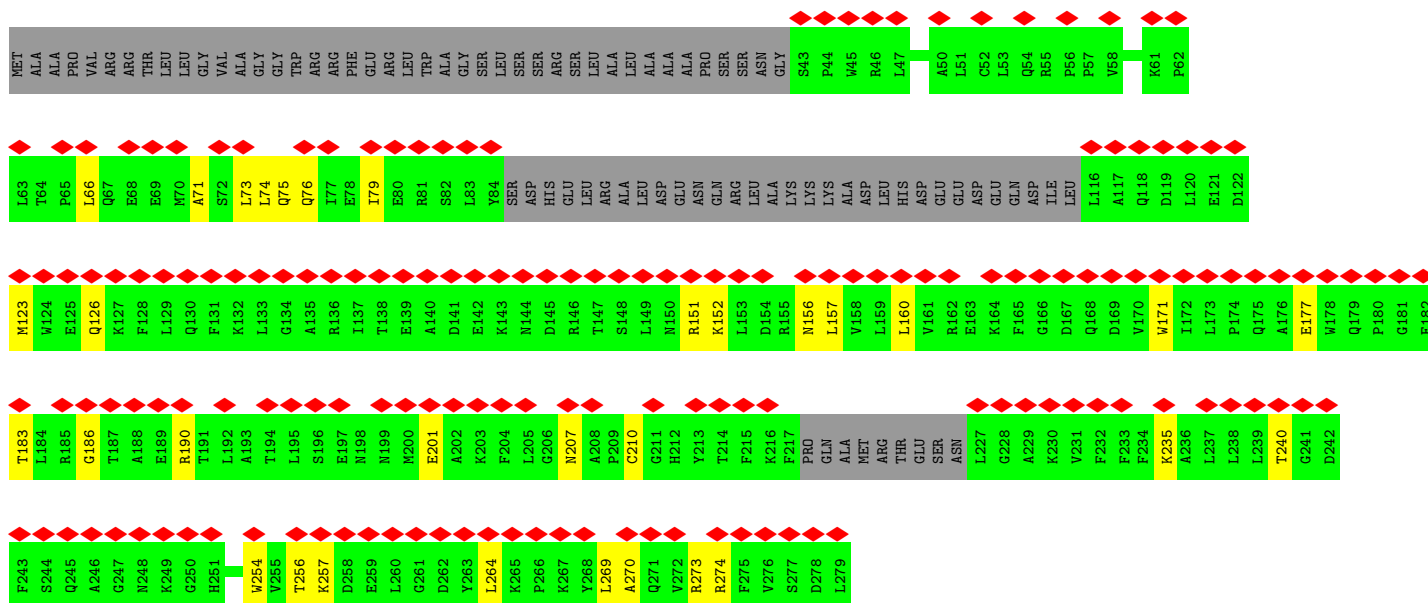


- Molecule 40: 39S ribosomal protein L45, mitochondrial

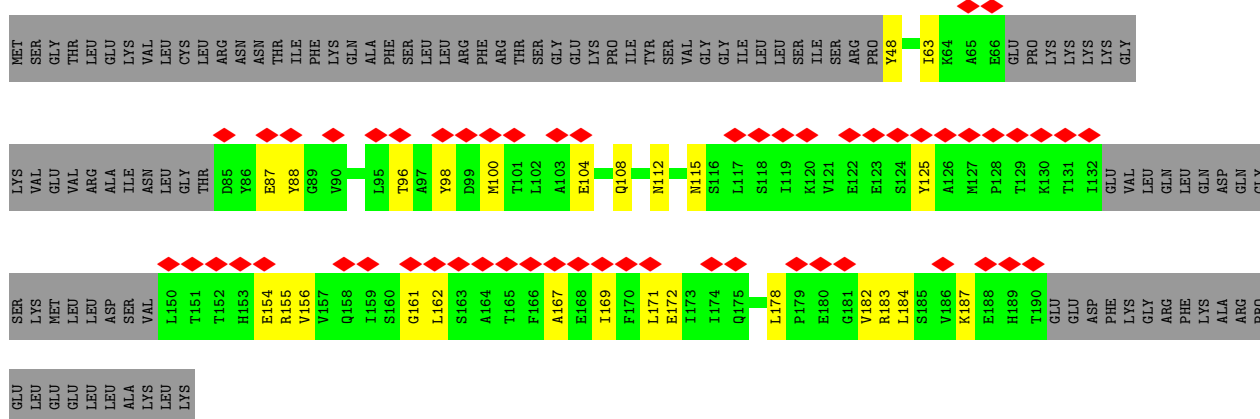
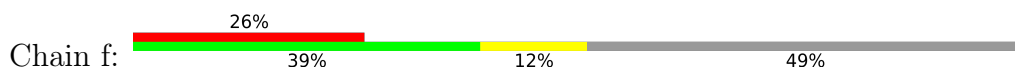


- Molecule 41: 39S ribosomal protein L46, mitochondrial

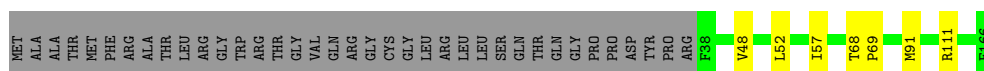




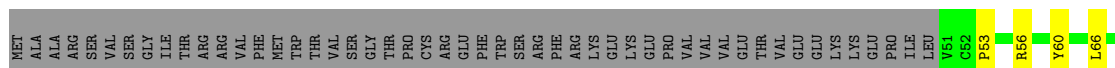
- Molecule 42: 39S ribosomal protein L48, mitochondrial



- Molecule 43: 39S ribosomal protein L49, mitochondrial



- Molecule 44: 39S ribosomal protein L50, mitochondrial





- Molecule 45: 39S ribosomal protein L51, mitochondrial

Chain i: 69% 7% 24%



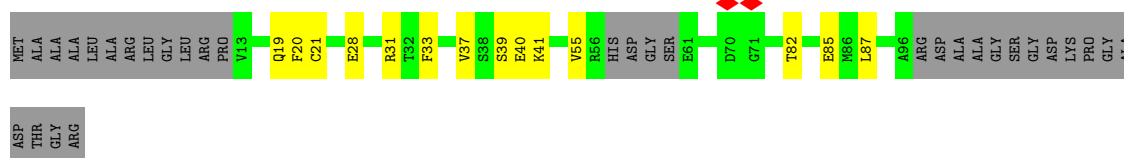
- Molecule 46: 39S ribosomal protein L52, mitochondrial

Chain j: 95% 5%



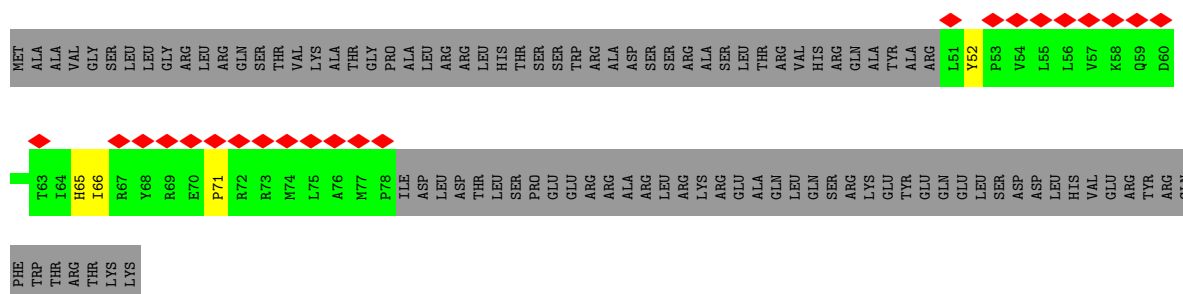
- Molecule 47: 39S ribosomal protein L53, mitochondrial

Chain k: 59% 12% 29%



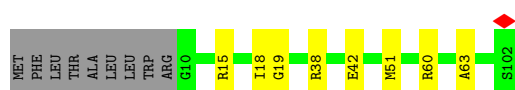
- Molecule 48: 39S ribosomal protein L55, mitochondrial

Chain m: 17% 19% 78%



- Molecule 49: Ribosomal protein 63, mitochondrial

Chain o: 83% 8% 9%



- Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial

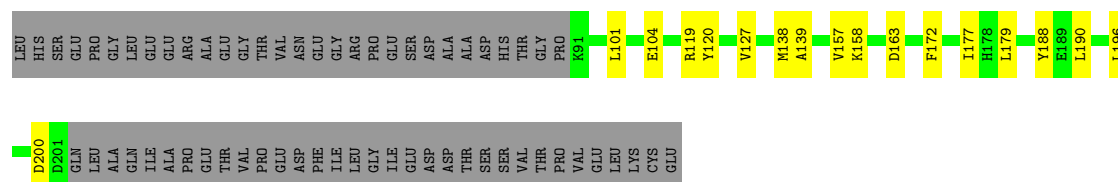
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | PRO | GLY | GLY | GLY | GLN | ASN | VAL | ASN | ARG | TRP | GLY | LEU | LEU | ARG | GLY | VAL | TRP | LEU | LEU | PRO | PRO | PRO | ALA | ARG | CYS | THR | THR | ASP | GLY | THR | E38 | D46 | K47 | V61 | PRO | ASN | GLY | ALA | LYS | GLN | ALA | ASP | ARG | D70 | I71 | P72 | R75 | S83 | GLY |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |     |     |     |      |     |     |
|-----|-----|-----|------|-----|-----|
| GLY | ALA | ALA | GLU  | ALA | MET |
| PRO | ALA | ALA | GLU  | ALA |     |
| SER | GLN | SER | GLN  | SER |     |
| SER | VAL | VAL | LEU  | ARG |     |
|     | LEU | LEU | GLY  | GLN |     |
|     | GLY | TYR | ALA  | ARG |     |
|     | GLN | VAL | VAL  | SER |     |
|     | ASP | PRO | GLY  | LEU |     |
|     | ARG | SER | VAL  | ALA |     |
|     | ALA | ALA | ARG  | THR |     |
|     | PHE | GLU | LEU  | LEU |     |
|     | GLN | PRO | ALA  | ALA |     |
|     | LEU | LEU | GLY  | PRO |     |
|     | GLN | LEU | SER  | GLY |     |
|     | ASP | GLN | ARG  | ARG |     |
|     | LEU | GLY | Y25  | GLY |     |
|     | GLU | LYS | D41  |     |     |
|     | LYS | LYS | D44  |     |     |
|     | ARG | ARG | T47  |     |     |
|     | LYS | ARG | P48  |     |     |
|     | LEU | LEU | R49  |     |     |
|     | LYS | LYS | W50  |     |     |
|     | GLU | GLU | K59  |     |     |
|     | GLU | LYS | A62  |     |     |
|     | GLN | LYS | V71  |     |     |
|     | ARG | LYS | S78  |     |     |
|     | LYS | GLU | P79  |     |     |
|     | ALA | ALA | R117 |     |     |
|     | ARG | ALA | I121 |     |     |
|     | ALA | ALA | M125 |     |     |
|     | LEU | ALA | Q130 |     |     |
|     | ALA | ALA | N134 |     |     |
|     | VAL | ALA | R152 |     |     |
|     | ALA | GLN | ARG  | ALA |     |
|     | ASP | PRO | ALA  | ARG |     |
|     | PRO | ALA | ALA  | LEU |     |
|     | SER | SER | GLN  | GLN |     |

- |      |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| R134 | LEU | ALA | LEU | LYS | ALA | LEU | VAL | PRO | LYS | LYS | LYS | PRO | R153 | R154 | A155 | P161 | W192 | H196 | F35 | F41 | GLN | GLU | GLY | LYS | THR | F47 | Q69 | C73 | I93 | R94 | R102 | R103 | I104 | Q109 | V119 | R126 |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|

- |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|
| D318 | D321 | F333 | R353 | P354 | F355 | V356 | V360 | D363 | Y366 | F369 | T376 | R389 | V410 | D415 | D416 | V417 | L418 | L419 | L426 | R427 | R428 | F429 | R430 | GLU  | GLU  | LYS  | SER  | GLN  | LEU  | LEU  | GLU  | ASN  |      |      |      |      |      |      |      |      |      |     |     |     |     |
| PRO  | GLU  | PRO  | GLU  | PRO  | GLU  | ASP  | LEU  | ALA  | R158 | R159 | R160 | R161 | R162 | V163 | R164 | R165 | V166 | E167 | E168 | V171 | I172 | S173 | L174 | P175 | V181 | L188 | H191 | L200 | Q232 | Q246 | E249 | F250 | V251 | P252 | L253 | D254 | L259 | L271 | P272 | D304 | P307 |     |     |     |     |
| MET  | ALA  | ALA  | ALA  | ARG  | CYS  | TRP  | PRO  | GLU  | ARG  | PRO  | ALA  | LEU  | LEU  | ASP  | LEU  | ALA  | ASN  | ALA  | ALA  | THR  | THR  | THR  | THR  | CYS  | GLN  | ASP  | VAL  | ALA  | ALA  | THR  | PRO  | V41  | S55  | R81  | K90  | A99  | T110 | P119 | PRO  | PRO  | PRO  | ALA | GLU | PRO | CYS |

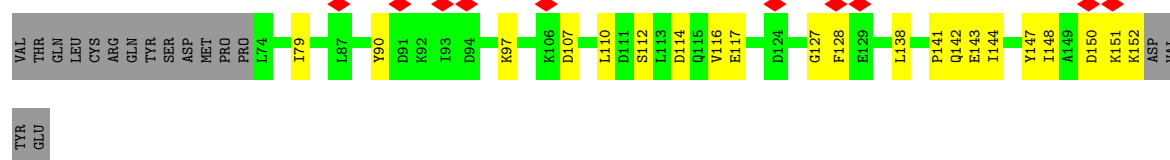
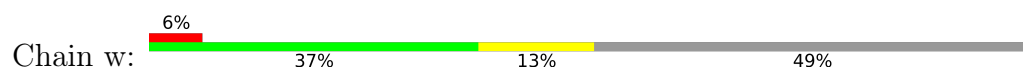
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | PRO | GLY | GLY | ARG | VAL | ALA | ALA | LEU | ARG | TRP | ARG | ARG | ALA | VAL | SER | SER | SER | VAL | VAL | ALA | GLY | GLU | PRO | GLY | LEU | ARG | LEU | LEU | VAL | VAL | GLN | ARG | ARG | LEU | PRO | VAL | GLY | ALA | PHE | CYS | ALA | ALA | CYS | GLN | THR | PRO | ASN | PHE | VAL | VAL | ARG | CYS | GLY |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



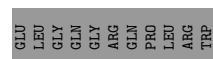
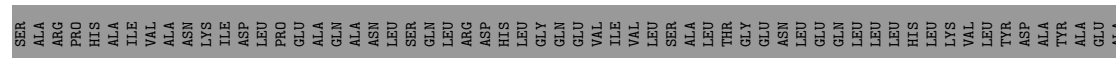
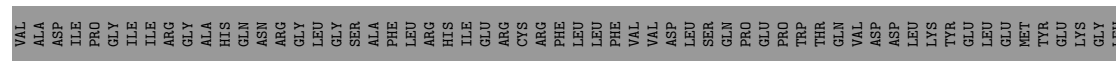
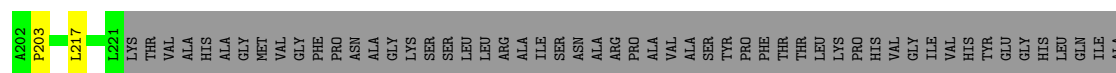
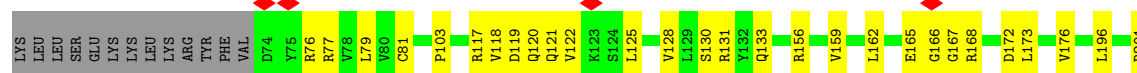
- Molecule 55: MIEF1 upstream open reading frame protein



- Molecule 56: Acyl carrier protein, mitochondrial



- Molecule 57: Mitochondrial ribosome-associated GTPase 2



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 98227                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 36                                      | Depositor |
| Minimum defocus (nm)                 | 300                                     | Depositor |
| Maximum defocus (nm)                 | 2800                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.113                                   | Depositor |
| Minimum map value                    | -0.035                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.004                                   | Depositor |
| Recommended contour level            | 0.006                                   | Depositor |
| Map size (Å)                         | 367.49997, 367.49997, 367.49997         | wwPDB     |
| Map dimensions                       | 350, 350, 350                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.05, 1.05, 1.05                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | 0     | 0.28         | 0/895       | 0.28        | 0/1201      |
| 2   | 1     | 0.11         | 0/438       | 0.26        | 0/583       |
| 3   | 2     | 0.38         | 0/373       | 0.35        | 0/496       |
| 4   | 3     | 0.34         | 0/852       | 0.31        | 0/1136      |
| 5   | 4     | 0.27         | 0/341       | 0.33        | 0/451       |
| 6   | 5     | 0.24         | 0/3294      | 0.33        | 0/4488      |
| 7   | 6     | 0.21         | 0/2809      | 0.32        | 0/3818      |
| 8   | 7     | 0.21         | 0/2391      | 0.32        | 0/3234      |
| 9   | 8     | 0.12         | 0/665       | 0.31        | 0/894       |
| 10  | 9     | 0.26         | 0/972       | 0.28        | 0/1306      |
| 11  | A     | 0.38         | 0/32605     | 0.33        | 0/50720     |
| 12  | B     | 0.12         | 0/1328      | 0.22        | 0/2056      |
| 13  | C     | 0.15         | 0/2754      | 0.29        | 0/3734      |
| 14  | D     | 0.29         | 0/1910      | 0.33        | 0/2569      |
| 15  | E     | 0.32         | 0/2497      | 0.33        | 0/3386      |
| 16  | F     | 0.33         | 0/2071      | 0.35        | 0/2817      |
| 17  | G     | 0.17         | 0/1974      | 0.28        | 0/2652      |
| 18  | H     | 0.23         | 0/798       | 0.29        | 0/1073      |
| 19  | I     | 0.15         | 0/1308      | 0.30        | 0/1761      |
| 20  | J     | 0.11         | 0/1077      | 0.26        | 0/1452      |
| 21  | K     | 0.33         | 0/1495      | 0.31        | 0/2029      |
| 22  | L     | 0.30         | 0/904       | 0.35        | 0/1218      |
| 23  | M     | 0.31         | 0/2359      | 0.31        | 0/3185      |
| 24  | N     | 0.24         | 0/1697      | 0.36        | 0/2281      |
| 25  | O     | 0.32         | 0/1269      | 0.32        | 0/1708      |
| 26  | P     | 0.23         | 0/1173      | 0.29        | 0/1588      |
| 27  | Q     | 0.28         | 0/1846      | 0.31        | 0/2487      |
| 28  | R     | 0.36         | 0/987       | 0.30        | 0/1320      |
| 29  | S     | 0.33         | 0/1276      | 0.33        | 0/1729      |
| 30  | T     | 0.33         | 0/1402      | 0.33        | 0/1886      |
| 31  | U     | 0.28         | 0/1183      | 0.29        | 0/1600      |
| 32  | V     | 0.22         | 0/404       | 0.24        | 0/545       |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 33  | W     | 0.33         | 0/881    | 0.30        | 0/1188   |
| 34  | X     | 0.27         | 0/2090   | 0.28        | 0/2825   |
| 35  | Y     | 0.29         | 0/1552   | 0.29        | 0/2079   |
| 36  | Z     | 0.30         | 0/960    | 0.34        | 0/1295   |
| 37  | a     | 0.29         | 0/616    | 0.28        | 0/833    |
| 38  | b     | 0.31         | 0/1202   | 0.34        | 0/1626   |
| 39  | c     | 0.27         | 0/2264   | 0.29        | 0/3059   |
| 40  | d     | 0.13         | 0/1702   | 0.28        | 0/2307   |
| 41  | e     | 0.10         | 0/1633   | 0.27        | 0/2204   |
| 42  | f     | 0.15         | 0/873    | 0.32        | 0/1180   |
| 43  | g     | 0.30         | 0/1102   | 0.33        | 0/1503   |
| 44  | h     | 0.19         | 0/884    | 0.27        | 0/1203   |
| 45  | i     | 0.37         | 0/849    | 0.32        | 0/1135   |
| 46  | j     | 0.26         | 0/698    | 0.29        | 0/940    |
| 47  | k     | 0.12         | 0/635    | 0.31        | 0/855    |
| 48  | m     | 0.12         | 0/239    | 0.37        | 0/322    |
| 49  | o     | 0.29         | 0/807    | 0.35        | 0/1083   |
| 50  | p     | 0.18         | 0/1071   | 0.27        | 0/1433   |
| 51  | q     | 0.19         | 0/1107   | 0.26        | 0/1498   |
| 52  | r     | 0.25         | 0/1238   | 0.28        | 0/1676   |
| 53  | s     | 0.31         | 0/3114   | 0.32        | 0/4225   |
| 54  | u     | 0.20         | 0/949    | 0.32        | 0/1281   |
| 55  | v     | 0.14         | 0/597    | 0.31        | 0/796    |
| 56  | w     | 0.11         | 0/647    | 0.31        | 0/871    |
| 57  | x     | 0.24         | 0/1091   | 0.38        | 0/1467   |
| All | All   | 0.30         | 0/106148 | 0.31        | 0/150287 |

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

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.

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 880   | 0        | 902      | 11      | 0            |
| 2   | 1     | 433   | 0        | 475      | 4       | 0            |
| 3   | 2     | 367   | 0        | 393      | 6       | 0            |
| 4   | 3     | 831   | 0        | 883      | 6       | 0            |
| 5   | 4     | 333   | 0        | 352      | 4       | 0            |
| 6   | 5     | 3199  | 0        | 3196     | 32      | 0            |
| 7   | 6     | 2723  | 0        | 2615     | 56      | 0            |
| 8   | 7     | 2334  | 0        | 2343     | 35      | 0            |
| 9   | 8     | 651   | 0        | 649      | 28      | 0            |
| 10  | 9     | 947   | 0        | 949      | 8       | 0            |
| 11  | A     | 29222 | 0        | 14853    | 362     | 0            |
| 12  | B     | 1191  | 0        | 607      | 14      | 0            |
| 13  | C     | 2690  | 0        | 2677     | 26      | 0            |
| 14  | D     | 1872  | 0        | 1932     | 23      | 0            |
| 15  | E     | 2427  | 0        | 2436     | 28      | 0            |
| 16  | F     | 2013  | 0        | 2044     | 27      | 0            |
| 17  | G     | 1943  | 0        | 2030     | 19      | 0            |
| 18  | H     | 784   | 0        | 832      | 9       | 0            |
| 19  | I     | 1283  | 0        | 1369     | 34      | 0            |
| 20  | J     | 1061  | 0        | 1141     | 20      | 0            |
| 21  | K     | 1451  | 0        | 1448     | 16      | 0            |
| 22  | L     | 889   | 0        | 941      | 22      | 0            |
| 23  | M     | 2305  | 0        | 2378     | 24      | 0            |
| 24  | N     | 1654  | 0        | 1681     | 32      | 0            |
| 25  | O     | 1245  | 0        | 1283     | 15      | 0            |
| 26  | P     | 1148  | 0        | 1148     | 17      | 0            |
| 27  | Q     | 1805  | 0        | 1841     | 15      | 0            |
| 28  | R     | 971   | 0        | 1045     | 15      | 0            |
| 29  | S     | 1251  | 0        | 1322     | 20      | 0            |
| 30  | T     | 1368  | 0        | 1410     | 19      | 0            |
| 31  | U     | 1154  | 0        | 1154     | 11      | 0            |
| 32  | V     | 395   | 0        | 392      | 2       | 0            |
| 33  | W     | 859   | 0        | 888      | 24      | 0            |
| 34  | X     | 2035  | 0        | 2054     | 20      | 0            |
| 35  | Y     | 1517  | 0        | 1561     | 9       | 0            |
| 36  | Z     | 937   | 0        | 983      | 9       | 0            |
| 37  | a     | 597   | 0        | 584      | 6       | 0            |
| 38  | b     | 1178  | 0        | 1180     | 20      | 0            |
| 39  | c     | 2217  | 0        | 2220     | 13      | 0            |
| 40  | d     | 1653  | 0        | 1632     | 15      | 0            |
| 41  | e     | 1599  | 0        | 1604     | 19      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 42  | f     | 857    | 0        | 852      | 22      | 0            |
| 43  | g     | 1067   | 0        | 1056     | 7       | 0            |
| 44  | h     | 862    | 0        | 845      | 8       | 0            |
| 45  | i     | 827    | 0        | 857      | 10      | 0            |
| 46  | j     | 684    | 0        | 673      | 3       | 0            |
| 47  | k     | 627    | 0        | 636      | 12      | 0            |
| 48  | m     | 234    | 0        | 250      | 3       | 0            |
| 49  | o     | 786    | 0        | 791      | 8       | 0            |
| 50  | p     | 1058   | 0        | 1083     | 9       | 0            |
| 51  | q     | 1076   | 0        | 1049     | 13      | 0            |
| 52  | r     | 1203   | 0        | 1219     | 11      | 0            |
| 53  | s     | 3036   | 0        | 3022     | 36      | 0            |
| 54  | u     | 927    | 0        | 921      | 15      | 0            |
| 55  | v     | 588    | 0        | 604      | 17      | 0            |
| 56  | w     | 638    | 0        | 637      | 15      | 0            |
| 57  | x     | 1073   | 0        | 1045     | 23      | 0            |
| 58  | 0     | 1      | 0        | 0        | 0       | 0            |
| 58  | 4     | 1      | 0        | 0        | 0       | 0            |
| 58  | r     | 1      | 0        | 0        | 0       | 0            |
| 59  | A     | 71     | 0        | 0        | 0       | 0            |
| 59  | E     | 1      | 0        | 0        | 0       | 0            |
| 59  | W     | 1      | 0        | 0        | 0       | 0            |
| 59  | g     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 101032 | 0        | 86967    | 1064    | 0            |

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

All (1064) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 11:A:3121:C:O2  | 11:A:3135:A:N6   | 1.97                     | 0.97              |
| 10:9:28:ARG:NH1 | 11:A:2376:A:O2'  | 2.00                     | 0.94              |
| 11:A:2182:G:O2' | 11:A:2183:C:OP1  | 1.85                     | 0.93              |
| 19:I:51:THR:OG1 | 24:N:250:ARG:NH2 | 2.00                     | 0.93              |
| 11:A:2528:G:OP1 | 14:D:135:ARG:NH2 | 2.02                     | 0.92              |
| 11:A:2472:A:OP1 | 22:L:56:ARG:NH2  | 2.06                     | 0.89              |
| 8:7:247:ASN:ND2 | 8:7:251:ILE:O    | 2.05                     | 0.89              |
| 11:A:1849:C:O2  | 11:A:2693:A:N6   | 2.06                     | 0.88              |
| 15:E:69:ASP:OD1 | 15:E:154:ARG:NH1 | 2.07                     | 0.88              |
| 11:A:2740:A:N3  | 11:A:2921:A:O2'  | 2.08                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:A:1747:G:N2   | 11:A:1750:G:O2'  | 2.09                     | 0.86              |
| 1:0:113:CYS:SG   | 1:0:115:HIS:ND1  | 2.49                     | 0.85              |
| 11:A:1837:C:OP1  | 38:b:4:ARG:NH2   | 2.10                     | 0.85              |
| 11:A:3088:C:O2'  | 57:x:201:ARG:NH2 | 2.10                     | 0.85              |
| 15:E:133:THR:OG1 | 15:E:144:THR:OG1 | 1.95                     | 0.85              |
| 22:L:128:ARG:NH1 | 54:u:120:TYR:O   | 2.10                     | 0.84              |
| 15:E:202:GLN:NE2 | 15:E:301:ASP:OD1 | 2.10                     | 0.84              |
| 2:1:25:GLY:O     | 51:q:117:ARG:NH2 | 2.10                     | 0.84              |
| 11:A:1823:A:O2'  | 11:A:1824:U:OP2  | 1.93                     | 0.84              |
| 15:E:63:GLN:NE2  | 15:E:67:ASP:OD2  | 2.12                     | 0.83              |
| 11:A:2643:G:O2'  | 11:A:2645:G:OP2  | 1.95                     | 0.82              |
| 19:I:105:SER:N   | 47:k:40:GLU:OE2  | 2.12                     | 0.81              |
| 11:A:3157:C:O2'  | 27:Q:84:ARG:O    | 1.98                     | 0.81              |
| 16:F:277:ASP:O   | 16:F:278:SER:OG  | 1.99                     | 0.80              |
| 11:A:1777:A:N6   | 11:A:1780:U:OP2  | 2.13                     | 0.80              |
| 11:A:3195:A:OP2  | 11:A:3196:G:O2'  | 1.98                     | 0.80              |
| 1:0:168:GLN:NE2  | 1:0:169:ASP:OD1  | 2.15                     | 0.80              |
| 2:1:39:GLU:OE1   | 13:C:146:ARG:NH2 | 2.15                     | 0.80              |
| 21:K:3:SER:O     | 39:c:302:ARG:NH1 | 2.15                     | 0.80              |
| 9:8:160:GLU:OE1  | 41:e:207:ASN:ND2 | 2.15                     | 0.79              |
| 11:A:2186:C:O2'  | 11:A:2187:C:O4'  | 1.99                     | 0.79              |
| 5:4:66:PHE:N     | 11:A:3013:G:HO2' | 1.80                     | 0.79              |
| 11:A:2256:U:O2'  | 29:S:118:ASN:ND2 | 2.15                     | 0.79              |
| 27:Q:131:SER:OG  | 54:u:119:ARG:NH1 | 2.15                     | 0.79              |
| 6:5:229:ARG:NH2  | 6:5:231:SER:OG   | 2.16                     | 0.78              |
| 11:A:2531:U:O4   | 14:D:246:ARG:NH2 | 2.15                     | 0.78              |
| 11:A:2166:C:O2'  | 11:A:2167:A:O4'  | 2.01                     | 0.78              |
| 11:A:3181:U:OP2  | 11:A:3182:A:O2'  | 2.02                     | 0.77              |
| 13:C:326:GLU:OE2 | 13:C:330:ASN:ND2 | 2.18                     | 0.77              |
| 11:A:2202:C:O2   | 11:A:2209:G:N2   | 2.17                     | 0.77              |
| 11:A:1671:G:O2'  | 11:A:1672:C:OP2  | 2.02                     | 0.77              |
| 42:f:104:GLU:OE2 | 42:f:108:GLN:NE2 | 2.17                     | 0.77              |
| 11:A:2152:A:OP1  | 49:o:38:ARG:NH2  | 2.19                     | 0.75              |
| 11:A:2167:A:N3   | 11:A:2213:A:N6   | 2.34                     | 0.75              |
| 24:N:137:GLY:O   | 24:N:138:HIS:ND1 | 2.20                     | 0.75              |
| 11:A:1678:C:O2'  | 11:A:1679:U:OP2  | 2.03                     | 0.75              |
| 11:A:2194:U:O2'  | 11:A:2195:A:O4'  | 2.04                     | 0.74              |
| 11:A:2754:A:OP1  | 18:H:91:LYS:NZ   | 2.20                     | 0.74              |
| 11:A:1794:A:OP1  | 16:F:142:ARG:NH2 | 2.20                     | 0.74              |
| 7:6:176:ALA:HB3  | 7:6:184:LEU:HD12 | 1.69                     | 0.74              |
| 29:S:112:ASP:OD1 | 29:S:113:LEU:N   | 2.21                     | 0.74              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:L:75:LEU:HD23 | 22:L:77:ILE:HD11  | 1.71                     | 0.73              |
| 12:B:1607:U:O2'  | 12:B:1608:G:OP1   | 2.05                     | 0.73              |
| 19:I:117:ARG:NH2 | 20:J:133:GLN:O    | 2.21                     | 0.73              |
| 11:A:1881:A:OP2  | 43:g:111:ARG:NH2  | 2.20                     | 0.73              |
| 11:A:2932:G:OP1  | 16:F:137:ARG:NH1  | 2.21                     | 0.73              |
| 7:6:114:ARG:NH1  | 12:B:1643:A:OP1   | 2.23                     | 0.72              |
| 39:c:183:GLU:OE1 | 39:c:183:GLU:N    | 2.22                     | 0.72              |
| 25:O:64:LYS:NZ   | 25:O:100:GLN:O    | 2.23                     | 0.72              |
| 1:0:96:ASN:OD1   | 11:A:2708:C:O2'   | 2.01                     | 0.72              |
| 41:e:75:GLN:O    | 41:e:79:ILE:HD12  | 1.88                     | 0.72              |
| 39:c:294:GLU:OE2 | 39:c:298:ARG:NE   | 2.23                     | 0.72              |
| 11:A:1962:A:OP2  | 11:A:2501:C:N4    | 2.22                     | 0.72              |
| 13:C:70:GLU:OE1  | 17:G:322:ARG:NH2  | 2.23                     | 0.72              |
| 5:4:85:ARG:N     | 11:A:3189:C:OP1   | 2.22                     | 0.71              |
| 19:I:114:HIS:ND1 | 20:J:128:GLU:OE2  | 2.23                     | 0.71              |
| 11:A:3116:C:H42  | 11:A:3140:A:H61   | 1.38                     | 0.71              |
| 7:6:187:VAL:O    | 7:6:317:SER:OG    | 2.09                     | 0.71              |
| 53:s:304:ASP:O   | 53:s:307:ARG:NH1  | 2.23                     | 0.71              |
| 34:X:35:GLU:N    | 34:X:35:GLU:OE1   | 2.24                     | 0.70              |
| 7:6:217:LEU:HD21 | 7:6:219:THR:HG23  | 1.72                     | 0.70              |
| 11:A:2065:A:OP1  | 42:f:48:TYR:N     | 2.24                     | 0.70              |
| 38:b:90:HIS:CE1  | 38:b:91:CYS:HG    | 2.10                     | 0.70              |
| 11:A:2386:C:OP2  | 14:D:71:LYS:NZ    | 2.21                     | 0.70              |
| 12:B:1609:U:O2   | 12:B:1616:A:N6    | 2.24                     | 0.70              |
| 19:I:148:VAL:O   | 47:k:31:ARG:NH1   | 2.24                     | 0.70              |
| 11:A:2204:U:O2'  | 11:A:2207:A:N7    | 2.23                     | 0.69              |
| 52:r:93:ILE:HD11 | 52:r:119:VAL:HG21 | 1.72                     | 0.69              |
| 11:A:3090:G:H4'  | 57:x:196:LEU:HD21 | 1.75                     | 0.69              |
| 24:N:216:GLU:OE2 | 24:N:238:LYS:NZ   | 2.25                     | 0.69              |
| 39:c:167:CYS:SG  | 39:c:171:ARG:NH1  | 2.66                     | 0.69              |
| 7:6:173:LEU:HD21 | 7:6:175:VAL:HG23  | 1.75                     | 0.69              |
| 18:H:84:GLU:OE1  | 34:X:44:ARG:NH2   | 2.25                     | 0.69              |
| 29:S:94:ARG:NH2  | 29:S:110:SER:O    | 2.26                     | 0.68              |
| 11:A:2111:C:OP1  | 19:I:35:ARG:NH1   | 2.24                     | 0.68              |
| 11:A:2164:C:O2'  | 11:A:2165:C:O4'   | 2.10                     | 0.68              |
| 11:A:2188:A:N6   | 11:A:2199:A:OP1   | 2.27                     | 0.68              |
| 11:A:2064:A:OP1  | 33:W:101:LYS:NZ   | 2.27                     | 0.68              |
| 31:U:150:TRP:NE1 | 40:d:172:MET:SD   | 2.66                     | 0.68              |
| 19:I:104:LEU:O   | 47:k:41:LYS:NZ    | 2.27                     | 0.68              |
| 24:N:205:ARG:NH2 | 24:N:249:LYS:O    | 2.26                     | 0.67              |
| 41:e:151:ARG:NH1 | 41:e:254:TRP:O    | 2.26                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:6:50:LYS:O      | 33:W:122:LYS:NZ   | 2.27                     | 0.67              |
| 11:A:1990:G:OP1   | 14:D:269:ARG:NH2  | 2.27                     | 0.67              |
| 11:A:2705:U:OP2   | 21:K:119:ARG:NH1  | 2.26                     | 0.67              |
| 11:A:1750:G:O2'   | 11:A:1751:A:OP2   | 2.11                     | 0.67              |
| 14:D:113:ARG:O    | 14:D:147:ARG:NH2  | 2.26                     | 0.67              |
| 40:d:86:ASP:O     | 40:d:198:ARG:NH2  | 2.28                     | 0.67              |
| 11:A:2191:A:HO2'  | 20:J:143:SER:HG   | 1.42                     | 0.67              |
| 6:5:68:PRO:O      | 11:A:1713:A:N6    | 2.28                     | 0.67              |
| 11:A:1953:A:O2'   | 11:A:2463:A:OP1   | 2.11                     | 0.66              |
| 41:e:177:GLU:O    | 41:e:190:ARG:NH2  | 2.28                     | 0.66              |
| 41:e:201:GLU:OE1  | 41:e:240:THR:OG1  | 2.13                     | 0.66              |
| 57:x:103:PRO:HD2  | 57:x:196:LEU:HD12 | 1.76                     | 0.66              |
| 11:A:1867:A:N1    | 11:A:2019:G:O2'   | 2.22                     | 0.66              |
| 7:6:239:ASN:OD1   | 7:6:275:GLN:NE2   | 2.27                     | 0.66              |
| 16:F:49:ARG:NH1   | 16:F:81:ASP:O     | 2.29                     | 0.66              |
| 1:0:127:TYR:OH    | 25:O:43:GLU:OE2   | 2.12                     | 0.65              |
| 11:A:1749:C:OP2   | 11:A:2899:C:O2'   | 2.13                     | 0.65              |
| 22:L:84:ALA:HB1   | 22:L:105:VAL:HG22 | 1.78                     | 0.65              |
| 32:V:171:ILE:O    | 35:Y:80:LYS:NZ    | 2.30                     | 0.65              |
| 12:B:1632:U:N3    | 12:B:1635:C:OP2   | 2.30                     | 0.65              |
| 30:T:133:ASN:ND2  | 40:d:226:ASP:OD2  | 2.29                     | 0.65              |
| 11:A:2635:G:O2'   | 11:A:2636:G:OP1   | 2.14                     | 0.64              |
| 34:X:61:ARG:NH2   | 34:X:63:GLU:OE2   | 2.30                     | 0.64              |
| 7:6:160:ASP:OD1   | 26:P:51:ARG:NH1   | 2.31                     | 0.64              |
| 8:7:231:GLN:N     | 8:7:231:GLN:OE1   | 2.30                     | 0.64              |
| 6:5:135:LYS:NZ    | 6:5:238:THR:O     | 2.31                     | 0.64              |
| 50:p:189:ARG:NH2  | 50:p:191:LYS:O    | 2.30                     | 0.64              |
| 13:C:84:ASP:OD1   | 13:C:85:HIS:N     | 2.31                     | 0.64              |
| 6:5:295:ASP:OD2   | 6:5:304:LEU:N     | 2.31                     | 0.63              |
| 21:K:110:GLY:O    | 21:K:114:LYS:NZ   | 2.29                     | 0.63              |
| 24:N:96:TYR:HB3   | 24:N:151:VAL:HG21 | 1.79                     | 0.63              |
| 11:A:3019:G:N2    | 11:A:3131:G:O2'   | 2.31                     | 0.63              |
| 39:c:227:GLU:OE2  | 39:c:302:ARG:NE   | 2.25                     | 0.63              |
| 26:P:167:GLU:O    | 50:p:187:ARG:NH1  | 2.31                     | 0.63              |
| 1:0:81:PRO:O      | 11:A:2679:U:O2'   | 2.17                     | 0.63              |
| 38:b:34:SER:OG    | 38:b:36:ASP:O     | 2.17                     | 0.63              |
| 29:S:108:VAL:HG13 | 29:S:195:ILE:HG13 | 1.81                     | 0.62              |
| 13:C:232:ARG:NH2  | 13:C:249:TYR:OH   | 2.31                     | 0.62              |
| 20:J:134:ASP:OD2  | 20:J:139:SER:OG   | 2.17                     | 0.62              |
| 11:A:1766:U:O2'   | 11:A:1767:G:O5'   | 2.17                     | 0.62              |
| 11:A:2755:A:O3'   | 34:X:112:ARG:NH2  | 2.31                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:6:268:LEU:HD12  | 7:6:319:PHE:CZ    | 2.35                     | 0.62              |
| 11:A:2531:U:O4'   | 14:D:253:ASN:ND2  | 2.33                     | 0.62              |
| 36:Z:64:HIS:HD1   | 49:o:51:MET:HE2   | 1.63                     | 0.62              |
| 8:7:199:LEU:O     | 8:7:203:THR:HG23  | 1.99                     | 0.62              |
| 33:W:60:TYR:OH    | 33:W:94:GLU:OE2   | 2.16                     | 0.62              |
| 52:r:102:ARG:NH1  | 52:r:109:GLN:OE1  | 2.32                     | 0.62              |
| 29:S:107:LYS:HD2  | 30:T:212:LEU:HD22 | 1.81                     | 0.62              |
| 43:g:68:THR:HG22  | 43:g:69:PRO:HD2   | 1.82                     | 0.62              |
| 27:Q:152:ARG:NH1  | 27:Q:198:SER:OG   | 2.33                     | 0.62              |
| 6:5:114:LEU:N     | 6:5:264:ASP:OD2   | 2.33                     | 0.62              |
| 34:X:16:LEU:HD21  | 34:X:208:LEU:HD11 | 1.82                     | 0.61              |
| 11:A:1787:G:N2    | 11:A:1790:A:OP2   | 2.32                     | 0.61              |
| 41:e:160:LEU:HD21 | 41:e:264:LEU:HD11 | 1.83                     | 0.61              |
| 11:A:2519:G:O2'   | 14:D:232:ARG:NH1  | 2.34                     | 0.61              |
| 39:c:161:THR:O    | 39:c:192:GLN:NE2  | 2.34                     | 0.61              |
| 34:X:81:GLY:N     | 34:X:131:THR:OG1  | 2.34                     | 0.61              |
| 11:A:2745:A:O2'   | 34:X:102:LYS:O    | 2.16                     | 0.60              |
| 40:d:129:ASP:OD1  | 40:d:130:ALA:N    | 2.34                     | 0.60              |
| 11:A:2453:G:O2'   | 25:O:116:ASP:OD2  | 2.19                     | 0.60              |
| 11:A:2837:A:O2'   | 11:A:2838:A:OP1   | 2.20                     | 0.60              |
| 11:A:2173:G:N7    | 11:A:2198:A:O2'   | 2.34                     | 0.60              |
| 24:N:199:ARG:O    | 24:N:203:GLU:OE1  | 2.20                     | 0.60              |
| 50:p:133:LEU:HD21 | 50:p:157:MET:HE1  | 1.84                     | 0.60              |
| 22:L:111:ASN:OD1  | 22:L:112:GLY:N    | 2.35                     | 0.60              |
| 8:7:203:THR:HG22  | 8:7:280:VAL:H     | 1.66                     | 0.60              |
| 11:A:1747:G:OP2   | 11:A:1749:C:N4    | 2.35                     | 0.59              |
| 11:A:2010:U:OP2   | 45:i:115:ARG:NH1  | 2.31                     | 0.59              |
| 23:M:62:ARG:HG2   | 45:i:128:ARG:HE   | 1.66                     | 0.59              |
| 11:A:2192:A:O2'   | 20:J:134:ASP:OD1  | 2.19                     | 0.59              |
| 4:3:153:THR:HG21  | 11:A:2044:A:OP1   | 2.02                     | 0.59              |
| 17:G:209:VAL:O    | 17:G:213:THR:HG23 | 2.03                     | 0.59              |
| 28:R:119:LEU:HD11 | 37:a:58:ILE:HD13  | 1.83                     | 0.59              |
| 11:A:1917:A:O2'   | 11:A:1983:U:O4    | 2.19                     | 0.59              |
| 28:R:112:THR:OG1  | 38:b:127:GLN:NE2  | 2.34                     | 0.59              |
| 11:A:2966:U:OP1   | 11:A:3024:U:O2'   | 2.20                     | 0.59              |
| 11:A:2896:G:O2'   | 11:A:2912:C:N4    | 2.36                     | 0.59              |
| 11:A:2143:G:OP1   | 29:S:173:ARG:NH2  | 2.36                     | 0.58              |
| 55:v:12:LEU:O     | 55:v:16:LEU:HD23  | 2.03                     | 0.58              |
| 11:A:2457:A:O2'   | 11:A:2458:A:OP2   | 2.13                     | 0.58              |
| 14:D:124:GLU:HB3  | 14:D:142:VAL:HG22 | 1.84                     | 0.58              |
| 33:W:120:LEU:HD12 | 42:f:63:ILE:HD11  | 1.85                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:5:145:ASN:OD1    | 6:5:195:HIS:NE2   | 2.29                     | 0.58              |
| 7:6:214:TRP:HB3    | 7:6:272:LEU:HD11  | 1.85                     | 0.58              |
| 16:F:48:LEU:HD11   | 44:h:95:ARG:HD2   | 1.86                     | 0.58              |
| 29:S:142:THR:HG23  | 37:a:62:HIS:NE2   | 2.19                     | 0.58              |
| 7:6:292:GLN:OE1    | 26:P:41:ASN:ND2   | 2.35                     | 0.58              |
| 8:7:52:LYS:HG2     | 8:7:219:LEU:HD21  | 1.84                     | 0.58              |
| 11:A:3127:G:N2     | 11:A:3130:A:OP2   | 2.37                     | 0.58              |
| 8:7:114:ASP:OD1    | 8:7:268:LEU:N     | 2.36                     | 0.58              |
| 28:R:64:MET:HE1    | 30:T:210:HIS:ND1  | 2.19                     | 0.58              |
| 11:A:2815:OMG:HM22 | 11:A:2816:G:O4'   | 2.04                     | 0.57              |
| 11:A:1718:A:OP2    | 11:A:1732:C:N4    | 2.37                     | 0.57              |
| 16:F:226:MET:SD    | 16:F:242:LEU:HD21 | 2.44                     | 0.57              |
| 19:I:101:ASN:OD1   | 19:I:174:LEU:HD21 | 2.05                     | 0.57              |
| 53:s:163:VAL:HG23  | 53:s:171:VAL:HG21 | 1.86                     | 0.57              |
| 11:A:2262:C:OP2    | 29:S:173:ARG:NH1  | 2.38                     | 0.57              |
| 38:b:45:GLU:HB2    | 38:b:94:VAL:HG22  | 1.87                     | 0.57              |
| 57:x:125:LEU:O     | 57:x:128:VAL:HG13 | 2.04                     | 0.57              |
| 41:e:264:LEU:HD23  | 41:e:269:LEU:HB3  | 1.85                     | 0.57              |
| 53:s:360:VAL:HG12  | 53:s:369:PHE:CD2  | 2.39                     | 0.57              |
| 42:f:100:MET:SD    | 42:f:155:ARG:NH2  | 2.78                     | 0.57              |
| 19:I:101:ASN:O     | 19:I:109:LYS:NZ   | 2.37                     | 0.57              |
| 17:G:137:ASN:O     | 17:G:141:VAL:HG23 | 2.05                     | 0.57              |
| 50:p:46:ASP:OD1    | 50:p:47:LYS:N     | 2.38                     | 0.57              |
| 15:E:119:VAL:HG21  | 15:E:284:TYR:HB3  | 1.87                     | 0.56              |
| 6:5:152:GLU:OE2    | 6:5:156:ASN:ND2   | 2.38                     | 0.56              |
| 15:E:347:PHE:O     | 27:Q:128:GLY:N    | 2.38                     | 0.56              |
| 16:F:175:LYS:O     | 16:F:179:THR:HG23 | 2.04                     | 0.56              |
| 11:A:2086:A:H2'    | 11:A:2087:U:C6    | 2.40                     | 0.56              |
| 39:c:124:GLU:OE1   | 39:c:124:GLU:N    | 2.35                     | 0.56              |
| 11:A:2836:C:OP1    | 33:W:47:SER:OG    | 2.23                     | 0.56              |
| 31:U:61:TYR:O      | 35:Y:63:GLY:N     | 2.38                     | 0.56              |
| 29:S:164:THR:HG22  | 29:S:165:GLU:H    | 1.70                     | 0.56              |
| 29:S:164:THR:HG22  | 29:S:165:GLU:N    | 2.20                     | 0.56              |
| 54:u:101:LEU:HD13  | 54:u:127:VAL:HG11 | 1.87                     | 0.56              |
| 7:6:217:LEU:HD12   | 7:6:236:LEU:HD13  | 1.87                     | 0.56              |
| 22:L:101:ASP:OD2   | 27:Q:152:ARG:NH2  | 2.39                     | 0.56              |
| 7:6:220:SER:HA     | 7:6:268:LEU:HD23  | 1.87                     | 0.56              |
| 11:A:2138:U:OP1    | 36:Z:73:LYS:NZ    | 2.27                     | 0.56              |
| 11:A:2191:A:O2'    | 20:J:143:SER:OG   | 2.15                     | 0.56              |
| 33:W:117:ILE:HA    | 33:W:120:LEU:HD13 | 1.88                     | 0.56              |
| 34:X:80:TRP:O      | 34:X:82:GLY:N     | 2.37                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:216:GLU:O     | 6:5:217:SER:OG    | 2.21                     | 0.56              |
| 6:5:280:GLN:OE1   | 53:s:158:ARG:NE   | 2.39                     | 0.56              |
| 11:A:1728:U:O2'   | 34:X:96:LYS:O     | 2.13                     | 0.56              |
| 11:A:3063:G:O2'   | 11:A:3066:C:OP2   | 2.18                     | 0.56              |
| 11:A:2374:A:N6    | 53:s:272:PRO:O    | 2.39                     | 0.55              |
| 22:L:144:PHE:O    | 54:u:119:ARG:NH2  | 2.40                     | 0.55              |
| 1:0:94:ARG:NH2    | 11:A:2310:G:OP2   | 2.38                     | 0.55              |
| 11:A:1713:A:HO2'  | 11:A:1714:C:P     | 2.30                     | 0.55              |
| 11:A:2202:C:N3    | 11:A:2209:G:N1    | 2.41                     | 0.55              |
| 11:A:2829:C:OP2   | 11:A:2830:A:O2'   | 2.15                     | 0.55              |
| 6:5:377:ASP:OD1   | 6:5:380:GLN:NE2   | 2.39                     | 0.55              |
| 11:A:2960:U:OP1   | 11:A:2962:C:N4    | 2.35                     | 0.55              |
| 13:C:252:VAL:HB   | 13:C:305:VAL:HG12 | 1.88                     | 0.55              |
| 17:G:301:PHE:O    | 17:G:305:THR:OG1  | 2.20                     | 0.55              |
| 24:N:218:ILE:HG22 | 24:N:226:ILE:HD13 | 1.89                     | 0.55              |
| 51:q:130:GLN:NE2  | 51:q:134:ASN:OD1  | 2.40                     | 0.55              |
| 9:8:136:ILE:O     | 9:8:140:LEU:HD23  | 2.07                     | 0.55              |
| 11:A:2970:C:N3    | 24:N:182:LYS:NZ   | 2.54                     | 0.55              |
| 15:E:120:THR:HG21 | 15:E:289:VAL:HG23 | 1.88                     | 0.55              |
| 31:U:22:THR:HG22  | 31:U:24:PHE:H     | 1.72                     | 0.55              |
| 11:A:2236:C:O2'   | 11:A:2237:A:O5'   | 2.25                     | 0.55              |
| 11:A:2837:A:H2'   | 11:A:2838:A:C8    | 2.41                     | 0.55              |
| 55:v:21:ARG:O     | 55:v:28:ARG:NH2   | 2.38                     | 0.55              |
| 9:8:145:GLU:OE2   | 41:e:274:ARG:NH2  | 2.40                     | 0.55              |
| 11:A:2180:A:O2'   | 11:A:2206:C:O3'   | 2.25                     | 0.55              |
| 21:K:90:VAL:HG22  | 21:K:94:GLN:HB2   | 1.89                     | 0.54              |
| 1:0:112:GLU:OE2   | 25:O:137:ARG:NH1  | 2.41                     | 0.54              |
| 10:9:41:ILE:HG23  | 10:9:57:VAL:HG22  | 1.88                     | 0.54              |
| 15:E:68:GLU:OE1   | 15:E:154:ARG:NH2  | 2.40                     | 0.54              |
| 23:M:233:ARG:HB3  | 23:M:244:LEU:HD11 | 1.89                     | 0.54              |
| 18:H:107:VAL:HG13 | 18:H:108:ARG:H    | 1.71                     | 0.54              |
| 22:L:41:VAL:HG11  | 22:L:121:THR:OG1  | 2.06                     | 0.54              |
| 8:7:193:MET:SD    | 8:7:295:ARG:NH2   | 2.80                     | 0.54              |
| 10:9:24:LYS:NZ    | 11:A:2422:U:OP2   | 2.39                     | 0.54              |
| 11:A:2112:A:N6    | 24:N:140:MET:SD   | 2.77                     | 0.54              |
| 53:s:90:LYS:HD2   | 53:s:232:GLN:HB2  | 1.90                     | 0.54              |
| 15:E:316:PHE:HB3  | 15:E:317:PRO:HD3  | 1.88                     | 0.54              |
| 9:8:143:GLN:O     | 9:8:147:LEU:HD23  | 2.08                     | 0.54              |
| 11:A:1784:A:O2'   | 31:U:84:ASN:ND2   | 2.40                     | 0.54              |
| 8:7:166:LEU:HD22  | 8:7:181:TYR:HE2   | 1.73                     | 0.54              |
| 13:C:70:GLU:O     | 13:C:371:ASN:ND2  | 2.39                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:J:138:SER:HA   | 20:J:141:VAL:HG12 | 1.90                     | 0.54              |
| 9:8:139:MET:SD    | 42:f:169:ILE:HD13 | 2.48                     | 0.54              |
| 35:Y:218:ARG:NH2  | 45:i:105:ASP:OD1  | 2.40                     | 0.54              |
| 11:A:2909:G:H2'   | 11:A:2910:A:C8    | 2.42                     | 0.54              |
| 11:A:2905:A:O2'   | 11:A:2906:C:O5'   | 2.22                     | 0.54              |
| 8:7:108:VAL:HB    | 8:7:113:TRP:CD1   | 2.43                     | 0.53              |
| 11:A:2214:A:H3'   | 11:A:2215:C:H5''  | 1.90                     | 0.53              |
| 11:A:3189:C:HO2'  | 52:r:155:ALA:H    | 1.57                     | 0.53              |
| 24:N:218:ILE:HG22 | 24:N:226:ILE:CD1  | 2.39                     | 0.53              |
| 51:q:44:ASP:O     | 51:q:47:THR:HG22  | 2.08                     | 0.53              |
| 52:r:93:ILE:HG22  | 52:r:94:ARG:O     | 2.07                     | 0.53              |
| 7:6:227:GLU:OE1   | 7:6:230:ALA:N     | 2.40                     | 0.53              |
| 35:Y:151:ASP:OD1  | 35:Y:154:ARG:NH2  | 2.39                     | 0.53              |
| 9:8:136:ILE:HD13  | 42:f:169:ILE:HD11 | 1.89                     | 0.53              |
| 7:6:235:TRP:HB3   | 7:6:254:TYR:HA    | 1.91                     | 0.53              |
| 11:A:2115:U:N3    | 11:A:2116:C:C5    | 2.77                     | 0.53              |
| 16:F:262:THR:O    | 16:F:265:THR:OG1  | 2.23                     | 0.53              |
| 24:N:218:ILE:HG23 | 24:N:223:MET:HB2  | 1.91                     | 0.53              |
| 8:7:79:PHE:HB3    | 8:7:81:MET:HE2    | 1.90                     | 0.53              |
| 8:7:186:ASP:OD1   | 8:7:187:SER:N     | 2.41                     | 0.53              |
| 11:A:3017:C:O2'   | 11:A:3021:C:N4    | 2.41                     | 0.53              |
| 17:G:196:ASP:OD1  | 17:G:197:THR:N    | 2.41                     | 0.53              |
| 29:S:96:PHE:HB3   | 38:b:126:ILE:HD13 | 1.91                     | 0.53              |
| 11:A:1713:A:O2'   | 11:A:1714:C:P     | 2.66                     | 0.53              |
| 11:A:2127:A:H4'   | 11:A:2251:A:C5    | 2.44                     | 0.53              |
| 11:A:2193:U:O2'   | 19:I:113:ARG:NH2  | 2.42                     | 0.53              |
| 11:A:3019:G:O2'   | 11:A:3125:A:N1    | 2.41                     | 0.53              |
| 11:A:3040:OMG:H2' | 11:A:3041:U:O4'   | 2.09                     | 0.53              |
| 19:I:171:VAL:HG23 | 19:I:171:VAL:O    | 2.08                     | 0.53              |
| 11:A:2104:A:OP1   | 24:N:73:ARG:NH1   | 2.40                     | 0.53              |
| 54:u:157:VAL:HG21 | 54:u:172:PHE:HD1  | 1.74                     | 0.53              |
| 7:6:157:LEU:HD23  | 7:6:221:LEU:HD22  | 1.91                     | 0.52              |
| 18:H:138:LYS:O    | 18:H:142:GLU:OE1  | 2.26                     | 0.52              |
| 24:N:133:ARG:NH1  | 24:N:134:LYS:O    | 2.42                     | 0.52              |
| 54:u:200:ASP:N    | 54:u:200:ASP:OD1  | 2.42                     | 0.52              |
| 11:A:3112:A:C2    | 11:A:3169:C:C2    | 2.98                     | 0.52              |
| 14:D:194:ASN:ND2  | 14:D:245:GLY:O    | 2.38                     | 0.52              |
| 57:x:165:GLU:HG2  | 57:x:166:GLY:H    | 1.73                     | 0.52              |
| 57:x:165:GLU:OE1  | 57:x:168:ARG:NH2  | 2.40                     | 0.52              |
| 7:6:51:TYR:OH     | 33:W:122:LYS:O    | 2.15                     | 0.52              |
| 1:0:153:THR:OG1   | 25:O:91:GLN:OE1   | 2.27                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:8:110:GLU:OE1   | 9:8:114:ARG:NH2   | 2.43                     | 0.52              |
| 41:e:152:LYS:HB2  | 41:e:157:LEU:HD11 | 1.90                     | 0.52              |
| 55:v:43:GLN:N     | 55:v:43:GLN:OE1   | 2.42                     | 0.52              |
| 11:A:2165:C:O2    | 11:A:2216:A:N6    | 2.25                     | 0.52              |
| 11:A:2458:A:OP1   | 25:O:9:ILE:N      | 2.43                     | 0.52              |
| 24:N:218:ILE:HA   | 24:N:223:MET:HG3  | 1.92                     | 0.52              |
| 41:e:156:ASN:C    | 41:e:157:LEU:HD12 | 2.35                     | 0.52              |
| 11:A:2182:G:HO2'  | 11:A:2183:C:P     | 2.25                     | 0.52              |
| 40:d:176:ILE:HD11 | 40:d:181:VAL:HB   | 1.92                     | 0.52              |
| 53:s:363:ASP:OD1  | 53:s:366:TYR:N    | 2.37                     | 0.52              |
| 4:3:148:VAL:HG13  | 7:6:360:ARG:HA    | 1.92                     | 0.52              |
| 39:c:228:LEU:HB2  | 39:c:307:PHE:CD2  | 2.45                     | 0.52              |
| 53:s:110:THR:HG23 | 53:s:333:PHE:CD1  | 2.44                     | 0.52              |
| 56:w:97:LYS:NZ    | 56:w:107:ASP:OD2  | 2.39                     | 0.52              |
| 9:8:129:ARG:HD3   | 12:B:1627:C:H4'   | 1.92                     | 0.51              |
| 11:A:2472:A:O2'   | 11:A:2478:G:N7    | 2.35                     | 0.51              |
| 35:Y:170:ARG:NH1  | 35:Y:174:GLY:O    | 2.43                     | 0.51              |
| 57:x:119:ASP:HB3  | 57:x:122:VAL:HG23 | 1.92                     | 0.51              |
| 3:2:69:ARG:NH2    | 11:A:1916:G:OP1   | 2.42                     | 0.51              |
| 11:A:3219:G:O2'   | 11:A:3221:A:OP2   | 2.22                     | 0.51              |
| 12:B:1607:U:O2'   | 12:B:1608:G:P     | 2.68                     | 0.51              |
| 18:H:107:VAL:HG13 | 18:H:108:ARG:N    | 2.25                     | 0.51              |
| 11:A:2408:U:O4    | 11:A:2409:A:N6    | 2.43                     | 0.51              |
| 53:s:251:VAL:HG22 | 53:s:252:PRO:HD2  | 1.92                     | 0.51              |
| 57:x:118:VAL:CG1  | 57:x:159:VAL:HG12 | 2.41                     | 0.51              |
| 11:A:1760:G:O2'   | 11:A:1761:A:N7    | 2.30                     | 0.51              |
| 14:D:74:ILE:HD11  | 14:D:149:ARG:HA   | 1.92                     | 0.51              |
| 6:5:79:ASP:OD1    | 6:5:80:ARG:N      | 2.43                     | 0.51              |
| 11:A:2092:C:H2'   | 11:A:2093:U:C6    | 2.45                     | 0.51              |
| 17:G:139:GLU:CG   | 17:G:140:PRO:HD3  | 2.39                     | 0.51              |
| 8:7:218:THR:O     | 8:7:219:LEU:HD23  | 2.11                     | 0.51              |
| 24:N:59:VAL:O     | 24:N:59:VAL:HG13  | 2.10                     | 0.51              |
| 27:Q:139:GLN:HB3  | 27:Q:150:ILE:CG2  | 2.41                     | 0.51              |
| 6:5:381:LEU:HD23  | 6:5:381:LEU:H     | 1.74                     | 0.51              |
| 11:A:2695:G:N2    | 15:E:247:ASP:OD1  | 2.44                     | 0.51              |
| 18:H:95:GLU:OE2   | 18:H:113:SER:OG   | 2.22                     | 0.51              |
| 38:b:141:ARG:NH2  | 38:b:149:GLN:O    | 2.40                     | 0.51              |
| 11:A:2215:C:H2'   | 11:A:2215:C:O2    | 2.11                     | 0.51              |
| 11:A:2615:A:N7    | 22:L:58:ILE:HD12  | 2.26                     | 0.51              |
| 11:A:2721:G:H5'   | 11:A:2722:A:OP2   | 2.10                     | 0.51              |
| 45:i:80:LEU:HD12  | 45:i:80:LEU:O     | 2.10                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:6:217:LEU:CD2    | 7:6:219:THR:HG23  | 2.41                     | 0.50              |
| 11:A:2239:A:O3'    | 21:K:29:GLY:HA3   | 2.11                     | 0.50              |
| 31:U:37:GLU:HB3    | 31:U:104:THR:HG23 | 1.93                     | 0.50              |
| 7:6:344:PHE:CE2    | 26:P:61:VAL:HG11  | 2.46                     | 0.50              |
| 14:D:96:ILE:O      | 14:D:269:ARG:NH1  | 2.42                     | 0.50              |
| 19:I:64:CYS:HB3    | 52:r:73:CYS:SG    | 2.50                     | 0.50              |
| 53:s:191:HIS:O     | 53:s:428:ARG:NH2  | 2.37                     | 0.50              |
| 53:s:416:ASP:OD1   | 53:s:417:VAL:N    | 2.44                     | 0.50              |
| 30:T:157:ARG:HB2   | 30:T:167:MET:HG3  | 1.91                     | 0.50              |
| 13:C:139:ILE:O     | 17:G:322:ARG:NH1  | 2.45                     | 0.50              |
| 53:s:376:THR:CG2   | 53:s:389:ARG:HB2  | 2.41                     | 0.50              |
| 11:A:3040:OMG:H2'  | 11:A:3041:U:C4'   | 2.41                     | 0.50              |
| 36:Z:36:PHE:HE2    | 36:Z:79:PRO:HG3   | 1.76                     | 0.50              |
| 4:3:108:LYS:NZ     | 11:A:1745:U:O4    | 2.43                     | 0.50              |
| 7:6:233:LEU:HB2    | 7:6:298:PHE:HE1   | 1.76                     | 0.50              |
| 11:A:1823:A:OP2    | 37:a:127:GLY:N    | 2.44                     | 0.50              |
| 11:A:1883:G:H5'    | 43:g:91:MET:HG3   | 1.92                     | 0.50              |
| 15:E:61:ILE:HD11   | 25:O:149:LEU:HD22 | 1.92                     | 0.50              |
| 33:W:67:ILE:HG21   | 33:W:131:VAL:HG11 | 1.94                     | 0.50              |
| 2:1:44:LEU:HD23    | 2:1:55:LEU:HD23   | 1.94                     | 0.50              |
| 11:A:3039:OMU:HM22 | 11:A:3040:OMG:C8  | 2.47                     | 0.50              |
| 17:G:136:LEU:HD23  | 17:G:141:VAL:HG22 | 1.94                     | 0.50              |
| 7:6:74:TYR:N       | 33:W:102:GLU:OE2  | 2.43                     | 0.50              |
| 11:A:3121:C:H5     | 11:A:3122:U:HO2'  | 1.60                     | 0.50              |
| 19:I:188:ARG:NE    | 47:k:55:VAL:HG13  | 2.27                     | 0.50              |
| 23:M:264:GLN:NE2   | 23:M:267:PHE:O    | 2.44                     | 0.50              |
| 11:A:3068:G:OP2    | 11:A:3068:G:N2    | 2.42                     | 0.49              |
| 13:C:183:ALA:CB    | 13:C:213:LEU:HD11 | 2.41                     | 0.49              |
| 9:8:173:LYS:O      | 42:f:183:ARG:NH2  | 2.45                     | 0.49              |
| 11:A:2841:U:O2     | 24:N:63:ARG:NH2   | 2.45                     | 0.49              |
| 11:A:1880:C:O2'    | 11:A:1884:G:OP1   | 2.28                     | 0.49              |
| 26:P:110:TRP:HA    | 26:P:113:LYS:HG2  | 1.94                     | 0.49              |
| 43:g:48:VAL:O      | 43:g:52:LEU:HD23  | 2.12                     | 0.49              |
| 43:g:57:ILE:HD13   | 43:g:91:MET:HE2   | 1.94                     | 0.49              |
| 11:A:2055:U:H2'    | 11:A:2056:G:H8    | 1.77                     | 0.49              |
| 11:A:2065:A:N1     | 33:W:72:HIS:NE2   | 2.60                     | 0.49              |
| 11:A:2112:A:C8     | 11:A:2114:C:C6    | 3.00                     | 0.49              |
| 11:A:2675:G:H4'    | 30:T:167:MET:HE3  | 1.92                     | 0.49              |
| 11:A:2910:A:H2'    | 11:A:2911:C:C1'   | 2.43                     | 0.49              |
| 7:6:218:LEU:HD22   | 7:6:234:HIS:HB2   | 1.94                     | 0.49              |
| 8:7:81:MET:HE1     | 8:7:94:HIS:HD2    | 1.76                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:T:55:ASN:O     | 40:d:227:ARG:NE   | 2.46                     | 0.49              |
| 54:u:138:MET:HG3  | 54:u:179:LEU:HD21 | 1.95                     | 0.49              |
| 8:7:81:MET:HE1    | 8:7:94:HIS:CD2    | 2.47                     | 0.49              |
| 19:I:121:ILE:HD11 | 19:I:154:LEU:HB3  | 1.95                     | 0.49              |
| 6:5:142:ASP:OD1   | 6:5:142:ASP:N     | 2.45                     | 0.49              |
| 6:5:177:CYS:O     | 6:5:180:ILE:HG22  | 2.11                     | 0.49              |
| 11:A:2151:A:H2'   | 11:A:2152:A:C8    | 2.48                     | 0.49              |
| 11:A:2853:A:O2'   | 11:A:2878:G:N2    | 2.45                     | 0.49              |
| 13:C:39:PRO:HD2   | 13:C:42:ARG:HD2   | 1.94                     | 0.49              |
| 23:M:111:ASP:O    | 23:M:116:ILE:HD11 | 2.13                     | 0.49              |
| 1:0:110:CYS:O     | 1:0:114:GLY:N     | 2.42                     | 0.49              |
| 11:A:1823:A:O2'   | 11:A:1824:U:P     | 2.70                     | 0.49              |
| 11:A:2191:A:N6    | 11:A:2198:A:OP1   | 2.46                     | 0.49              |
| 3:2:62:ASN:O      | 3:2:68:ARG:HD2    | 2.13                     | 0.49              |
| 11:A:1740:A:OP2   | 11:A:1741:A:O2'   | 2.27                     | 0.49              |
| 38:b:43:ALA:HB2   | 38:b:89:ILE:HD12  | 1.94                     | 0.49              |
| 44:h:60:TYR:OH    | 44:h:130:TYR:O    | 2.30                     | 0.49              |
| 11:A:1680:A:H2'   | 11:A:1681:G:O4'   | 2.13                     | 0.49              |
| 11:A:2145:G:N3    | 29:S:104:ARG:NH2  | 2.59                     | 0.49              |
| 11:A:2938:A:H2'   | 11:A:2939:C:O2    | 2.12                     | 0.49              |
| 16:F:191:ASP:OD1  | 16:F:192:SER:N    | 2.46                     | 0.49              |
| 22:L:32:ILE:HG23  | 22:L:36:THR:OG1   | 2.13                     | 0.49              |
| 7:6:218:LEU:HD12  | 7:6:270:PHE:CE2   | 2.48                     | 0.48              |
| 7:6:253:PRO:O     | 7:6:296:ARG:NH2   | 2.45                     | 0.48              |
| 11:A:2754:A:N3    | 34:X:108:GLN:NE2  | 2.58                     | 0.48              |
| 16:F:211:ARG:NH1  | 44:h:56:ARG:O     | 2.46                     | 0.48              |
| 16:F:237:LEU:O    | 51:q:25:TYR:N     | 2.46                     | 0.48              |
| 32:V:178:SER:OG   | 32:V:181:ASP:OD2  | 2.29                     | 0.48              |
| 53:s:174:LEU:HB3  | 53:s:175:PRO:HD3  | 1.95                     | 0.48              |
| 11:A:1713:A:O2'   | 11:A:1714:C:OP1   | 2.25                     | 0.48              |
| 11:A:2241:A:H2'   | 52:r:192:TRP:HB2  | 1.96                     | 0.48              |
| 11:A:2815:OMG:N1  | 11:A:2816:G:O6    | 2.46                     | 0.48              |
| 11:A:2905:A:O2'   | 11:A:2906:C:P     | 2.70                     | 0.48              |
| 15:E:121:LEU:HD22 | 15:E:284:TYR:CE1  | 2.48                     | 0.48              |
| 24:N:223:MET:O    | 36:Z:115:HIS:HB3  | 2.12                     | 0.48              |
| 27:Q:168:ASN:O    | 27:Q:171:VAL:HG22 | 2.13                     | 0.48              |
| 36:Z:114:LYS:NZ   | 49:o:42:GLU:OE2   | 2.45                     | 0.48              |
| 53:s:171:VAL:HG23 | 53:s:172:ILE:HG12 | 1.95                     | 0.48              |
| 55:v:23:LEU:O     | 55:v:28:ARG:NH2   | 2.46                     | 0.48              |
| 11:A:2456:U:O2'   | 11:A:2457:A:H5'   | 2.12                     | 0.48              |
| 15:E:111:THR:OG1  | 15:E:113:ASP:OD1  | 2.24                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:E:204:VAL:HG21  | 15:E:299:VAL:CG1  | 2.44                     | 0.48              |
| 16:F:91:PRO:HB3    | 23:M:16:LEU:HD11  | 1.95                     | 0.48              |
| 29:S:194:ARG:NH2   | 38:b:13:SER:OG    | 2.46                     | 0.48              |
| 8:7:148:MET:HE2    | 8:7:257:ILE:HG13  | 1.95                     | 0.48              |
| 11:A:2952:U:C2     | 11:A:2953:U:C5    | 3.01                     | 0.48              |
| 11:A:3208:C:O4'    | 11:A:3208:C:O2    | 2.32                     | 0.48              |
| 53:s:167:GLU:O     | 53:s:171:VAL:HG22 | 2.14                     | 0.48              |
| 11:A:1822:U:O2     | 11:A:2707:A:O2'   | 2.30                     | 0.48              |
| 11:A:2959:G:H4'    | 57:x:130:SER:HB2  | 1.96                     | 0.48              |
| 13:C:302:GLY:N     | 13:C:382:ARG:O    | 2.35                     | 0.48              |
| 30:T:155:ARG:O     | 30:T:167:MET:N    | 2.46                     | 0.48              |
| 11:A:1672:C:O2'    | 30:T:149:ARG:O    | 2.28                     | 0.48              |
| 11:A:3054:G:H2'    | 11:A:3055:U:C6    | 2.49                     | 0.48              |
| 7:6:233:LEU:HB2    | 7:6:298:PHE:CE1   | 2.47                     | 0.48              |
| 20:J:102:ARG:N     | 20:J:107:GLU:OE1  | 2.42                     | 0.48              |
| 24:N:216:GLU:OE1   | 24:N:238:LYS:HG2  | 2.13                     | 0.48              |
| 39:c:46:GLU:OE1    | 39:c:49:ARG:NH1   | 2.46                     | 0.48              |
| 11:A:2081:U:OP1    | 49:o:63:ALA:N     | 2.40                     | 0.48              |
| 19:I:168:LEU:HD11  | 19:I:174:LEU:HD23 | 1.95                     | 0.48              |
| 22:L:39:ARG:NH2    | 27:Q:158:GLN:OE1  | 2.47                     | 0.48              |
| 40:d:50:PHE:HA     | 40:d:53:GLU:HG3   | 1.95                     | 0.48              |
| 11:A:1714:C:OP2    | 11:A:1715:C:N4    | 2.47                     | 0.48              |
| 11:A:2113:G:N1     | 49:o:15:ARG:HB2   | 2.28                     | 0.48              |
| 15:E:230:THR:O     | 15:E:231:HIS:HB2  | 2.14                     | 0.48              |
| 40:d:258:SER:OG    | 40:d:259:TRP:N    | 2.46                     | 0.48              |
| 11:A:1766:U:O2'    | 11:A:1767:G:P     | 2.72                     | 0.48              |
| 11:A:2194:U:O2     | 19:I:125:VAL:O    | 2.31                     | 0.48              |
| 19:I:98:VAL:HG13   | 19:I:177:LEU:HB3  | 1.96                     | 0.48              |
| 33:W:61:VAL:HG21   | 33:W:97:VAL:CG2   | 2.44                     | 0.48              |
| 7:6:377:TYR:CD1    | 23:M:141:VAL:HG11 | 2.49                     | 0.47              |
| 9:8:134:ASP:OD1    | 9:8:137:ARG:NH2   | 2.43                     | 0.47              |
| 9:8:169:PHE:HB2    | 9:8:170:PRO:HD3   | 1.96                     | 0.47              |
| 11:A:2911:C:O2     | 11:A:2911:C:O4'   | 2.31                     | 0.47              |
| 13:C:350:ASP:OD1   | 13:C:351:THR:N    | 2.47                     | 0.47              |
| 19:I:188:ARG:HE    | 47:k:55:VAL:HG13  | 1.79                     | 0.47              |
| 28:R:112:THR:HG23  | 29:S:142:THR:HG21 | 1.96                     | 0.47              |
| 6:5:270:ILE:HG23   | 6:5:270:ILE:O     | 2.14                     | 0.47              |
| 7:6:186:PRO:O      | 7:6:191:ASN:ND2   | 2.46                     | 0.47              |
| 11:A:2093:U:O2     | 11:A:2266:U:O2'   | 2.32                     | 0.47              |
| 11:A:3039:OMU:HM23 | 11:A:3041:U:C6    | 2.49                     | 0.47              |
| 20:J:33:PRO:N      | 20:J:34:PRO:HD2   | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:X:178:PRO:O    | 34:X:179:GLU:HG2  | 2.15                     | 0.47              |
| 11:A:2635:G:O2'   | 11:A:2636:G:P     | 2.72                     | 0.47              |
| 11:A:2954:C:O2    | 24:N:182:LYS:NZ   | 2.40                     | 0.47              |
| 30:T:174:TYR:CE2  | 30:T:176:VAL:HG13 | 2.49                     | 0.47              |
| 8:7:70:VAL:HG22   | 8:7:70:VAL:O      | 2.14                     | 0.47              |
| 20:J:26:ALA:HB1   | 20:J:57:THR:HG23  | 1.97                     | 0.47              |
| 34:X:20:ILE:HA    | 34:X:23:ARG:HE    | 1.80                     | 0.47              |
| 55:v:10:LEU:HD11  | 56:w:112:SER:CB   | 2.44                     | 0.47              |
| 56:w:90:TYR:OH    | 56:w:117:GLU:OE2  | 2.31                     | 0.47              |
| 11:A:2081:U:H2'   | 11:A:2082:G:C8    | 2.50                     | 0.47              |
| 11:A:2129:G:O4'   | 11:A:2152:A:H2    | 1.98                     | 0.47              |
| 11:A:2181:A:O2'   | 11:A:2182:G:OP1   | 2.32                     | 0.47              |
| 11:A:3157:C:O4'   | 11:A:3157:C:OP2   | 2.32                     | 0.47              |
| 14:D:207:ILE:HG12 | 14:D:229:PRO:HD3  | 1.96                     | 0.47              |
| 17:G:310:VAL:O    | 17:G:314:GLN:HG2  | 2.14                     | 0.47              |
| 8:7:81:MET:HB3    | 8:7:86:SER:OG     | 2.14                     | 0.47              |
| 11:A:2052:A:O2'   | 11:A:2053:U:H5'   | 2.15                     | 0.47              |
| 11:A:2099:U:H2'   | 11:A:2100:C:C6    | 2.49                     | 0.47              |
| 11:A:2615:A:C5    | 22:L:58:ILE:HD12  | 2.49                     | 0.47              |
| 30:T:87:MET:HE3   | 30:T:117:ILE:CG1  | 2.43                     | 0.47              |
| 33:W:61:VAL:HG13  | 33:W:65:ASN:HB2   | 1.96                     | 0.47              |
| 42:f:178:LEU:HD13 | 42:f:184:LEU:HD21 | 1.96                     | 0.47              |
| 53:s:250:PHE:CE2  | 53:s:356:VAL:HG13 | 2.49                     | 0.47              |
| 7:6:334:LEU:HD23  | 7:6:334:LEU:H     | 1.80                     | 0.47              |
| 8:7:276:PHE:HB2   | 8:7:304:VAL:HG12  | 1.95                     | 0.47              |
| 9:8:122:SER:HA    | 9:8:125:LYS:HE3   | 1.96                     | 0.47              |
| 11:A:1884:G:N3    | 11:A:1895:C:O2'   | 2.46                     | 0.47              |
| 11:A:2114:C:C2    | 11:A:2115:U:C5    | 3.02                     | 0.47              |
| 16:F:89:THR:H     | 16:F:179:THR:HG21 | 1.80                     | 0.47              |
| 17:G:137:ASN:C    | 17:G:140:PRO:HD2  | 2.40                     | 0.47              |
| 22:L:55:PRO:HB3   | 22:L:77:ILE:HG12  | 1.97                     | 0.47              |
| 23:M:62:ARG:CG    | 45:i:128:ARG:HE   | 2.26                     | 0.47              |
| 24:N:80:THR:O     | 24:N:80:THR:HG22  | 2.14                     | 0.47              |
| 27:Q:77:SER:OG    | 27:Q:79:GLU:OE1   | 2.31                     | 0.47              |
| 27:Q:240:ILE:HG21 | 27:Q:243:ILE:HD12 | 1.96                     | 0.47              |
| 30:T:195:HIS:CD2  | 37:a:123:TRP:HE3  | 2.32                     | 0.47              |
| 33:W:99:TYR:CE2   | 33:W:131:VAL:HG22 | 2.49                     | 0.47              |
| 57:x:117:ARG:HB3  | 57:x:156:ARG:HD2  | 1.95                     | 0.47              |
| 11:A:2080:U:O2'   | 49:o:60:ARG:HA    | 2.14                     | 0.47              |
| 11:A:2367:A:N3    | 35:Y:123:ARG:NH2  | 2.61                     | 0.47              |
| 6:5:95:GLU:N      | 6:5:95:GLU:OE1    | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:2209:G:C2'   | 11:A:2210:C:OP1   | 2.62                     | 0.47              |
| 42:f:161:GLY:C    | 42:f:162:LEU:HD22 | 2.40                     | 0.47              |
| 55:v:20:GLY:O     | 55:v:28:ARG:NH1   | 2.48                     | 0.47              |
| 9:8:110:GLU:OE2   | 9:8:111:THR:HG23  | 2.15                     | 0.47              |
| 10:9:57:VAL:O     | 31:U:16:GLN:NE2   | 2.48                     | 0.47              |
| 11:A:2116:C:C2    | 11:A:2117:U:C5    | 3.03                     | 0.47              |
| 11:A:2331:C:H4'   | 11:A:2332:C:O5'   | 2.15                     | 0.47              |
| 11:A:2523:C:C2'   | 11:A:2523:C:O2    | 2.63                     | 0.47              |
| 11:A:2896:G:N2    | 11:A:2917:G:O4'   | 2.48                     | 0.47              |
| 11:A:3169:C:H2'   | 11:A:3170:C:O2    | 2.15                     | 0.47              |
| 13:C:192:LEU:HD11 | 13:C:231:VAL:HG22 | 1.97                     | 0.47              |
| 16:F:249:ASN:ND2  | 45:i:55:GLY:C     | 2.73                     | 0.47              |
| 17:G:112:LEU:HD13 | 17:G:128:ILE:HD11 | 1.95                     | 0.47              |
| 21:K:8:PRO:HG2    | 39:c:295:GLU:HG3  | 1.97                     | 0.47              |
| 11:A:2292:G:C8    | 28:R:11:ARG:HB2   | 2.51                     | 0.46              |
| 11:A:2939:C:O2    | 11:A:2939:C:O4'   | 2.31                     | 0.46              |
| 25:O:38:ARG:NE    | 25:O:82:GLU:OE1   | 2.44                     | 0.46              |
| 11:A:2470:G:O2'   | 22:L:36:THR:HG22  | 2.15                     | 0.46              |
| 33:W:100:THR:OG1  | 33:W:132:HIS:NE2  | 2.33                     | 0.46              |
| 42:f:125:TYR:CE1  | 42:f:156:VAL:HG11 | 2.51                     | 0.46              |
| 53:s:415:ASP:O    | 53:s:419:LEU:HD23 | 2.16                     | 0.46              |
| 56:w:141:PRO:HA   | 56:w:144:ILE:HG22 | 1.98                     | 0.46              |
| 13:C:183:ALA:N    | 13:C:184:PRO:CD   | 2.78                     | 0.46              |
| 45:i:79:TRP:O     | 45:i:93:ARG:NE    | 2.39                     | 0.46              |
| 53:s:110:THR:HG22 | 53:s:110:THR:O    | 2.15                     | 0.46              |
| 8:7:230:PHE:HD2   | 8:7:240:ILE:HD11  | 1.80                     | 0.46              |
| 11:A:2165:C:H3'   | 11:A:2166:C:C2    | 2.50                     | 0.46              |
| 11:A:2868:C:H2'   | 11:A:2869:A:O4'   | 2.15                     | 0.46              |
| 57:x:120:GLN:OE1  | 57:x:176:VAL:HG13 | 2.16                     | 0.46              |
| 6:5:123:LEU:HD22  | 6:5:220:LEU:HD13  | 1.98                     | 0.46              |
| 11:A:2187:C:O2    | 20:J:104:THR:OG1  | 2.32                     | 0.46              |
| 11:A:2803:A:H2'   | 11:A:2804:A:O4'   | 2.15                     | 0.46              |
| 23:M:44:ARG:HD3   | 23:M:45:ARG:HG3   | 1.97                     | 0.46              |
| 53:s:188:LEU:HD12 | 53:s:426:LEU:HD21 | 1.97                     | 0.46              |
| 11:A:2009:G:OP1   | 45:i:112:LYS:HD3  | 2.15                     | 0.46              |
| 11:A:2853:A:H4'   | 11:A:2854:U:H3'   | 1.97                     | 0.46              |
| 13:C:336:VAL:HG11 | 13:C:380:MET:HE2  | 1.98                     | 0.46              |
| 50:p:192:ARG:O    | 50:p:193:ILE:C    | 2.58                     | 0.46              |
| 55:v:47:ASP:OD1   | 55:v:48:ALA:N     | 2.44                     | 0.46              |
| 2:1:54:VAL:CG1    | 51:q:125:MET:HE1  | 2.46                     | 0.46              |
| 9:8:124:TYR:OH    | 9:8:128:GLU:OE2   | 2.33                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:2274:A:H5'   | 28:R:16:ASP:OD2   | 2.16                     | 0.46              |
| 11:A:2458:A:O2'   | 15:E:215:PHE:O    | 2.32                     | 0.46              |
| 24:N:51:ARG:NH1   | 24:N:52:PHE:O     | 2.49                     | 0.46              |
| 43:g:68:THR:CG2   | 43:g:69:PRO:HD2   | 2.46                     | 0.46              |
| 11:A:1718:A:H2'   | 11:A:1719:G:O4'   | 2.15                     | 0.46              |
| 11:A:2429:A:N1    | 11:A:2433:C:O2'   | 2.46                     | 0.46              |
| 11:A:2615:A:C6    | 22:L:58:ILE:HG23  | 2.51                     | 0.46              |
| 21:K:7:ALA:HB3    | 21:K:8:PRO:HD3    | 1.98                     | 0.46              |
| 46:j:99:GLN:O     | 46:j:102:GLN:HG3  | 2.16                     | 0.46              |
| 50:p:136:THR:O    | 50:p:153:LYS:NZ   | 2.49                     | 0.46              |
| 51:q:47:THR:HG23  | 51:q:47:THR:O     | 2.16                     | 0.46              |
| 3:2:78:VAL:HG22   | 3:2:81:ARG:HH21   | 1.81                     | 0.46              |
| 11:A:3112:A:C8    | 11:A:3201:A:C6    | 3.03                     | 0.46              |
| 17:G:162:ARG:NH1  | 17:G:189:MET:O    | 2.48                     | 0.46              |
| 25:O:110:ILE:HG23 | 25:O:111:PRO:HD2  | 1.98                     | 0.46              |
| 29:S:159:THR:OG1  | 29:S:196:ASN:OD1  | 2.25                     | 0.46              |
| 34:X:222:ASP:OD1  | 34:X:222:ASP:N    | 2.48                     | 0.46              |
| 23:M:110:VAL:HG13 | 23:M:116:ILE:HD12 | 1.98                     | 0.46              |
| 25:O:77:ASP:O     | 25:O:83:LYS:NZ    | 2.49                     | 0.46              |
| 8:7:108:VAL:HG13  | 8:7:123:CYS:SG    | 2.57                     | 0.45              |
| 11:A:1861:U:H2'   | 11:A:1862:U:C6    | 2.51                     | 0.45              |
| 8:7:167:VAL:HG12  | 8:7:182:ASP:O     | 2.16                     | 0.45              |
| 11:A:2382:A:H2'   | 11:A:2383:U:C6    | 2.51                     | 0.45              |
| 19:I:161:VAL:HG23 | 19:I:195:SER:OG   | 2.17                     | 0.45              |
| 40:d:266:VAL:HG13 | 40:d:266:VAL:O    | 2.15                     | 0.45              |
| 42:f:96:THR:OG1   | 42:f:154:GLU:OE2  | 2.25                     | 0.45              |
| 42:f:167:ALA:O    | 42:f:171:LEU:HD23 | 2.16                     | 0.45              |
| 7:6:64:GLU:HG3    | 33:W:125:VAL:HG21 | 1.97                     | 0.45              |
| 9:8:138:ALA:O     | 9:8:141:GLU:HG3   | 2.16                     | 0.45              |
| 11:A:2905:A:H2'   | 11:A:2906:C:O4'   | 2.16                     | 0.45              |
| 21:K:144:GLU:OE2  | 38:b:146:ARG:NH1  | 2.50                     | 0.45              |
| 38:b:33:VAL:O     | 38:b:67:SER:HA    | 2.17                     | 0.45              |
| 6:5:107:PHE:CE1   | 6:5:113:LEU:HD11  | 2.50                     | 0.45              |
| 11:A:3112:A:N7    | 11:A:3200:U:C2    | 2.84                     | 0.45              |
| 13:C:166:VAL:HG13 | 13:C:191:LEU:HD23 | 1.96                     | 0.45              |
| 53:s:110:THR:HG23 | 53:s:333:PHE:CG   | 2.51                     | 0.45              |
| 7:6:222:ASP:OD1   | 7:6:222:ASP:N     | 2.47                     | 0.45              |
| 7:6:299:ARG:O     | 7:6:302:ASP:OD1   | 2.35                     | 0.45              |
| 11:A:2056:G:H2'   | 11:A:2057:C:C6    | 2.52                     | 0.45              |
| 13:C:28:LYS:NZ    | 13:C:30:LYS:O     | 2.44                     | 0.45              |
| 17:G:139:GLU:HG3  | 17:G:140:PRO:HD3  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:G:264:ARG:O    | 17:G:268:LEU:HD23 | 2.16                     | 0.45              |
| 23:M:94:LYS:NZ    | 23:M:135:ASP:OD2  | 2.46                     | 0.45              |
| 6:5:380:GLN:HB3   | 6:5:410:THR:HG22  | 1.98                     | 0.45              |
| 11:A:1877:U:O3'   | 23:M:30:ASN:ND2   | 2.49                     | 0.45              |
| 11:A:2177:U:N3    | 11:A:2180:A:OP2   | 2.48                     | 0.45              |
| 11:A:2494:C:O2    | 11:A:2494:C:H2'   | 2.16                     | 0.45              |
| 11:A:2925:U:O2'   | 11:A:2926:A:O5'   | 2.33                     | 0.45              |
| 31:U:42:PHE:HB3   | 31:U:44:ILE:HD11  | 1.98                     | 0.45              |
| 38:b:72:VAL:HG13  | 38:b:74:ARG:HG3   | 1.98                     | 0.45              |
| 55:v:10:LEU:HD12  | 56:w:116:VAL:CG2  | 2.47                     | 0.45              |
| 11:A:1986:A:H1'   | 11:A:1987:G:OP2   | 2.17                     | 0.45              |
| 19:I:181:ILE:O    | 19:I:184:THR:OG1  | 2.28                     | 0.45              |
| 36:Z:101:LYS:NZ   | 46:j:83:GLU:OE1   | 2.49                     | 0.45              |
| 54:u:188:TYR:HB3  | 54:u:190:LEU:HD12 | 1.98                     | 0.45              |
| 7:6:238:THR:HG21  | 7:6:281:PHE:CE2   | 2.52                     | 0.45              |
| 15:E:135:LYS:HZ2  | 15:E:142:MET:HA   | 1.82                     | 0.45              |
| 17:G:268:LEU:HD21 | 17:G:301:PHE:CE1  | 2.51                     | 0.45              |
| 20:J:60:ILE:HG13  | 20:J:61:LYS:H     | 1.82                     | 0.45              |
| 26:P:94:VAL:HG22  | 26:P:144:MET:SD   | 2.57                     | 0.45              |
| 57:x:81:CYS:SG    | 57:x:133:GLN:OE1  | 2.74                     | 0.45              |
| 9:8:171:PHE:O     | 42:f:187:LYS:NZ   | 2.50                     | 0.45              |
| 11:A:1707:C:C4'   | 11:A:1708:A:OP1   | 2.65                     | 0.45              |
| 11:A:1878:U:O3'   | 16:F:92:ARG:NH2   | 2.49                     | 0.45              |
| 11:A:2016:C:OP2   | 23:M:59:ARG:NH1   | 2.43                     | 0.45              |
| 11:A:2079:C:O2    | 11:A:2079:C:O4'   | 2.32                     | 0.45              |
| 12:B:1603:A:N6    | 12:B:1669:G:C6    | 2.85                     | 0.45              |
| 13:C:183:ALA:N    | 13:C:184:PRO:HD3  | 2.32                     | 0.45              |
| 13:C:296:LEU:HB2  | 13:C:328:LEU:HD13 | 1.99                     | 0.45              |
| 42:f:183:ARG:HE   | 42:f:184:LEU:N    | 2.14                     | 0.45              |
| 53:s:249:GLU:HG2  | 53:s:354:PRO:HG2  | 1.99                     | 0.45              |
| 57:x:130:SER:O    | 57:x:131:ARG:C    | 2.60                     | 0.45              |
| 7:6:147:HIS:O     | 7:6:151:LEU:HD23  | 2.17                     | 0.45              |
| 8:7:319:ARG:CZ    | 25:O:155:ASP:OD2  | 2.65                     | 0.45              |
| 10:9:103:ASP:OD2  | 10:9:116:LYS:NZ   | 2.45                     | 0.45              |
| 11:A:1942:C:H2'   | 11:A:1943:A:O4'   | 2.16                     | 0.45              |
| 11:A:2110:A:O2'   | 19:I:33:VAL:O     | 2.18                     | 0.45              |
| 11:A:2326:C:OP2   | 53:s:55:SER:OG    | 2.23                     | 0.45              |
| 11:A:2993:U:H5    | 11:A:3070:G:O6    | 2.00                     | 0.45              |
| 22:L:96:MET:HE2   | 27:Q:165:GLU:H    | 1.81                     | 0.45              |
| 27:Q:87:THR:HG21  | 27:Q:92:PHE:CZ    | 2.52                     | 0.45              |
| 53:s:259:ILE:HD12 | 53:s:259:ILE:H    | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:4:96:PRO:HB2    | 11:A:3014:G:H5'   | 1.99                     | 0.44              |
| 11:A:2937:A:C2    | 11:A:2938:A:C8    | 3.06                     | 0.44              |
| 47:k:82:THR:N     | 47:k:85:GLU:OE1   | 2.48                     | 0.44              |
| 56:w:147:TYR:O    | 56:w:150:ASP:OD1  | 2.35                     | 0.44              |
| 6:5:208:THR:HG21  | 53:s:160:ARG:HG2  | 1.99                     | 0.44              |
| 16:F:99:VAL:HG21  | 16:F:173:GLY:HA3  | 1.99                     | 0.44              |
| 18:H:102:VAL:HG13 | 18:H:105:VAL:HB   | 2.00                     | 0.44              |
| 41:e:183:THR:HG23 | 41:e:186:GLY:H    | 1.82                     | 0.44              |
| 57:x:118:VAL:CG2  | 57:x:173:LEU:HB3  | 2.47                     | 0.44              |
| 4:3:116:ARG:NH1   | 4:3:159:ASP:OD1   | 2.50                     | 0.44              |
| 11:A:3187:C:O2'   | 11:A:3188:U:H2'   | 2.17                     | 0.44              |
| 17:G:240:ARG:NH2  | 17:G:269:GLU:OE1  | 2.51                     | 0.44              |
| 21:K:143:GLU:OE1  | 38:b:136:LYS:NZ   | 2.45                     | 0.44              |
| 22:L:38:VAL:HG12  | 22:L:75:LEU:HD11  | 1.99                     | 0.44              |
| 24:N:172:VAL:HG12 | 24:N:176:LEU:HG   | 1.98                     | 0.44              |
| 34:X:80:TRP:CD1   | 34:X:80:TRP:N     | 2.85                     | 0.44              |
| 6:5:173:ARG:HA    | 6:5:176:TYR:CE2   | 2.53                     | 0.44              |
| 34:X:6:TYR:CG     | 34:X:14:LEU:HD11  | 2.51                     | 0.44              |
| 35:Y:151:ASP:OD1  | 35:Y:154:ARG:NH1  | 2.49                     | 0.44              |
| 38:b:71:CYS:O     | 38:b:72:VAL:HB    | 2.17                     | 0.44              |
| 54:u:196:LEU:HD23 | 55:v:57:LYS:HB2   | 1.99                     | 0.44              |
| 6:5:145:ASN:O     | 6:5:191:GLN:NE2   | 2.49                     | 0.44              |
| 11:A:2677:A:H2'   | 11:A:2678:A:C8    | 2.53                     | 0.44              |
| 14:D:290:PRO:HA   | 14:D:293:LYS:HG3  | 1.98                     | 0.44              |
| 19:I:101:ASN:N    | 19:I:152:MET:HE3  | 2.32                     | 0.44              |
| 36:Z:69:VAL:HG12  | 36:Z:119:ILE:HG12 | 1.99                     | 0.44              |
| 8:7:81:MET:HE3    | 8:7:91:CYS:SG     | 2.57                     | 0.44              |
| 11:A:1839:C:C6    | 21:K:50:LEU:HD21  | 2.53                     | 0.44              |
| 11:A:1881:A:O2'   | 11:A:1893:A:N1    | 2.50                     | 0.44              |
| 11:A:2059:C:H1'   | 11:A:2080:U:O4    | 2.18                     | 0.44              |
| 11:A:3155:C:O2'   | 11:A:3156:A:H5'   | 2.18                     | 0.44              |
| 15:E:275:ARG:HD2  | 15:E:333:TYR:CE2  | 2.52                     | 0.44              |
| 16:F:72:PHE:HD2   | 44:h:53:PRO:HD3   | 1.83                     | 0.44              |
| 33:W:105:VAL:HG23 | 33:W:105:VAL:O    | 2.18                     | 0.44              |
| 37:a:140:LYS:NZ   | 37:a:142:ARG:O    | 2.50                     | 0.44              |
| 38:b:26:LEU:HD22  | 38:b:105:ALA:HA   | 1.99                     | 0.44              |
| 47:k:33:PHE:O     | 47:k:37:VAL:HG12  | 2.17                     | 0.44              |
| 7:6:268:LEU:HD12  | 7:6:319:PHE:CE2   | 2.52                     | 0.44              |
| 10:9:28:ARG:NH1   | 11:A:2376:A:HO2'  | 2.11                     | 0.44              |
| 11:A:1707:C:H4'   | 11:A:1708:A:OP1   | 2.17                     | 0.44              |
| 11:A:2053:U:O2'   | 11:A:2054:U:H6    | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:2114:C:N3    | 11:A:2115:U:C5    | 2.86                     | 0.44              |
| 11:A:2379:C:H2'   | 11:A:2380:C:O4'   | 2.18                     | 0.44              |
| 13:C:176:ILE:HG23 | 13:C:250:ASP:H    | 1.83                     | 0.44              |
| 20:J:25:ARG:HA    | 20:J:65:PRO:HA    | 1.99                     | 0.44              |
| 41:e:73:LEU:O     | 41:e:76:GLN:HG3   | 2.17                     | 0.44              |
| 57:x:79:LEU:O     | 57:x:131:ARG:HA   | 2.17                     | 0.44              |
| 8:7:148:MET:HE1   | 8:7:255:HIS:C     | 2.42                     | 0.44              |
| 11:A:1917:A:C8    | 11:A:1983:U:C4    | 3.05                     | 0.44              |
| 11:A:2116:C:O2'   | 11:A:2837:A:N3    | 2.45                     | 0.44              |
| 11:A:2124:A:H5'   | 11:A:2125:C:H5''  | 2.00                     | 0.44              |
| 11:A:2261:C:O2'   | 29:S:184:ARG:NH1  | 2.49                     | 0.44              |
| 14:D:293:LYS:HA   | 14:D:296:VAL:HG23 | 2.00                     | 0.44              |
| 19:I:150:HIS:HB3  | 19:I:152:MET:HE1  | 2.00                     | 0.44              |
| 19:I:161:VAL:HA   | 19:I:164:MET:HE3  | 2.00                     | 0.44              |
| 21:K:90:VAL:O     | 21:K:90:VAL:HG13  | 2.18                     | 0.44              |
| 22:L:38:VAL:CG1   | 22:L:75:LEU:HD11  | 2.48                     | 0.44              |
| 25:O:30:ARG:HD2   | 25:O:78:PHE:O     | 2.17                     | 0.44              |
| 26:P:72:PHE:HB2   | 33:W:107:HIS:HA   | 1.99                     | 0.44              |
| 41:e:256:THR:OG1  | 41:e:257:LYS:N    | 2.50                     | 0.44              |
| 53:s:271:LEU:O    | 53:s:272:PRO:C    | 2.61                     | 0.44              |
| 57:x:103:PRO:CG   | 57:x:203:PRO:HD2  | 2.48                     | 0.44              |
| 4:3:127:ALA:HA    | 23:M:79:PRO:HD3   | 2.00                     | 0.44              |
| 7:6:257:PRO:HB3   | 7:6:268:LEU:HD11  | 2.00                     | 0.44              |
| 7:6:275:GLN:HG3   | 7:6:311:MET:SD    | 2.58                     | 0.44              |
| 11:A:1795:A:H2'   | 11:A:1796:A:O4'   | 2.17                     | 0.44              |
| 11:A:2117:U:H5'   | 11:A:2837:A:H1'   | 2.00                     | 0.44              |
| 11:A:2135:A:N3    | 11:A:2135:A:H2'   | 2.32                     | 0.44              |
| 11:A:2144:A:OP1   | 28:R:57:ARG:NH1   | 2.48                     | 0.44              |
| 11:A:2635:G:HO2'  | 11:A:2636:G:P     | 2.37                     | 0.44              |
| 11:A:2837:A:H4'   | 11:A:2838:A:OP1   | 2.18                     | 0.44              |
| 15:E:204:VAL:HG23 | 15:E:300:LYS:O    | 2.18                     | 0.44              |
| 29:S:133:VAL:O    | 29:S:133:VAL:HG13 | 2.17                     | 0.44              |
| 47:k:19:GLN:NE2   | 47:k:21:CYS:SG    | 2.91                     | 0.44              |
| 47:k:20:PHE:O     | 47:k:55:VAL:HG23  | 2.18                     | 0.44              |
| 11:A:2124:A:C5'   | 11:A:2125:C:H5''  | 2.48                     | 0.43              |
| 11:A:2322:C:O2    | 11:A:2322:C:O4'   | 2.33                     | 0.43              |
| 11:A:2442:U:OP1   | 53:s:81:ARG:NH2   | 2.37                     | 0.43              |
| 41:e:270:ALA:O    | 41:e:273:ARG:NH1  | 2.51                     | 0.43              |
| 54:u:196:LEU:HD12 | 54:u:196:LEU:N    | 2.33                     | 0.43              |
| 8:7:73:THR:HG23   | 8:7:99:TYR:OH     | 2.17                     | 0.43              |
| 9:8:178:TYR:HE2   | 48:m:65:HIS:ND1   | 2.16                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:1823:A:C2'   | 11:A:1824:U:OP2   | 2.64                     | 0.43              |
| 11:A:2523:C:O2    | 11:A:2523:C:H2'   | 2.17                     | 0.43              |
| 51:q:48:PRO:HB2   | 51:q:50:TRP:CD1   | 2.54                     | 0.43              |
| 11:A:1939:G:O2'   | 11:A:1973:G:H4'   | 2.18                     | 0.43              |
| 12:B:1631:C:H2'   | 12:B:1632:U:O4'   | 2.18                     | 0.43              |
| 19:I:139:LYS:HD2  | 19:I:139:LYS:O    | 2.18                     | 0.43              |
| 28:R:75:ALA:HB2   | 28:R:106:ALA:HB1  | 2.00                     | 0.43              |
| 30:T:91:ALA:O     | 30:T:95:ARG:HG3   | 2.17                     | 0.43              |
| 55:v:10:LEU:HD12  | 56:w:116:VAL:HG21 | 2.00                     | 0.43              |
| 55:v:46:GLU:HB2   | 55:v:51:ARG:HE    | 1.82                     | 0.43              |
| 3:2:87:ARG:NH2    | 11:A:1792:G:N7    | 2.57                     | 0.43              |
| 6:5:355:LEU:HD21  | 6:5:357:PHE:HB2   | 2.00                     | 0.43              |
| 8:7:221:VAL:CG1   | 8:7:225:VAL:HB    | 2.49                     | 0.43              |
| 9:8:128:GLU:O     | 9:8:131:MET:HG2   | 2.18                     | 0.43              |
| 9:8:132:GLU:O     | 9:8:136:ILE:HG12  | 2.19                     | 0.43              |
| 11:A:1760:G:OP2   | 51:q:59:LYS:NZ    | 2.33                     | 0.43              |
| 11:A:2171:U:O4    | 20:J:147:SER:OG   | 2.33                     | 0.43              |
| 11:A:2194:U:OP1   | 19:I:124:LYS:HD3  | 2.19                     | 0.43              |
| 11:A:2409:A:H2'   | 11:A:2410:U:C6    | 2.52                     | 0.43              |
| 11:A:3092:U:O2'   | 11:A:3093:C:O5'   | 2.37                     | 0.43              |
| 11:A:3116:C:H2'   | 11:A:3117:C:H6    | 1.83                     | 0.43              |
| 13:C:280:GLU:HA   | 13:C:283:ILE:HG12 | 2.01                     | 0.43              |
| 14:D:139:ILE:HD12 | 14:D:150:TRP:CE3  | 2.53                     | 0.43              |
| 16:F:292:ASP:OD1  | 16:F:292:ASP:N    | 2.48                     | 0.43              |
| 21:K:91:THR:HG22  | 52:r:161:PRO:HB3  | 2.00                     | 0.43              |
| 25:O:94:ALA:HB3   | 25:O:95:PRO:HD3   | 2.00                     | 0.43              |
| 8:7:293:LEU:CD2   | 8:7:295:ARG:HG2   | 2.49                     | 0.43              |
| 11:A:1750:G:O2'   | 11:A:1751:A:P     | 2.76                     | 0.43              |
| 11:A:2413:C:N3    | 53:s:161:ARG:NH1  | 2.49                     | 0.43              |
| 11:A:2416:U:H3    | 53:s:166:TYR:HB3  | 1.84                     | 0.43              |
| 11:A:2956:A:C6    | 11:A:2969:A:C8    | 3.07                     | 0.43              |
| 11:A:3115:U:H2'   | 11:A:3116:C:C6    | 2.53                     | 0.43              |
| 26:P:91:GLU:HG2   | 26:P:106:SER:HB3  | 2.00                     | 0.43              |
| 49:o:18:ILE:HG13  | 49:o:19:GLY:N     | 2.33                     | 0.43              |
| 8:7:144:ARG:NE    | 8:7:171:GLU:OE2   | 2.51                     | 0.43              |
| 11:A:1814:A:C8    | 45:i:32:ILE:HG21  | 2.54                     | 0.43              |
| 11:A:2164:C:O2'   | 11:A:2165:C:O5'   | 2.36                     | 0.43              |
| 11:A:2182:G:O2'   | 11:A:2183:C:P     | 2.76                     | 0.43              |
| 16:F:262:THR:OG1  | 16:F:265:THR:HG23 | 2.18                     | 0.43              |
| 57:x:118:VAL:HG23 | 57:x:173:LEU:HB3  | 2.00                     | 0.43              |
| 8:7:167:VAL:HG23  | 8:7:235:TYR:CD1   | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:8:126:GLN:HA    | 9:8:129:ARG:NH1   | 2.34                     | 0.43              |
| 11:A:1882:A:N1    | 11:A:1891:A:O2'   | 2.47                     | 0.43              |
| 11:A:2053:U:O2'   | 11:A:2054:U:C6    | 2.71                     | 0.43              |
| 11:A:2134:A:N6    | 11:A:2135:A:H62   | 2.16                     | 0.43              |
| 11:A:2959:G:O6    | 11:A:2962:C:H3'   | 2.18                     | 0.43              |
| 24:N:168:GLU:OE1  | 24:N:170:GLU:N    | 2.45                     | 0.43              |
| 26:P:72:PHE:O     | 33:W:105:VAL:HG23 | 2.17                     | 0.43              |
| 28:R:109:GLU:OE2  | 29:S:107:LYS:NZ   | 2.47                     | 0.43              |
| 31:U:143:ARG:HE   | 40:d:282:ILE:CD1  | 2.30                     | 0.43              |
| 34:X:127:VAL:HG22 | 34:X:131:THR:HB   | 2.00                     | 0.43              |
| 7:6:233:LEU:O     | 7:6:296:ARG:NH1   | 2.47                     | 0.43              |
| 7:6:238:THR:HG21  | 7:6:281:PHE:CD2   | 2.54                     | 0.43              |
| 7:6:330:ILE:HG22  | 7:6:335:LEU:HD13  | 2.00                     | 0.43              |
| 11:A:1872:U:H2'   | 11:A:1873:A:O4'   | 2.19                     | 0.43              |
| 15:E:269:TYR:HB3  | 15:E:304:LEU:CD1  | 2.49                     | 0.43              |
| 19:I:181:ILE:O    | 19:I:182:ASP:OD1  | 2.36                     | 0.43              |
| 55:v:10:LEU:HD11  | 56:w:112:SER:HB3  | 2.00                     | 0.43              |
| 7:6:276:ASP:HB2   | 7:6:310:THR:OG1   | 2.19                     | 0.43              |
| 11:A:1671:G:O2'   | 11:A:1672:C:P     | 2.76                     | 0.43              |
| 11:A:2519:G:N7    | 14:D:230:SER:OG   | 2.46                     | 0.43              |
| 15:E:340:PRO:C    | 27:Q:101:GLU:OE1  | 2.62                     | 0.43              |
| 23:M:106:ASP:HB3  | 43:g:68:THR:HG21  | 1.99                     | 0.43              |
| 46:j:96:GLN:OE1   | 46:j:99:GLN:NE2   | 2.51                     | 0.43              |
| 3:2:92:HIS:CD2    | 10:9:17:ARG:HG2   | 2.54                     | 0.43              |
| 11:A:2187:C:H2'   | 11:A:2188:A:C8    | 2.54                     | 0.43              |
| 11:A:2286:A:H2'   | 11:A:2287:U:C6    | 2.54                     | 0.43              |
| 11:A:3203:A:C5    | 11:A:3204:C:C5    | 3.06                     | 0.43              |
| 17:G:169:LEU:O    | 17:G:213:THR:HG22 | 2.19                     | 0.43              |
| 23:M:162:LEU:HD11 | 50:p:144:PHE:CB   | 2.49                     | 0.43              |
| 26:P:61:VAL:O     | 26:P:61:VAL:HG12  | 2.18                     | 0.43              |
| 41:e:160:LEU:HG   | 41:e:171:TRP:CD1  | 2.54                     | 0.43              |
| 47:k:33:PHE:HD1   | 47:k:87:LEU:HD12  | 1.83                     | 0.43              |
| 55:v:15:ALA:CB    | 55:v:62:LEU:HD11  | 2.49                     | 0.43              |
| 7:6:51:TYR:CZ     | 33:W:122:LYS:O    | 2.71                     | 0.42              |
| 8:7:107:LEU:HG    | 8:7:128:LEU:HD11  | 2.00                     | 0.42              |
| 11:A:2123:C:C3'   | 11:A:2124:A:H5''  | 2.49                     | 0.42              |
| 11:A:2383:U:H2'   | 11:A:2384:A:O4'   | 2.18                     | 0.42              |
| 11:A:2696:A:H1'   | 11:A:2698:G:OP2   | 2.19                     | 0.42              |
| 11:A:3048:A:O3'   | 22:L:74:LEU:HD11  | 2.19                     | 0.42              |
| 11:A:3212:C:O2    | 11:A:3212:C:O4'   | 2.37                     | 0.42              |
| 28:R:78:GLU:OE1   | 38:b:135:ASN:ND2  | 2.47                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:b:6:THR:HG23   | 38:b:7:PRO:HD2    | 2.01                     | 0.42              |
| 52:r:124:ARG:NH1  | 52:r:153:ARG:O    | 2.49                     | 0.42              |
| 6:5:208:THR:O     | 6:5:208:THR:HG23  | 2.19                     | 0.42              |
| 11:A:2387:U:H3'   | 14:D:75:THR:HG22  | 2.00                     | 0.42              |
| 24:N:172:VAL:HG13 | 24:N:175:PHE:CZ   | 2.54                     | 0.42              |
| 24:N:222:ASN:ND2  | 36:Z:39:SER:OG    | 2.51                     | 0.42              |
| 28:R:109:GLU:HG2  | 29:S:96:PHE:CE1   | 2.55                     | 0.42              |
| 30:T:90:LEU:HB3   | 30:T:117:ILE:HD12 | 2.01                     | 0.42              |
| 31:U:9:LEU:N      | 35:Y:183:GLN:OE1  | 2.51                     | 0.42              |
| 33:W:106:PRO:CD   | 33:W:117:ILE:HD11 | 2.49                     | 0.42              |
| 48:m:52:TYR:CG    | 48:m:71:PRO:HG3   | 2.54                     | 0.42              |
| 12:B:1628:C:N4    | 12:B:1640:A:N1    | 2.66                     | 0.42              |
| 27:Q:154:VAL:HG22 | 27:Q:199:THR:HA   | 2.01                     | 0.42              |
| 9:8:125:LYS:HA    | 9:8:128:GLU:HB2   | 2.01                     | 0.42              |
| 11:A:1958:G:N7    | 30:T:160:GLY:O    | 2.52                     | 0.42              |
| 11:A:1986:A:H4'   | 11:A:1987:G:O5'   | 2.18                     | 0.42              |
| 11:A:2002:G:H4'   | 11:A:2003:A:N3    | 2.34                     | 0.42              |
| 11:A:2215:C:C6    | 11:A:2216:A:C8    | 3.07                     | 0.42              |
| 11:A:2385:U:O5'   | 14:D:71:LYS:NZ    | 2.52                     | 0.42              |
| 11:A:2694:A:C6    | 11:A:2985:C:H1'   | 2.55                     | 0.42              |
| 11:A:2847:C:H2'   | 11:A:2848:A:C8    | 2.54                     | 0.42              |
| 23:M:187:VAL:CG2  | 23:M:265:ILE:HG23 | 2.50                     | 0.42              |
| 40:d:42:THR:O     | 40:d:42:THR:HG23  | 2.19                     | 0.42              |
| 42:f:98:TYR:CG    | 48:m:66:ILE:HG22  | 2.54                     | 0.42              |
| 53:s:99:ALA:HB1   | 53:s:271:LEU:HD11 | 2.00                     | 0.42              |
| 54:u:177:ILE:HG22 | 54:u:179:LEU:HD12 | 2.02                     | 0.42              |
| 57:x:165:GLU:O    | 57:x:167:GLY:N    | 2.52                     | 0.42              |
| 11:A:2176:C:H1'   | 20:J:102:ARG:NH1  | 2.34                     | 0.42              |
| 11:A:2196:A:H2'   | 11:A:2196:A:N3    | 2.35                     | 0.42              |
| 11:A:3007:C:C5    | 11:A:3054:G:C4    | 3.08                     | 0.42              |
| 11:A:3148:C:O2'   | 11:A:3149:C:H5'   | 2.19                     | 0.42              |
| 11:A:3170:C:O2    | 11:A:3170:C:O4'   | 2.37                     | 0.42              |
| 14:D:141:LEU:HB2  | 14:D:150:TRP:CZ3  | 2.54                     | 0.42              |
| 16:F:79:LEU:HD11  | 44:h:117:LEU:HD21 | 2.01                     | 0.42              |
| 40:d:287:LEU:HD11 | 40:d:293:TYR:HB2  | 2.01                     | 0.42              |
| 56:w:127:GLY:O    | 56:w:128:PHE:HB2  | 2.20                     | 0.42              |
| 7:6:173:LEU:HD12  | 7:6:272:LEU:HD22  | 2.02                     | 0.42              |
| 7:6:176:ALA:CB    | 7:6:184:LEU:HD12  | 2.45                     | 0.42              |
| 7:6:224:HIS:HA    | 7:6:232:TYR:CE2   | 2.54                     | 0.42              |
| 7:6:346:ARG:NH2   | 26:P:178:ILE:O    | 2.51                     | 0.42              |
| 11:A:2381:A:N6    | 11:A:2412:A:C6    | 2.88                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:C:345:ARG:NH2  | 13:C:362:GLU:OE1  | 2.52                     | 0.42              |
| 15:E:87:ILE:HG23  | 15:E:317:PRO:HG2  | 2.02                     | 0.42              |
| 41:e:71:ALA:O     | 41:e:74:LEU:HG    | 2.20                     | 0.42              |
| 53:s:253:LEU:O    | 53:s:254:ASP:HB2  | 2.19                     | 0.42              |
| 57:x:119:ASP:OD1  | 57:x:121:GLN:N    | 2.36                     | 0.42              |
| 6:5:157:VAL:HG12  | 6:5:180:ILE:HD12  | 2.00                     | 0.42              |
| 9:8:121:TRP:HD1   | 41:e:66:LEU:HD21  | 1.84                     | 0.42              |
| 11:A:2292:G:C8    | 28:R:11:ARG:CB    | 3.03                     | 0.42              |
| 11:A:2333:G:H2'   | 11:A:2334:C:C6    | 2.54                     | 0.42              |
| 11:A:3032:G:H2'   | 11:A:3033:U:O4'   | 2.20                     | 0.42              |
| 14:D:288:PRO:HG3  | 14:D:296:VAL:HG21 | 2.00                     | 0.42              |
| 16:F:249:ASN:ND2  | 45:i:55:GLY:O     | 2.52                     | 0.42              |
| 19:I:132:LYS:HB2  | 19:I:133:PRO:HD3  | 2.02                     | 0.42              |
| 21:K:5:SER:HB2    | 21:K:8:PRO:HD2    | 2.02                     | 0.42              |
| 21:K:136:ASP:OD1  | 21:K:137:ILE:N    | 2.52                     | 0.42              |
| 44:h:66:LEU:CD2   | 44:h:127:LEU:HD12 | 2.50                     | 0.42              |
| 53:s:165:ARG:HA   | 53:s:168:GLU:HG3  | 2.02                     | 0.42              |
| 56:w:138:LEU:HD13 | 56:w:144:ILE:HD13 | 2.01                     | 0.42              |
| 8:7:167:VAL:HG12  | 8:7:182:ASP:C     | 2.45                     | 0.42              |
| 11:A:2313:A:H2'   | 11:A:2314:C:C6    | 2.55                     | 0.42              |
| 11:A:3122:U:H4'   | 11:A:3123:G:OP1   | 2.20                     | 0.42              |
| 11:A:3212:C:H2'   | 11:A:3213:A:O4'   | 2.20                     | 0.42              |
| 13:C:247:ASP:OD1  | 13:C:382:ARG:NH1  | 2.53                     | 0.42              |
| 19:I:53:TYR:CD1   | 24:N:209:ASN:HB3  | 2.55                     | 0.42              |
| 28:R:64:MET:HE1   | 30:T:210:HIS:CG   | 2.55                     | 0.42              |
| 34:X:96:LYS:HG3   | 34:X:97:LEU:HD12  | 2.02                     | 0.42              |
| 51:q:41:ASP:OD1   | 51:q:41:ASP:N     | 2.49                     | 0.42              |
| 56:w:148:ILE:HA   | 56:w:151:LYS:HG2  | 2.02                     | 0.42              |
| 6:5:308:GLN:HE22  | 11:A:2389:C:H42   | 1.67                     | 0.42              |
| 7:6:323:TRP:HH2   | 7:6:328:THR:HG1   | 1.65                     | 0.42              |
| 9:8:164:ARG:HD3   | 42:f:88:TYR:CE1   | 2.55                     | 0.42              |
| 16:F:184:GLN:NE2  | 23:M:20:PRO:O     | 2.53                     | 0.42              |
| 23:M:177:ALA:HA   | 23:M:222:TYR:CD1  | 2.55                     | 0.42              |
| 30:T:48:SER:O     | 30:T:49:ARG:NH1   | 2.49                     | 0.42              |
| 34:X:81:GLY:O     | 34:X:130:ARG:NE   | 2.44                     | 0.42              |
| 39:c:86:ASP:OD1   | 39:c:87:LEU:N     | 2.49                     | 0.42              |
| 50:p:72:PRO:HG2   | 50:p:75:ARG:HB2   | 2.02                     | 0.42              |
| 51:q:71:VAL:HG13  | 51:q:71:VAL:O     | 2.18                     | 0.42              |
| 53:s:304:ASP:O    | 53:s:307:ARG:HG3  | 2.20                     | 0.42              |
| 1:0:185:PHE:CE1   | 25:O:131:PRO:HA   | 2.55                     | 0.42              |
| 3:2:78:VAL:O      | 3:2:82:ARG:HG2    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:2143:G:C5    | 11:A:2258:A:C2    | 3.07                     | 0.42              |
| 11:A:2171:U:N3    | 11:A:2173:G:H4'   | 2.35                     | 0.42              |
| 16:F:110:SER:O    | 16:F:158:PRO:HA   | 2.19                     | 0.42              |
| 16:F:220:ASP:O    | 16:F:245:ALA:N    | 2.52                     | 0.42              |
| 19:I:103:ALA:HB1  | 47:k:39:SER:HA    | 2.02                     | 0.42              |
| 21:K:178:LEU:HD13 | 52:r:35:PHE:CZ    | 2.55                     | 0.42              |
| 22:L:121:THR:HB   | 22:L:122:PRO:HD2  | 2.01                     | 0.42              |
| 23:M:254:LYS:O    | 23:M:258:THR:HG23 | 2.20                     | 0.42              |
| 41:e:123:MET:O    | 41:e:126:GLN:HG3  | 2.19                     | 0.42              |
| 57:x:162:LEU:HG   | 57:x:172:ASP:OD1  | 2.20                     | 0.42              |
| 8:7:223:ALA:N     | 8:7:250:ARG:O     | 2.51                     | 0.41              |
| 11:A:2056:G:H2'   | 11:A:2057:C:H6    | 1.83                     | 0.41              |
| 11:A:2118:U:C2    | 11:A:2119:U:C5    | 3.08                     | 0.41              |
| 11:A:2186:C:O5'   | 11:A:2186:C:H6    | 2.03                     | 0.41              |
| 11:A:2331:C:N3    | 11:A:2443:C:H5    | 2.17                     | 0.41              |
| 11:A:2965:A:N7    | 11:A:3016:G:C6    | 2.88                     | 0.41              |
| 15:E:204:VAL:HG12 | 15:E:271:LEU:O    | 2.20                     | 0.41              |
| 31:U:80:ARG:HD3   | 31:U:84:ASN:OD1   | 2.20                     | 0.41              |
| 34:X:127:VAL:CG2  | 34:X:131:THR:HB   | 2.50                     | 0.41              |
| 56:w:110:LEU:HB3  | 56:w:114:ASP:HB2  | 2.02                     | 0.41              |
| 57:x:76:ARG:NE    | 57:x:128:VAL:HG21 | 2.35                     | 0.41              |
| 6:5:82:TYR:CG     | 6:5:89:ARG:HG3    | 2.55                     | 0.41              |
| 8:7:80:VAL:O      | 8:7:80:VAL:HG23   | 2.20                     | 0.41              |
| 11:A:1771:C:O2'   | 11:A:1772:A:H5'   | 2.20                     | 0.41              |
| 11:A:1821:A:H2'   | 11:A:1822:U:O4'   | 2.19                     | 0.41              |
| 11:A:2082:G:H2'   | 11:A:2083:U:O4'   | 2.20                     | 0.41              |
| 11:A:2188:A:N6    | 11:A:2189:C:O2    | 2.53                     | 0.41              |
| 11:A:2333:G:O2'   | 11:A:2447:A:O2'   | 2.34                     | 0.41              |
| 11:A:2668:A:H2'   | 11:A:2669:A:C8    | 2.54                     | 0.41              |
| 19:I:79:ILE:HG23  | 19:I:80:ARG:N     | 2.35                     | 0.41              |
| 24:N:224:LEU:HB2  | 24:N:226:ILE:HG23 | 2.02                     | 0.41              |
| 34:X:127:VAL:HG22 | 34:X:128:THR:N    | 2.36                     | 0.41              |
| 57:x:77:ARG:HA    | 57:x:217:LEU:O    | 2.21                     | 0.41              |
| 9:8:155:PRO:O     | 9:8:158:HIS:NE2   | 2.53                     | 0.41              |
| 11:A:2034:A:H2'   | 11:A:2035:U:O4'   | 2.20                     | 0.41              |
| 11:A:2408:U:C4    | 11:A:2409:A:N6    | 2.88                     | 0.41              |
| 56:w:79:ILE:CD1   | 56:w:152:LYS:HZ3  | 2.33                     | 0.41              |
| 7:6:218:LEU:HD12  | 7:6:270:PHE:CZ    | 2.54                     | 0.41              |
| 11:A:2072:A:H2'   | 11:A:2073:A:C8    | 2.55                     | 0.41              |
| 11:A:2802:A:H2'   | 11:A:2803:A:O4'   | 2.21                     | 0.41              |
| 12:B:1623:G:OP1   | 26:P:86:THR:OG1   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:M:197:GLY:CA   | 51:q:62:ALA:HB2   | 2.50                     | 0.41              |
| 26:P:156:ASP:OD1  | 26:P:157:SER:N    | 2.53                     | 0.41              |
| 30:T:202:GLN:OE1  | 37:a:122:ARG:NH2  | 2.38                     | 0.41              |
| 53:s:181:VAL:HG12 | 53:s:200:LEU:HD11 | 2.03                     | 0.41              |
| 53:s:410:VAL:O    | 53:s:410:VAL:HG23 | 2.20                     | 0.41              |
| 55:v:5:SER:OG     | 55:v:8:ALA:HB2    | 2.20                     | 0.41              |
| 55:v:23:LEU:HD21  | 55:v:26:THR:OG1   | 2.21                     | 0.41              |
| 55:v:43:GLN:HA    | 55:v:46:GLU:OE2   | 2.20                     | 0.41              |
| 5:4:88:TRP:CE2    | 11:A:2160:A:H2'   | 2.56                     | 0.41              |
| 7:6:218:LEU:C     | 7:6:218:LEU:HD23  | 2.45                     | 0.41              |
| 10:9:39:LYS:HG3   | 11:A:1705:A:N7    | 2.36                     | 0.41              |
| 11:A:1741:A:O4'   | 11:A:1743:U:C6    | 2.73                     | 0.41              |
| 11:A:2111:C:H2'   | 11:A:2112:A:C8    | 2.55                     | 0.41              |
| 11:A:2493:C:O2    | 11:A:2493:C:O4'   | 2.35                     | 0.41              |
| 13:C:262:ARG:NH2  | 13:C:371:ASN:OD1  | 2.51                     | 0.41              |
| 19:I:96:ILE:HG22  | 19:I:180:CYS:O    | 2.19                     | 0.41              |
| 20:J:24:VAL:HG12  | 20:J:25:ARG:N     | 2.35                     | 0.41              |
| 27:Q:154:VAL:HG23 | 27:Q:154:VAL:O    | 2.20                     | 0.41              |
| 29:S:108:VAL:CG1  | 29:S:195:ILE:HG21 | 2.51                     | 0.41              |
| 30:T:61:PRO:HA    | 40:d:229:GLY:CA   | 2.51                     | 0.41              |
| 35:Y:205:VAL:HG12 | 35:Y:205:VAL:O    | 2.21                     | 0.41              |
| 38:b:47:VAL:O     | 38:b:51:VAL:HG12  | 2.20                     | 0.41              |
| 50:p:75:ARG:NH1   | 50:p:109:GLU:OE1  | 2.53                     | 0.41              |
| 53:s:318:ASP:O    | 53:s:321:GLU:HG2  | 2.20                     | 0.41              |
| 15:E:121:LEU:CD2  | 15:E:284:TYR:CE1  | 3.03                     | 0.41              |
| 20:J:103:GLN:O    | 20:J:104:THR:OG1  | 2.24                     | 0.41              |
| 28:R:17:ARG:O     | 28:R:21:ILE:HG12  | 2.21                     | 0.41              |
| 39:c:220:ILE:O    | 39:c:223:MET:HG2  | 2.20                     | 0.41              |
| 11:A:1839:C:H2'   | 11:A:1840:C:C6    | 2.55                     | 0.41              |
| 11:A:2343:G:H3'   | 11:A:2343:G:N3    | 2.35                     | 0.41              |
| 11:A:2898:U:H2'   | 11:A:2899:C:O4'   | 2.19                     | 0.41              |
| 11:A:3065:U:O2'   | 15:E:236:THR:HG21 | 2.21                     | 0.41              |
| 11:A:3118:U:O2'   | 54:u:158:LYS:NZ   | 2.42                     | 0.41              |
| 12:B:1643:A:N7    | 26:P:120:ARG:NH2  | 2.67                     | 0.41              |
| 13:C:182:ALA:HB2  | 13:C:255:ASP:HB3  | 2.03                     | 0.41              |
| 19:I:64:CYS:HA    | 52:r:69:GLN:OE1   | 2.21                     | 0.41              |
| 19:I:148:VAL:HG13 | 47:k:28:GLU:OE1   | 2.20                     | 0.41              |
| 24:N:226:ILE:HD12 | 24:N:230:LEU:HD11 | 2.03                     | 0.41              |
| 26:P:94:VAL:HG21  | 26:P:136:CYS:SG   | 2.61                     | 0.41              |
| 51:q:78:SER:HB2   | 51:q:79:PRO:HD2   | 2.03                     | 0.41              |
| 7:6:106:ARG:NH1   | 12:B:1621:A:OP2   | 2.38                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:1848:U:O2'   | 11:A:1849:C:OP1   | 2.32                     | 0.41              |
| 11:A:2179:A:H3'   | 11:A:2180:A:H5''  | 2.03                     | 0.41              |
| 11:A:3116:C:H2'   | 11:A:3117:C:C6    | 2.55                     | 0.41              |
| 16:F:177:ALA:O    | 16:F:181:LYS:HG2  | 2.21                     | 0.41              |
| 23:M:156:VAL:O    | 23:M:176:THR:HA   | 2.20                     | 0.41              |
| 33:W:70:GLN:HG3   | 33:W:72:HIS:O     | 2.20                     | 0.41              |
| 38:b:90:HIS:NE2   | 38:b:91:CYS:SG    | 2.75                     | 0.41              |
| 42:f:169:ILE:HD12 | 42:f:172:GLU:OE2  | 2.20                     | 0.41              |
| 56:w:114:ASP:O    | 56:w:117:GLU:HG2  | 2.21                     | 0.41              |
| 4:3:148:VAL:CG1   | 7:6:360:ARG:HA    | 2.51                     | 0.41              |
| 6:5:300:ARG:N     | 6:5:301:PRO:HD2   | 2.36                     | 0.41              |
| 6:5:354:PHE:HB3   | 6:5:417:LEU:HD11  | 2.03                     | 0.41              |
| 7:6:181:GLU:OE1   | 7:6:181:GLU:N     | 2.54                     | 0.41              |
| 8:7:194:PRO:HG2   | 8:7:283:VAL:HG21  | 2.02                     | 0.41              |
| 9:8:129:ARG:CZ    | 12:B:1627:C:O4'   | 2.68                     | 0.41              |
| 9:8:142:ALA:O     | 9:8:145:GLU:HG3   | 2.21                     | 0.41              |
| 9:8:173:LYS:H     | 42:f:183:ARG:HH22 | 1.67                     | 0.41              |
| 11:A:1907:A:N3    | 11:A:2930:U:O2'   | 2.42                     | 0.41              |
| 11:A:2091:A:H2'   | 11:A:2092:C:O4'   | 2.21                     | 0.41              |
| 11:A:2292:G:C8    | 16:F:155:PRO:HD3  | 2.56                     | 0.41              |
| 11:A:2695:G:O6    | 11:A:3059:A:C4    | 2.74                     | 0.41              |
| 11:A:2838:A:C5    | 11:A:2840:C:C5    | 3.09                     | 0.41              |
| 11:A:2853:A:H5'   | 11:A:2854:U:H2'   | 2.03                     | 0.41              |
| 11:A:2934:G:H1    | 11:A:2938:A:H62   | 1.68                     | 0.41              |
| 14:D:247:VAL:HG12 | 14:D:248:SER:N    | 2.36                     | 0.41              |
| 15:E:122:LEU:HD22 | 15:E:297:VAL:HG21 | 2.03                     | 0.41              |
| 16:F:87:PHE:C     | 16:F:179:THR:HG22 | 2.46                     | 0.41              |
| 22:L:84:ALA:HB1   | 22:L:105:VAL:CG2  | 2.48                     | 0.41              |
| 39:c:173:LEU:O    | 39:c:174:ALA:HB3  | 2.21                     | 0.41              |
| 40:d:122:ILE:O    | 40:d:125:ILE:HG22 | 2.21                     | 0.41              |
| 41:e:210:CYS:SG   | 41:e:235:LYS:HB2  | 2.61                     | 0.41              |
| 42:f:87:GLU:OE1   | 42:f:88:TYR:O     | 2.39                     | 0.41              |
| 42:f:178:LEU:HD11 | 42:f:182:VAL:HB   | 2.03                     | 0.41              |
| 54:u:163:ASP:OD1  | 54:u:163:ASP:N    | 2.54                     | 0.41              |
| 56:w:142:GLN:HG2  | 56:w:143:GLU:N    | 2.36                     | 0.41              |
| 6:5:105:TYR:CD2   | 6:5:262:ILE:HD12  | 2.57                     | 0.41              |
| 7:6:60:ARG:NH1    | 7:6:64:GLU:OE2    | 2.53                     | 0.41              |
| 7:6:320:GLN:OE1   | 26:P:52:ASN:ND2   | 2.54                     | 0.41              |
| 8:7:192:TRP:O     | 8:7:295:ARG:NH2   | 2.53                     | 0.41              |
| 11:A:1739:A:O2'   | 11:A:1888:G:H1'   | 2.21                     | 0.41              |
| 11:A:2045:A:H2'   | 11:A:2046:C:O4'   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:2096:U:O2    | 11:A:2096:U:O4'   | 2.37                     | 0.41              |
| 11:A:2174:G:C5    | 11:A:2175:C:C5    | 3.08                     | 0.41              |
| 11:A:2194:U:O2'   | 11:A:2195:A:C8    | 2.74                     | 0.41              |
| 11:A:2688:C:H2'   | 11:A:2689:C:C6    | 2.56                     | 0.41              |
| 11:A:2851:A:H2'   | 11:A:2852:C:O4'   | 2.21                     | 0.41              |
| 20:J:57:THR:O     | 20:J:60:ILE:O     | 2.39                     | 0.41              |
| 21:K:176:TYR:CE1  | 52:r:104:ILE:HG13 | 2.56                     | 0.41              |
| 23:M:118:LEU:CD2  | 23:M:184:LEU:HD11 | 2.51                     | 0.41              |
| 24:N:152:THR:HG23 | 24:N:152:THR:O    | 2.20                     | 0.41              |
| 30:T:94:ILE:HD11  | 30:T:174:TYR:OH   | 2.21                     | 0.41              |
| 36:Z:69:VAL:HG23  | 36:Z:91:LEU:HD21  | 2.03                     | 0.41              |
| 55:v:15:ALA:HB3   | 55:v:62:LEU:HD11  | 2.02                     | 0.41              |
| 11:A:1731:A:C6    | 18:H:75:ARG:NH1   | 2.89                     | 0.40              |
| 11:A:2466:A:O2'   | 11:A:2467:A:H5'   | 2.21                     | 0.40              |
| 11:A:2998:U:H2'   | 11:A:2999:C:O4'   | 2.21                     | 0.40              |
| 24:N:172:VAL:CG1  | 24:N:176:LEU:HG   | 2.51                     | 0.40              |
| 38:b:90:HIS:CE1   | 38:b:91:CYS:SG    | 3.12                     | 0.40              |
| 53:s:246:GLN:OE1  | 53:s:353:ARG:NH1  | 2.47                     | 0.40              |
| 57:x:117:ARG:O    | 57:x:156:ARG:HA   | 2.21                     | 0.40              |
| 6:5:219:LEU:HD23  | 6:5:219:LEU:H     | 1.85                     | 0.40              |
| 7:6:217:LEU:HD21  | 7:6:219:THR:CG2   | 2.47                     | 0.40              |
| 11:A:1865:C:OP1   | 28:R:13:ARG:HD2   | 2.21                     | 0.40              |
| 11:A:2332:C:O2    | 11:A:2445:U:H5    | 2.04                     | 0.40              |
| 11:A:2838:A:C8    | 11:A:2840:C:C5    | 3.09                     | 0.40              |
| 11:A:2898:U:O2    | 11:A:2898:U:O4'   | 2.37                     | 0.40              |
| 11:A:2917:G:O6    | 23:M:77:ARG:NH2   | 2.52                     | 0.40              |
| 11:A:2949:C:H1'   | 11:A:2978:U:O4    | 2.21                     | 0.40              |
| 11:A:3045:A:H2'   | 11:A:3046:C:O4'   | 2.21                     | 0.40              |
| 13:C:342:THR:HG22 | 13:C:346:ARG:NE   | 2.36                     | 0.40              |
| 33:W:106:PRO:HD3  | 33:W:117:ILE:HD11 | 2.03                     | 0.40              |
| 42:f:167:ALA:O    | 42:f:171:LEU:CD2  | 2.69                     | 0.40              |
| 44:h:69:ARG:HD3   | 44:h:107:ASP:OD2  | 2.21                     | 0.40              |
| 44:h:92:GLU:OE1   | 44:h:92:GLU:N     | 2.49                     | 0.40              |
| 51:q:117:ARG:O    | 51:q:121:ILE:HG12 | 2.21                     | 0.40              |
| 54:u:104:GLU:OE2  | 54:u:138:MET:HE3  | 2.21                     | 0.40              |
| 6:5:262:ILE:O     | 6:5:262:ILE:HG22  | 2.21                     | 0.40              |
| 11:A:1826:G:N2    | 11:A:2686:G:C8    | 2.88                     | 0.40              |
| 11:A:2172:A:OP1   | 20:J:21:ARG:NH2   | 2.55                     | 0.40              |
| 11:A:2993:U:O2    | 11:A:2993:U:O4'   | 2.38                     | 0.40              |
| 11:A:3165:C:H2'   | 11:A:3166:U:C6    | 2.56                     | 0.40              |
| 15:E:106:MET:HE2  | 15:E:118:VAL:HG12 | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:E:208:ALA:HB2  | 15:E:297:VAL:HG12 | 2.04                     | 0.40              |
| 20:J:60:ILE:HG13  | 20:J:61:LYS:N     | 2.35                     | 0.40              |
| 22:L:84:ALA:HB2   | 22:L:107:LEU:HD23 | 2.03                     | 0.40              |
| 33:W:99:TYR:CD2   | 33:W:131:VAL:HG22 | 2.57                     | 0.40              |
| 1:O:154:ILE:HD12  | 1:O:154:ILE:HA    | 1.99                     | 0.40              |
| 9:8:129:ARG:CD    | 12:B:1627:C:H4'   | 2.51                     | 0.40              |
| 11:A:2053:U:HO2'  | 11:A:2054:U:H6    | 1.60                     | 0.40              |
| 11:A:2397:C:N4    | 11:A:2398:A:H62   | 2.19                     | 0.40              |
| 11:A:3155:C:H2'   | 11:A:3156:A:C8    | 2.56                     | 0.40              |
| 11:A:3169:C:H5    | 11:A:3198:A:N1    | 2.20                     | 0.40              |
| 14:D:138:ASP:OD1  | 14:D:248:SER:OG   | 2.34                     | 0.40              |
| 17:G:237:ALA:HB2  | 17:G:253:TYR:CE1  | 2.56                     | 0.40              |
| 40:d:211:GLN:HA   | 40:d:248:PHE:O    | 2.22                     | 0.40              |
| 54:u:139:ALA:HB2  | 54:u:179:LEU:HD22 | 2.03                     | 0.40              |
| 7:6:216:LEU:O     | 7:6:236:LEU:HD12  | 2.22                     | 0.40              |
| 11:A:2171:U:C2    | 11:A:2173:G:H4'   | 2.57                     | 0.40              |
| 11:A:2275:U:H2'   | 11:A:2276:C:H6    | 1.86                     | 0.40              |
| 11:A:2397:C:N4    | 11:A:2398:A:N6    | 2.70                     | 0.40              |
| 11:A:3040:OMG:H3' | 11:A:3041:U:H5''  | 2.03                     | 0.40              |
| 14:D:164:LEU:HD21 | 14:D:166:SER:HB3  | 2.03                     | 0.40              |
| 17:G:237:ALA:HB2  | 17:G:253:TYR:CZ   | 2.56                     | 0.40              |
| 18:H:78:ARG:HG3   | 18:H:78:ARG:O     | 2.22                     | 0.40              |
| 23:M:288:GLU:HG2  | 23:M:289:ASN:N    | 2.37                     | 0.40              |
| 24:N:133:ARG:HD3  | 24:N:134:LYS:O    | 2.22                     | 0.40              |
| 24:N:223:MET:O    | 49:o:42:GLU:OE1   | 2.38                     | 0.40              |
| 25:O:70:GLU:HG2   | 25:O:71:ARG:N     | 2.36                     | 0.40              |
| 26:P:67:GLY:HA3   | 33:W:78:GLY:O     | 2.21                     | 0.40              |
| 31:U:134:ARG:HA   | 31:U:137:ARG:HG3  | 2.04                     | 0.40              |
| 42:f:112:ASN:O    | 42:f:115:ASN:OD1  | 2.40                     | 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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 0     | 106/108 (98%) | 105 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 2   | 1     | 50/65 (77%)   | 49 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 3   | 2     | 43/92 (47%)   | 42 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 4   | 3     | 93/188 (50%)  | 90 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 5   | 4     | 35/103 (34%)  | 34 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 6   | 5     | 390/423 (92%) | 376 (96%) | 14 (4%) | 0        | 100         | 100 |
| 7   | 6     | 316/380 (83%) | 303 (96%) | 13 (4%) | 0        | 100         | 100 |
| 8   | 7     | 285/338 (84%) | 268 (94%) | 17 (6%) | 0        | 100         | 100 |
| 9   | 8     | 75/206 (36%)  | 72 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 10  | 9     | 113/137 (82%) | 112 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 13  | C     | 335/384 (87%) | 317 (95%) | 18 (5%) | 0        | 100         | 100 |
| 14  | D     | 238/305 (78%) | 232 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 15  | E     | 306/348 (88%) | 296 (97%) | 10 (3%) | 0        | 100         | 100 |
| 16  | F     | 248/311 (80%) | 242 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 17  | G     | 236/381 (62%) | 225 (95%) | 11 (5%) | 0        | 100         | 100 |
| 18  | H     | 93/267 (35%)  | 88 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 19  | I     | 154/261 (59%) | 146 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 20  | J     | 138/192 (72%) | 126 (91%) | 12 (9%) | 0        | 100         | 100 |
| 21  | K     | 175/178 (98%) | 171 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 22  | L     | 113/145 (78%) | 109 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 23  | M     | 285/296 (96%) | 282 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 24  | N     | 203/251 (81%) | 191 (94%) | 12 (6%) | 0        | 100         | 100 |
| 25  | O     | 150/175 (86%) | 147 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 26  | P     | 139/180 (77%) | 134 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 27  | Q     | 215/292 (74%) | 212 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 28  | R     | 114/149 (76%) | 113 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 29  | S     | 154/205 (75%) | 151 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 30  | T     | 164/206 (80%) | 161 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 31  | U     | 135/153 (88%) | 133 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 32  | V     | 45/216 (21%)  | 45 (100%) | 0       | 0        | 100         | 100 |
| 33  | W     | 107/148 (72%) | 105 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 34  | X     | 241/256 (94%) | 236 (98%) | 5 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 35  | Y     | 174/250 (70%)    | 170 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 36  | Z     | 113/161 (70%)    | 110 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 37  | a     | 67/142 (47%)     | 67 (100%)  | 0        | 0        | 100         | 100 |
| 38  | b     | 146/215 (68%)    | 141 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 39  | c     | 271/332 (82%)    | 267 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 40  | d     | 189/306 (62%)    | 183 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 41  | e     | 191/279 (68%)    | 179 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 42  | f     | 102/212 (48%)    | 94 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| 43  | g     | 127/166 (76%)    | 120 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 44  | h     | 101/158 (64%)    | 99 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 45  | i     | 95/128 (74%)     | 94 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 46  | j     | 83/85 (98%)      | 83 (100%)  | 0        | 0        | 100         | 100 |
| 47  | k     | 76/112 (68%)     | 70 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 48  | m     | 26/128 (20%)     | 20 (77%)   | 6 (23%)  | 0        | 100         | 100 |
| 49  | o     | 91/102 (89%)     | 89 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 50  | p     | 119/206 (58%)    | 116 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 51  | q     | 126/222 (57%)    | 126 (100%) | 0        | 0        | 100         | 100 |
| 52  | r     | 140/196 (71%)    | 133 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 53  | s     | 366/439 (83%)    | 358 (98%)  | 8 (2%)   | 0        | 100         | 100 |
| 54  | u     | 109/234 (47%)    | 100 (92%)  | 9 (8%)   | 0        | 100         | 100 |
| 55  | v     | 67/70 (96%)      | 65 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 56  | w     | 77/156 (49%)     | 73 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 57  | x     | 146/406 (36%)    | 138 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| All | All   | 8496/12044 (70%) | 8208 (97%) | 288 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 0     | 97/97 (100%)  | 97 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 49/60 (82%)   | 49 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 39/72 (54%)   | 39 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 88/166 (53%)  | 88 (100%)  | 0        | 100         | 100 |
| 5   | 4     | 36/89 (40%)   | 36 (100%)  | 0        | 100         | 100 |
| 6   | 5     | 353/368 (96%) | 353 (100%) | 0        | 100         | 100 |
| 7   | 6     | 286/332 (86%) | 286 (100%) | 0        | 100         | 100 |
| 8   | 7     | 263/303 (87%) | 263 (100%) | 0        | 100         | 100 |
| 9   | 8     | 70/190 (37%)  | 70 (100%)  | 0        | 100         | 100 |
| 10  | 9     | 99/112 (88%)  | 99 (100%)  | 0        | 100         | 100 |
| 13  | C     | 293/328 (89%) | 293 (100%) | 0        | 100         | 100 |
| 14  | D     | 194/245 (79%) | 194 (100%) | 0        | 100         | 100 |
| 15  | E     | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 16  | F     | 217/262 (83%) | 217 (100%) | 0        | 100         | 100 |
| 17  | G     | 221/350 (63%) | 221 (100%) | 0        | 100         | 100 |
| 18  | H     | 86/228 (38%)  | 86 (100%)  | 0        | 100         | 100 |
| 19  | I     | 145/232 (62%) | 145 (100%) | 0        | 100         | 100 |
| 20  | J     | 113/150 (75%) | 113 (100%) | 0        | 100         | 100 |
| 21  | K     | 155/156 (99%) | 155 (100%) | 0        | 100         | 100 |
| 22  | L     | 98/124 (79%)  | 98 (100%)  | 0        | 100         | 100 |
| 23  | M     | 245/249 (98%) | 245 (100%) | 0        | 100         | 100 |
| 24  | N     | 172/211 (82%) | 172 (100%) | 0        | 100         | 100 |
| 25  | O     | 133/150 (89%) | 133 (100%) | 0        | 100         | 100 |
| 26  | P     | 123/155 (79%) | 123 (100%) | 0        | 100         | 100 |
| 27  | Q     | 199/256 (78%) | 199 (100%) | 0        | 100         | 100 |
| 28  | R     | 101/126 (80%) | 101 (100%) | 0        | 100         | 100 |
| 29  | S     | 141/180 (78%) | 141 (100%) | 0        | 100         | 100 |
| 30  | T     | 146/176 (83%) | 146 (100%) | 0        | 100         | 100 |
| 31  | U     | 124/135 (92%) | 124 (100%) | 0        | 100         | 100 |
| 32  | V     | 43/191 (22%)  | 43 (100%)  | 0        | 100         | 100 |
| 33  | W     | 89/119 (75%)  | 89 (100%)  | 0        | 100         | 100 |
| 34  | X     | 219/229 (96%) | 219 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 35  | Y     | 159/223 (71%)    | 159 (100%)  | 0        | 100         | 100 |
| 36  | Z     | 106/147 (72%)    | 106 (100%)  | 0        | 100         | 100 |
| 37  | a     | 67/133 (50%)     | 67 (100%)   | 0        | 100         | 100 |
| 38  | b     | 130/186 (70%)    | 130 (100%)  | 0        | 100         | 100 |
| 39  | c     | 241/288 (84%)    | 241 (100%)  | 0        | 100         | 100 |
| 40  | d     | 184/274 (67%)    | 184 (100%)  | 0        | 100         | 100 |
| 41  | e     | 171/236 (72%)    | 171 (100%)  | 0        | 100         | 100 |
| 42  | f     | 95/188 (50%)     | 95 (100%)   | 0        | 100         | 100 |
| 43  | g     | 119/148 (80%)    | 119 (100%)  | 0        | 100         | 100 |
| 44  | h     | 100/148 (68%)    | 100 (100%)  | 0        | 100         | 100 |
| 45  | i     | 86/110 (78%)     | 86 (100%)   | 0        | 100         | 100 |
| 46  | j     | 68/68 (100%)     | 68 (100%)   | 0        | 100         | 100 |
| 47  | k     | 71/90 (79%)      | 71 (100%)   | 0        | 100         | 100 |
| 48  | m     | 26/113 (23%)     | 26 (100%)   | 0        | 100         | 100 |
| 49  | o     | 79/87 (91%)      | 79 (100%)   | 0        | 100         | 100 |
| 50  | p     | 117/181 (65%)    | 117 (100%)  | 0        | 100         | 100 |
| 51  | q     | 110/178 (62%)    | 110 (100%)  | 0        | 100         | 100 |
| 52  | r     | 133/169 (79%)    | 133 (100%)  | 0        | 100         | 100 |
| 53  | s     | 326/381 (86%)    | 326 (100%)  | 0        | 100         | 100 |
| 54  | u     | 105/200 (52%)    | 105 (100%)  | 0        | 100         | 100 |
| 55  | v     | 59/60 (98%)      | 59 (100%)   | 0        | 100         | 100 |
| 56  | w     | 73/136 (54%)     | 73 (100%)   | 0        | 100         | 100 |
| 57  | x     | 109/320 (34%)    | 109 (100%)  | 0        | 100         | 100 |
| All | All   | 7633/10395 (73%) | 7633 (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 (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 140 | GLN  |
| 1   | 0     | 170 | GLN  |
| 6   | 5     | 94  | HIS  |
| 13  | C     | 314 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | E     | 88  | HIS  |
| 15  | E     | 336 | ASN  |
| 16  | F     | 105 | ASN  |
| 16  | F     | 188 | HIS  |
| 16  | F     | 208 | HIS  |
| 16  | F     | 228 | GLN  |
| 20  | J     | 133 | GLN  |
| 23  | M     | 53  | HIS  |
| 23  | M     | 219 | ASN  |
| 27  | Q     | 252 | GLN  |
| 27  | Q     | 258 | GLN  |
| 28  | R     | 94  | GLN  |
| 29  | S     | 75  | HIS  |
| 29  | S     | 118 | ASN  |
| 33  | W     | 62  | HIS  |
| 34  | X     | 93  | ASN  |
| 34  | X     | 240 | GLN  |
| 35  | Y     | 89  | GLN  |
| 35  | Y     | 117 | GLN  |
| 35  | Y     | 147 | GLN  |
| 35  | Y     | 225 | ASN  |
| 36  | Z     | 136 | ASN  |
| 38  | b     | 16  | HIS  |
| 38  | b     | 58  | ASN  |
| 38  | b     | 129 | GLN  |
| 39  | c     | 69  | HIS  |
| 39  | c     | 123 | GLN  |
| 41  | e     | 271 | GLN  |
| 43  | g     | 92  | HIS  |
| 44  | h     | 110 | HIS  |
| 45  | i     | 59  | ASN  |
| 46  | j     | 99  | GLN  |
| 47  | k     | 19  | GLN  |
| 50  | p     | 104 | HIS  |
| 51  | q     | 130 | GLN  |
| 52  | r     | 65  | ASN  |
| 52  | r     | 131 | HIS  |
| 53  | s     | 107 | GLN  |
| 53  | s     | 179 | GLN  |
| 54  | u     | 134 | HIS  |
| 54  | u     | 136 | HIS  |
| 54  | u     | 156 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | A     | 1359/1559 (87%) | 294 (21%)         | 21 (1%)         |
| 12  | B     | 51/69 (73%)     | 16 (31%)          | 1 (1%)          |
| All | All   | 1410/1628 (86%) | 310 (21%)         | 22 (1%)         |

All (310) RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1672 | C    |
| 11  | A     | 1676 | A    |
| 11  | A     | 1677 | C    |
| 11  | A     | 1679 | U    |
| 11  | A     | 1680 | A    |
| 11  | A     | 1681 | G    |
| 11  | A     | 1689 | C    |
| 11  | A     | 1690 | C    |
| 11  | A     | 1699 | C    |
| 11  | A     | 1700 | U    |
| 11  | A     | 1704 | U    |
| 11  | A     | 1708 | A    |
| 11  | A     | 1714 | C    |
| 11  | A     | 1715 | C    |
| 11  | A     | 1724 | A    |
| 11  | A     | 1727 | A    |
| 11  | A     | 1728 | U    |
| 11  | A     | 1731 | A    |
| 11  | A     | 1732 | C    |
| 11  | A     | 1748 | G    |
| 11  | A     | 1750 | G    |
| 11  | A     | 1751 | A    |
| 11  | A     | 1767 | G    |
| 11  | A     | 1770 | G    |
| 11  | A     | 1777 | A    |
| 11  | A     | 1794 | A    |
| 11  | A     | 1817 | C    |
| 11  | A     | 1819 | U    |
| 11  | A     | 1821 | A    |
| 11  | A     | 1823 | A    |
| 11  | A     | 1824 | U    |
| 11  | A     | 1827 | C    |
| 11  | A     | 1828 | A    |
| 11  | A     | 1829 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1832 | A    |
| 11  | A     | 1836 | A    |
| 11  | A     | 1844 | A    |
| 11  | A     | 1849 | C    |
| 11  | A     | 1853 | A    |
| 11  | A     | 1854 | U    |
| 11  | A     | 1855 | A    |
| 11  | A     | 1856 | A    |
| 11  | A     | 1869 | A    |
| 11  | A     | 1878 | U    |
| 11  | A     | 1882 | A    |
| 11  | A     | 1883 | G    |
| 11  | A     | 1887 | A    |
| 11  | A     | 1888 | G    |
| 11  | A     | 1892 | A    |
| 11  | A     | 1893 | A    |
| 11  | A     | 1902 | C    |
| 11  | A     | 1903 | C    |
| 11  | A     | 1918 | G    |
| 11  | A     | 1938 | A    |
| 11  | A     | 1940 | A    |
| 11  | A     | 1958 | G    |
| 11  | A     | 1972 | A    |
| 11  | A     | 1974 | A    |
| 11  | A     | 1985 | G    |
| 11  | A     | 1987 | G    |
| 11  | A     | 1992 | C    |
| 11  | A     | 1994 | A    |
| 11  | A     | 1995 | A    |
| 11  | A     | 2001 | C    |
| 11  | A     | 2002 | G    |
| 11  | A     | 2015 | G    |
| 11  | A     | 2021 | U    |
| 11  | A     | 2022 | G    |
| 11  | A     | 2029 | A    |
| 11  | A     | 2030 | U    |
| 11  | A     | 2036 | C    |
| 11  | A     | 2037 | U    |
| 11  | A     | 2039 | A    |
| 11  | A     | 2054 | U    |
| 11  | A     | 2055 | U    |
| 11  | A     | 2060 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2065 | A    |
| 11  | A     | 2074 | A    |
| 11  | A     | 2079 | C    |
| 11  | A     | 2083 | U    |
| 11  | A     | 2085 | A    |
| 11  | A     | 2093 | U    |
| 11  | A     | 2097 | A    |
| 11  | A     | 2098 | G    |
| 11  | A     | 2113 | G    |
| 11  | A     | 2114 | C    |
| 11  | A     | 2124 | A    |
| 11  | A     | 2126 | U    |
| 11  | A     | 2132 | A    |
| 11  | A     | 2141 | U    |
| 11  | A     | 2147 | G    |
| 11  | A     | 2154 | A    |
| 11  | A     | 2155 | A    |
| 11  | A     | 2157 | U    |
| 11  | A     | 2159 | U    |
| 11  | A     | 2163 | A    |
| 11  | A     | 2164 | C    |
| 11  | A     | 2165 | C    |
| 11  | A     | 2166 | C    |
| 11  | A     | 2172 | A    |
| 11  | A     | 2173 | G    |
| 11  | A     | 2177 | U    |
| 11  | A     | 2180 | A    |
| 11  | A     | 2182 | G    |
| 11  | A     | 2183 | C    |
| 11  | A     | 2184 | A    |
| 11  | A     | 2187 | C    |
| 11  | A     | 2193 | U    |
| 11  | A     | 2194 | U    |
| 11  | A     | 2197 | G    |
| 11  | A     | 2198 | A    |
| 11  | A     | 2199 | A    |
| 11  | A     | 2200 | A    |
| 11  | A     | 2210 | C    |
| 11  | A     | 2212 | C    |
| 11  | A     | 2213 | A    |
| 11  | A     | 2215 | C    |
| 11  | A     | 2216 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2233 | U    |
| 11  | A     | 2237 | A    |
| 11  | A     | 2239 | A    |
| 11  | A     | 2241 | A    |
| 11  | A     | 2242 | U    |
| 11  | A     | 2243 | A    |
| 11  | A     | 2246 | A    |
| 11  | A     | 2262 | C    |
| 11  | A     | 2263 | C    |
| 11  | A     | 2282 | C    |
| 11  | A     | 2285 | U    |
| 11  | A     | 2297 | A    |
| 11  | A     | 2300 | G    |
| 11  | A     | 2316 | U    |
| 11  | A     | 2322 | C    |
| 11  | A     | 2331 | C    |
| 11  | A     | 2332 | C    |
| 11  | A     | 2335 | A    |
| 11  | A     | 2345 | G    |
| 11  | A     | 2349 | G    |
| 11  | A     | 2369 | A    |
| 11  | A     | 2371 | U    |
| 11  | A     | 2374 | A    |
| 11  | A     | 2381 | A    |
| 11  | A     | 2384 | A    |
| 11  | A     | 2386 | C    |
| 11  | A     | 2387 | U    |
| 11  | A     | 2390 | A    |
| 11  | A     | 2393 | C    |
| 11  | A     | 2399 | A    |
| 11  | A     | 2404 | U    |
| 11  | A     | 2408 | U    |
| 11  | A     | 2415 | C    |
| 11  | A     | 2427 | C    |
| 11  | A     | 2432 | A    |
| 11  | A     | 2434 | A    |
| 11  | A     | 2444 | A    |
| 11  | A     | 2446 | A    |
| 11  | A     | 2451 | A    |
| 11  | A     | 2458 | A    |
| 11  | A     | 2478 | G    |
| 11  | A     | 2485 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2493 | C    |
| 11  | A     | 2496 | G    |
| 11  | A     | 2500 | A    |
| 11  | A     | 2502 | C    |
| 11  | A     | 2507 | A    |
| 11  | A     | 2508 | C    |
| 11  | A     | 2511 | C    |
| 11  | A     | 2520 | C    |
| 11  | A     | 2521 | A    |
| 11  | A     | 2527 | A    |
| 11  | A     | 2528 | G    |
| 11  | A     | 2531 | U    |
| 11  | A     | 2540 | C    |
| 11  | A     | 2618 | U    |
| 11  | A     | 2635 | G    |
| 11  | A     | 2636 | G    |
| 11  | A     | 2637 | C    |
| 11  | A     | 2639 | C    |
| 11  | A     | 2645 | G    |
| 11  | A     | 2654 | U    |
| 11  | A     | 2656 | U    |
| 11  | A     | 2660 | U    |
| 11  | A     | 2683 | C    |
| 11  | A     | 2684 | C    |
| 11  | A     | 2686 | G    |
| 11  | A     | 2694 | A    |
| 11  | A     | 2696 | A    |
| 11  | A     | 2706 | A    |
| 11  | A     | 2709 | A    |
| 11  | A     | 2718 | C    |
| 11  | A     | 2719 | G    |
| 11  | A     | 2721 | G    |
| 11  | A     | 2722 | A    |
| 11  | A     | 2724 | G    |
| 11  | A     | 2732 | G    |
| 11  | A     | 2739 | U    |
| 11  | A     | 2748 | A    |
| 11  | A     | 2750 | U    |
| 11  | A     | 2756 | C    |
| 11  | A     | 2804 | A    |
| 11  | A     | 2810 | G    |
| 11  | A     | 2815 | OMG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2819 | G    |
| 11  | A     | 2831 | G    |
| 11  | A     | 2832 | A    |
| 11  | A     | 2833 | A    |
| 11  | A     | 2836 | C    |
| 11  | A     | 2837 | A    |
| 11  | A     | 2838 | A    |
| 11  | A     | 2839 | C    |
| 11  | A     | 2846 | G    |
| 11  | A     | 2847 | C    |
| 11  | A     | 2853 | A    |
| 11  | A     | 2854 | U    |
| 11  | A     | 2855 | G    |
| 11  | A     | 2857 | U    |
| 11  | A     | 2859 | A    |
| 11  | A     | 2864 | U    |
| 11  | A     | 2865 | C    |
| 11  | A     | 2871 | U    |
| 11  | A     | 2890 | U    |
| 11  | A     | 2895 | U    |
| 11  | A     | 2896 | G    |
| 11  | A     | 2906 | C    |
| 11  | A     | 2911 | C    |
| 11  | A     | 2912 | C    |
| 11  | A     | 2913 | A    |
| 11  | A     | 2917 | G    |
| 11  | A     | 2918 | A    |
| 11  | A     | 2919 | A    |
| 11  | A     | 2922 | A    |
| 11  | A     | 2926 | A    |
| 11  | A     | 2928 | C    |
| 11  | A     | 2932 | G    |
| 11  | A     | 2935 | A    |
| 11  | A     | 2936 | U    |
| 11  | A     | 2943 | G    |
| 11  | A     | 2955 | U    |
| 11  | A     | 2956 | A    |
| 11  | A     | 2958 | A    |
| 11  | A     | 2962 | C    |
| 11  | A     | 2963 | A    |
| 11  | A     | 2965 | A    |
| 11  | A     | 2971 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2989 | G    |
| 11  | A     | 2990 | A    |
| 11  | A     | 2991 | U    |
| 11  | A     | 3005 | A    |
| 11  | A     | 3016 | G    |
| 11  | A     | 3022 | G    |
| 11  | A     | 3041 | U    |
| 11  | A     | 3042 | U    |
| 11  | A     | 3043 | C    |
| 11  | A     | 3051 | A    |
| 11  | A     | 3053 | A    |
| 11  | A     | 3054 | G    |
| 11  | A     | 3060 | C    |
| 11  | A     | 3063 | G    |
| 11  | A     | 3068 | G    |
| 11  | A     | 3073 | C    |
| 11  | A     | 3089 | A    |
| 11  | A     | 3093 | C    |
| 11  | A     | 3096 | U    |
| 11  | A     | 3097 | U    |
| 11  | A     | 3100 | U    |
| 11  | A     | 3102 | U    |
| 11  | A     | 3108 | U    |
| 11  | A     | 3109 | U    |
| 11  | A     | 3113 | A    |
| 11  | A     | 3123 | G    |
| 11  | A     | 3124 | U    |
| 11  | A     | 3129 | A    |
| 11  | A     | 3134 | C    |
| 11  | A     | 3141 | A    |
| 11  | A     | 3150 | U    |
| 11  | A     | 3155 | C    |
| 11  | A     | 3157 | C    |
| 11  | A     | 3158 | A    |
| 11  | A     | 3162 | C    |
| 11  | A     | 3168 | C    |
| 11  | A     | 3169 | C    |
| 11  | A     | 3172 | C    |
| 11  | A     | 3173 | G    |
| 11  | A     | 3180 | A    |
| 11  | A     | 3189 | C    |
| 11  | A     | 3190 | A    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 3197 | U    |
| 11  | A     | 3198 | A    |
| 11  | A     | 3200 | U    |
| 11  | A     | 3202 | U    |
| 11  | A     | 3207 | A    |
| 11  | A     | 3217 | A    |
| 11  | A     | 3218 | A    |
| 11  | A     | 3220 | A    |
| 12  | B     | 1607 | U    |
| 12  | B     | 1608 | G    |
| 12  | B     | 1609 | U    |
| 12  | B     | 1611 | G    |
| 12  | B     | 1614 | U    |
| 12  | B     | 1615 | A    |
| 12  | B     | 1625 | A    |
| 12  | B     | 1631 | C    |
| 12  | B     | 1632 | U    |
| 12  | B     | 1633 | U    |
| 12  | B     | 1641 | G    |
| 12  | B     | 1644 | G    |
| 12  | B     | 1645 | A    |
| 12  | B     | 1649 | C    |
| 12  | B     | 1651 | A    |
| 12  | B     | 1669 | G    |

All (22) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1707 | C    |
| 11  | A     | 1713 | A    |
| 11  | A     | 1766 | U    |
| 11  | A     | 1823 | A    |
| 11  | A     | 1986 | A    |
| 11  | A     | 2164 | C    |
| 11  | A     | 2182 | G    |
| 11  | A     | 2186 | C    |
| 11  | A     | 2209 | G    |
| 11  | A     | 2284 | C    |
| 11  | A     | 2457 | A    |
| 11  | A     | 2507 | A    |
| 11  | A     | 2530 | A    |
| 11  | A     | 2635 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2695 | G    |
| 11  | A     | 2836 | C    |
| 11  | A     | 2837 | A    |
| 11  | A     | 2905 | A    |
| 11  | A     | 3092 | U    |
| 11  | A     | 3122 | U    |
| 11  | A     | 3196 | G    |
| 12  | B     | 1607 | U    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | OMG  | A     | 3040 | 11   | 23,26,27     | 1.26 | 4 (17%)  | 32,38,41    | 2.05 | 7 (21%)  |
| 11  | OMG  | A     | 2815 | 11   | 23,26,27     | 1.18 | 2 (8%)   | 32,38,41    | 2.12 | 7 (21%)  |
| 11  | OMU  | A     | 3039 | 11   | 19,22,23     | 1.33 | 3 (15%)  | 25,31,34    | 2.08 | 5 (20%)  |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 11  | OMG  | A     | 3040 | 11   | -       | 0/9/27/28 | 0/3/3/3 |
| 11  | OMG  | A     | 2815 | 11   | -       | 2/9/27/28 | 0/3/3/3 |
| 11  | OMU  | A     | 3039 | 11   | -       | 0/9/27/28 | 0/2/2/2 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A     | 3039 | OMU  | C4-N3 | -3.18 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A     | 2815 | OMG  | C5-C4 | 2.92  | 1.46        | 1.38     |
| 11  | A     | 3040 | OMG  | C6-N1 | -2.76 | 1.33        | 1.38     |
| 11  | A     | 3039 | OMU  | C2-N3 | -2.76 | 1.33        | 1.38     |
| 11  | A     | 3040 | OMG  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 11  | A     | 2815 | OMG  | C6-N1 | -2.44 | 1.34        | 1.38     |
| 11  | A     | 3039 | OMU  | C5-C4 | -2.42 | 1.38        | 1.43     |
| 11  | A     | 3040 | OMG  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 11  | A     | 3040 | OMG  | C4-N9 | -2.06 | 1.32        | 1.38     |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11  | A     | 3040 | OMG  | C5-C4-N3   | -6.02 | 118.81      | 128.39   |
| 11  | A     | 2815 | OMG  | C5-C4-N3   | -5.79 | 119.17      | 128.39   |
| 11  | A     | 3040 | OMG  | C2-N3-C4   | 5.08  | 121.05      | 112.30   |
| 11  | A     | 2815 | OMG  | C2-N3-C4   | 5.04  | 120.98      | 112.30   |
| 11  | A     | 3039 | OMU  | C4-N3-C2   | -4.88 | 120.55      | 126.61   |
| 11  | A     | 3040 | OMG  | N9-C4-N3   | 4.43  | 134.81      | 125.95   |
| 11  | A     | 3039 | OMU  | C5-C4-N3   | 4.35  | 120.89      | 114.80   |
| 11  | A     | 2815 | OMG  | N9-C4-N3   | 4.24  | 134.44      | 125.95   |
| 11  | A     | 3039 | OMU  | N3-C2-N1   | 4.22  | 120.39      | 114.89   |
| 11  | A     | 2815 | OMG  | C2'-C1'-N9 | -4.02 | 106.62      | 114.24   |
| 11  | A     | 3039 | OMU  | C2'-C1'-N1 | -3.80 | 107.03      | 114.24   |
| 11  | A     | 2815 | OMG  | C6-C5-N7   | 3.52  | 136.69      | 130.29   |
| 11  | A     | 3040 | OMG  | C6-C5-N7   | 3.35  | 136.39      | 130.29   |
| 11  | A     | 3039 | OMU  | O4-C4-C5   | -3.01 | 119.97      | 125.16   |
| 11  | A     | 3040 | OMG  | C2'-C1'-N9 | -3.00 | 108.54      | 114.24   |
| 11  | A     | 2815 | OMG  | C4-C5-N7   | -2.60 | 106.55      | 110.67   |
| 11  | A     | 3040 | OMG  | C4-C5-N7   | -2.51 | 106.69      | 110.67   |
| 11  | A     | 3040 | OMG  | O6-C6-C5   | -2.28 | 120.51      | 126.53   |
| 11  | A     | 2815 | OMG  | O6-C6-C5   | -2.14 | 120.89      | 126.53   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | A     | 2815 | OMG  | O4'-C4'-C5'-O5' |
| 11  | A     | 2815 | OMG  | C3'-C4'-C5'-O5' |

There are no ring outliers.

3 monomers are involved in 7 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 11  | A     | 3040 | OMG  | 4       | 0            |
| 11  | A     | 2815 | OMG  | 2       | 0            |
| 11  | A     | 3039 | OMU  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 77 ligands modelled in this entry, 77 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

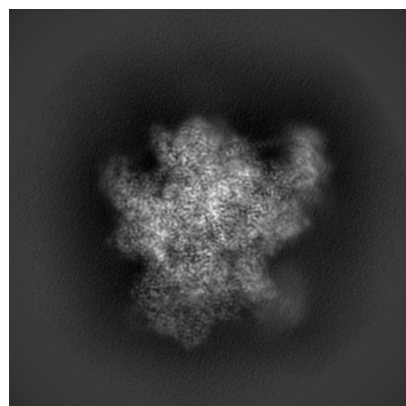
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12872. These allow visual inspection of the internal detail of the map and identification of artifacts.

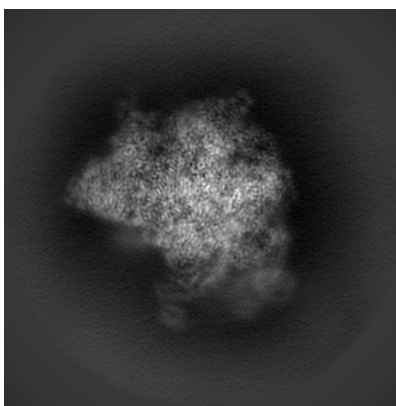
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

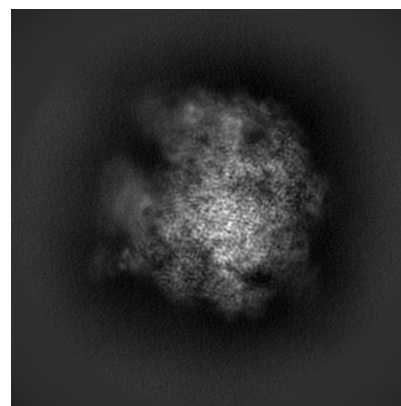
#### 6.1.1 Primary map



X

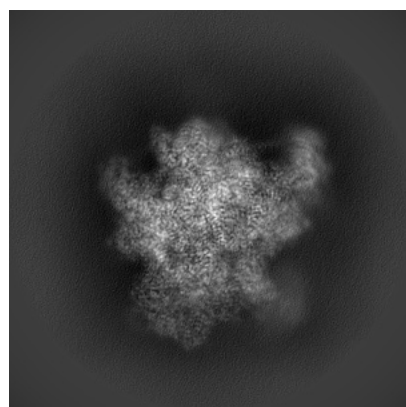


Y

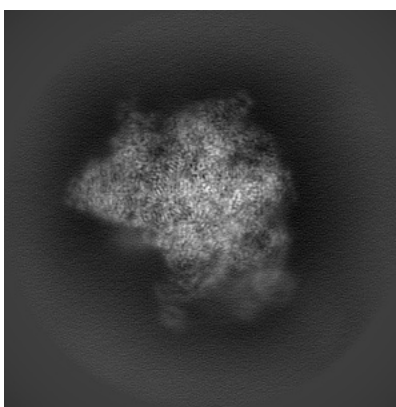


Z

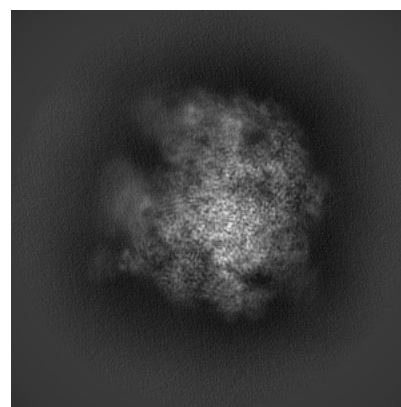
#### 6.1.2 Raw map



X



Y

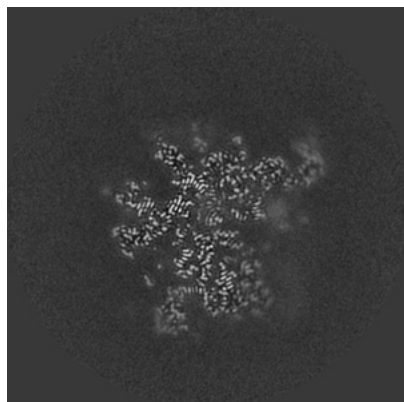


Z

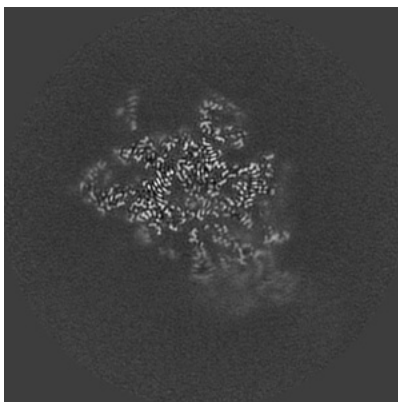
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

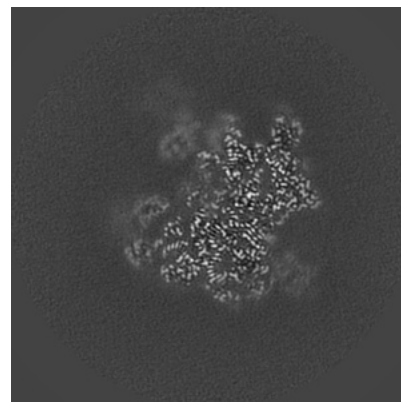
### 6.2.1 Primary map



X Index: 175

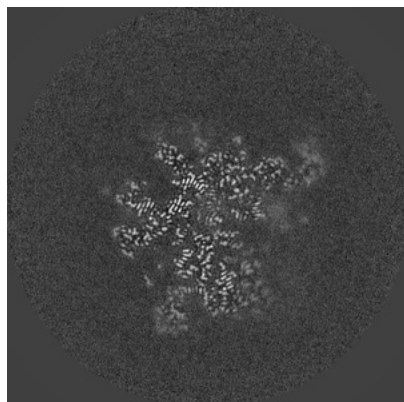


Y Index: 175

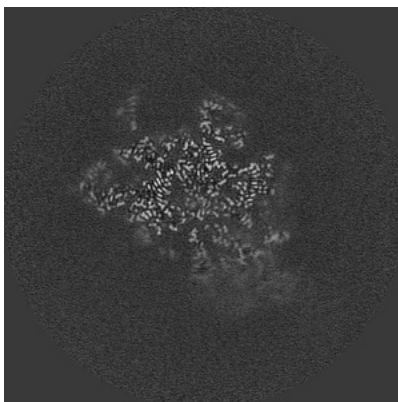


Z Index: 175

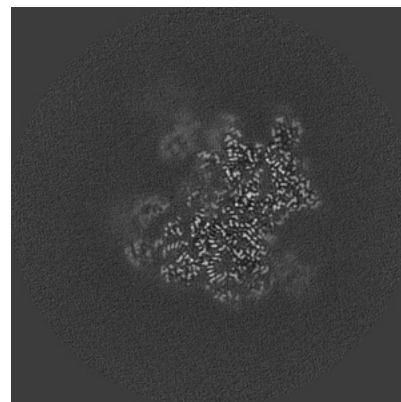
### 6.2.2 Raw map



X Index: 175



Y Index: 175

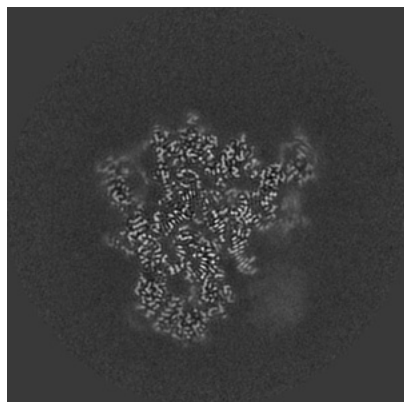


Z Index: 175

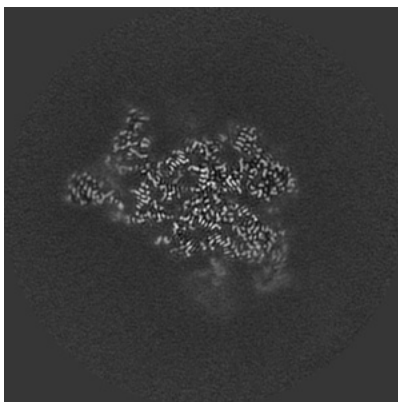
The images above show central slices of the map in three orthogonal directions.

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

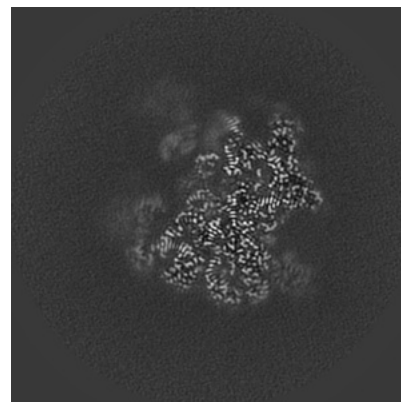
### 6.3.1 Primary map



X Index: 188

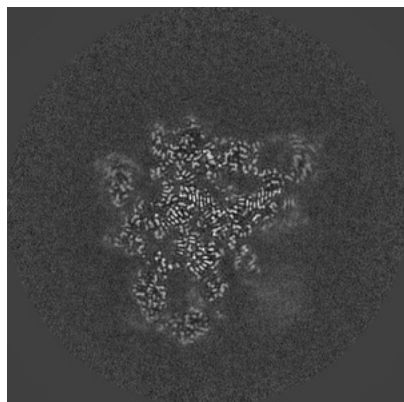


Y Index: 159

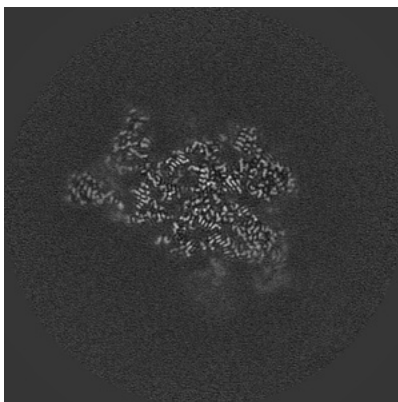


Z Index: 178

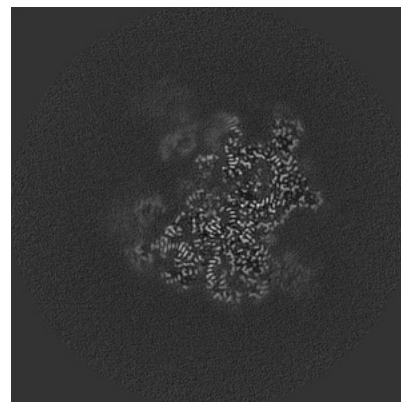
### 6.3.2 Raw map



X Index: 192



Y Index: 159

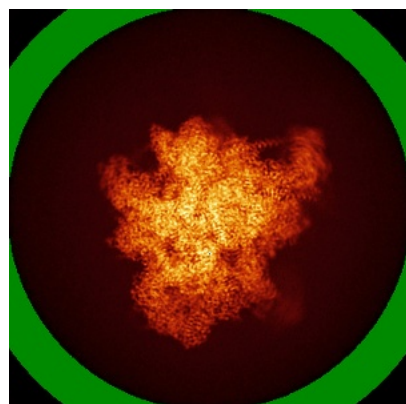


Z Index: 177

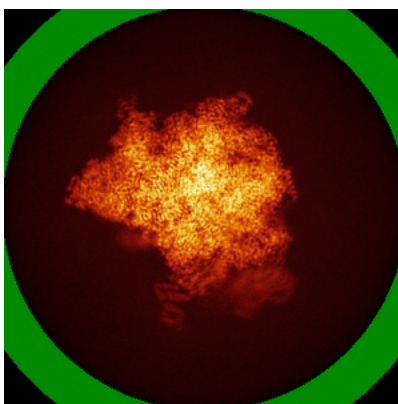
The images above show the largest variance slices of the map in three orthogonal directions.

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

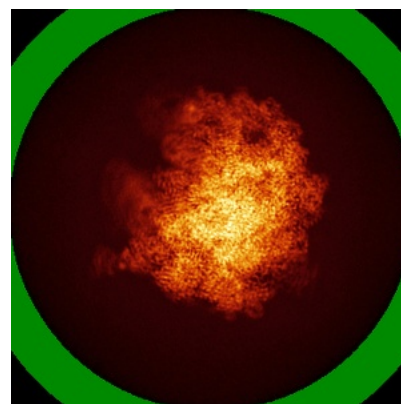
### 6.4.1 Primary map



X

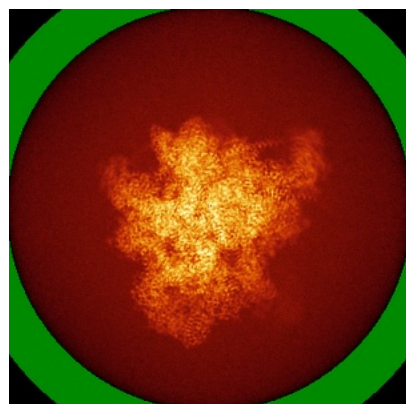


Y

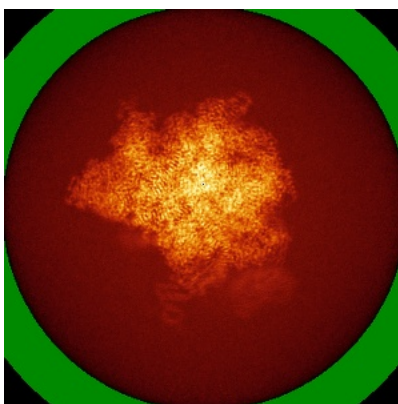


Z

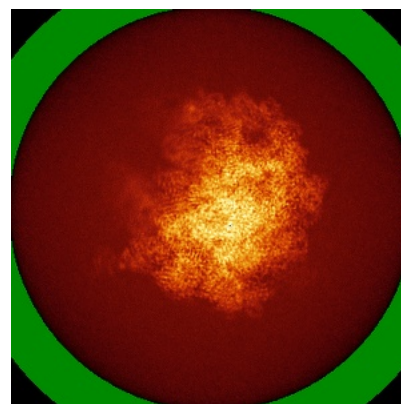
### 6.4.2 Raw map



X



Y

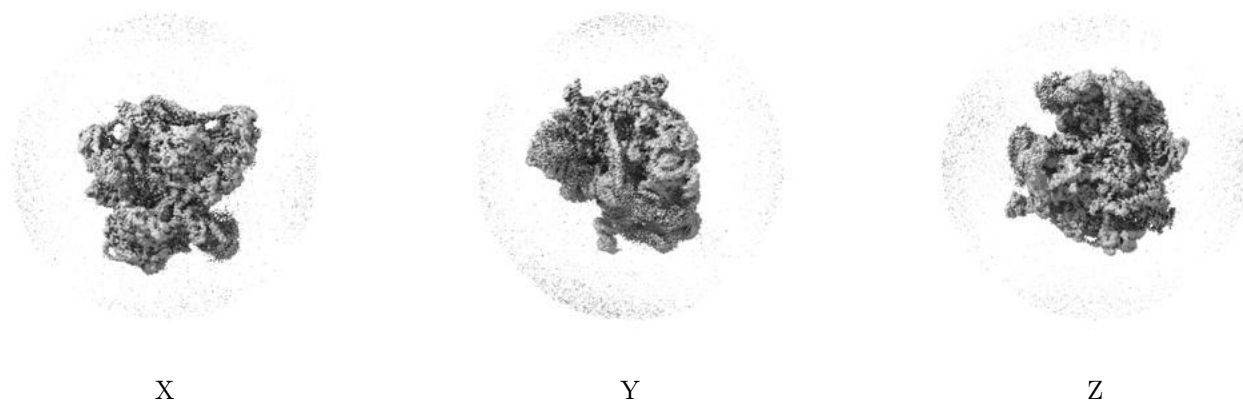


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

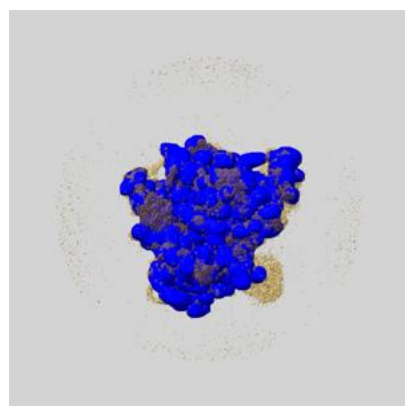
## 6.6 Mask visualisation [i](#)

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

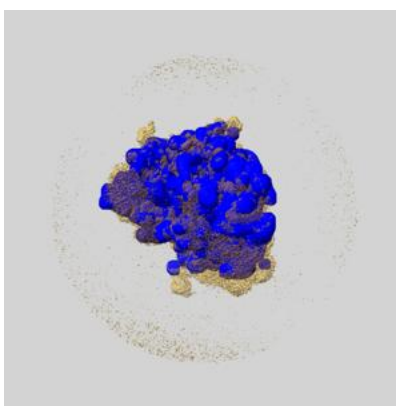
A mask typically either:

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

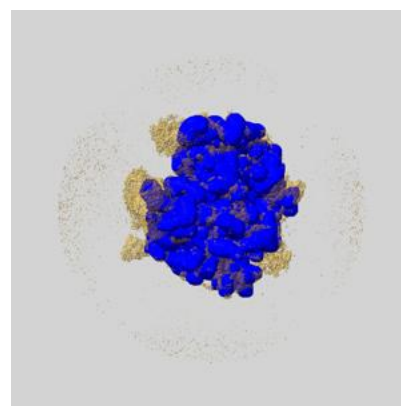
### 6.6.1 emd\_12872\_msk\_1.map [i](#)



X



Y

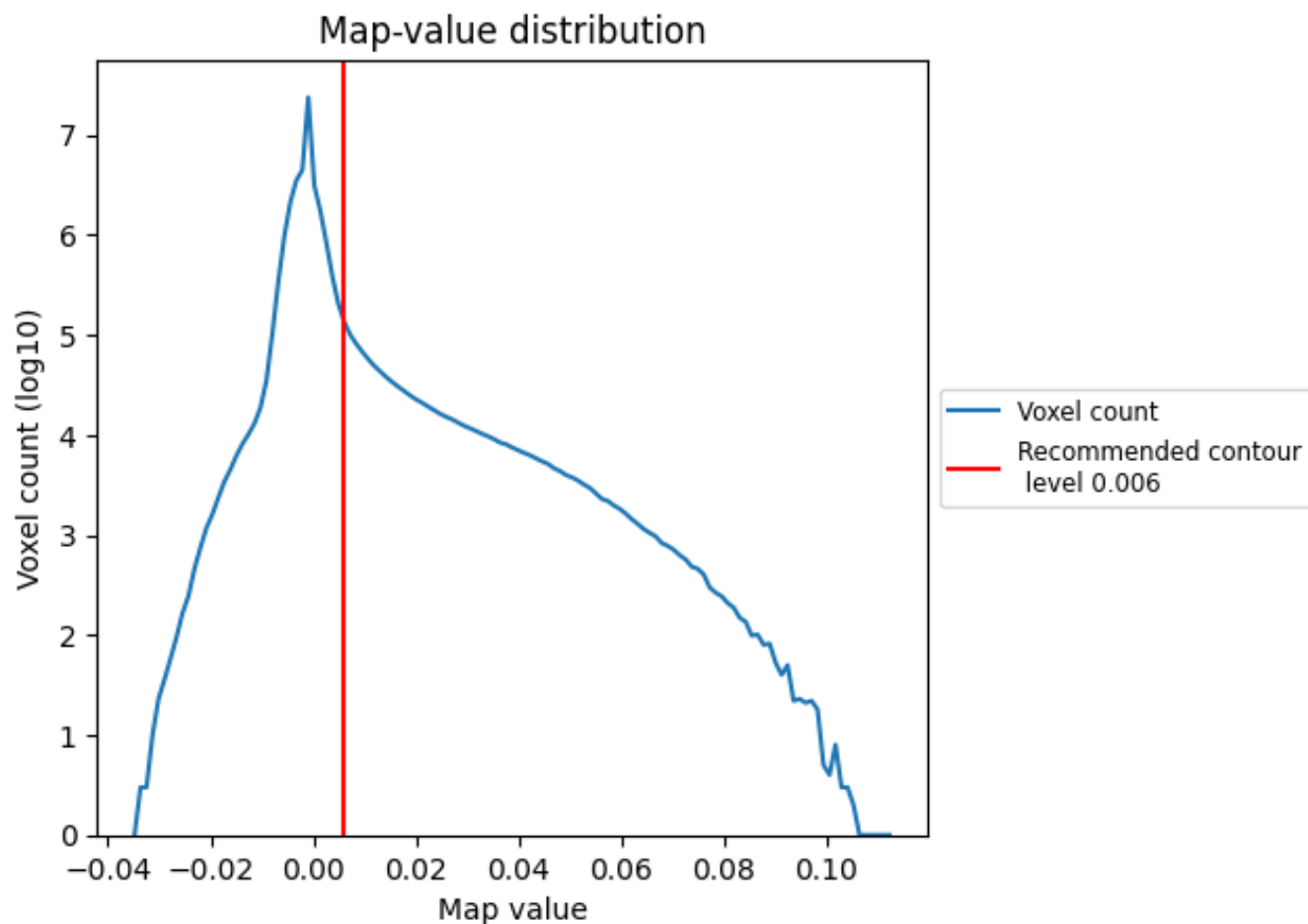


Z

## 7 Map analysis [i](#)

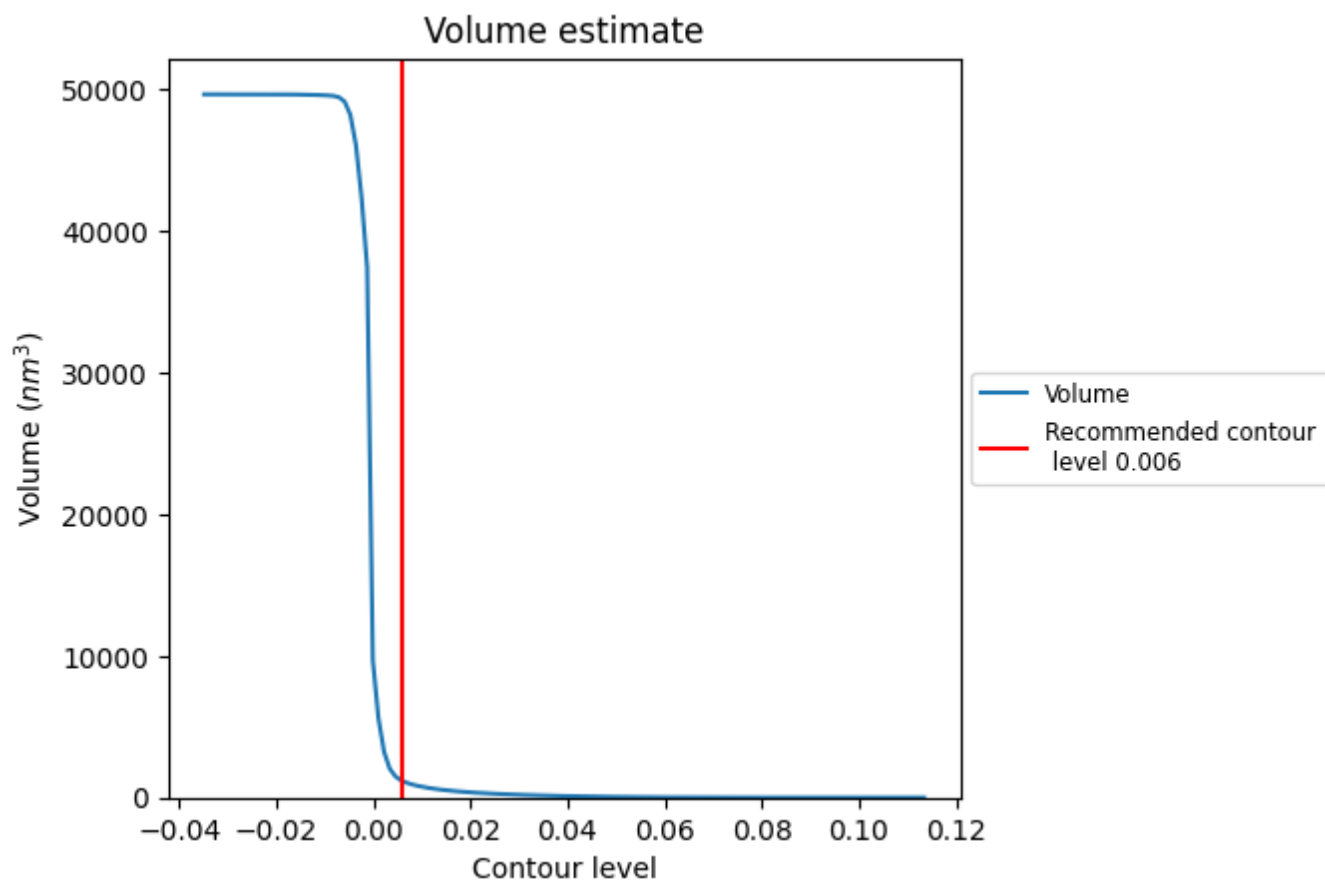
This section contains the results of statistical analysis of the map.

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



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

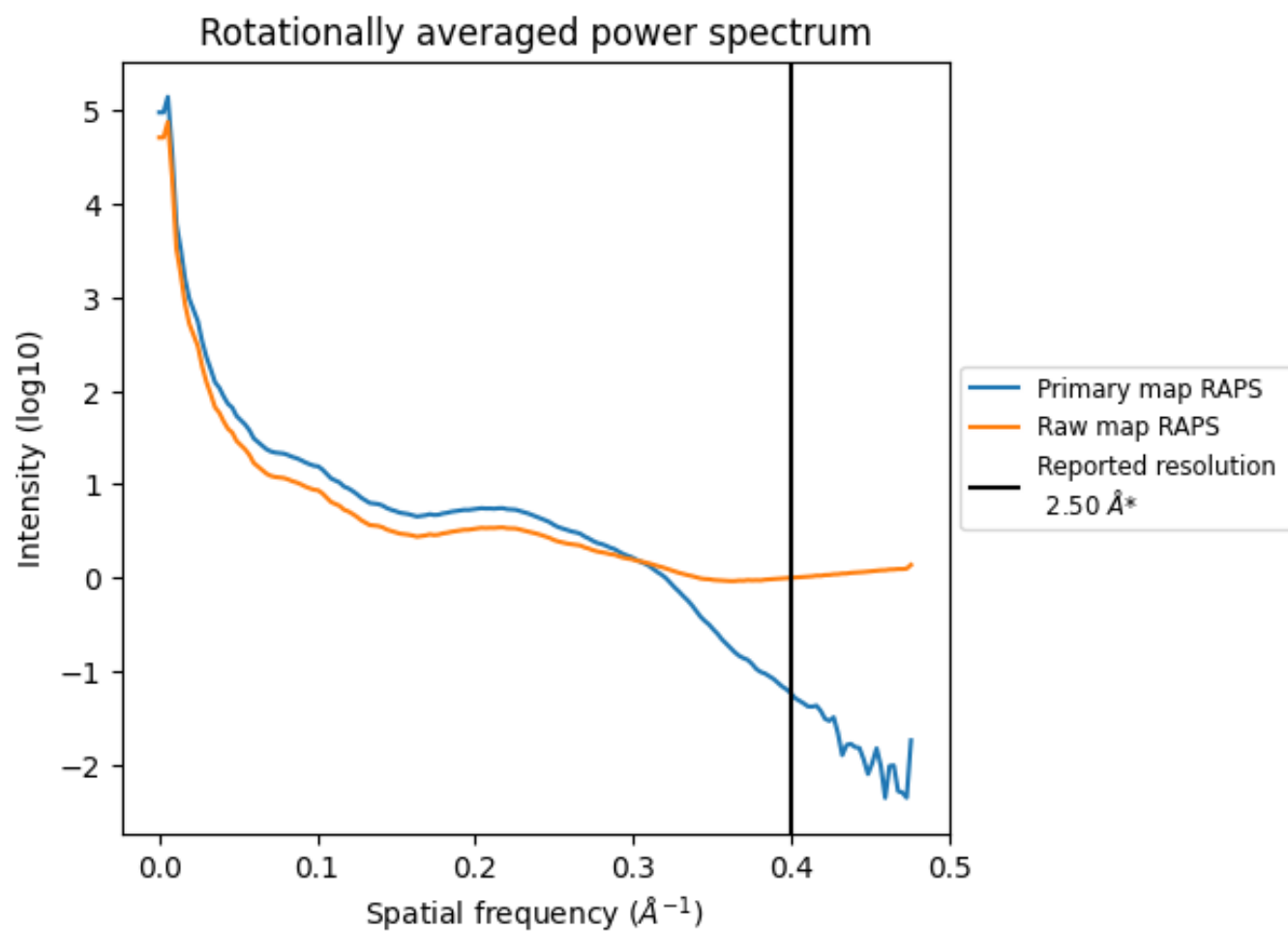
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1175 nm<sup>3</sup>; this corresponds to an approximate mass of 1062 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 ⓘ

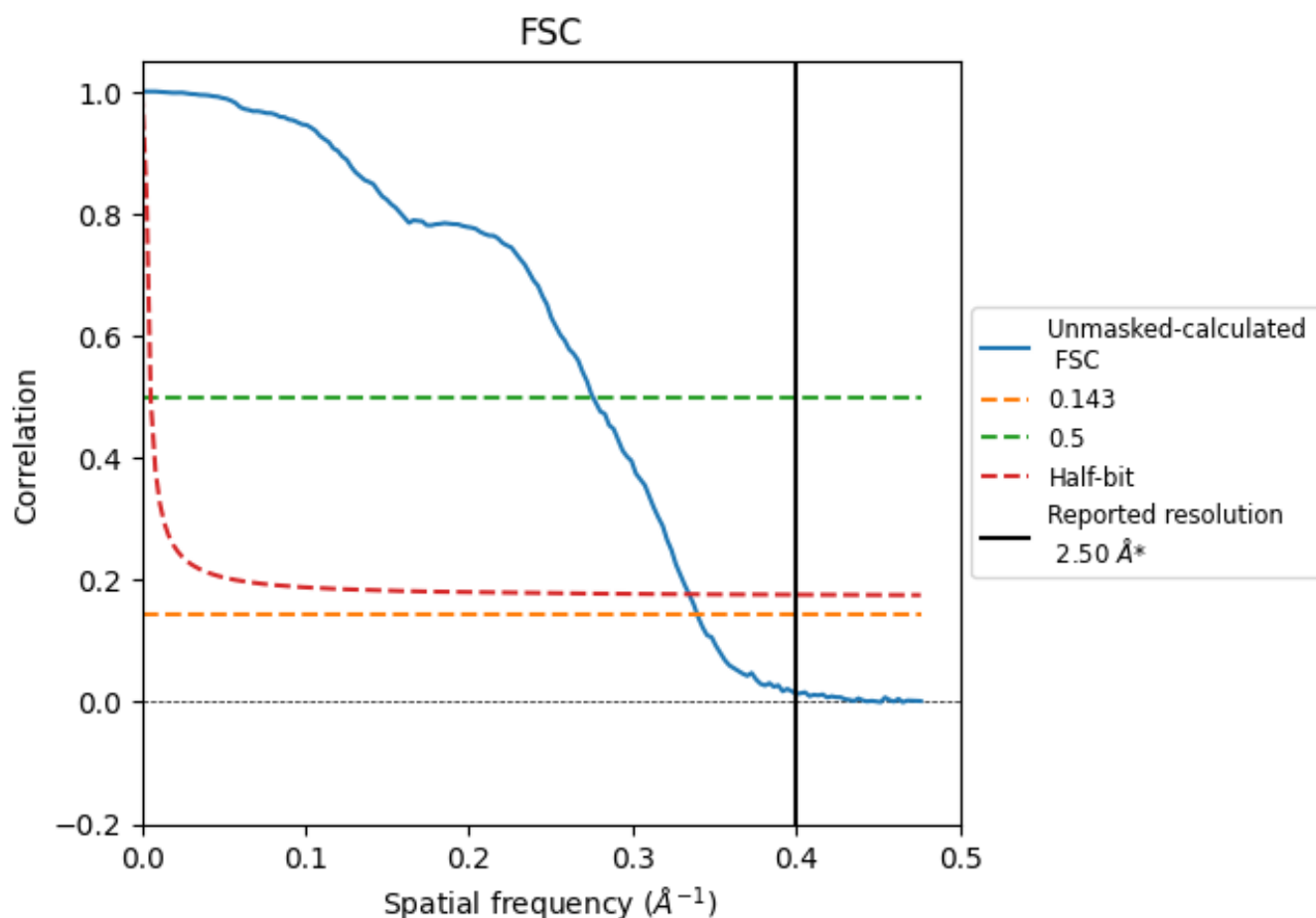


\*Reported resolution corresponds to spatial frequency of 0.400  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

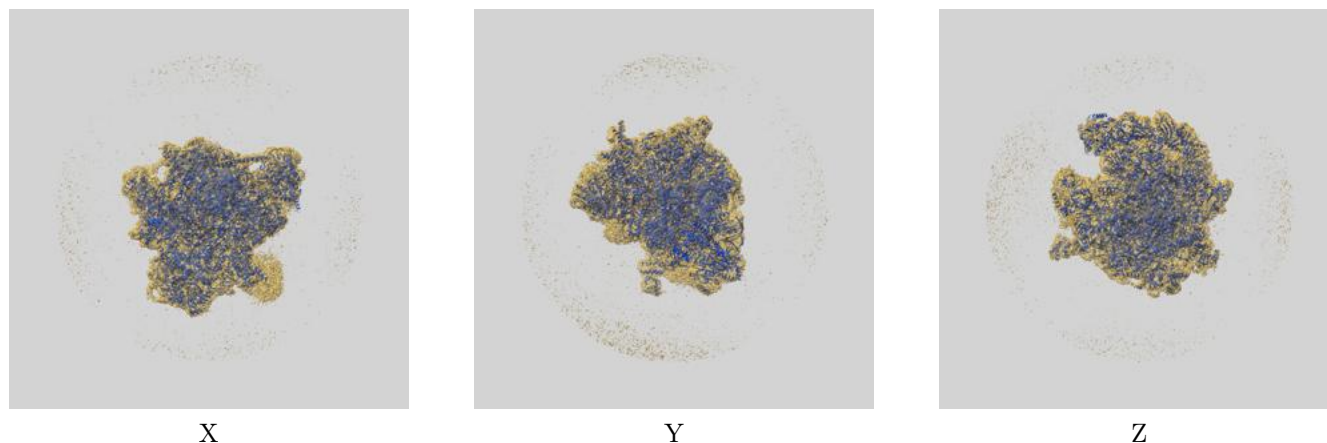
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.50                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 2.94                               | 3.63 | 2.99     |

\*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 2.94 differs from the reported value 2.5 by more than 10 %

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

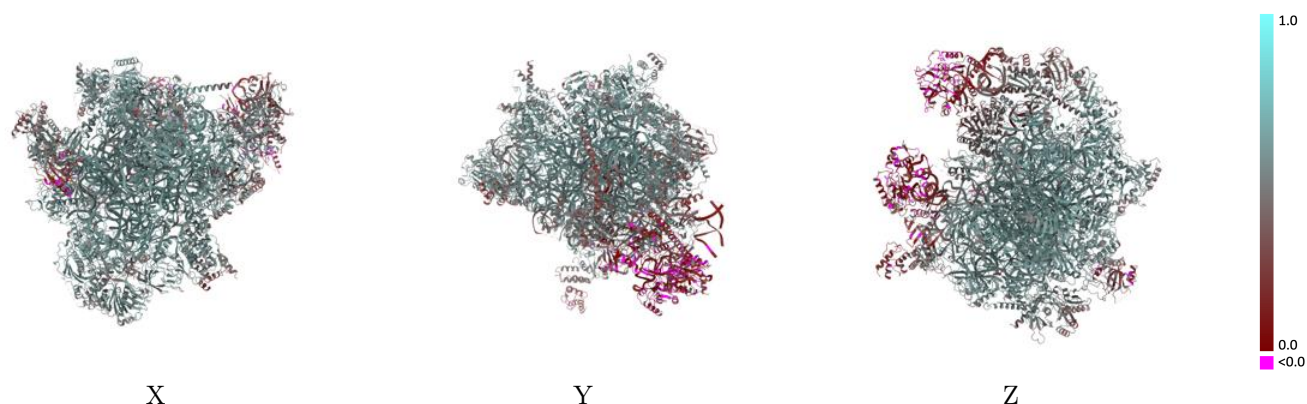
This section contains information regarding the fit between EMDB map EMD-12872 and PDB model 7OF7. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



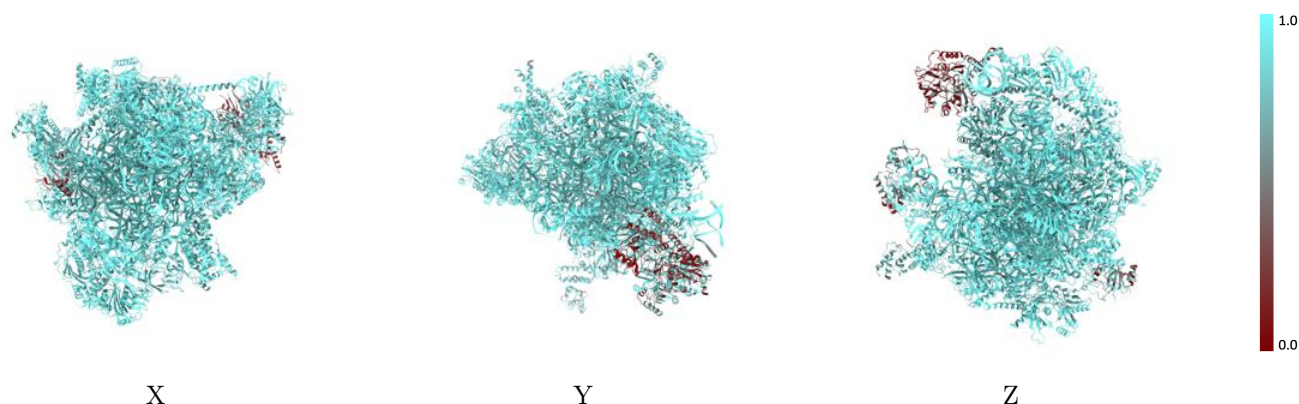
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



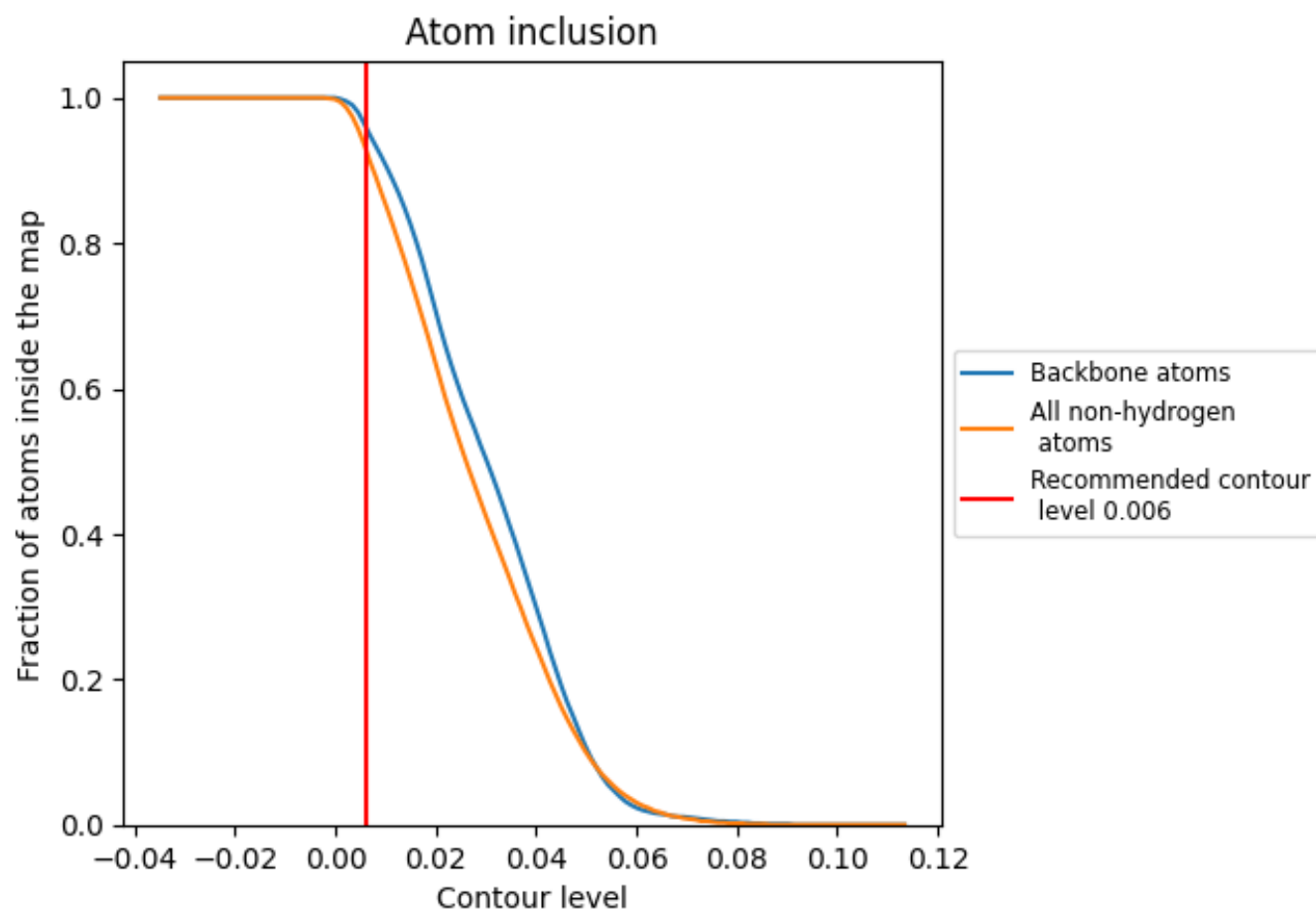
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9310   |  0.5230   |
| 0     |  0.9640   |  0.5670   |
| 1     |  0.8860   |  0.3710   |
| 2     |  1.0000   |  0.6420   |
| 3     |  0.9840   |  0.6260   |
| 4     |  0.9750   |  0.5650   |
| 5     |  0.9590   |  0.5370   |
| 6     |  0.9460   |  0.4560   |
| 7     |  0.9360   |  0.4950   |
| 8     |  0.3370   |  0.1560   |
| 9     |  0.9510   |  0.5530   |
| A     |  0.9950   |  0.5800   |
| B     |  0.9350   |  0.2930   |
| C     |  0.9100   |  0.4110   |
| D     |  0.9610  |  0.5800  |
| E     |  0.9720 |  0.5880 |
| F     |  0.9840 |  0.6080 |
| G     |  0.9000 |  0.4410 |
| H     |  0.9260 |  0.5320 |
| I     |  0.8200 |  0.2460 |
| J     |  0.5860 |  0.0940 |
| K     |  0.9840 |  0.6050 |
| L     |  0.9690 |  0.5830 |
| M     |  0.9740 |  0.5980 |
| N     |  0.9480 |  0.5390 |
| O     |  0.9800 |  0.5950 |
| P     |  0.9670 |  0.5120 |
| Q     |  0.9610 |  0.5710 |
| R     |  0.9870 |  0.6170 |
| S     |  0.9690 |  0.5900 |
| T     |  0.9740 |  0.6050 |
| U     |  0.8710 |  0.5420 |
| V     |  0.9560 |  0.5360 |
| W     |  0.9790 |  0.5970 |
| X     |  0.9570 |  0.5700 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Y     |  0.9630   |  0.5840   |
| Z     |  0.9660   |  0.5910   |
| a     |  0.9690   |  0.5940   |
| b     |  0.9800   |  0.5990   |
| c     |  0.9590   |  0.5590   |
| d     |  0.6550   |  0.3280   |
| e     |  0.1900   |  0.0940   |
| f     |  0.4250   |  0.2540   |
| g     |  0.9830   |  0.5930   |
| h     |  0.9300   |  0.4890   |
| i     |  0.9870   |  0.6300   |
| j     |  0.9620   |  0.5720   |
| k     |  0.8780   |  0.2730   |
| m     |  0.2140   |  0.1370   |
| o     |  0.9730   |  0.6040   |
| p     |  0.9240   |  0.4990   |
| q     |  0.8860   |  0.4520   |
| r     |  0.9700  |  0.5440  |
| s     |  0.9680 |  0.5800 |
| u     |  0.9450 |  0.4580 |
| v     |  0.8790 |  0.3490 |
| w     |  0.6790 |  0.1820 |
| x     |  0.8820 |  0.3910 |