



## Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 08:35 PM EDT

PDB ID : 8FKP / pdb\_00008fkp  
EMDB ID : EMD-29252  
Title : Human nucleolar pre-60S ribosomal subunit (State A1)  
Authors : Vanden Broeck, A.; Klinge, S.  
Deposited on : 2022-12-21  
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

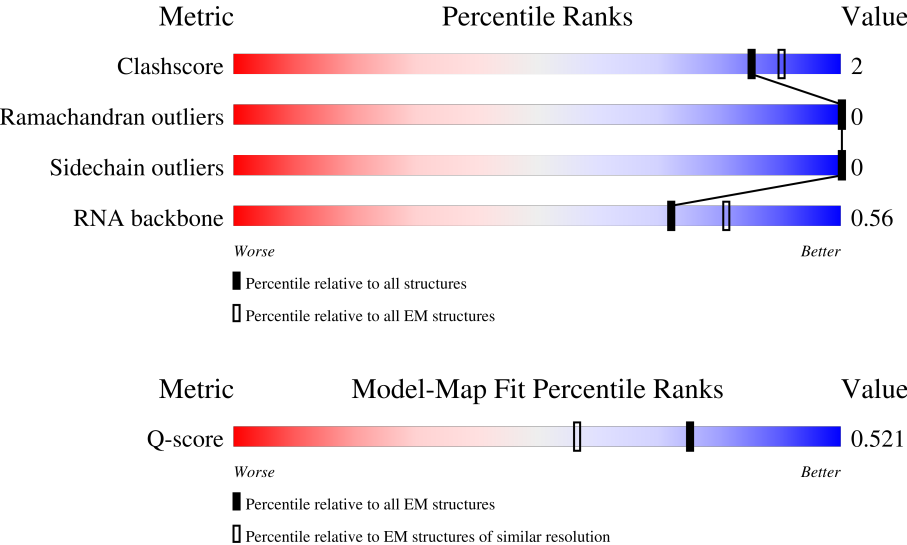
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11965 ( 2.35 - 3.35 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 1   | L1    | 157    | <div> <div>26%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div> |
| 2   | L2    | 1167   | <div> <div>94%</div> <div>• •</div> </div>                               |
| 3   | L3    | 5070   | <div> <div>24%</div> <div>5%</div> <div>70%</div> <div>•</div> </div>    |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | L6    | 211    |                  |
| 5   | L7    | 203    |                  |
| 6   | L8    | 215    |                  |
| 7   | L9    | 204    |                  |
| 8   | LA    | 184    |                  |
| 9   | LB    | 188    |                  |
| 10  | LC    | 176    |                  |
| 11  | LE    | 160    |                  |
| 12  | LG    | 140    |                  |
| 13  | LH    | 156    |                  |
| 14  | LI    | 145    |                  |
| 15  | LK    | 148    |                  |
| 16  | LN    | 403    |                  |
| 17  | LQ    | 135    |                  |
| 18  | LS    | 123    |                  |
| 19  | LT    | 110    |                  |
| 20  | LU    | 105    |                  |
| 21  | LW    | 97     |                  |
| 22  | NB    | 549    |                  |
| 23  | NE    | 361    |                  |
| 24  | NG    | 282    |                  |
| 25  | NM    | 300    |                  |
| 26  | NN    | 473    |                  |
| 27  | NO    | 461    |                  |
| 28  | NQ    | 385    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | NS    | 349    |                  |
| 30  | SA    | 427    |                  |
| 31  | SC    | 288    |                  |
| 32  | SD    | 248    |                  |
| 33  | SE    | 266    |                  |
| 34  | SH    | 293    |                  |
| 35  | SI    | 255    |                  |
| 36  | SJ    | 847    |                  |
| 37  | SK    | 245    |                  |
| 38  | SL    | 490    |                  |
| 39  | SM    | 588    |                  |
| 40  | SN    | 306    |                  |
| 41  | SO    | 353    |                  |
| 42  | SR    | 634    |                  |
| 43  | SS    | 746    |                  |
| 44  | ST    | 365    |                  |
| 45  | SV    | 163    |                  |
| 46  | SW    | 670    |                  |
| 47  | SZ    | 178    |                  |

## 2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 101451 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 1   | L1    | 152      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3234  | 1443 | 571 | 1068 | 152 |         |       |

- Molecule 2 is a RNA chain called ITS2 rRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | L2    | 69       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1468  | 653 | 263 | 483 | 69 |         |       |

- Molecule 3 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 3   | L3    | 1507     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32319 | 14383 | 5932 | 10497 | 1507 |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | L6    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 936   | 583 | 206 | 146 | 1 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | L7    | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1507  | 976 | 290 | 237 | 4 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | L8    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 713 | 213 | 178 | 7 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | L9    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1546  | 974 | 325 | 243 | 4 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | LA    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1161  | 732 | 214 | 208 | 7 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | LB    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1223  | 768 | 247 | 203 | 5 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10  | LC    | 174      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1438  | 912 | 282 | 233 | 11 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 11  | LE    | 108      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 702   | 430 | 138 | 134 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | LG    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 844   | 532 | 155 | 152 | 5 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 13  | LH    | 20       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 146   | 95 | 29 | 22 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | LI    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | LK    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 388 | 137 | 115 | 2 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | LN    | 377      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3044  | 1937 | 566 | 527 | 14 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | LQ    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1096  | 690 | 225 | 176 | 5 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | LS    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LT    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | LU    | 102      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 840   | 526 | 180 | 129 | 5 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 21  | LW    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 563   | 346 | 126 | 86 | 5 |         |       |

- Molecule 22 is a protein called Guanine nucleotide-binding protein-like 3.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | NB    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 257   | 164 | 49 | 43 | 1 |         |       |

- Molecule 23 is a protein called Surfeit locus protein 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | NE    | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1331  | 810 | 293 | 226 | 2 |         |       |

- Molecule 24 is a protein called RRP15-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | NG    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 456 | 145 | 133 | 4 |         |       |

- Molecule 25 is a protein called Protein MAK16 homolog.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | NM    | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1550  | 983 | 286 | 273 | 8 |         |       |

- Molecule 26 is a protein called Suppressor of SWI4 1 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | NN    | 244      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1950  | 1230 | 371 | 338 | 11 |         |       |

- Molecule 27 is a protein called Ribosomal RNA processing protein 1 homolog A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27  | NO    | 305      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2487  | 1577 | 437 | 461 | 12 |         |       |

- Molecule 28 is a protein called WD repeat-containing protein 74.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | NQ    | 324      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2502  | 1559 | 471 | 457 | 15 |         |       |

- Molecule 29 is a protein called Ribosome production factor 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29  | NS    | 305      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2529  | 1607 | 472 | 444 | 6 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 30  | SA    | 331      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2656  | 1681 | 524 | 437 | 14 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | SC    | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1627  | 1046 | 305 | 274 | 2 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | SD    | 239      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1985  | 1275 | 381 | 320 | 9 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | SE    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1498  | 951 | 290 | 253 | 4 |         |       |

- Molecule 34 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | SH    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1267  | 819 | 224 | 220 | 4 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L7-like 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | SI    | 199      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1661  | 1076 | 311 | 270 | 4 |         |       |

- Molecule 36 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 36  | SJ    | 72       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 609   | 385 | 114 | 110 |  |         |       |

- Molecule 37 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | SK    | 226      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1721  | 1070 | 296 | 343 | 12 |         |       |

- Molecule 38 is a protein called Ribosomal L1 domain-containing protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | SL    | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1960  | 1254 | 344 | 356 | 6 |         |       |

- Molecule 39 is a protein called Pescadillo homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39  | SM    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3452  | 2229 | 603 | 609 | 11 |         |       |

- Molecule 40 is a protein called Probable rRNA-processing protein EBP2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | SN    | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1308  | 821 | 247 | 235 | 5 |         |       |

- Molecule 41 is a protein called Ribosome biogenesis protein BRX1 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41  | SO    | 307      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2544  | 1637 | 458 | 434 | 15 |         |       |

- Molecule 42 is a protein called GTP-binding protein 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | SR    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 411 | 107 | 122 | 2 |         |       |

- Molecule 43 is a protein called Ribosome biogenesis protein BOP1.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 43  | SS    | 235      | Total | C    | N   | O   | P S | 0       | 0     |
|     |       |          | 1955  | 1238 | 348 | 360 | 2 7 |         |       |

- Molecule 44 is a protein called Ribosome biogenesis regulatory protein homolog.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | ST    | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 263   | 160 | 51 | 51 | 1 |         |       |

- Molecule 45 is a protein called Probable ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 45  | SV    | 137      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1171  | 745 | 227 | 189 | 10 |         |       |

- Molecule 46 is a protein called ATP-dependent RNA helicase DDX18.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46  | SW    | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3560  | 2288 | 609 | 646 | 17 |         |       |

- Molecule 47 is a protein called Nucleolar protein 16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | SZ    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1338  | 835 | 260 | 238 | 5 |         |       |

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 48  | L1    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |
| 48  | L2    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 48  | L3    | 46       | Total | Mg | 0       |
|     |       |          | 46    | 46 |         |

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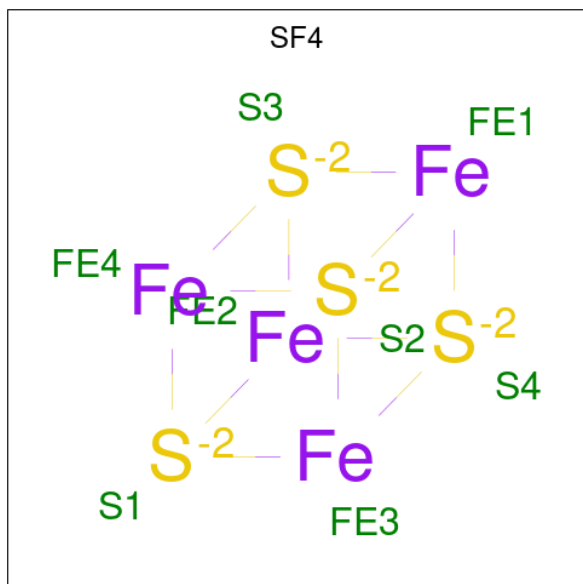
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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 48  | L9    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 48  | LQ    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 48  | LT    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 48  | SA    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 49  | LW    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 49  | SV    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 50 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

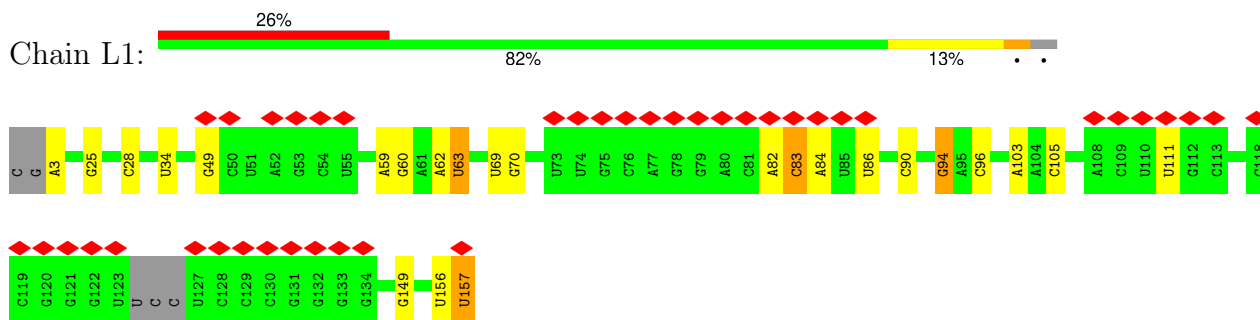


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 50  | NM    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

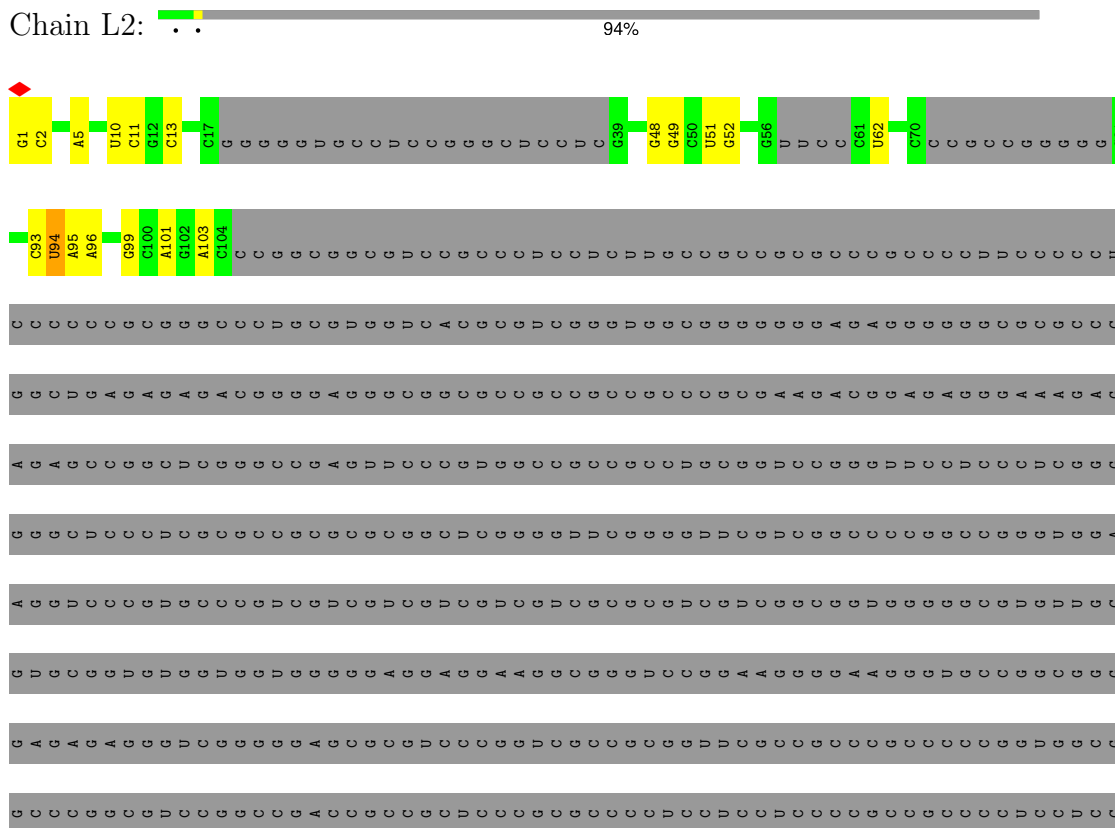
### 3 Residue-property plots [i](#)

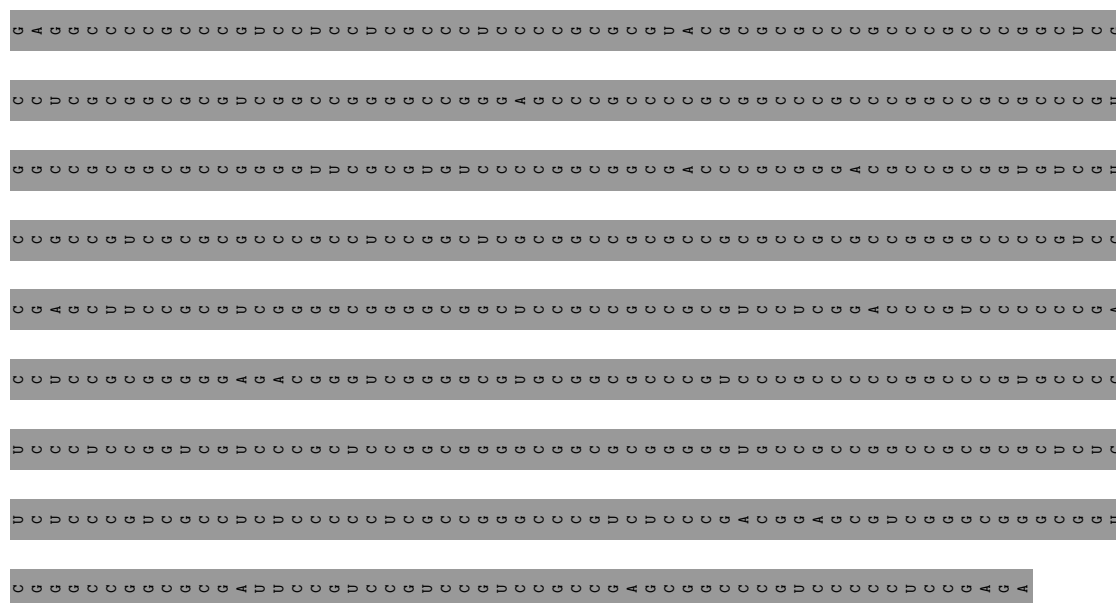
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 5.8S rRNA

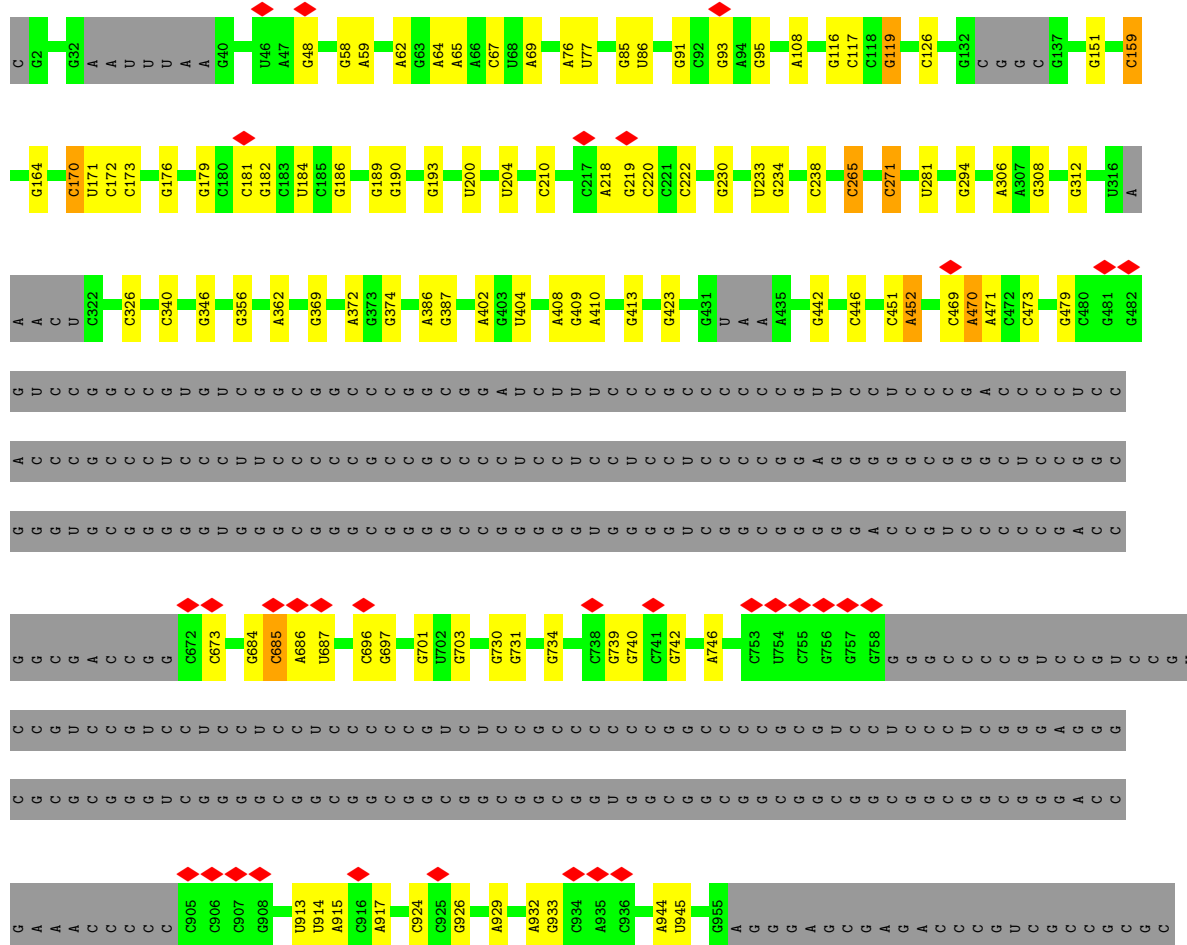


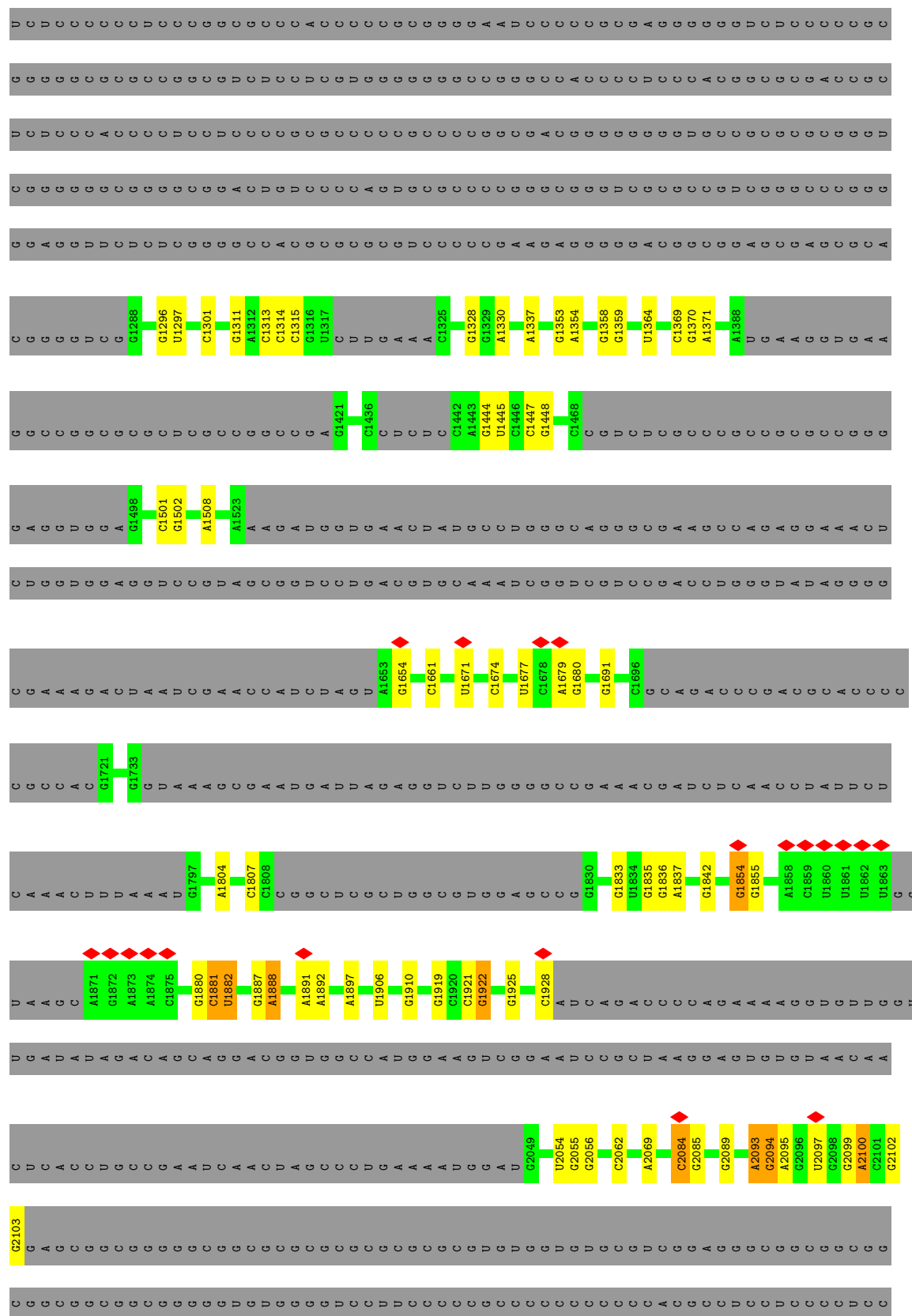
#### • Molecule 2: ITS2 rRNA





• Molecule 3: 28S rRNA



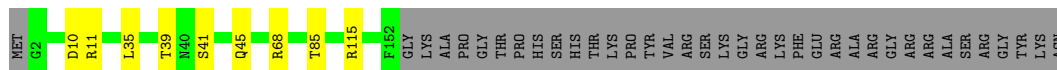
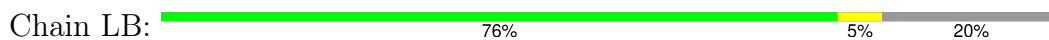




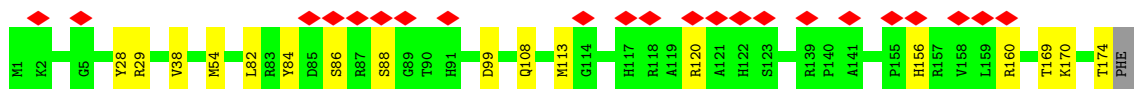
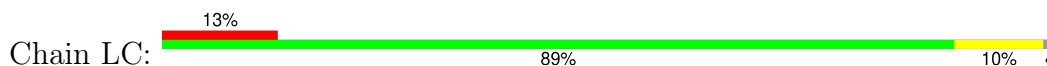




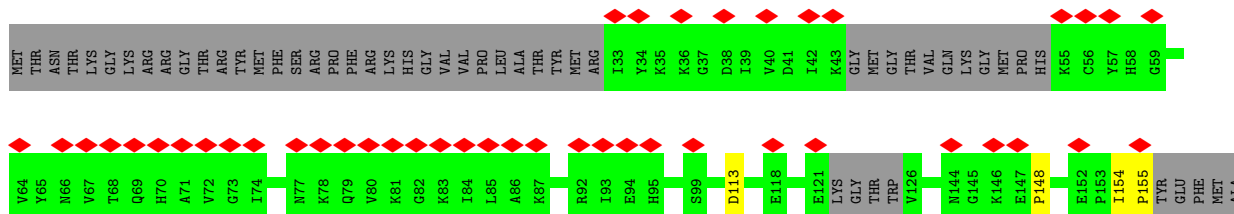
- Molecule 9: 60S ribosomal protein L18



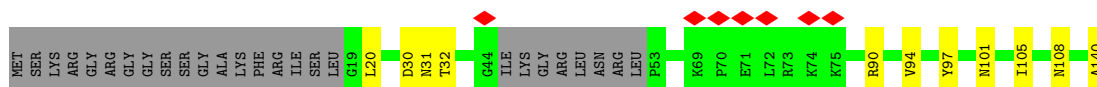
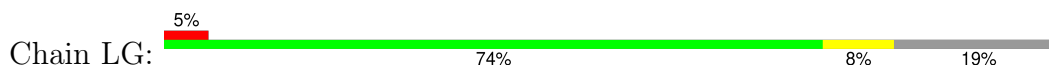
- Molecule 10: 60S ribosomal protein L18a



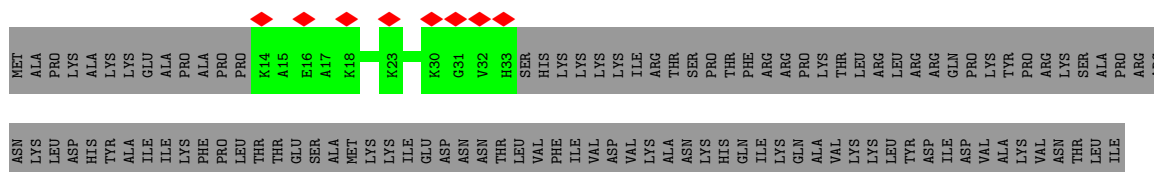
- Molecule 11: 60S ribosomal protein L21



- Molecule 12: 60S ribosomal protein L23



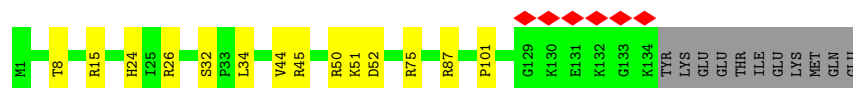
- Molecule 13: 60S ribosomal protein L23a



ARG  
PRO  
ASP  
GLY  
GLU  
LYS  
LYS  
ALA  
TYR  
VAL  
ARG  
LEU  
ALA  
PRO  
ASP  
TYR  
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ASP  
VAL  
ALA  
ASN  
LYS  
ILE  
GLY  
ILE

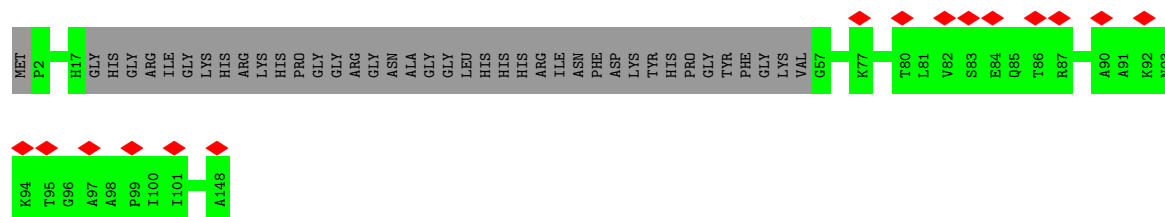
- Molecule 14: 60S ribosomal protein L26

Chain LI:  83% 10% 8%



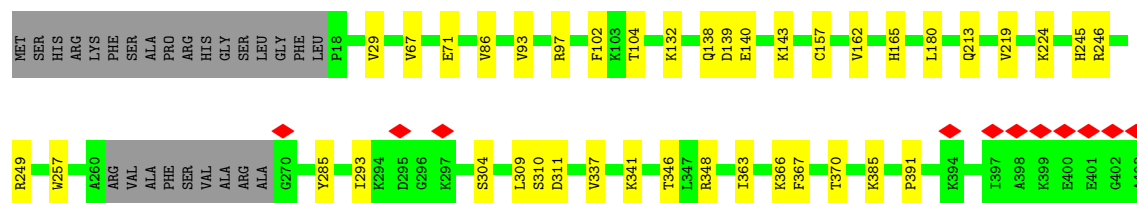
- Molecule 15: 60S ribosomal protein L27a

Chain LK:  10% 73% 27%

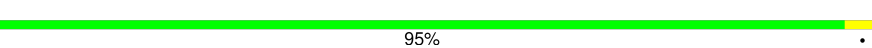


- Molecule 16: 60S ribosomal protein L3

Chain LN:  84% 10% 6%



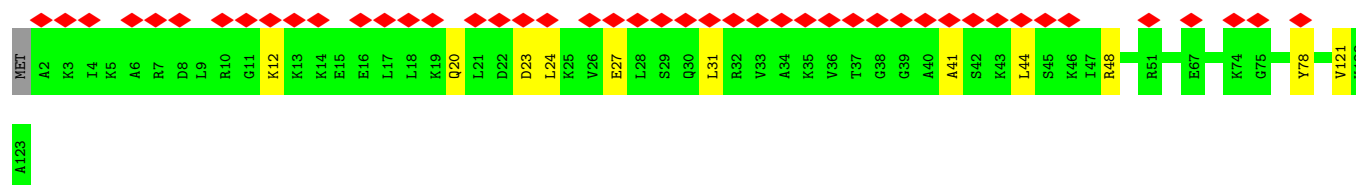
- Molecule 17: 60S ribosomal protein L32

Chain LQ:  95% 5% 0%



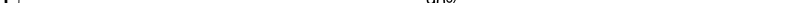
- Molecule 18: 60S ribosomal protein L35

Chain LS:  37% 90% 9% 0%



- Molecule 19: 60S ribosomal protein L35a

Diagram illustrating a protein structure with residues MET, S2, V33, D37, E38, R68, S108, R109, and I110. The residues are represented by colored blocks (grey, yellow, and red) connected by green bars, indicating interactions or structural elements.

- Chain LU:  8% 90% 7%

- Chain LW:

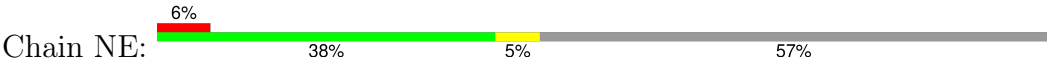
Sequence logo for the 1000bp upstream region of the human HNF1A gene. The y-axis represents information content in bits (0.00 to 0.03). The x-axis shows amino acid positions from -1000 to +100. The logo shows a high degree of conservation for the first 100 amino acids, with a peak at position 100 (Glu, Glu, Glu, Glu, Glu, Glu, Glu, Glu, Glu, Glu). The conservation drops significantly after position 100, with a small peak around position 200 (Glu, Glu, Glu, Glu, Glu, Glu, Glu, Glu, Glu, Glu). The sequence ends with a stop codon (TGA) at position 200.

- Chain NB:  5% 94%

[illegible]

PHE  
SER  
THR  
ASP  
TYR  
VAL

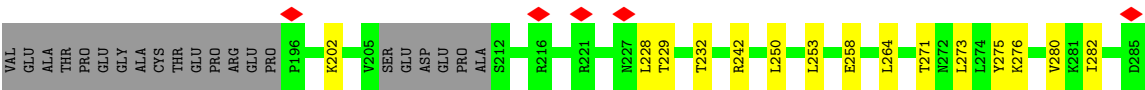
• Molecule 23: Surfeit locus protein 6



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

LYS  
ALA  
ALA  
GLU  
LYS  
HIS  
ILE  
GLN  
GLY  
SER  
SER  
PRO  
ALA  
LYS  
SER  
SER  
GLY  
ALA  
ARG  
ALA  
TRP  
ALA  
SER  
SER  
SER  
GLY  
ASN  
PRO  
ALA  
GLY  
ASP  
GLY  
LEU  
ARG  
ALA  
LYS  
LYS  
GLU  
THR  
PRO  
GLU  
SER  
VAL  
PHE  
GLN  
ALA  
LEU  
ARG  
GLN  
VAL  
ARG

LEU  
HIS  
GLU  
LYS  
ILE  
GLN  
GLY  
SER  
SER  
ALA  
LYS  
GLU  
LYS  
SER  
PRO  
ALA  
LYS  
SER  
SER  
PRO  
ALA  
ARG  
ARG  
ARG  
LYS  
LYS  
GLN  
GLY  
ARG  
GLY  
ARG  
LYS  
ARG  
LYS  
LYS  
GLU  
THR  
ALA  
LYS  
ARG  
LYS  
VAL  
ALA  
GLU  
GLU  
THR  
THR  
GLU  
ALA  
GLN  
VAL

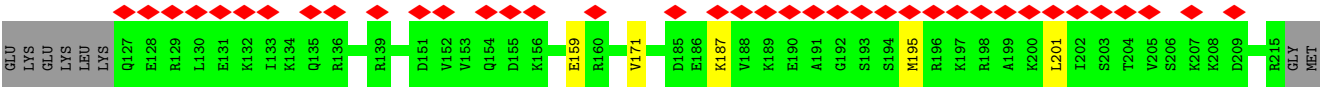


• Molecule 24: RRP15-like protein



MET  
ALA  
ALA  
GLU  
ALA  
PRO  
ASP  
SER  
SER  
VAL  
SER  
GLU  
GLU  
GLU  
ASN  
LYS  
LYS  
THR  
PRO  
ASP  
LYS  
LYS  
GLY  
MET  
LYS  
MET  
VAL  
THR  
GLY  
GLY  
ALA  
VAL  
SER  
ASP  
VAL  
LEU  
GLU  
ASP  
GLY  
ALA  
THR  
THR  
LYS  
LYS  
ASP  
SER  
SER  
GLY  
GLY  
CYS  
GLY  
SER  
SER  
GLU  
LEU  
VAL  
LYS  
ASP  
HIS  
PHE  
TYR  
SER  
ASP  
ASP

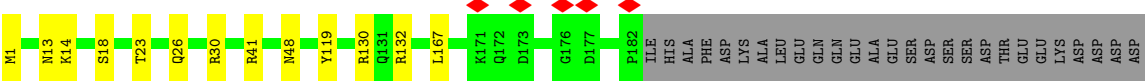
ASP  
ALA  
ILE  
GLU  
ALA  
ASP  
SER  
GLY  
GLY  
ASP  
GLU  
ALA  
PRO  
CYS  
ASP  
LYS  
LYS  
ASN  
GLY  
ASP  
GLY  
THR  
ASP  
GLY  
TRP  
ALA  
SER  
VAL  
ALA  
LEU  
MET  
LYS  
VAL  
VAL  
ASN  
LYS  
LYS  
THR  
THR  
PRO  
GLY  
SER  
GLY  
LYS  
CYS  
PRO  
THR  
ILE  
LEU  
VAL  
LYS  
VAL  
ASP  
HIS  
PHE  
TYR  
SER  
ASP  
ASP



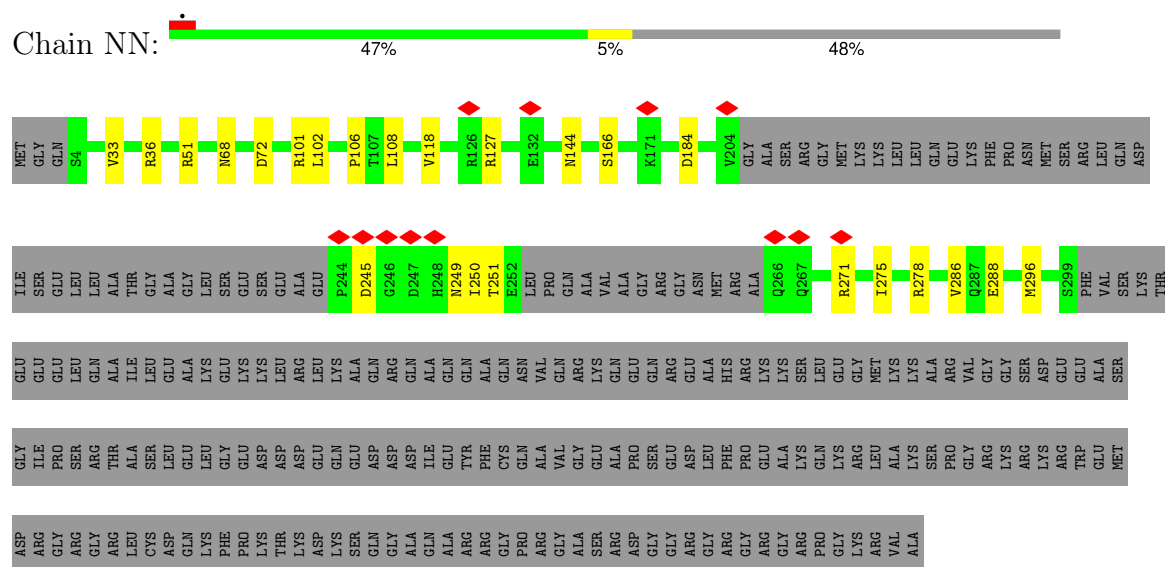
ASP  
GLY  
SER  
THR  
ASN  
GLU  
THR  
ALA  
SER  
SER  
ARG  
SER  
LYS  
PRO  
LYS  
LYS  
ALA  
LYS  
GLN  
THR  
GLU  
VAL  
VAL  
LYS  
SER  
SER  
GLY  
GLU  
GLY  
PRO  
TRP  
THR  
ILE  
LEU  
ARG  
ASP  
PHE  
MET  
MET  
GLY  
ALA  
SER  
MET  
LYS  
LYS  
ASP  
LEU  
GLY  
GLN  
GLY  
ALA  
GLY  
SER  
SER  
SER  
TRP  
ASP  
LYS  
LYS  
GLY  
GLY  
SER  
SER  
ASP  
GLY  
PRO  
SER  
ASP  
ASP  
ASP  
THR  
ALA  
GLY  
HIS  
LYS  
LYS  
GLY  
ASP  
ASP  
ASP  
ASP

SER  
ASP  
SER  
ASP  
THR

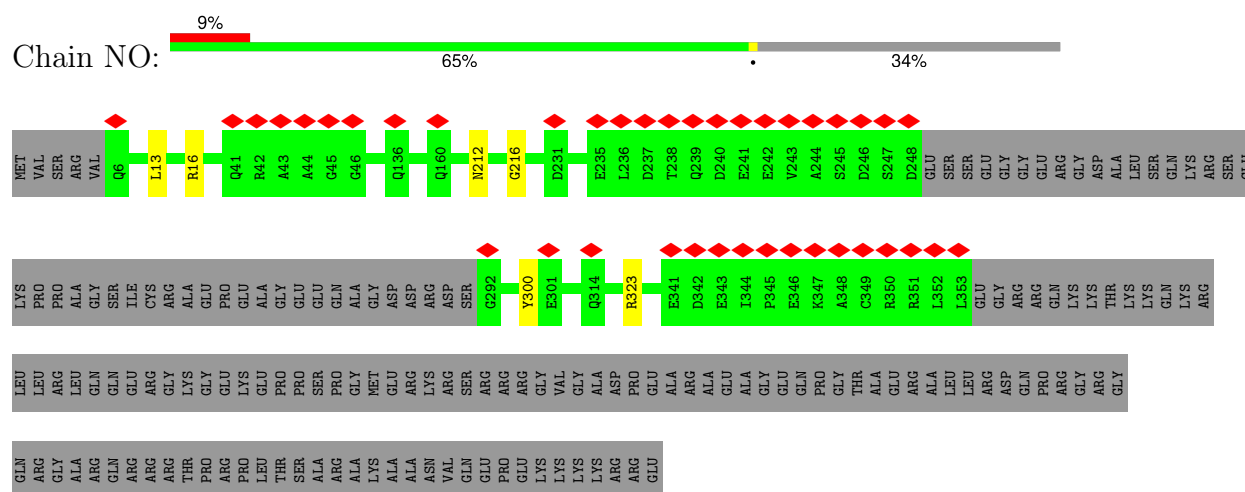
• Molecule 25: Protein MAK16 homolog



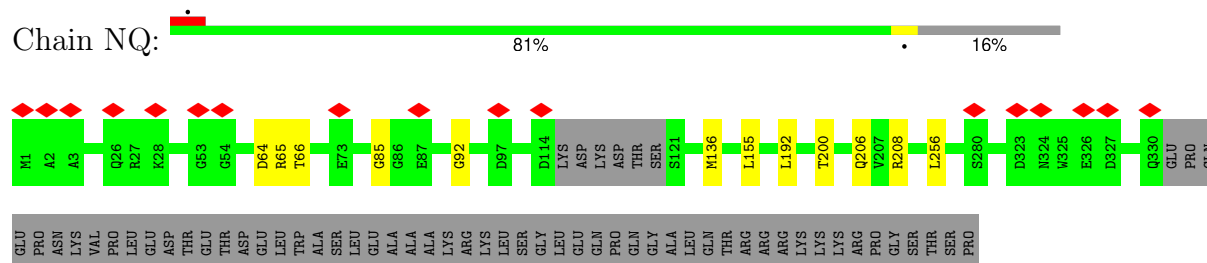
- Molecule 26: Suppressor of SWI4 1 homolog



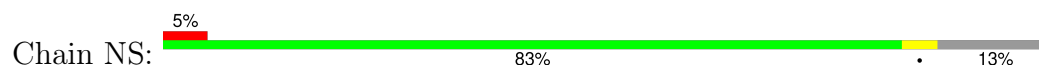
- Molecule 27: Ribosomal RNA processing protein 1 homolog A

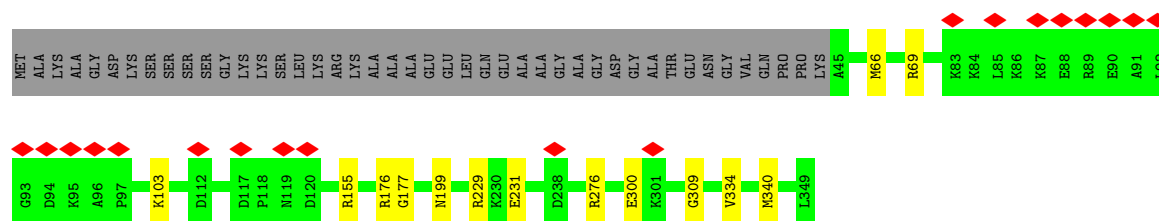


- Molecule 28: WD repeat-containing protein 74

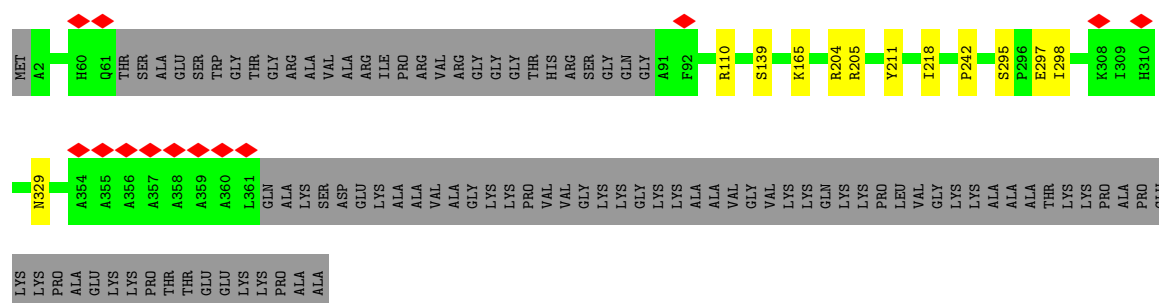
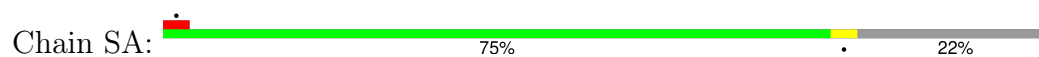


- Molecule 29: Ribosome production factor 1

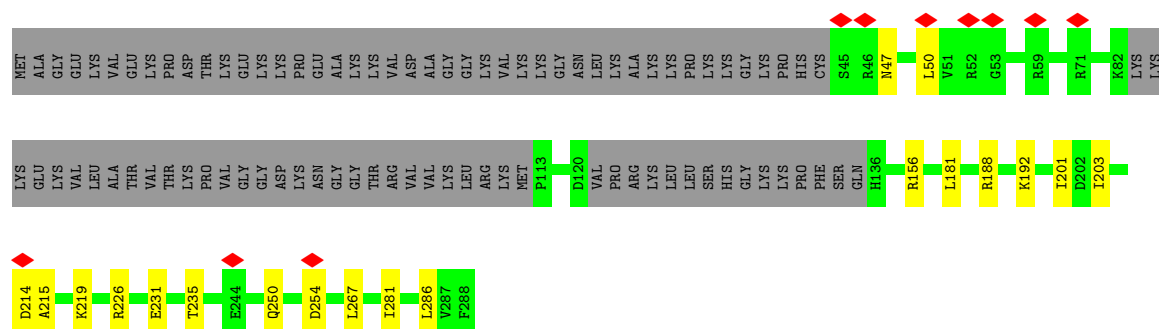




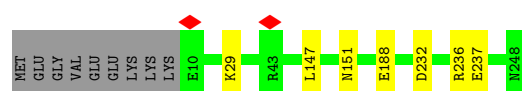
• Molecule 30: 60S ribosomal protein L4



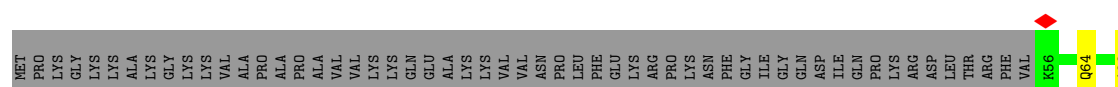
• Molecule 31: 60S ribosomal protein L6

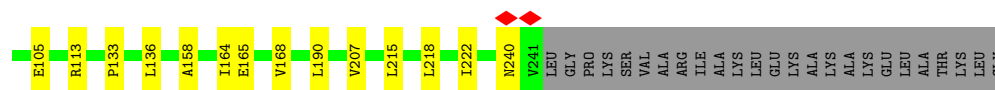


• Molecule 32: 60S ribosomal protein L7

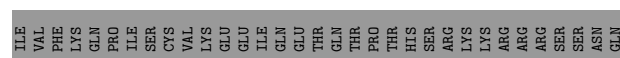
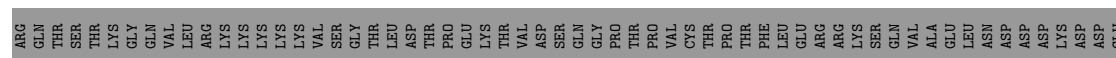
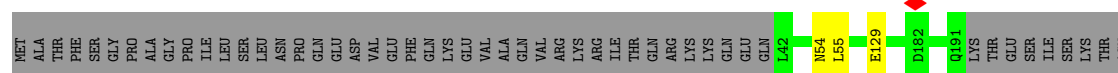


• Molecule 33: 60S ribosomal protein L7a

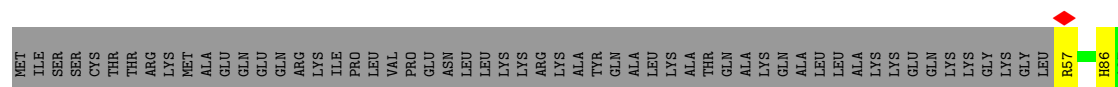




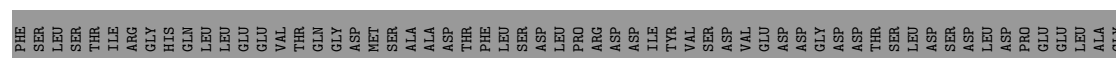
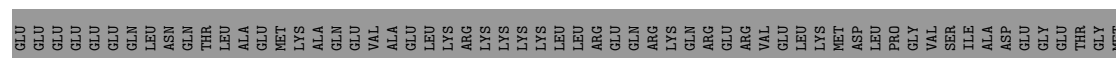
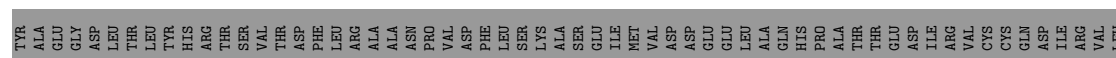
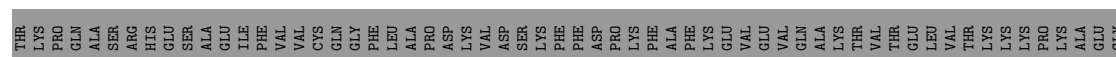
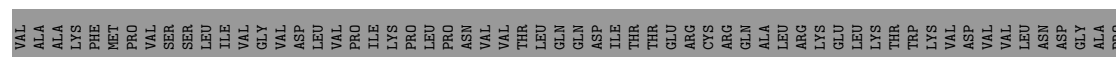
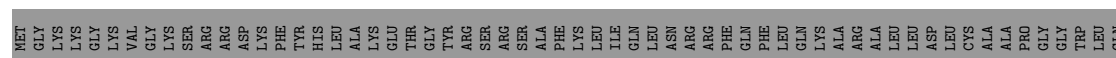
- Molecule 34: MKI67 FHA domain-interacting nucleolar phosphoprotein



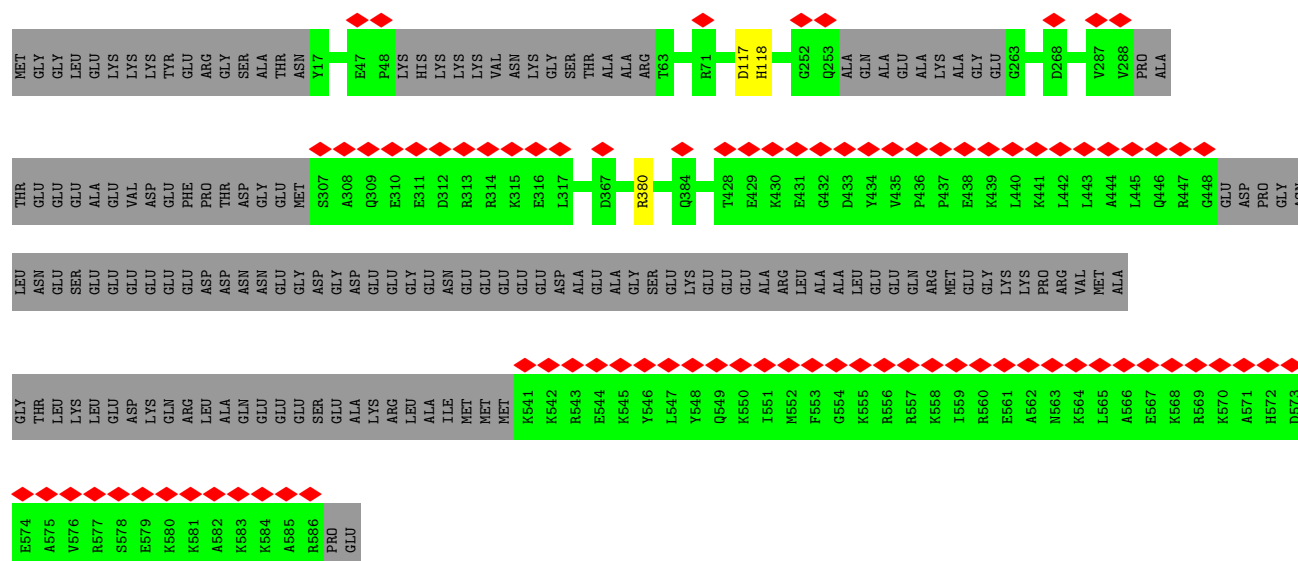
- Molecule 35: 60S ribosomal protein L7-like 1



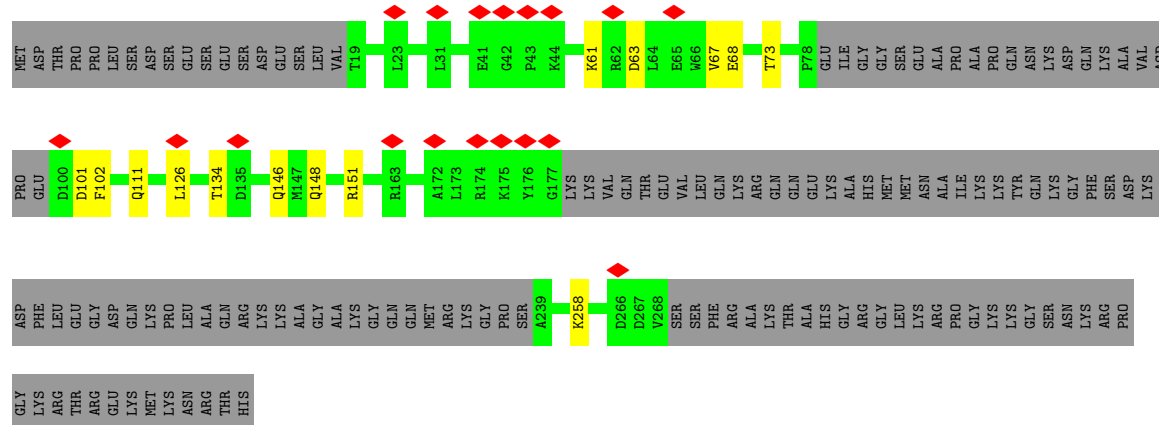
- Molecule 36: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3



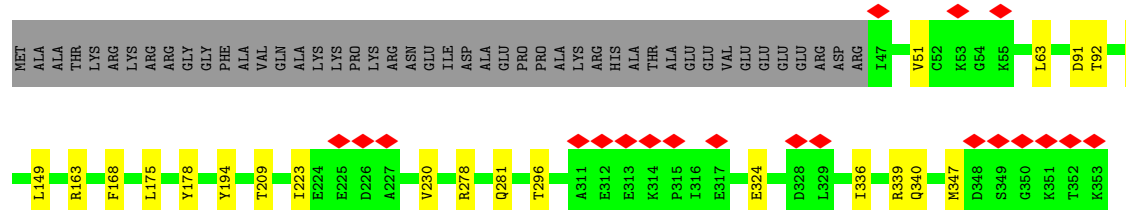
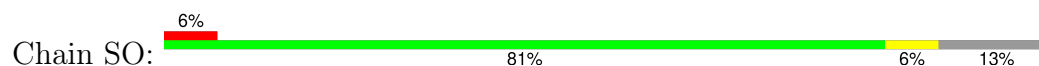




• Molecule 40: Probable rRNA-processing protein EBP2



• Molecule 41: Ribosome biogenesis protein BRX1 homolog



• Molecule 42: GTP-binding protein 4





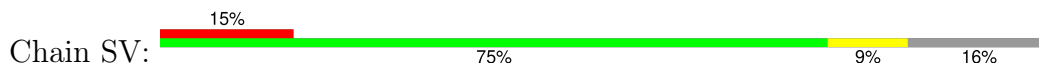
[illegible]

- Molecule 44: Ribosome biogenesis regulatory protein homolog



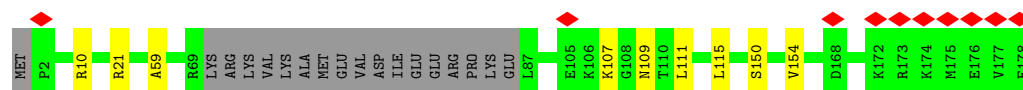
|     |     |     |      |     |     |     |
|-----|-----|-----|------|-----|-----|-----|
| GLY | ARG | PHE | ARG  | LVS | LEU | MET |
| LYS | ALA | ALA | VAL  | GLY | GLN | GLY |
| GLY | GLU | GLU | LYS  | PRO | ALA | GLN |
| GLY | LYS | LYS | ASN  | ASN | ALA | SER |
| PRO | ASN | GLN | GLU  | LYS | ARG | VAL |
| PRO | GLN | LEU | ASN  | THR | ASN | GLU |
| SER | LEU | GLU | ARG  | THR | THR | LEU |
| GLN | GLU | GLU | LEU  | ASN | GLN | LEU |
| GLY | LEU | LEU | ARG  | VAL | LEU | ALA |
| GLY | LEU | LEU | ASN  | VAL | LEU | LYS |
| LYS | ARG | ARG | LEU  | TRP | ILE | ALA |
| ARG | VAL | VAL | ALA  | ASP | ASN | GLU |
| LYS | MET | MET | ARG  | GLU | GLN | GLN |
| GLY | ASN | SER | ALA  | VAL | LEU | ASP |
| GLY | SER | LYS | HIS  | SER | TRP | GLU |
| LEU | LYS | LYS | LYS  | GLY | GLN | GLU |
| GLY | LYS | LYS | MET  | GLY | LEU | GLU |
| GLY | PRO | PRO | GLN  | TRP | PRO | LYS |
| LYS | GLN | GLN | LEU  | ARG | THR | LEU |
| MET | LEU | LEU | P202 | ARG | GLY | GLN |
| ASN | ASP | VAL | S203 | ARG | ARG | ARG |
| SER | THR | THR | A204 | TRP | VAL | ILE |
| GLY | ARG | ARG | A205 | GLY | GLU | THR |
| PRO | ALA | ALA |      | TYR | VAL | HIS |
| GLY | THR | THR | E216 | GLN | ALA | LYS |
| LEU | ASN | ASN | E217 | ALA | VAL | LEU |
| GLY | LYS | LYS |      | ARG | ALA | GLU |
| GLY | GLN | GLN | R220 | ASP | ARG | LEU |
| LYS | MET | MET |      | ASP | LEU | LEU |
| ARG | ARG | ARG | V227 | THR | PRO | GLN |
| GLY | GLU | GLU |      | LYS | GLU | GLN |
| LYS | GLY | GLU |      | GLU | PRO | PHE |
| GLY | ASP | ASP | R234 | TRP | THR | ASP |
| GLN | GLN | GLN | F235 | LEU | THR | LEU |
| ARG | GLU | GLU | Q236 | ILE | ARG | GLY |
| PRO | GLU | GLU | E237 | GLU | LEU | LEU |
| GLY | ALA | ALA |      | VAL | PRO | ALA |
| LYS | ALA | LYS | ARG  | PRO | ARG | SER |
| ARG | ARG | ARG | PRO  | ASN | LYS | ASP |
| ARG | LYS | LYS | LYS  | ALA | PRO | ASP |
| LYS | LYS | MET | GLU  | ASP | LEU | ASN |
|     | SER | SER | VAL  | PRO | PRO | PRO |
|     | GLN | GLN | ARG  | GLU | ARG | THR |
|     | LYS | LYS | PRO  | ASP | ARG | GLY |
|     | GLY | GLY | GLY  | GLN | PRO | LEU |
|     | LYS | ARG | SER  | PHE | LEU | ARG |
|     | ARG | LYS | GLY  | ALA | THR | CYS |
|     | GLY | GLY | LYS  | LYS | ARG | ALA |
|     | GLY | GLY | ARG  | ARG | TRP | GLY |
|     | ARG | LYS | ILE  | ILE | GLN | THR |
|     | ARG | LYS | GLN  | GLN | GLN | PRO |
|     | GLY | GLN | ALA  | ALA | PHE | GLU |
|     | GLY | PRO | GLN  | LYS | ALA | ALA |
|     | PRO | PRO | LEU  | LYS | ARG |     |

- Molecule 45: Probable ribosome biogenesis protein RLP24

[illegible]

- Molecule 46: ATP-dependent RNA helicase DDX18

[illegible]



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 42413                                   | 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 ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 64000                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 5.947                                   | Depositor |
| Minimum map value                    | -0.089                                  | Depositor |
| Average map value                    | 0.033                                   | Depositor |
| Map value standard deviation         | 0.131                                   | Depositor |
| Recommended contour level            | 0.75                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 514.56, 514.56, 514.56                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.072, 1.072, 1.072                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, HIC, AME, SF4, SEP

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   | L1    | 0.20         | 0/3611  | 0.26        | 0/5623  |
| 2   | L2    | 0.27         | 0/1634  | 0.30        | 0/2538  |
| 3   | L3    | 0.23         | 0/36123 | 0.29        | 0/56296 |
| 4   | L6    | 0.24         | 0/953   | 0.38        | 0/1276  |
| 5   | L7    | 0.18         | 0/1534  | 0.34        | 0/2049  |
| 6   | L8    | 0.17         | 0/1133  | 0.34        | 0/1516  |
| 7   | L9    | 0.23         | 0/1584  | 0.36        | 0/2117  |
| 8   | LA    | 0.18         | 0/1179  | 0.35        | 0/1575  |
| 9   | LB    | 0.23         | 0/1239  | 0.37        | 0/1658  |
| 10  | LC    | 0.21         | 0/1476  | 0.40        | 0/1981  |
| 11  | LE    | 0.16         | 0/708   | 0.36        | 0/958   |
| 12  | LG    | 0.20         | 0/856   | 0.37        | 0/1149  |
| 13  | LH    | 0.16         | 0/146   | 0.28        | 0/190   |
| 14  | LI    | 0.24         | 0/1132  | 0.37        | 0/1504  |
| 15  | LK    | 0.18         | 0/648   | 0.41        | 0/880   |
| 16  | LN    | 0.26         | 0/3092  | 0.38        | 0/4133  |
| 17  | LQ    | 0.23         | 0/1114  | 0.34        | 0/1486  |
| 18  | LS    | 0.18         | 0/1023  | 0.38        | 0/1351  |
| 19  | LT    | 0.22         | 0/895   | 0.37        | 0/1198  |
| 20  | LU    | 0.20         | 0/854   | 0.34        | 0/1129  |
| 21  | LW    | 0.15         | 0/573   | 0.39        | 0/755   |
| 22  | NB    | 0.13         | 0/262   | 0.26        | 0/352   |
| 23  | NE    | 0.22         | 0/1339  | 0.39        | 0/1767  |
| 24  | NG    | 0.16         | 0/743   | 0.32        | 0/986   |
| 25  | NM    | 0.22         | 0/1566  | 0.31        | 0/2097  |
| 26  | NN    | 0.28         | 0/1988  | 0.42        | 0/2678  |
| 27  | NO    | 0.15         | 0/2530  | 0.28        | 0/3412  |
| 28  | NQ    | 0.18         | 0/2556  | 0.32        | 0/3466  |
| 29  | NS    | 0.19         | 0/2592  | 0.33        | 0/3487  |
| 30  | SA    | 0.23         | 0/2705  | 0.34        | 0/3632  |
| 31  | SC    | 0.16         | 0/1657  | 0.33        | 0/2219  |
| 32  | SD    | 0.21         | 0/2022  | 0.34        | 0/2696  |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 33  | SE    | 0.23         | 0/1524   | 0.36        | 0/2056   |
| 34  | SH    | 0.24         | 0/1298   | 0.32        | 0/1742   |
| 35  | SI    | 0.21         | 0/1702   | 0.32        | 0/2289   |
| 36  | SJ    | 0.17         | 0/623    | 0.31        | 0/836    |
| 37  | SK    | 0.22         | 0/1745   | 0.43        | 0/2374   |
| 38  | SL    | 0.24         | 0/1994   | 0.38        | 0/2684   |
| 39  | SM    | 0.18         | 0/3530   | 0.27        | 0/4779   |
| 40  | SN    | 0.16         | 0/1327   | 0.33        | 0/1774   |
| 41  | SO    | 0.20         | 0/2608   | 0.32        | 0/3506   |
| 42  | SR    | 0.24         | 0/657    | 0.48        | 0/887    |
| 43  | SS    | 0.18         | 0/1994   | 0.32        | 0/2703   |
| 44  | ST    | 0.14         | 0/267    | 0.31        | 0/357    |
| 45  | SV    | 0.25         | 0/1194   | 0.44        | 0/1582   |
| 46  | SW    | 0.18         | 0/3631   | 0.32        | 0/4900   |
| 47  | SZ    | 0.20         | 0/1364   | 0.31        | 0/1826   |
| All | All   | 0.21         | 0/106925 | 0.32        | 0/152449 |

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.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | L1    | 3234  | 0        | 1639     | 14      | 0            |
| 2   | L2    | 1468  | 0        | 755      | 8       | 0            |
| 3   | L3    | 32319 | 0        | 16377    | 104     | 0            |
| 4   | L6    | 936   | 0        | 1017     | 9       | 0            |
| 5   | L7    | 1507  | 0        | 1649     | 11      | 0            |
| 6   | L8    | 1111  | 0        | 1174     | 7       | 0            |
| 7   | L9    | 1546  | 0        | 1585     | 6       | 0            |
| 8   | LA    | 1161  | 0        | 1221     | 8       | 0            |
| 9   | LB    | 1223  | 0        | 1330     | 7       | 0            |
| 10  | LC    | 1438  | 0        | 1484     | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | LE    | 702   | 0        | 561      | 4       | 0            |
| 12  | LG    | 844   | 0        | 883      | 8       | 0            |
| 13  | LH    | 146   | 0        | 176      | 0       | 0            |
| 14  | LI    | 1115  | 0        | 1205     | 12      | 0            |
| 15  | LK    | 642   | 0        | 455      | 0       | 0            |
| 16  | LN    | 3044  | 0        | 3178     | 32      | 0            |
| 17  | LQ    | 1096  | 0        | 1183     | 6       | 0            |
| 18  | LS    | 1015  | 0        | 1148     | 9       | 0            |
| 19  | LT    | 876   | 0        | 912      | 6       | 0            |
| 20  | LU    | 840   | 0        | 930      | 6       | 0            |
| 21  | LW    | 563   | 0        | 596      | 9       | 0            |
| 22  | NB    | 257   | 0        | 259      | 1       | 0            |
| 23  | NE    | 1331  | 0        | 1430     | 19      | 0            |
| 24  | NG    | 738   | 0        | 786      | 4       | 0            |
| 25  | NM    | 1550  | 0        | 1599     | 12      | 0            |
| 26  | NN    | 1950  | 0        | 2005     | 17      | 0            |
| 27  | NO    | 2487  | 0        | 2506     | 5       | 0            |
| 28  | NQ    | 2502  | 0        | 2481     | 6       | 0            |
| 29  | NS    | 2529  | 0        | 2563     | 10      | 0            |
| 30  | SA    | 2656  | 0        | 2833     | 9       | 0            |
| 31  | SC    | 1627  | 0        | 1751     | 17      | 0            |
| 32  | SD    | 1985  | 0        | 2128     | 6       | 0            |
| 33  | SE    | 1498  | 0        | 1601     | 10      | 0            |
| 34  | SH    | 1267  | 0        | 1291     | 2       | 0            |
| 35  | SI    | 1661  | 0        | 1752     | 11      | 0            |
| 36  | SJ    | 609   | 0        | 600      | 2       | 0            |
| 37  | SK    | 1721  | 0        | 1695     | 28      | 0            |
| 38  | SL    | 1960  | 0        | 2052     | 8       | 0            |
| 39  | SM    | 3452  | 0        | 3376     | 3       | 0            |
| 40  | SN    | 1308  | 0        | 1286     | 10      | 0            |
| 41  | SO    | 2544  | 0        | 2631     | 18      | 0            |
| 42  | SR    | 642   | 0        | 630      | 12      | 0            |
| 43  | SS    | 1955  | 0        | 1871     | 13      | 0            |
| 44  | ST    | 263   | 0        | 260      | 1       | 0            |
| 45  | SV    | 1171  | 0        | 1232     | 19      | 0            |
| 46  | SW    | 3560  | 0        | 3641     | 14      | 0            |
| 47  | SZ    | 1338  | 0        | 1352     | 8       | 0            |
| 48  | L1    | 3     | 0        | 0        | 0       | 0            |
| 48  | L2    | 1     | 0        | 0        | 0       | 0            |
| 48  | L3    | 46    | 0        | 0        | 0       | 0            |
| 48  | L9    | 1     | 0        | 0        | 0       | 0            |
| 48  | LQ    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 48  | LT    | 1      | 0        | 0        | 0       | 0            |
| 48  | SA    | 1      | 0        | 0        | 0       | 0            |
| 49  | LW    | 1      | 0        | 0        | 0       | 0            |
| 49  | SV    | 1      | 0        | 0        | 0       | 0            |
| 50  | NM    | 8      | 0        | 0        | 0       | 0            |
| All | All   | 101451 | 0        | 85069    | 397     | 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 2.

All (397) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:LA:42:ARG:NH1    | 24:NG:195:MET:SD   | 2.49                     | 0.85              |
| 3:L3:4598:C:O2     | 3:L3:4612:C:N4     | 2.13                     | 0.82              |
| 30:SA:295:SER:OG   | 30:SA:297:GLU:OE1  | 1.96                     | 0.82              |
| 30:SA:329:ASN:ND2  | 32:SD:188:GLU:OE1  | 2.12                     | 0.82              |
| 7:L9:16:SER:OG     | 20:LU:48:CYS:SG    | 2.36                     | 0.81              |
| 3:L3:271:C:OP1     | 46:SW:297:LYS:NZ   | 2.13                     | 0.81              |
| 42:SR:453:LEU:HD21 | 45:SV:99:ILE:HD11  | 1.64                     | 0.79              |
| 3:L3:2100:A:OP1    | 32:SD:29:LYS:NZ    | 2.15                     | 0.79              |
| 3:L3:2084:C:O2     | 9:LB:45:GLN:NE2    | 2.16                     | 0.78              |
| 3:L3:470:A:N6      | 3:L3:685:C:O2      | 2.16                     | 0.77              |
| 3:L3:4940:C:OP1    | 31:SC:156:ARG:NH1  | 2.17                     | 0.77              |
| 37:SK:95:ARG:NH1   | 45:SV:77:GLU:OE2   | 2.18                     | 0.75              |
| 3:L3:306:A:OP1     | 20:LU:53:TYR:OH    | 2.04                     | 0.75              |
| 3:L3:4946:U:HO2'   | 19:LT:2:SER:N      | 1.84                     | 0.75              |
| 3:L3:116:G:O2'     | 43:SS:239:ARG:NH1  | 2.19                     | 0.74              |
| 16:LN:304:SER:OG   | 16:LN:310:SER:O    | 2.06                     | 0.74              |
| 3:L3:2836:A:O2'    | 3:L3:2837:U:O5'    | 2.04                     | 0.73              |
| 37:SK:119:PRO:O    | 37:SK:139:ARG:NH2  | 2.21                     | 0.73              |
| 23:NE:228:LEU:HD21 | 23:NE:271:THR:HG21 | 1.69                     | 0.73              |
| 16:LN:309:LEU:HD11 | 42:SR:430:PRO:HB3  | 1.69                     | 0.73              |
| 46:SW:241:ILE:HD11 | 46:SW:254:VAL:HG23 | 1.70                     | 0.73              |
| 3:L3:62:A:N3       | 3:L3:77:U:O2'      | 2.22                     | 0.73              |
| 3:L3:151:G:OP2     | 7:L9:4:TYR:OH      | 2.06                     | 0.73              |
| 26:NN:36:ARG:NH1   | 26:NN:68:ASN:O     | 2.22                     | 0.73              |
| 3:L3:126:C:OP1     | 18:LS:78:TYR:OH    | 2.07                     | 0.72              |
| 3:L3:4598:C:OP2    | 3:L3:4599:A:O2'    | 2.06                     | 0.72              |
| 3:L3:3856:A:OP1    | 8:LA:82:ARG:NE     | 2.23                     | 0.71              |
| 3:L3:5058:A:OP1    | 26:NN:127:ARG:NH1  | 2.23                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:NG:159:GLU:OE1  | 26:NN:278:ARG:NH2  | 2.24                     | 0.71              |
| 1:L1:94:G:O2'      | 21:LW:82:THR:O     | 2.04                     | 0.70              |
| 40:SN:67:VAL:HG22  | 40:SN:126:LEU:HD13 | 1.72                     | 0.70              |
| 37:SK:201:ASP:OD1  | 37:SK:202:TRP:N    | 2.26                     | 0.69              |
| 23:NE:275:TYR:HB2  | 23:NE:282:ILE:HD11 | 1.75                     | 0.69              |
| 3:L3:2361:G:O2'    | 3:L3:3859:G:O6     | 2.09                     | 0.69              |
| 3:L3:238:C:OP2     | 14:LI:45:ARG:NH2   | 2.26                     | 0.68              |
| 3:L3:4763:U:C6     | 10:LC:174:THR:HA   | 2.27                     | 0.68              |
| 3:L3:2054:U:O2'    | 5:L7:133:ARG:NH1   | 2.26                     | 0.68              |
| 16:LN:165:HIS:HB3  | 16:LN:180:LEU:HD23 | 1.75                     | 0.68              |
| 2:L2:10:U:OP2      | 38:SL:163:ARG:NH2  | 2.26                     | 0.68              |
| 3:L3:423:G:OP1     | 8:LA:62:ARG:NH1    | 2.26                     | 0.68              |
| 3:L3:1508:A:OP1    | 30:SA:110:ARG:NH2  | 2.27                     | 0.68              |
| 3:L3:374:G:OP2     | 21:LW:56:ARG:NH1   | 2.26                     | 0.67              |
| 3:L3:4759:C:O2     | 5:L7:165:LYS:NZ    | 2.15                     | 0.67              |
| 3:L3:1922:G:OP1    | 10:LC:160:ARG:NH1  | 2.28                     | 0.67              |
| 3:L3:182:G:N7      | 41:SO:339:ARG:NH1  | 2.43                     | 0.67              |
| 7:L9:96:ARG:NH2    | 7:L9:104:GLU:OE1   | 2.28                     | 0.67              |
| 16:LN:219:VAL:HG11 | 16:LN:337:VAL:HG21 | 1.75                     | 0.67              |
| 31:SC:250:GLN:NE2  | 31:SC:254:ASP:OD1  | 2.28                     | 0.67              |
| 1:L1:63:U:OP1      | 18:LS:48:ARG:NH2   | 2.28                     | 0.67              |
| 26:NN:101:ARG:NH1  | 26:NN:102:LEU:O    | 2.28                     | 0.67              |
| 35:SI:143:VAL:O    | 35:SI:147:VAL:HG12 | 1.94                     | 0.66              |
| 3:L3:1833:G:N2     | 3:L3:1835:G:O4'    | 2.28                     | 0.66              |
| 16:LN:138:GLN:O    | 16:LN:143:LYS:NZ   | 2.29                     | 0.66              |
| 3:L3:308:G:OP2     | 3:L3:308:G:N2      | 2.21                     | 0.66              |
| 37:SK:107:VAL:HG11 | 37:SK:121:LEU:HD21 | 1.77                     | 0.65              |
| 9:LB:115:ARG:NH1   | 41:SO:296:THR:OG1  | 2.29                     | 0.65              |
| 3:L3:1369:C:OP2    | 3:L3:1370:G:O2'    | 2.09                     | 0.65              |
| 3:L3:4760:G:OP1    | 5:L7:117:ARG:NH2   | 2.29                     | 0.65              |
| 18:LS:23:ASP:OD1   | 18:LS:24:LEU:N     | 2.30                     | 0.65              |
| 20:LU:74:LYS:HD3   | 41:SO:109:MET:HE1  | 1.79                     | 0.65              |
| 26:NN:245:ASP:OD1  | 26:NN:271:ARG:NH2  | 2.30                     | 0.65              |
| 3:L3:369:G:N2      | 3:L3:372:A:OP2     | 2.21                     | 0.64              |
| 46:SW:327:LEU:HD22 | 46:SW:354:LEU:HD22 | 1.79                     | 0.64              |
| 35:SI:101:ARG:NH1  | 35:SI:122:LYS:O    | 2.31                     | 0.64              |
| 9:LB:35:LEU:HD21   | 30:SA:298:ILE:HD11 | 1.80                     | 0.64              |
| 3:L3:2062:C:OP1    | 10:LC:120:ARG:NH1  | 2.31                     | 0.64              |
| 37:SK:112:ASP:OD2  | 37:SK:156:ASN:ND2  | 2.30                     | 0.63              |
| 3:L3:402:A:O2'     | 29:NS:103:LYS:O    | 2.16                     | 0.63              |
| 3:L3:4583:C:O4'    | 16:LN:97:ARG:NH1   | 2.31                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 46:SW:182:LEU:HD22 | 46:SW:185:LEU:HD12  | 1.79                     | 0.63              |
| 14:LI:32:SER:OG    | 14:LI:101:PRO:O     | 2.12                     | 0.63              |
| 45:SV:110:ASN:OD1  | 45:SV:111:ARG:N     | 2.31                     | 0.63              |
| 3:L3:184:U:O2'     | 3:L3:189:G:OP2      | 2.16                     | 0.63              |
| 3:L3:404:U:O3'     | 14:LI:87:ARG:NH2    | 2.32                     | 0.62              |
| 3:L3:1447:C:OP2    | 27:NO:323:ARG:NH2   | 2.32                     | 0.62              |
| 11:LE:154:ILE:HD12 | 11:LE:155:PRO:HD2   | 1.81                     | 0.62              |
| 12:LG:30:ASP:OD1   | 12:LG:31:ASN:N      | 2.31                     | 0.62              |
| 4:L6:62:PRO:O      | 4:L6:63:THR:OG1     | 2.15                     | 0.62              |
| 4:L6:100:PRO:O     | 20:LU:25[B]:ARG:NH2 | 2.33                     | 0.61              |
| 37:SK:1:MET:N      | 37:SK:219:GLU:OE1   | 2.33                     | 0.61              |
| 38:SL:57:LEU:HD11  | 46:SW:527:LEU:HD22  | 1.80                     | 0.61              |
| 3:L3:230:G:OP1     | 14:LI:15:ARG:NH1    | 2.32                     | 0.61              |
| 3:L3:471:A:N7      | 3:L3:684:G:N2       | 2.49                     | 0.61              |
| 4:L6:50:PRO:HG3    | 18:LS:121:VAL:HG12  | 1.82                     | 0.61              |
| 3:L3:222:C:OP2     | 30:SA:165:LYS:NZ    | 2.26                     | 0.61              |
| 3:L3:4971:A:OP1    | 16:LN:246:ARG:NH1   | 2.33                     | 0.61              |
| 23:NE:202:LYS:O    | 26:NN:166:SER:OG    | 2.16                     | 0.60              |
| 37:SK:177:LEU:HD22 | 37:SK:181:LEU:HD21  | 1.83                     | 0.60              |
| 16:LN:219:VAL:HG11 | 16:LN:337:VAL:CG2   | 2.32                     | 0.60              |
| 46:SW:314:ASP:OD1  | 46:SW:318:ASN:ND2   | 2.35                     | 0.60              |
| 3:L3:4763:U:O2'    | 10:LC:156:HIS:ND1   | 2.32                     | 0.60              |
| 25:NM:13:ASN:OD1   | 25:NM:14:LYS:N      | 2.35                     | 0.59              |
| 1:L1:157:U:OP2     | 35:SI:57:ARG:NH1    | 2.35                     | 0.59              |
| 8:LA:158:PRO:O     | 29:NS:276:ARG:NH2   | 2.36                     | 0.59              |
| 16:LN:257:TRP:N    | 26:NN:72:ASP:OD2    | 2.34                     | 0.59              |
| 37:SK:142:VAL:HG23 | 37:SK:148:VAL:HG12  | 1.84                     | 0.59              |
| 3:L3:2836:A:HO2'   | 3:L3:2837:U:P       | 2.26                     | 0.59              |
| 40:SN:148:GLN:OE1  | 40:SN:151:ARG:NH2   | 2.35                     | 0.59              |
| 3:L3:740:G:N2      | 3:L3:924:C:O2       | 2.35                     | 0.59              |
| 12:LG:90:ARG:NH2   | 12:LG:140:ALA:OXT   | 2.33                     | 0.59              |
| 31:SC:281:ILE:CG2  | 31:SC:286:LEU:HD11  | 2.33                     | 0.59              |
| 37:SK:177:LEU:CD2  | 37:SK:181:LEU:HD21  | 2.33                     | 0.58              |
| 18:LS:27:GLU:O     | 18:LS:31:LEU:HD23   | 2.02                     | 0.58              |
| 21:LW:17:THR:OG1   | 21:LW:29:LEU:HD21   | 2.03                     | 0.58              |
| 1:L1:94:G:H21      | 21:LW:82:THR:HG21   | 1.67                     | 0.58              |
| 26:NN:249:ASN:OD1  | 26:NN:250:ILE:N     | 2.36                     | 0.58              |
| 26:NN:250:ILE:HG23 | 26:NN:250:ILE:O     | 2.04                     | 0.57              |
| 8:LA:94:MET:HG2    | 8:LA:148:MET:HE3    | 1.85                     | 0.57              |
| 3:L3:452:A:N3      | 31:SC:226:ARG:NH2   | 2.53                     | 0.57              |
| 3:L3:2318:G:N2     | 3:L3:2321:G:OP2     | 2.32                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L3:4724:A:O2'    | 16:LN:104:THR:HG22 | 2.04                     | 0.57              |
| 6:L8:62:LEU:HD21   | 6:L8:82:ILE:HD11   | 1.87                     | 0.57              |
| 3:L3:119:G:OP2     | 43:SS:249:SER:OG   | 2.05                     | 0.57              |
| 16:LN:309:LEU:HD11 | 42:SR:430:PRO:CB   | 2.35                     | 0.57              |
| 29:NS:334:VAL:O    | 29:NS:340:MET:HE1  | 2.05                     | 0.57              |
| 23:NE:275:TYR:CB   | 23:NE:282:ILE:HD11 | 2.34                     | 0.56              |
| 18:LS:12:LYS:NZ    | 18:LS:20:GLN:OE1   | 2.39                     | 0.56              |
| 14:LI:26:ARG:NH1   | 14:LI:75:ARG:O     | 2.39                     | 0.56              |
| 32:SD:232:ASP:OD1  | 32:SD:236:ARG:NH2  | 2.39                     | 0.56              |
| 3:L3:4972:U:OP1    | 16:LN:249:ARG:NH1  | 2.36                     | 0.56              |
| 16:LN:86:VAL:HG13  | 16:LN:162:VAL:HG13 | 1.88                     | 0.56              |
| 39:SM:117:ASP:OD1  | 39:SM:118:HIS:N    | 2.39                     | 0.56              |
| 6:L8:15:VAL:HG22   | 6:L8:50:MET:HE1    | 1.88                     | 0.55              |
| 40:SN:111:GLN:OE1  | 41:SO:209:THR:HG22 | 2.07                     | 0.55              |
| 1:L1:3:A:O2'       | 8:LA:61:ARG:NH1    | 2.39                     | 0.55              |
| 5:L7:141:LEU:O     | 5:L7:145:VAL:HG23  | 2.07                     | 0.55              |
| 30:SA:204:ARG:NH1  | 30:SA:205:ARG:O    | 2.38                     | 0.55              |
| 30:SA:211:TYR:OH   | 30:SA:218:ILE:HD11 | 2.06                     | 0.55              |
| 34:SH:54:ASN:OD1   | 34:SH:55:LEU:HD12  | 2.06                     | 0.55              |
| 12:LG:97:TYR:OH    | 45:SV:37:HIS:NE2   | 2.34                     | 0.55              |
| 42:SR:453:LEU:HD21 | 45:SV:99:ILE:CD1   | 2.36                     | 0.55              |
| 3:L3:265:C:N4      | 47:SZ:154:VAL:HG21 | 2.22                     | 0.54              |
| 46:SW:285:ILE:HD11 | 46:SW:298:LEU:HD21 | 1.89                     | 0.54              |
| 8:LA:53:LEU:O      | 8:LA:55:LYS:NZ     | 2.40                     | 0.54              |
| 37:SK:107:VAL:CG1  | 37:SK:121:LEU:HD21 | 2.37                     | 0.54              |
| 40:SN:146:GLN:NE2  | 41:SO:149:LEU:O    | 2.41                     | 0.54              |
| 37:SK:72:VAL:HB    | 37:SK:76:THR:HG21  | 1.90                     | 0.54              |
| 47:SZ:111:LEU:HD11 | 47:SZ:115:LEU:HD23 | 1.90                     | 0.53              |
| 3:L3:5010:U:O2'    | 45:SV:122:GLN:OE1  | 2.27                     | 0.53              |
| 5:L7:185:VAL:HG12  | 5:L7:185:VAL:O     | 2.09                     | 0.53              |
| 16:LN:213:GLN:NE2  | 16:LN:285:TYR:O    | 2.41                     | 0.53              |
| 46:SW:504:ASP:OD1  | 46:SW:505:ASP:N    | 2.42                     | 0.53              |
| 23:NE:273:LEU:HD11 | 26:NN:296:MET:SD   | 2.49                     | 0.53              |
| 25:NM:130:ARG:NH2  | 29:NS:177:GLY:O    | 2.42                     | 0.53              |
| 31:SC:281:ILE:HG21 | 31:SC:286:LEU:HD11 | 1.91                     | 0.53              |
| 37:SK:99:GLU:OE1   | 37:SK:125:THR:OG1  | 2.23                     | 0.53              |
| 3:L3:76:A:N7       | 4:L6:74:ARG:NH2    | 2.55                     | 0.53              |
| 3:L3:4875:G:H2'    | 10:LC:169:THR:HG22 | 1.90                     | 0.53              |
| 24:NG:171:VAL:HG13 | 26:NN:251:THR:OG1  | 2.09                     | 0.53              |
| 28:NQ:192:LEU:HD21 | 28:NQ:256:LEU:HD13 | 1.90                     | 0.53              |
| 16:LN:93:VAL:HG12  | 16:LN:157:CYS:HA   | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:NB:346:ALA:O    | 22:NB:350:VAL:HG23 | 2.09                     | 0.52              |
| 40:SN:101:ASP:OD1  | 40:SN:102:PHE:N    | 2.42                     | 0.52              |
| 3:L3:4589:A:N1     | 3:L3:4621:C:O2'    | 2.34                     | 0.52              |
| 2:L2:1:G:O2'       | 2:L2:2:C:OP1       | 2.21                     | 0.52              |
| 12:LG:94:VAL:HG11  | 45:SV:20:MET:HE3   | 1.92                     | 0.52              |
| 23:NE:228:LEU:HD21 | 23:NE:271:THR:CG2  | 2.39                     | 0.52              |
| 38:SL:67:MET:HE3   | 38:SL:212:SER:O    | 2.09                     | 0.52              |
| 1:L1:49:G:H1'      | 18:LS:44:LEU:HD13  | 1.92                     | 0.52              |
| 33:SE:164:ILE:O    | 33:SE:168:VAL:HG13 | 2.09                     | 0.52              |
| 37:SK:155:SER:OG   | 37:SK:156:ASN:N    | 2.41                     | 0.52              |
| 33:SE:218:LEU:O    | 33:SE:222:ILE:HD12 | 2.10                     | 0.52              |
| 23:NE:258:GLU:OE1  | 23:NE:258:GLU:N    | 2.43                     | 0.52              |
| 26:NN:118:VAL:HG23 | 26:NN:275:ILE:O    | 2.09                     | 0.52              |
| 3:L3:346:G:OP1     | 14:LI:8:THR:HG23   | 2.10                     | 0.52              |
| 3:L3:1311:G:OP2    | 40:SN:258:LYS:NZ   | 2.43                     | 0.52              |
| 43:SS:296:HIS:NE2  | 43:SS:298:MET:O    | 2.43                     | 0.52              |
| 7:L9:26:ARG:NH2    | 33:SE:165:GLU:OE1  | 2.42                     | 0.51              |
| 23:NE:276:LYS:HG3  | 23:NE:282:ILE:HD12 | 1.93                     | 0.51              |
| 35:SI:192:ILE:HD12 | 43:SS:351:ARG:NH1  | 2.25                     | 0.51              |
| 3:L3:170:C:O2      | 47:SZ:109:ASN:ND2  | 2.39                     | 0.51              |
| 14:LI:34:LEU:HD22  | 14:LI:44:VAL:HG13  | 1.92                     | 0.51              |
| 35:SI:192:ILE:HD11 | 39:SM:380:ARG:HE   | 1.75                     | 0.51              |
| 45:SV:104:GLN:O    | 45:SV:108:ILE:HG22 | 2.10                     | 0.51              |
| 28:NQ:206:GLN:OE1  | 28:NQ:208:ARG:NH2  | 2.43                     | 0.51              |
| 1:L1:90:C:O2'      | 14:LI:24:HIS:ND1   | 2.35                     | 0.51              |
| 37:SK:28:ILE:HG23  | 37:SK:28:ILE:O     | 2.10                     | 0.51              |
| 3:L3:4583:C:O2'    | 3:L3:4584:A:OP2    | 2.25                     | 0.51              |
| 31:SC:47:ASN:ND2   | 31:SC:50:LEU:HD22  | 2.25                     | 0.51              |
| 3:L3:2269:C:O2'    | 25:NM:13:ASN:ND2   | 2.45                     | 0.50              |
| 25:NM:23:THR:OG1   | 25:NM:26:GLN:O     | 2.27                     | 0.50              |
| 42:SR:453:LEU:HD22 | 45:SV:71:PHE:CE2   | 2.46                     | 0.50              |
| 3:L3:1501:C:O2'    | 9:LB:68:ARG:NH1    | 2.44                     | 0.50              |
| 31:SC:203:ILE:O    | 31:SC:203:ILE:HG22 | 2.12                     | 0.50              |
| 3:L3:193:G:OP2     | 47:SZ:21:ARG:NH1   | 2.44                     | 0.50              |
| 10:LC:86:SER:OG    | 10:LC:88:SER:O     | 2.30                     | 0.50              |
| 3:L3:734:G:H22     | 3:L3:929:A:H2      | 1.57                     | 0.50              |
| 12:LG:20:LEU:HD21  | 12:LG:101:ASN:CG   | 2.36                     | 0.50              |
| 46:SW:316:MET:HE1  | 46:SW:350:ILE:HG23 | 1.94                     | 0.50              |
| 3:L3:1364:U:OP2    | 4:L6:36:ARG:NH1    | 2.44                     | 0.50              |
| 1:L1:25:G:N3       | 3:L3:356:G:O2'     | 2.44                     | 0.50              |
| 33:SE:207:VAL:HG21 | 33:SE:215:LEU:HD22 | 1.92                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:SO:324:GLU:OE1  | 41:SO:324:GLU:N    | 2.45                     | 0.50              |
| 8:LA:10:ASN:OD1    | 8:LA:12:THR:OG1    | 2.30                     | 0.50              |
| 3:L3:4662:C:OP2    | 3:L3:4663:G:N2     | 2.46                     | 0.49              |
| 10:LC:38:VAL:HG22  | 32:SD:237:GLU:OE1  | 2.12                     | 0.49              |
| 37:SK:161:VAL:HG22 | 37:SK:162:HIS:H    | 1.76                     | 0.49              |
| 46:SW:336:ASP:OD1  | 46:SW:337:ARG:N    | 2.43                     | 0.49              |
| 3:L3:5005:G:N2     | 3:L3:5041:G:O2'    | 2.45                     | 0.49              |
| 41:SO:347:MET:HE2  | 41:SO:347:MET:HA   | 1.95                     | 0.49              |
| 25:NM:167:LEU:HD22 | 29:NS:300:GLU:O    | 2.12                     | 0.49              |
| 3:L3:4993:G:H22    | 3:L3:5058:A:H2     | 1.60                     | 0.49              |
| 9:LB:39:THR:HG22   | 9:LB:41:SER:H      | 1.78                     | 0.49              |
| 16:LN:139:ASP:OD1  | 16:LN:140:GLU:N    | 2.46                     | 0.49              |
| 35:SI:196:ASP:OD2  | 39:SM:380:ARG:NH2  | 2.46                     | 0.49              |
| 3:L3:4728:U:OP2    | 16:LN:132:LYS:NZ   | 2.38                     | 0.49              |
| 6:L8:131:GLN:O     | 6:L8:135:LEU:HD23  | 2.13                     | 0.48              |
| 42:SR:432:ILE:HD13 | 45:SV:1:MET:HE3    | 1.95                     | 0.48              |
| 3:L3:4940:C:OP2    | 31:SC:219:LYS:NZ   | 2.42                     | 0.48              |
| 31:SC:201:ILE:HD11 | 31:SC:267:LEU:HD21 | 1.95                     | 0.48              |
| 37:SK:103:ALA:O    | 37:SK:107:VAL:HG23 | 2.13                     | 0.48              |
| 3:L3:4880:C:OP1    | 6:L8:124:LYS:NZ    | 2.28                     | 0.48              |
| 3:L3:1881:C:O2'    | 3:L3:1882:U:O5'    | 2.27                     | 0.48              |
| 29:NS:155:ARG:NH1  | 29:NS:231:GLU:OE2  | 2.41                     | 0.48              |
| 43:SS:265:MET:HE2  | 43:SS:265:MET:N    | 2.28                     | 0.48              |
| 26:NN:144:ASN:ND2  | 26:NN:184:ASP:OD1  | 2.47                     | 0.48              |
| 37:SK:166:SER:OG   | 37:SK:168:GLU:OE2  | 2.31                     | 0.48              |
| 37:SK:2:ALA:HB3    | 37:SK:215:LEU:HD11 | 1.96                     | 0.48              |
| 41:SO:278:ARG:NH1  | 41:SO:281:GLN:OE1  | 2.46                     | 0.48              |
| 9:LB:10:ASP:OD2    | 9:LB:11:ARG:N      | 2.47                     | 0.48              |
| 16:LN:370:THR:O    | 16:LN:370:THR:HG22 | 2.14                     | 0.47              |
| 35:SI:251:ILE:O    | 35:SI:255:ASN:N    | 2.47                     | 0.47              |
| 3:L3:5052:C:H2'    | 3:L3:5053:U:O4'    | 2.14                     | 0.47              |
| 10:LC:84:TYR:CD1   | 10:LC:113:MET:HE1  | 2.49                     | 0.47              |
| 12:LG:20:LEU:HD21  | 12:LG:101:ASN:ND2  | 2.29                     | 0.47              |
| 16:LN:29:VAL:HG23  | 16:LN:346:THR:HG21 | 1.96                     | 0.47              |
| 28:NQ:65:ARG:NH1   | 28:NQ:85:GLY:O     | 2.46                     | 0.47              |
| 28:NQ:64:ASP:O     | 28:NQ:66:THR:N     | 2.45                     | 0.47              |
| 28:NQ:92:GLY:HA3   | 28:NQ:136:MET:HE3  | 1.96                     | 0.47              |
| 37:SK:121:LEU:O    | 37:SK:139:ARG:NH2  | 2.48                     | 0.47              |
| 33:SE:105:GLU:OE1  | 33:SE:113:ARG:NH1  | 2.48                     | 0.47              |
| 21:LW:17:THR:HG22  | 21:LW:18:LEU:N     | 2.30                     | 0.47              |
| 37:SK:173:LEU:O    | 37:SK:177:LEU:N    | 2.41                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:NM:132:ARG:NH2  | 29:NS:199:ASN:OD1  | 2.48                     | 0.47              |
| 42:SR:442:ILE:CG2  | 45:SV:79:ILE:HD11  | 2.44                     | 0.47              |
| 14:LI:52:ASP:O     | 14:LI:52:ASP:OD2   | 2.33                     | 0.47              |
| 16:LN:367:PHE:HB2  | 45:SV:1:MET:HE1    | 1.97                     | 0.47              |
| 29:NS:66:MET:SD    | 29:NS:69:ARG:NH2   | 2.88                     | 0.47              |
| 40:SN:73:THR:HG22  | 41:SO:168:PHE:HB2  | 1.97                     | 0.47              |
| 47:SZ:107:LYS:HE3  | 47:SZ:107:LYS:HA   | 1.95                     | 0.47              |
| 2:L2:99:G:N2       | 34:SH:129:GLU:OE1  | 2.48                     | 0.47              |
| 41:SO:223:ILE:HD11 | 41:SO:230:VAL:HG23 | 1.96                     | 0.46              |
| 2:L2:13:C:OP1      | 35:SI:86:HIS:NE2   | 2.35                     | 0.46              |
| 16:LN:29:VAL:HG13  | 16:LN:348:ARG:HD3  | 1.96                     | 0.46              |
| 2:L2:5:A:N6        | 2:L2:95:A:O2'      | 2.49                     | 0.46              |
| 23:NE:228:LEU:HD23 | 23:NE:228:LEU:H    | 1.81                     | 0.46              |
| 23:NE:341:LEU:HD11 | 23:NE:351:LEU:HD13 | 1.97                     | 0.46              |
| 25:NM:18:SER:OG    | 30:SA:139:SER:O    | 2.22                     | 0.46              |
| 33:SE:99:ALA:HB1   | 33:SE:136:LEU:HD11 | 1.97                     | 0.46              |
| 37:SK:53:ILE:HG23  | 37:SK:76:THR:HG22  | 1.96                     | 0.46              |
| 41:SO:63:LEU:HD11  | 41:SO:91:ASP:HB2   | 1.98                     | 0.46              |
| 16:LN:71:GLU:OE2   | 16:LN:366:LYS:NZ   | 2.27                     | 0.46              |
| 23:NE:229:THR:OG1  | 23:NE:242:ARG:NH2  | 2.48                     | 0.46              |
| 38:SL:67:MET:HE3   | 38:SL:67:MET:HA    | 1.97                     | 0.46              |
| 3:L3:1925:G:OP1    | 6:L8:33:GLN:NE2    | 2.49                     | 0.46              |
| 3:L3:4626:A:OP2    | 16:LN:224:LYS:NZ   | 2.38                     | 0.46              |
| 17:LQ:84:GLU:OE1   | 25:NM:30:ARG:NH2   | 2.45                     | 0.46              |
| 21:LW:36:LYS:O     | 21:LW:45:ARG:NH1   | 2.46                     | 0.46              |
| 19:LT:37:ASP:OD1   | 19:LT:38:GLU:N     | 2.49                     | 0.46              |
| 27:NO:13:LEU:HD23  | 27:NO:16:ARG:HH21  | 1.81                     | 0.46              |
| 5:L7:178:ARG:NH1   | 6:L8:123:ILE:HG21  | 2.30                     | 0.46              |
| 43:SS:150:VAL:HG23 | 43:SS:150:VAL:O    | 2.16                     | 0.46              |
| 10:LC:38:VAL:HG13  | 32:SD:237:GLU:OE1  | 2.15                     | 0.46              |
| 20:LU:77:VAL:HG11  | 20:LU:82:ARG:HB3   | 1.96                     | 0.46              |
| 21:LW:53:ALA:O     | 21:LW:57:ASN:ND2   | 2.49                     | 0.45              |
| 27:NO:300:TYR:CE2  | 31:SC:50:LEU:HD21  | 2.51                     | 0.45              |
| 3:L3:1928:C:N4     | 3:L3:2054:U:O2     | 2.49                     | 0.45              |
| 19:LT:108:SER:OG   | 31:SC:192:LYS:O    | 2.30                     | 0.45              |
| 36:SJ:709:GLU:O    | 36:SJ:713:ARG:N    | 2.37                     | 0.45              |
| 41:SO:91:ASP:OD1   | 41:SO:92:THR:N     | 2.48                     | 0.45              |
| 3:L3:4632:U:H3'    | 3:L3:4633:G:H5''   | 1.98                     | 0.45              |
| 16:LN:391:PRO:HD2  | 45:SV:108:ILE:HG21 | 1.97                     | 0.45              |
| 40:SN:61:LYS:NZ    | 40:SN:63:ASP:OD1   | 2.48                     | 0.45              |
| 3:L3:2303:C:OP1    | 17:LQ:107:ASN:ND2  | 2.45                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:SK:100:ARG:NH1  | 45:SV:26:CYS:SG    | 2.90                     | 0.45              |
| 42:SR:442:ILE:HD13 | 45:SV:86:TRP:CZ2   | 2.52                     | 0.45              |
| 12:LG:32:THR:HG21  | 12:LG:105:ILE:HD12 | 1.98                     | 0.45              |
| 37:SK:162:HIS:NE2  | 37:SK:191:GLU:OE2  | 2.49                     | 0.45              |
| 7:L9:97:SER:O      | 7:L9:100:SER:OG    | 2.33                     | 0.45              |
| 16:LN:29:VAL:CG2   | 16:LN:346:THR:HG21 | 2.47                     | 0.45              |
| 16:LN:93:VAL:HG13  | 16:LN:102:PHE:HB2  | 1.99                     | 0.45              |
| 38:SL:203:LEU:HD23 | 38:SL:214:ILE:HD13 | 1.98                     | 0.45              |
| 1:L1:149:G:H21     | 33:SE:64:GLN:HE22  | 1.65                     | 0.45              |
| 3:L3:4883:C:N4     | 31:SC:181:LEU:O    | 2.48                     | 0.45              |
| 21:LW:60:GLY:O     | 47:SZ:10:ARG:NH1   | 2.50                     | 0.45              |
| 23:NE:273:LEU:HD21 | 26:NN:288:GLU:HG2  | 1.97                     | 0.45              |
| 6:L8:40:GLY:O      | 6:L8:43:THR:N      | 2.49                     | 0.45              |
| 25:NM:41:ARG:NH1   | 25:NM:48:ASN:OD1   | 2.50                     | 0.45              |
| 43:SS:368:LEU:HD22 | 43:SS:372:LEU:HD12 | 1.99                     | 0.45              |
| 17:LQ:84:GLU:O     | 17:LQ:87:VAL:HG22  | 2.17                     | 0.44              |
| 11:LE:154:ILE:HD12 | 11:LE:155:PRO:CD   | 2.47                     | 0.44              |
| 18:LS:121:VAL:HG13 | 47:SZ:59:ALA:HB3   | 1.99                     | 0.44              |
| 29:NS:176:ARG:NH2  | 31:SC:231:GLU:O    | 2.43                     | 0.44              |
| 31:SC:235:THR:O    | 31:SC:235:THR:HG23 | 2.18                     | 0.44              |
| 3:L3:442:G:OP1     | 19:LT:68:ARG:NH1   | 2.42                     | 0.44              |
| 16:LN:311:ASP:OD1  | 16:LN:311:ASP:O    | 2.35                     | 0.44              |
| 23:NE:273:LEU:HD22 | 26:NN:106:PRO:HG3  | 1.99                     | 0.44              |
| 3:L3:67:C:OP2      | 3:L3:312:G:N2      | 2.45                     | 0.44              |
| 3:L3:4761:G:O6     | 10:LC:170:LYS:NZ   | 2.50                     | 0.44              |
| 19:LT:33:VAL:HG23  | 19:LT:38:GLU:HB2   | 1.99                     | 0.44              |
| 3:L3:4626:A:OP1    | 16:LN:341:LYS:NZ   | 2.48                     | 0.44              |
| 42:SR:418:ASP:C    | 42:SR:419:LEU:HD12 | 2.43                     | 0.44              |
| 1:L1:28:C:O2'      | 3:L3:1371:A:N1     | 2.49                     | 0.43              |
| 33:SE:158:ALA:HB2  | 33:SE:190:LEU:HD12 | 2.00                     | 0.43              |
| 27:NO:212:ASN:O    | 27:NO:216:GLY:N    | 2.40                     | 0.43              |
| 42:SR:453:LEU:HD22 | 45:SV:71:PHE:HE2   | 1.82                     | 0.43              |
| 26:NN:108:LEU:HD22 | 26:NN:286:VAL:HG22 | 1.99                     | 0.43              |
| 31:SC:214:ASP:OD1  | 31:SC:215:ALA:N    | 2.51                     | 0.43              |
| 36:SJ:664:ASP:OD1  | 36:SJ:667:GLY:N    | 2.48                     | 0.43              |
| 2:L2:93:C:O2'      | 2:L2:94:U:O5'      | 2.36                     | 0.43              |
| 3:L3:1807:C:O2'    | 11:LE:113:ASP:OD2  | 2.31                     | 0.43              |
| 3:L3:4763:U:H5     | 5:L7:126:VAL:HG21  | 1.82                     | 0.43              |
| 16:LN:293:ILE:N    | 16:LN:293:ILE:HD12 | 2.34                     | 0.43              |
| 37:SK:116:LEU:HD21 | 37:SK:176:LEU:HD22 | 2.00                     | 0.43              |
| 3:L3:1854:G:H1'    | 3:L3:1855:G:C8     | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:SR:432:ILE:CD1  | 45:SV:1:MET:HE3    | 2.49                     | 0.43              |
| 1:L1:83:C:H42      | 14:LI:50:ARG:NE    | 2.16                     | 0.43              |
| 27:NO:13:LEU:HD23  | 27:NO:16:ARG:NH2   | 2.34                     | 0.43              |
| 1:L1:60:G:O6       | 1:L1:96:C:O2'      | 2.31                     | 0.42              |
| 3:L3:119:G:N3      | 3:L3:119:G:H2'     | 2.34                     | 0.42              |
| 47:SZ:150:SER:O    | 47:SZ:154:VAL:HG23 | 2.18                     | 0.42              |
| 1:L1:69:U:H2'      | 1:L1:70:G:O4'      | 2.19                     | 0.42              |
| 5:L7:54:TYR:HD1    | 5:L7:145:VAL:HG21  | 1.84                     | 0.42              |
| 17:LQ:118:LEU:HD12 | 25:NM:119:TYR:HE1  | 1.84                     | 0.42              |
| 3:L3:116:G:H2'     | 3:L3:117:C:C6      | 2.54                     | 0.42              |
| 3:L3:1887:G:H3'    | 3:L3:1888:A:C5'    | 2.48                     | 0.42              |
| 3:L3:4761:G:OP1    | 5:L7:37:ARG:NH2    | 2.52                     | 0.42              |
| 37:SK:107:VAL:HG12 | 37:SK:108:THR:HG23 | 2.00                     | 0.42              |
| 3:L3:164:G:O2'     | 46:SW:577:LYS:NZ   | 2.41                     | 0.42              |
| 10:LC:28:TYR:CD2   | 10:LC:54:MET:HE2   | 2.55                     | 0.42              |
| 21:LW:17:THR:HG22  | 21:LW:18:LEU:H     | 1.84                     | 0.42              |
| 41:SO:194:TYR:HA   | 43:SS:154:LEU:HD13 | 2.02                     | 0.42              |
| 2:L2:52:G:N7       | 38:SL:171:ARG:NH1  | 2.68                     | 0.42              |
| 16:LN:67:VAL:O     | 16:LN:67:VAL:HG22  | 2.19                     | 0.42              |
| 46:SW:219:LEU:HD12 | 46:SW:384:LEU:O    | 2.19                     | 0.42              |
| 3:L3:119:G:N2      | 33:SE:133:PRO:O    | 2.41                     | 0.42              |
| 35:SI:135:GLN:OE1  | 35:SI:135:GLN:N    | 2.49                     | 0.42              |
| 1:L1:83:C:N4       | 14:LI:50:ARG:HE    | 2.18                     | 0.42              |
| 3:L3:5039:U:OP1    | 45:SV:111:ARG:NH1  | 2.52                     | 0.42              |
| 12:LG:108:ASN:HD22 | 12:LG:108:ASN:C    | 2.25                     | 0.42              |
| 10:LC:99:ASP:OD1   | 10:LC:108:GLN:NE2  | 2.53                     | 0.42              |
| 29:NS:229:ARG:HE   | 29:NS:309:GLY:HA2  | 1.85                     | 0.42              |
| 40:SN:68:GLU:O     | 41:SO:163:ARG:NH2  | 2.52                     | 0.42              |
| 43:SS:298:MET:SD   | 43:SS:298:MET:N    | 2.93                     | 0.42              |
| 38:SL:149:LEU:HD21 | 38:SL:176:ARG:HG3  | 2.01                     | 0.42              |
| 23:NE:250:LEU:HD23 | 23:NE:264:LEU:HD23 | 2.02                     | 0.42              |
| 35:SI:98:PHE:HB2   | 35:SI:152:PRO:HG3  | 2.02                     | 0.42              |
| 3:L3:1353:G:O6     | 9:LB:85:THR:HG21   | 2.20                     | 0.41              |
| 3:L3:4941:G:OP2    | 31:SC:188:ARG:NH2  | 2.50                     | 0.41              |
| 3:L3:5001:U:OP1    | 16:LN:385:LYS:NZ   | 2.48                     | 0.41              |
| 46:SW:284:LEU:HD12 | 46:SW:306:VAL:O    | 2.20                     | 0.41              |
| 5:L7:20:ALA:HB3    | 5:L7:87:MET:HE1    | 2.02                     | 0.41              |
| 38:SL:122:GLY:O    | 38:SL:124:LYS:NZ   | 2.50                     | 0.41              |
| 2:L2:2:C:C6        | 35:SI:230:ARG:HD3  | 2.56                     | 0.41              |
| 3:L3:159:C:O2      | 4:L6:88:LYS:NZ     | 2.47                     | 0.41              |
| 10:LC:82:LEU:HD12  | 10:LC:82:LEU:C     | 2.46                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:LI:50:ARG:NH1   | 14:LI:51:LYS:O     | 2.46                     | 0.41              |
| 18:LS:41:ALA:HA    | 18:LS:44:LEU:HD12  | 2.01                     | 0.41              |
| 23:NE:228:LEU:CD2  | 23:NE:271:THR:HG21 | 2.44                     | 0.41              |
| 37:SK:96:ARG:O     | 45:SV:76:ASN:ND2   | 2.50                     | 0.41              |
| 42:SR:369:ASP:OD2  | 42:SR:370:ASP:N    | 2.53                     | 0.41              |
| 17:LQ:114:ARG:NH1  | 25:NM:119:TYR:OH   | 2.53                     | 0.41              |
| 31:SC:281:ILE:HG23 | 31:SC:286:LEU:HD21 | 2.02                     | 0.41              |
| 32:SD:147:LEU:O    | 32:SD:151:ASN:ND2  | 2.53                     | 0.41              |
| 37:SK:199:VAL:HG21 | 37:SK:222:PHE:CE2  | 2.55                     | 0.41              |
| 41:SO:175:LEU:HD12 | 41:SO:178:TYR:HD1  | 1.86                     | 0.41              |
| 41:SO:336:ILE:HG23 | 41:SO:340:GLN:HB2  | 2.02                     | 0.41              |
| 46:SW:209:SER:O    | 46:SW:213:LEU:HD13 | 2.21                     | 0.41              |
| 17:LQ:118:LEU:HD12 | 25:NM:119:TYR:CE1  | 2.56                     | 0.41              |
| 33:SE:240:ASN:O    | 33:SE:240:ASN:ND2  | 2.53                     | 0.41              |
| 3:L3:2093:A:O2'    | 3:L3:2094:G:H4'    | 2.20                     | 0.41              |
| 3:L3:2296:G:O2'    | 30:SA:242:PRO:O    | 2.37                     | 0.41              |
| 23:NE:232:THR:HG21 | 23:NE:280:VAL:HG12 | 2.03                     | 0.41              |
| 23:NE:253:LEU:HD12 | 23:NE:264:LEU:HD22 | 2.02                     | 0.41              |
| 24:NG:187:LYS:HB3  | 24:NG:201:LEU:HD23 | 2.03                     | 0.41              |
| 40:SN:134:THR:O    | 44:ST:234:ARG:NH2  | 2.45                     | 0.41              |
| 43:SS:265:MET:HE2  | 43:SS:265:MET:CA   | 2.51                     | 0.41              |
| 3:L3:1854:G:C8     | 3:L3:1855:G:N7     | 2.89                     | 0.41              |
| 3:L3:2100:A:OP2    | 3:L3:2262:G:N2     | 2.54                     | 0.41              |
| 3:L3:4763:U:C5     | 5:L7:126:VAL:HG21  | 2.56                     | 0.41              |
| 3:L3:4946:U:O2'    | 19:LT:2:SER:N      | 2.50                     | 0.41              |
| 41:SO:51:VAL:HG23  | 43:SS:132:ILE:O    | 2.21                     | 0.41              |
| 41:SO:175:LEU:HD12 | 41:SO:178:TYR:CD1  | 2.56                     | 0.41              |
| 37:SK:126:GLU:OE2  | 37:SK:139:ARG:NH1  | 2.54                     | 0.40              |
| 4:L6:64:VAL:O      | 4:L6:67:HIS:ND1    | 2.54                     | 0.40              |
| 20:LU:71:LYS:NZ    | 43:SS:127:SEP:O3P  | 2.39                     | 0.40              |
| 23:NE:341:LEU:HD11 | 23:NE:351:LEU:CD1  | 2.51                     | 0.40              |
| 43:SS:125:ASP:OD1  | 43:SS:126:SEP:N    | 2.55                     | 0.40              |
| 7:L9:94:PHE:CE2    | 7:L9:96:ARG:HB2    | 2.56                     | 0.40              |
| 10:LC:29:ARG:NH1   | 11:LE:148:PRO:O    | 2.54                     | 0.40              |
| 26:NN:33:VAL:O     | 26:NN:51:ARG:NH2   | 2.52                     | 0.40              |
| 28:NQ:155:LEU:HD22 | 28:NQ:200:THR:HG21 | 2.03                     | 0.40              |
| 3:L3:1444:G:HO2'   | 3:L3:1448:G:HO2'   | 1.63                     | 0.40              |
| 4:L6:63:THR:HG22   | 4:L6:64:VAL:N      | 2.36                     | 0.40              |
| 4:L6:94:ILE:HD11   | 4:L6:96:ILE:HD12   | 2.02                     | 0.40              |
| 16:LN:285:TYR:HA   | 16:LN:363:ILE:HD11 | 2.04                     | 0.40              |
| 23:NE:350:ILE:HG21 | 23:NE:355:LEU:HD21 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 4   | L6    | 112/211 (53%) | 110 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 5   | L7    | 180/203 (89%) | 178 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 6   | L8    | 133/215 (62%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 7   | L9    | 179/204 (88%) | 177 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 8   | LA    | 137/184 (74%) | 135 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 9   | LB    | 149/188 (79%) | 149 (100%) | 0       | 0        | 100         | 100 |
| 10  | LC    | 172/176 (98%) | 169 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 11  | LE    | 102/160 (64%) | 102 (100%) | 0       | 0        | 100         | 100 |
| 12  | LG    | 110/140 (79%) | 110 (100%) | 0       | 0        | 100         | 100 |
| 13  | LH    | 18/156 (12%)  | 18 (100%)  | 0       | 0        | 100         | 100 |
| 14  | LI    | 132/145 (91%) | 132 (100%) | 0       | 0        | 100         | 100 |
| 15  | LK    | 104/148 (70%) | 100 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 16  | LN    | 372/403 (92%) | 365 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 17  | LQ    | 131/135 (97%) | 130 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 18  | LS    | 120/123 (98%) | 120 (100%) | 0       | 0        | 100         | 100 |
| 19  | LT    | 107/110 (97%) | 107 (100%) | 0       | 0        | 100         | 100 |
| 20  | LU    | 101/105 (96%) | 100 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 21  | LW    | 65/97 (67%)   | 64 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 22  | NB    | 29/549 (5%)   | 29 (100%)  | 0       | 0        | 100         | 100 |
| 23  | NE    | 152/361 (42%) | 149 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 24  | NG    | 87/282 (31%)  | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 25  | NM    | 180/300 (60%) | 176 (98%)  | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|------------------|------------|---------|----------|-------------|-----|
| 26  | NN    | 238/473 (50%)    | 233 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 27  | NO    | 301/461 (65%)    | 300 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 28  | NQ    | 320/385 (83%)    | 315 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 29  | NS    | 303/349 (87%)    | 302 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 30  | SA    | 327/427 (77%)    | 323 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 31  | SC    | 193/288 (67%)    | 188 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 32  | SD    | 237/248 (96%)    | 232 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 33  | SE    | 184/266 (69%)    | 182 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 34  | SH    | 148/293 (50%)    | 147 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 35  | SI    | 198/255 (78%)    | 195 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 36  | SJ    | 70/847 (8%)      | 68 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 37  | SK    | 224/245 (91%)    | 221 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 38  | SL    | 241/490 (49%)    | 238 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 39  | SM    | 427/588 (73%)    | 427 (100%) | 0       | 0        | 100         | 100 |
| 40  | SN    | 162/306 (53%)    | 161 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 41  | SO    | 305/353 (86%)    | 302 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 42  | SR    | 73/634 (12%)     | 71 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 43  | SS    | 227/746 (30%)    | 227 (100%) | 0       | 0        | 100         | 100 |
| 44  | ST    | 34/365 (9%)      | 33 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 45  | SV    | 135/163 (83%)    | 133 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 46  | SW    | 441/670 (66%)    | 434 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 47  | SZ    | 156/178 (88%)    | 155 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| All | All   | 7816/13625 (57%) | 7724 (99%) | 92 (1%) | 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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 4   | L6    | 98/177 (55%)  | 98 (100%)  | 0        | 100         | 100 |
| 5   | L7    | 157/174 (90%) | 157 (100%) | 0        | 100         | 100 |
| 6   | L8    | 115/161 (71%) | 115 (100%) | 0        | 100         | 100 |
| 7   | L9    | 155/172 (90%) | 155 (100%) | 0        | 100         | 100 |
| 8   | LA    | 132/163 (81%) | 132 (100%) | 0        | 100         | 100 |
| 9   | LB    | 136/165 (82%) | 136 (100%) | 0        | 100         | 100 |
| 10  | LC    | 155/157 (99%) | 155 (100%) | 0        | 100         | 100 |
| 11  | LE    | 47/140 (34%)  | 47 (100%)  | 0        | 100         | 100 |
| 12  | LG    | 87/107 (81%)  | 87 (100%)  | 0        | 100         | 100 |
| 13  | LH    | 13/133 (10%)  | 13 (100%)  | 0        | 100         | 100 |
| 14  | LI    | 124/135 (92%) | 124 (100%) | 0        | 100         | 100 |
| 15  | LK    | 29/121 (24%)  | 29 (100%)  | 0        | 100         | 100 |
| 16  | LN    | 328/348 (94%) | 328 (100%) | 0        | 100         | 100 |
| 17  | LQ    | 119/121 (98%) | 119 (100%) | 0        | 100         | 100 |
| 18  | LS    | 109/110 (99%) | 109 (100%) | 0        | 100         | 100 |
| 19  | LT    | 88/89 (99%)   | 88 (100%)  | 0        | 100         | 100 |
| 20  | LU    | 87/89 (98%)   | 87 (100%)  | 0        | 100         | 100 |
| 21  | LW    | 58/80 (72%)   | 58 (100%)  | 0        | 100         | 100 |
| 22  | NB    | 27/485 (6%)   | 27 (100%)  | 0        | 100         | 100 |
| 23  | NE    | 136/294 (46%) | 136 (100%) | 0        | 100         | 100 |
| 24  | NG    | 83/246 (34%)  | 83 (100%)  | 0        | 100         | 100 |
| 25  | NM    | 168/272 (62%) | 168 (100%) | 0        | 100         | 100 |
| 26  | NN    | 218/398 (55%) | 218 (100%) | 0        | 100         | 100 |
| 27  | NO    | 269/392 (69%) | 269 (100%) | 0        | 100         | 100 |
| 28  | NQ    | 265/318 (83%) | 265 (100%) | 0        | 100         | 100 |
| 29  | NS    | 276/305 (90%) | 276 (100%) | 0        | 100         | 100 |
| 30  | SA    | 280/348 (80%) | 280 (100%) | 0        | 100         | 100 |
| 31  | SC    | 178/252 (71%) | 178 (100%) | 0        | 100         | 100 |
| 32  | SD    | 207/215 (96%) | 207 (100%) | 0        | 100         | 100 |
| 33  | SE    | 159/223 (71%) | 159 (100%) | 0        | 100         | 100 |
| 34  | SH    | 140/274 (51%) | 140 (100%) | 0        | 100         | 100 |
| 35  | SI    | 182/228 (80%) | 182 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 36  | SJ    | 64/733 (9%)      | 64 (100%)   | 0        | 100         | 100 |
| 37  | SK    | 196/213 (92%)    | 196 (100%)  | 0        | 100         | 100 |
| 38  | SL    | 226/437 (52%)    | 226 (100%)  | 0        | 100         | 100 |
| 39  | SM    | 350/509 (69%)    | 350 (100%)  | 0        | 100         | 100 |
| 40  | SN    | 126/260 (48%)    | 126 (100%)  | 0        | 100         | 100 |
| 41  | SO    | 283/319 (89%)    | 283 (100%)  | 0        | 100         | 100 |
| 42  | SR    | 69/574 (12%)     | 69 (100%)   | 0        | 100         | 100 |
| 43  | SS    | 208/648 (32%)    | 208 (100%)  | 0        | 100         | 100 |
| 44  | ST    | 27/300 (9%)      | 27 (100%)   | 0        | 100         | 100 |
| 45  | SV    | 127/149 (85%)    | 127 (100%)  | 0        | 100         | 100 |
| 46  | SW    | 394/591 (67%)    | 394 (100%)  | 0        | 100         | 100 |
| 47  | SZ    | 141/158 (89%)    | 141 (100%)  | 0        | 100         | 100 |
| All | All   | 6836/11783 (58%) | 6836 (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 (64) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L6    | 104 | ASN  |
| 5   | L7    | 90  | HIS  |
| 5   | L7    | 199 | HIS  |
| 6   | L8    | 34  | ASN  |
| 7   | L9    | 8   | GLN  |
| 7   | L9    | 158 | HIS  |
| 7   | L9    | 201 | HIS  |
| 9   | LB    | 7   | HIS  |
| 10  | LC    | 37  | HIS  |
| 10  | LC    | 91  | HIS  |
| 10  | LC    | 122 | HIS  |
| 14  | LI    | 96  | HIS  |
| 16  | LN    | 68  | ASN  |
| 16  | LN    | 184 | GLN  |
| 17  | LQ    | 52  | GLN  |
| 17  | LQ    | 102 | ASN  |
| 17  | LQ    | 107 | ASN  |
| 19  | LT    | 21  | GLN  |
| 19  | LT    | 99  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | LU    | 12  | ASN  |
| 20  | LU    | 15  | HIS  |
| 20  | LU    | 26  | HIS  |
| 20  | LU    | 36  | HIS  |
| 23  | NE    | 235 | ASN  |
| 26  | NN    | 170 | HIS  |
| 28  | NQ    | 113 | HIS  |
| 29  | NS    | 153 | HIS  |
| 29  | NS    | 162 | GLN  |
| 29  | NS    | 206 | ASN  |
| 29  | NS    | 257 | HIS  |
| 29  | NS    | 335 | HIS  |
| 30  | SA    | 38  | ASN  |
| 30  | SA    | 231 | ASN  |
| 30  | SA    | 245 | HIS  |
| 31  | SC    | 190 | HIS  |
| 31  | SC    | 227 | HIS  |
| 32  | SD    | 56  | HIS  |
| 32  | SD    | 99  | ASN  |
| 32  | SD    | 151 | ASN  |
| 33  | SE    | 64  | GLN  |
| 33  | SE    | 206 | GLN  |
| 33  | SE    | 208 | ASN  |
| 33  | SE    | 240 | ASN  |
| 34  | SH    | 51  | HIS  |
| 34  | SH    | 60  | GLN  |
| 34  | SH    | 119 | HIS  |
| 35  | SI    | 66  | HIS  |
| 36  | SJ    | 726 | HIS  |
| 37  | SK    | 68  | HIS  |
| 37  | SK    | 74  | ASN  |
| 37  | SK    | 79  | GLN  |
| 37  | SK    | 83  | HIS  |
| 38  | SL    | 35  | GLN  |
| 38  | SL    | 218 | HIS  |
| 39  | SM    | 191 | GLN  |
| 39  | SM    | 211 | HIS  |
| 39  | SM    | 253 | GLN  |
| 39  | SM    | 375 | HIS  |
| 40  | SN    | 113 | GLN  |
| 40  | SN    | 124 | HIS  |
| 41  | SO    | 340 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | SS    | 211 | GLN  |
| 46  | SW    | 187 | ASN  |
| 46  | SW    | 525 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | L1    | 150/157 (95%)   | 14 (9%)           | 0               |
| 2   | L2    | 65/1167 (5%)    | 9 (13%)           | 0               |
| 3   | L3    | 1477/5070 (29%) | 208 (14%)         | 2 (0%)          |
| All | All   | 1692/6394 (26%) | 231 (13%)         | 2 (0%)          |

All (231) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L1    | 34  | U    |
| 1   | L1    | 59  | A    |
| 1   | L1    | 62  | A    |
| 1   | L1    | 63  | U    |
| 1   | L1    | 82  | A    |
| 1   | L1    | 83  | C    |
| 1   | L1    | 84  | A    |
| 1   | L1    | 86  | U    |
| 1   | L1    | 94  | G    |
| 1   | L1    | 103 | A    |
| 1   | L1    | 105 | C    |
| 1   | L1    | 111 | U    |
| 1   | L1    | 156 | U    |
| 1   | L1    | 157 | U    |
| 2   | L2    | 11  | C    |
| 2   | L2    | 48  | G    |
| 2   | L2    | 49  | G    |
| 2   | L2    | 51  | U    |
| 2   | L2    | 62  | U    |
| 2   | L2    | 94  | U    |
| 2   | L2    | 96  | A    |
| 2   | L2    | 101 | A    |
| 2   | L2    | 103 | A    |
| 3   | L3    | 48  | G    |
| 3   | L3    | 58  | G    |
| 3   | L3    | 59  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L3    | 64  | A    |
| 3   | L3    | 65  | A    |
| 3   | L3    | 69  | A    |
| 3   | L3    | 85  | G    |
| 3   | L3    | 86  | U    |
| 3   | L3    | 91  | G    |
| 3   | L3    | 93  | G    |
| 3   | L3    | 95  | G    |
| 3   | L3    | 108 | A    |
| 3   | L3    | 119 | G    |
| 3   | L3    | 159 | C    |
| 3   | L3    | 170 | C    |
| 3   | L3    | 171 | U    |
| 3   | L3    | 172 | C    |
| 3   | L3    | 173 | C    |
| 3   | L3    | 176 | G    |
| 3   | L3    | 179 | G    |
| 3   | L3    | 181 | C    |
| 3   | L3    | 186 | G    |
| 3   | L3    | 190 | G    |
| 3   | L3    | 200 | U    |
| 3   | L3    | 204 | U    |
| 3   | L3    | 210 | C    |
| 3   | L3    | 218 | A    |
| 3   | L3    | 219 | G    |
| 3   | L3    | 220 | C    |
| 3   | L3    | 233 | U    |
| 3   | L3    | 234 | G    |
| 3   | L3    | 265 | C    |
| 3   | L3    | 271 | C    |
| 3   | L3    | 281 | U    |
| 3   | L3    | 294 | G    |
| 3   | L3    | 326 | C    |
| 3   | L3    | 340 | C    |
| 3   | L3    | 362 | A    |
| 3   | L3    | 386 | A    |
| 3   | L3    | 387 | G    |
| 3   | L3    | 408 | A    |
| 3   | L3    | 409 | G    |
| 3   | L3    | 410 | A    |
| 3   | L3    | 413 | G    |
| 3   | L3    | 446 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 451  | C    |
| 3   | L3    | 452  | A    |
| 3   | L3    | 469  | C    |
| 3   | L3    | 470  | A    |
| 3   | L3    | 473  | C    |
| 3   | L3    | 479  | G    |
| 3   | L3    | 673  | C    |
| 3   | L3    | 685  | C    |
| 3   | L3    | 686  | A    |
| 3   | L3    | 687  | U    |
| 3   | L3    | 696  | C    |
| 3   | L3    | 697  | G    |
| 3   | L3    | 701  | G    |
| 3   | L3    | 703  | G    |
| 3   | L3    | 730  | G    |
| 3   | L3    | 731  | G    |
| 3   | L3    | 739  | G    |
| 3   | L3    | 742  | G    |
| 3   | L3    | 746  | A    |
| 3   | L3    | 913  | U    |
| 3   | L3    | 914  | U    |
| 3   | L3    | 915  | A    |
| 3   | L3    | 917  | A    |
| 3   | L3    | 926  | G    |
| 3   | L3    | 932  | A    |
| 3   | L3    | 933  | G    |
| 3   | L3    | 944  | A    |
| 3   | L3    | 945  | U    |
| 3   | L3    | 1296 | G    |
| 3   | L3    | 1297 | U    |
| 3   | L3    | 1301 | C    |
| 3   | L3    | 1313 | C    |
| 3   | L3    | 1314 | C    |
| 3   | L3    | 1315 | C    |
| 3   | L3    | 1328 | G    |
| 3   | L3    | 1330 | A    |
| 3   | L3    | 1337 | A    |
| 3   | L3    | 1354 | A    |
| 3   | L3    | 1358 | G    |
| 3   | L3    | 1359 | G    |
| 3   | L3    | 1445 | U    |
| 3   | L3    | 1502 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 1654 | G    |
| 3   | L3    | 1661 | C    |
| 3   | L3    | 1671 | U    |
| 3   | L3    | 1674 | C    |
| 3   | L3    | 1677 | U    |
| 3   | L3    | 1679 | A    |
| 3   | L3    | 1680 | G    |
| 3   | L3    | 1691 | G    |
| 3   | L3    | 1804 | A    |
| 3   | L3    | 1836 | G    |
| 3   | L3    | 1837 | A    |
| 3   | L3    | 1842 | G    |
| 3   | L3    | 1854 | G    |
| 3   | L3    | 1881 | C    |
| 3   | L3    | 1882 | U    |
| 3   | L3    | 1888 | A    |
| 3   | L3    | 1891 | A    |
| 3   | L3    | 1892 | A    |
| 3   | L3    | 1897 | A    |
| 3   | L3    | 1906 | U    |
| 3   | L3    | 1910 | G    |
| 3   | L3    | 1919 | G    |
| 3   | L3    | 1921 | C    |
| 3   | L3    | 1922 | G    |
| 3   | L3    | 2055 | G    |
| 3   | L3    | 2056 | G    |
| 3   | L3    | 2069 | A    |
| 3   | L3    | 2084 | C    |
| 3   | L3    | 2085 | G    |
| 3   | L3    | 2089 | G    |
| 3   | L3    | 2094 | G    |
| 3   | L3    | 2095 | A    |
| 3   | L3    | 2097 | U    |
| 3   | L3    | 2099 | G    |
| 3   | L3    | 2100 | A    |
| 3   | L3    | 2102 | G    |
| 3   | L3    | 2103 | G    |
| 3   | L3    | 2261 | G    |
| 3   | L3    | 2265 | G    |
| 3   | L3    | 2266 | C    |
| 3   | L3    | 2267 | U    |
| 3   | L3    | 2289 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 2300 | A    |
| 3   | L3    | 2301 | G    |
| 3   | L3    | 2313 | A    |
| 3   | L3    | 2314 | G    |
| 3   | L3    | 2348 | G    |
| 3   | L3    | 2351 | C    |
| 3   | L3    | 2364 | G    |
| 3   | L3    | 2826 | U    |
| 3   | L3    | 2829 | U    |
| 3   | L3    | 2836 | A    |
| 3   | L3    | 2837 | U    |
| 3   | L3    | 2838 | G    |
| 3   | L3    | 3852 | A    |
| 3   | L3    | 3895 | G    |
| 3   | L3    | 4584 | A    |
| 3   | L3    | 4589 | A    |
| 3   | L3    | 4590 | A    |
| 3   | L3    | 4618 | G    |
| 3   | L3    | 4621 | C    |
| 3   | L3    | 4629 | U    |
| 3   | L3    | 4633 | G    |
| 3   | L3    | 4640 | C    |
| 3   | L3    | 4641 | U    |
| 3   | L3    | 4642 | U    |
| 3   | L3    | 4647 | G    |
| 3   | L3    | 4648 | A    |
| 3   | L3    | 4649 | G    |
| 3   | L3    | 4651 | A    |
| 3   | L3    | 4657 | U    |
| 3   | L3    | 4658 | G    |
| 3   | L3    | 4661 | G    |
| 3   | L3    | 4671 | C    |
| 3   | L3    | 4672 | A    |
| 3   | L3    | 4673 | U    |
| 3   | L3    | 4719 | G    |
| 3   | L3    | 4737 | G    |
| 3   | L3    | 4740 | G    |
| 3   | L3    | 4741 | C    |
| 3   | L3    | 4742 | G    |
| 3   | L3    | 4745 | G    |
| 3   | L3    | 4747 | C    |
| 3   | L3    | 4754 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 4757 | C    |
| 3   | L3    | 4759 | C    |
| 3   | L3    | 4761 | G    |
| 3   | L3    | 4763 | U    |
| 3   | L3    | 4765 | G    |
| 3   | L3    | 4773 | C    |
| 3   | L3    | 4870 | G    |
| 3   | L3    | 4871 | C    |
| 3   | L3    | 4882 | U    |
| 3   | L3    | 4883 | C    |
| 3   | L3    | 4910 | G    |
| 3   | L3    | 4912 | G    |
| 3   | L3    | 4914 | C    |
| 3   | L3    | 4943 | A    |
| 3   | L3    | 4949 | G    |
| 3   | L3    | 4950 | U    |
| 3   | L3    | 4951 | G    |
| 3   | L3    | 4955 | A    |
| 3   | L3    | 4958 | C    |
| 3   | L3    | 4960 | G    |
| 3   | L3    | 4966 | A    |
| 3   | L3    | 4976 | U    |
| 3   | L3    | 5013 | C    |
| 3   | L3    | 5022 | U    |
| 3   | L3    | 5025 | C    |
| 3   | L3    | 5026 | U    |
| 3   | L3    | 5027 | C    |
| 3   | L3    | 5028 | G    |
| 3   | L3    | 5030 | U    |
| 3   | L3    | 5031 | G    |
| 3   | L3    | 5040 | U    |
| 3   | L3    | 5041 | G    |
| 3   | L3    | 5045 | G    |
| 3   | L3    | 5053 | U    |
| 3   | L3    | 5059 | C    |
| 3   | L3    | 5064 | G    |
| 3   | L3    | 5065 | U    |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 1880 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 2093 | A    |

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

4 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 |
| 25  | AME  | NM    | 1   | 25   | 9,10,11      | 1.52 | 2 (22%)  | 9,11,13     | 1.37 | 1 (11%)  |
| 43  | SEP  | SS    | 127 | 43   | 8,9,10       | 1.57 | 1 (12%)  | 7,12,14     | 1.13 | 1 (14%)  |
| 43  | SEP  | SS    | 126 | 43   | 8,9,10       | 1.57 | 1 (12%)  | 7,12,14     | 1.22 | 1 (14%)  |
| 16  | HIC  | LN    | 245 | 16   | 10,11,12     | 1.44 | 1 (10%)  | 9,14,16     | 1.19 | 2 (22%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 25  | AME  | NM    | 1   | 25   | -       | 1/9/10/12 | -       |
| 43  | SEP  | SS    | 127 | 43   | -       | 2/6/8/10  | -       |
| 43  | SEP  | SS    | 126 | 43   | -       | 0/6/8/10  | -       |
| 16  | HIC  | LN    | 245 | 16   | -       | 0/5/6/8   | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 43  | SS    | 126 | SEP  | P-O1P  | 3.47  | 1.61        | 1.50     |
| 43  | SS    | 127 | SEP  | P-O1P  | 3.44  | 1.61        | 1.50     |
| 25  | NM    | 1   | AME  | CT1-N  | 3.43  | 1.45        | 1.34     |
| 16  | LN    | 245 | HIC  | CD2-CG | 2.77  | 1.41        | 1.36     |
| 25  | NM    | 1   | AME  | OT-CT1 | -2.13 | 1.18        | 1.23     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | LN    | 245 | HIC  | NE2-CE1-ND1 | -2.68 | 111.64      | 112.66   |
| 43  | SS    | 126 | SEP  | OG-CB-CA    | 2.66  | 110.73      | 108.14   |
| 25  | NM    | 1   | AME  | CT2-CT1-N   | 2.40  | 120.09      | 116.12   |
| 16  | LN    | 245 | HIC  | CB-CG-CD2   | -2.03 | 125.06      | 129.96   |
| 43  | SS    | 127 | SEP  | OG-CB-CA    | 2.02  | 110.11      | 108.14   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 25  | NM    | 1   | AME  | C-CA-N-CT1 |
| 43  | SS    | 127 | SEP  | N-CA-CB-OG |
| 43  | SS    | 127 | SEP  | CA-CB-OG-P |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 43  | SS    | 127 | SEP  | 1       | 0            |
| 43  | SS    | 126 | SEP  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 56 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 50  | SF4  | NM    | 401 | 25   | 0,12,12      | -    | -           | -           |      |             |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 50  | SF4  | NM    | 401 | 25   | -       | -        | 0/6/5/5 |

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.

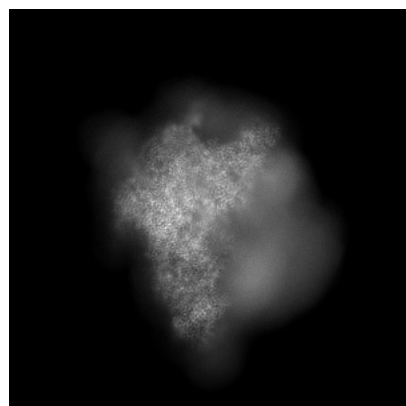
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29252. These allow visual inspection of the internal detail of the map and identification of artifacts.

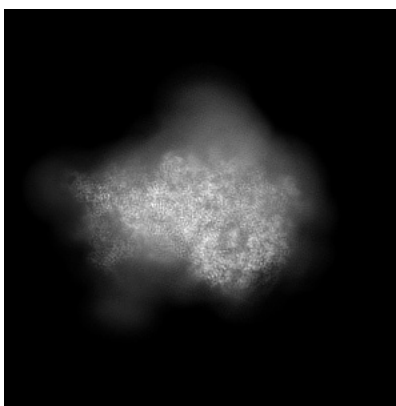
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

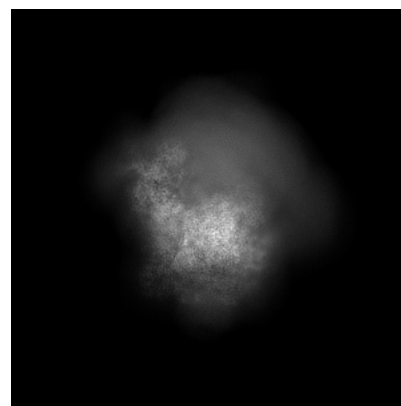
#### 6.1.1 Primary map



X

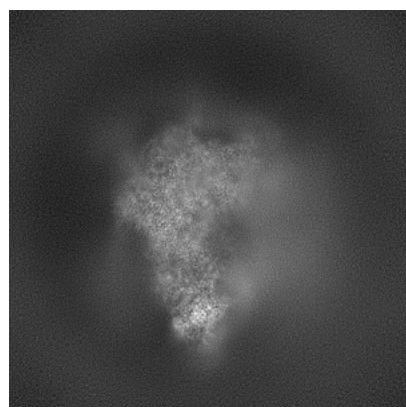


Y

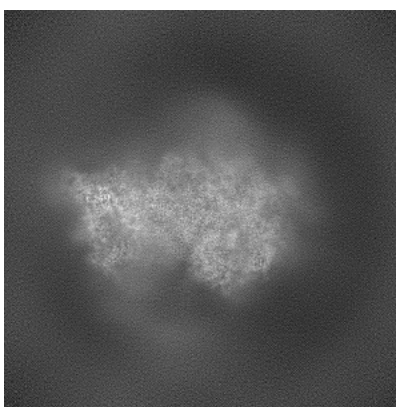


Z

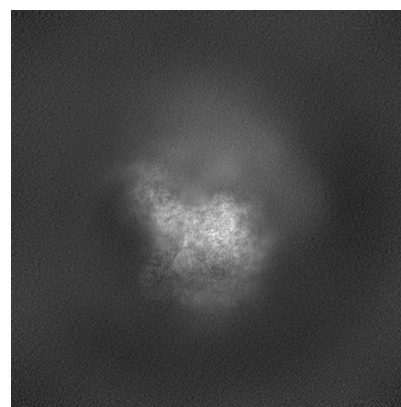
#### 6.1.2 Raw map



X



Y

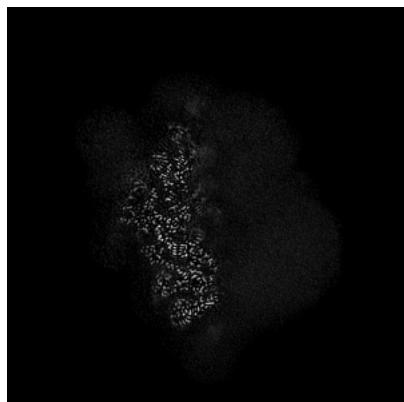


Z

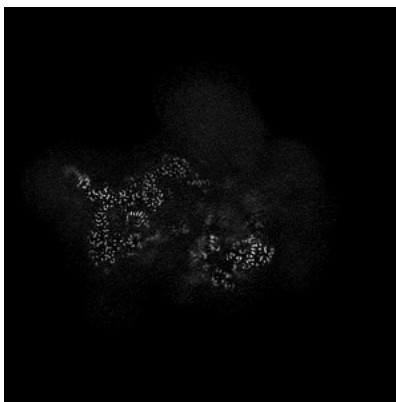
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

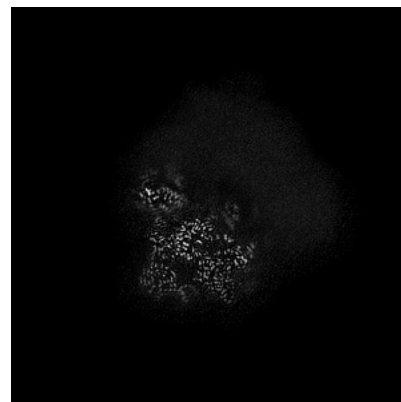
### 6.2.1 Primary map



X Index: 240

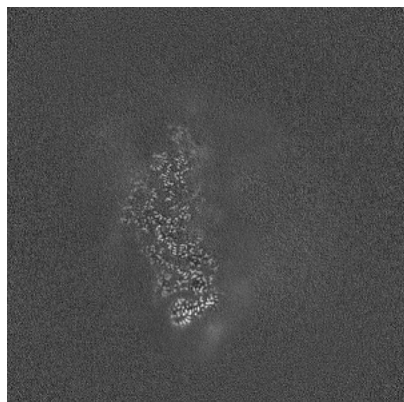


Y Index: 240

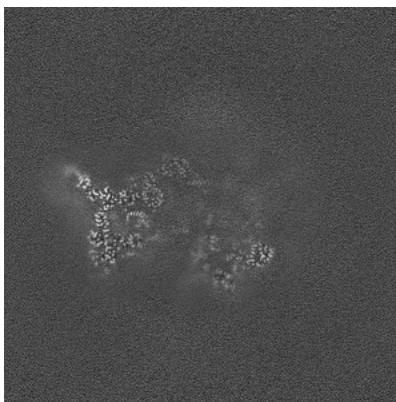


Z Index: 240

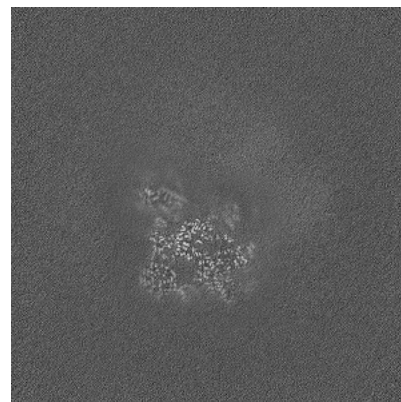
### 6.2.2 Raw map



X Index: 240



Y Index: 240

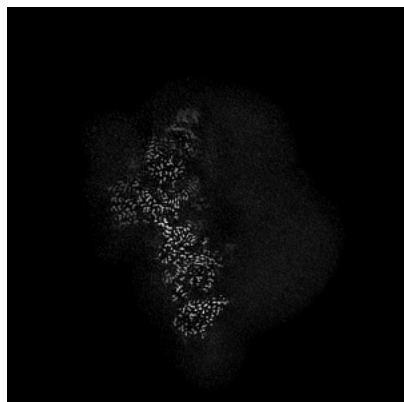


Z Index: 240

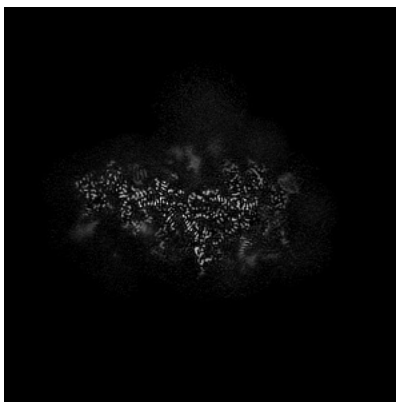
The images above show central slices of the map in three orthogonal directions.

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

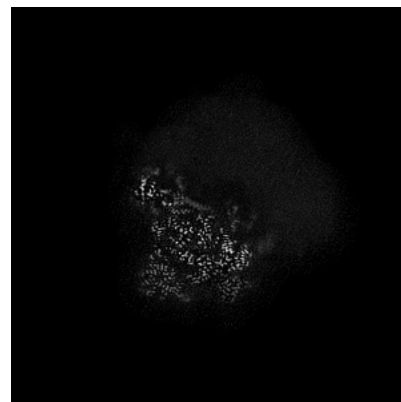
### 6.3.1 Primary map



X Index: 257

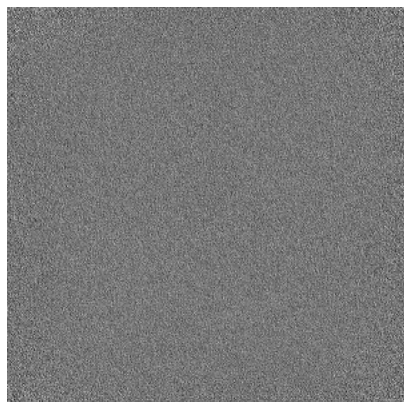


Y Index: 205

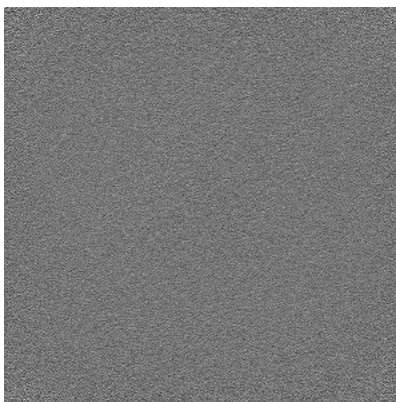


Z Index: 245

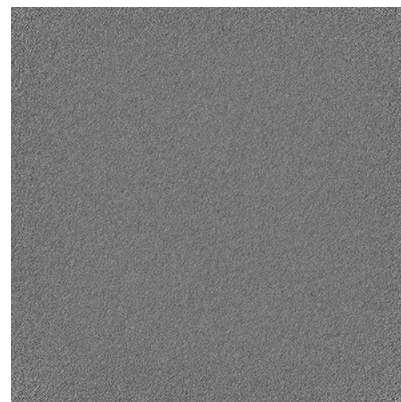
### 6.3.2 Raw map



X Index: 0



Y Index: 0

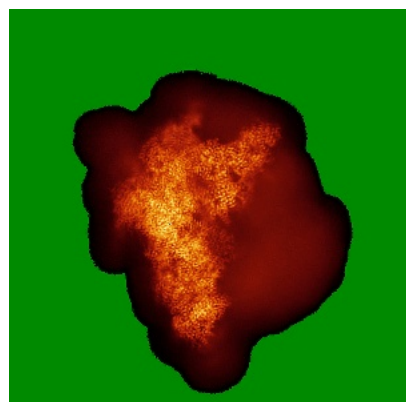


Z Index: 0

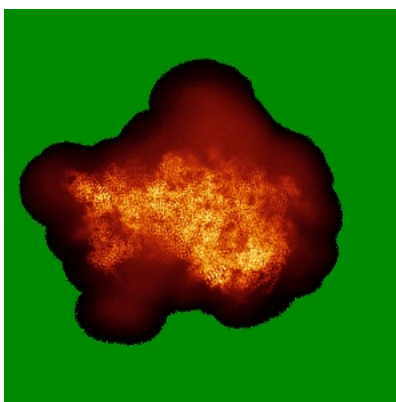
The images above show the largest variance slices of the map in three orthogonal directions.

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

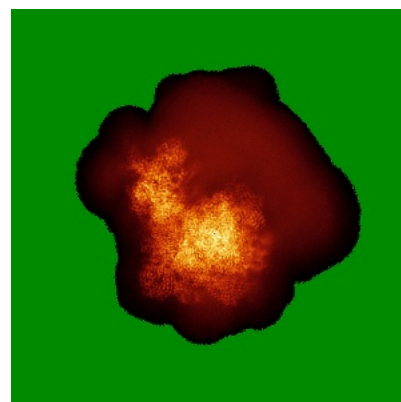
### 6.4.1 Primary map



X

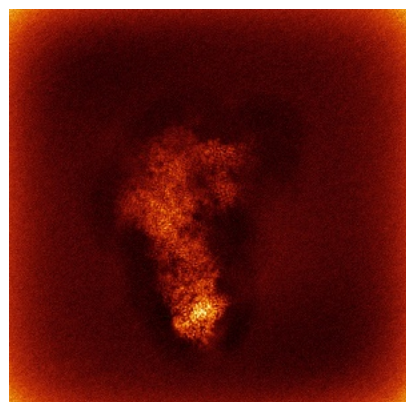


Y

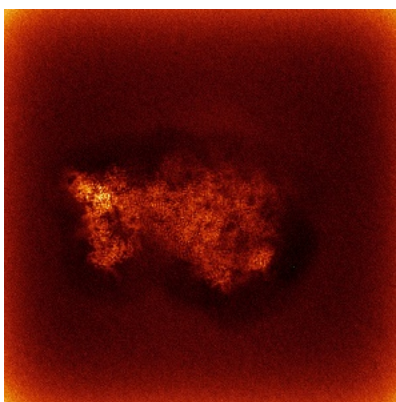


Z

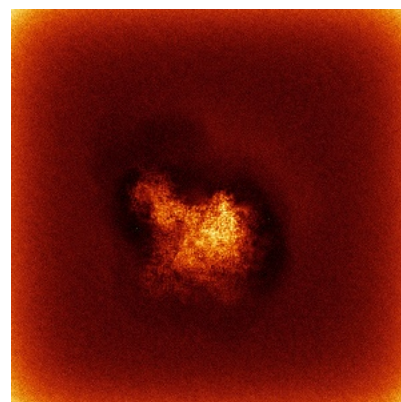
### 6.4.2 Raw map



X



Y



Z

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

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

### 6.5.1 Primary map



X



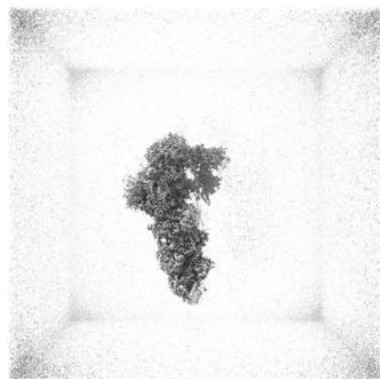
Y



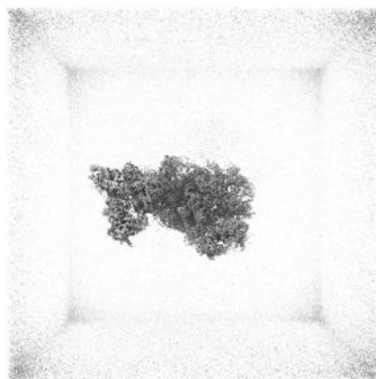
Z

The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

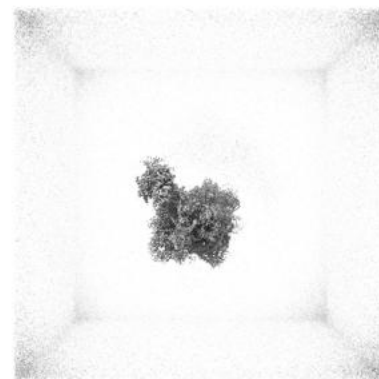
### 6.5.2 Raw map



X



Y



Z

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

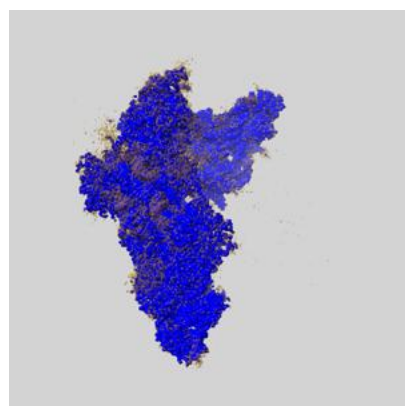
## 6.6 Mask visualisation [i](#)

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

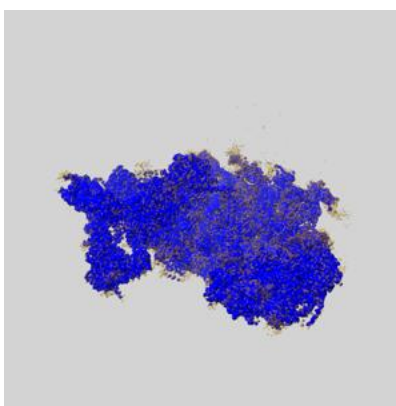
A mask typically either:

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

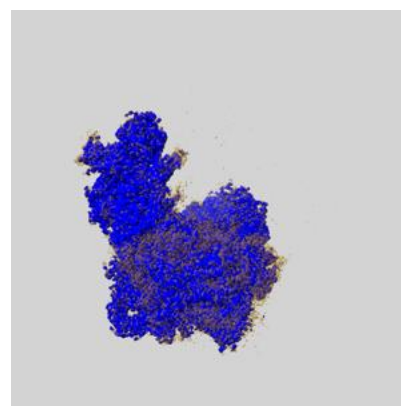
### 6.6.1 emd\_29252\_msk\_1.map [i](#)



X



Y

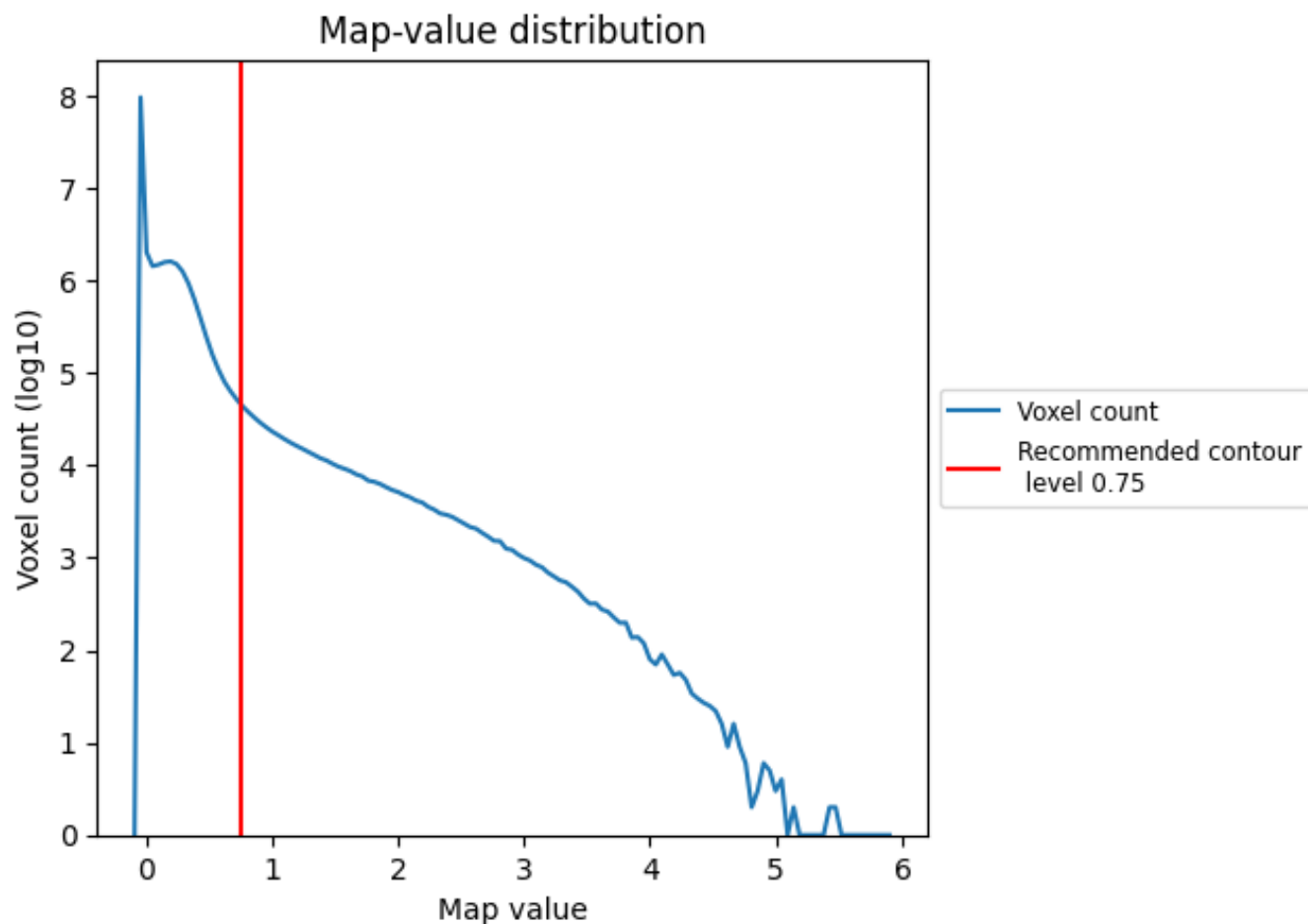


Z

## 7 Map analysis [i](#)

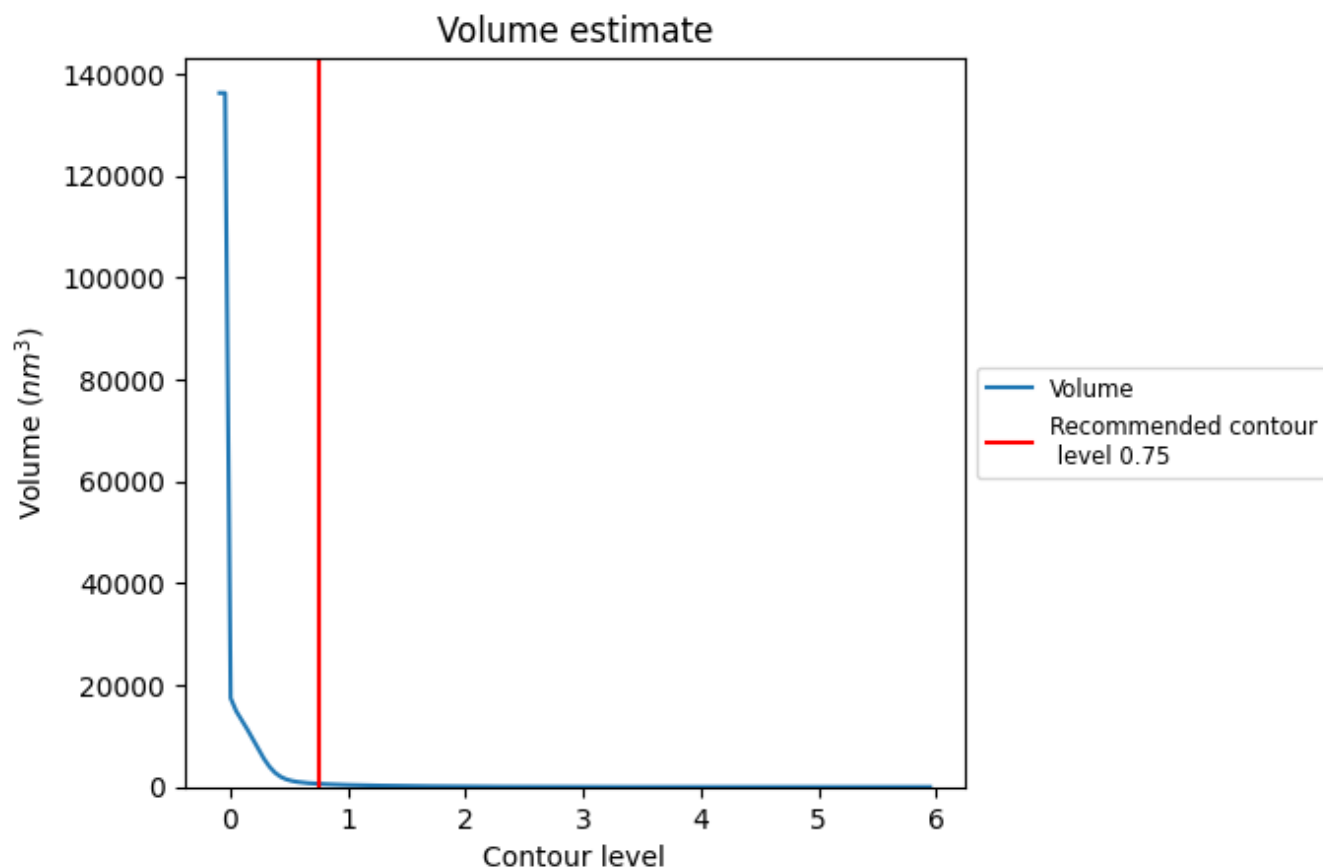
This section contains the results of statistical analysis of the map.

### 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.

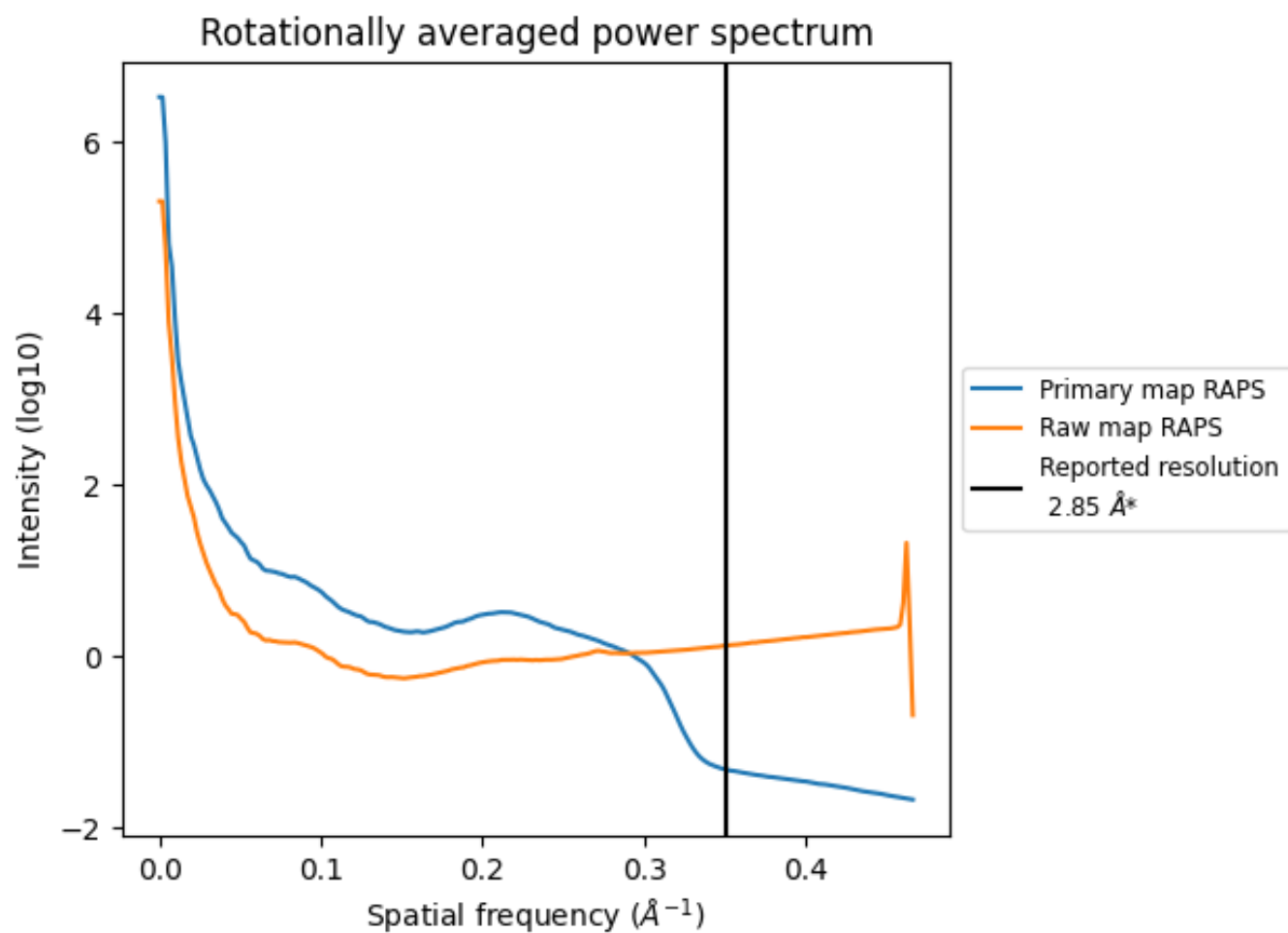
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621  $\text{nm}^3$ ; this corresponds to an approximate mass of 561 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

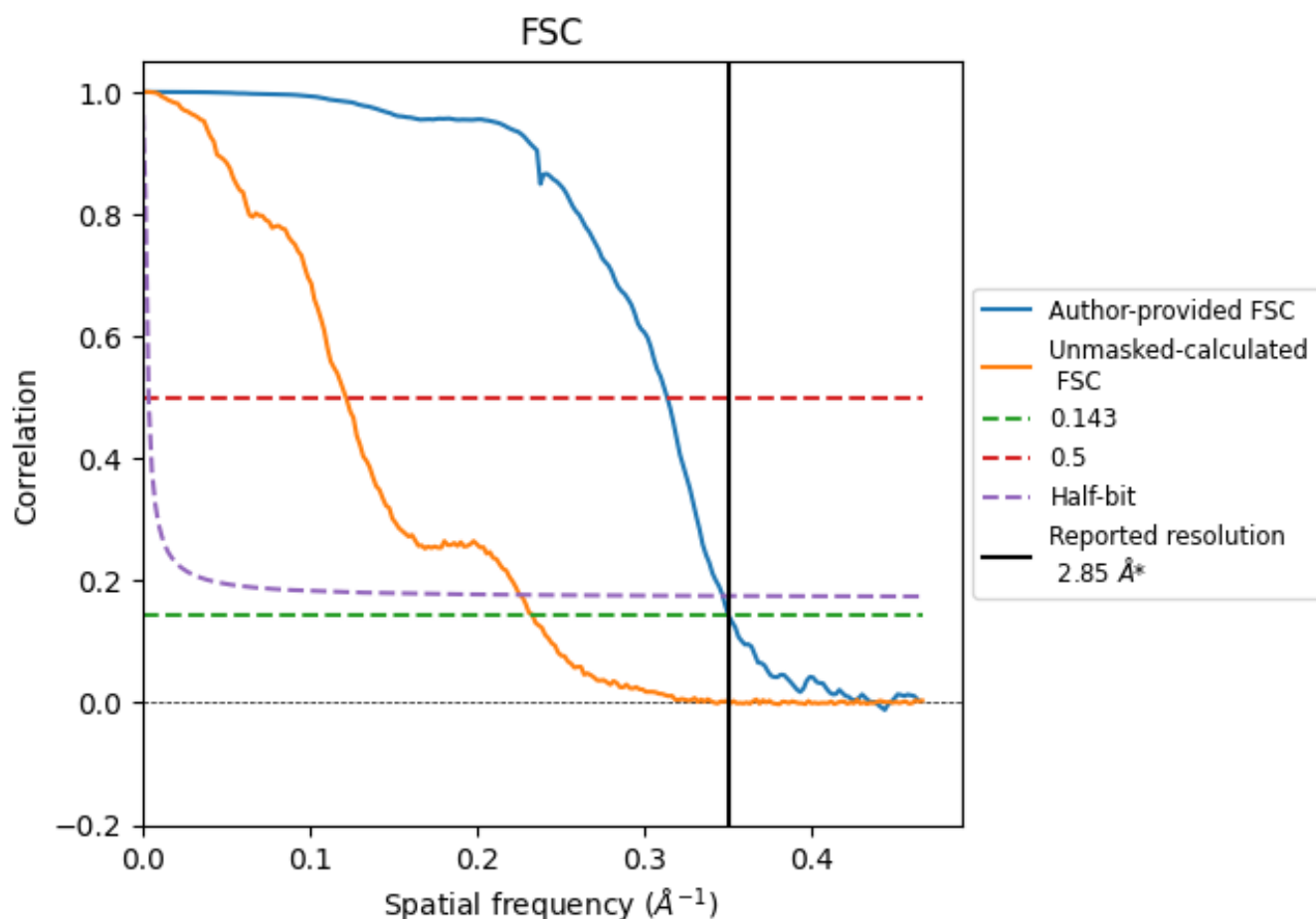


\*Reported resolution corresponds to spatial frequency of 0.351 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

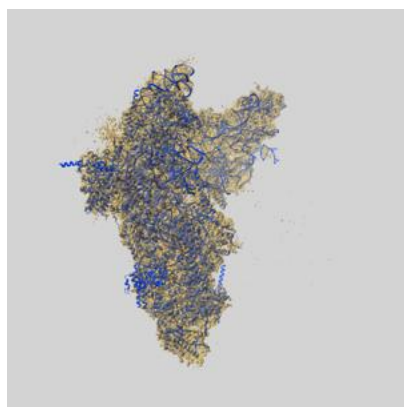
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.85                               | -    | -        |
| Author-provided FSC curve | 2.85                               | 3.19 | 2.88     |
| Unmasked-calculated*      | 4.28                               | 8.21 | 4.43     |

\*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 4.28 differs from the reported value 2.85 by more than 10 %

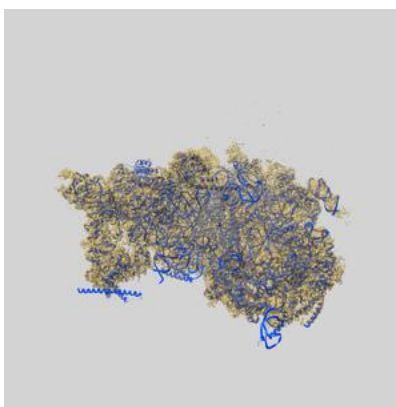
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29252 and PDB model 8FKP. Per-residue inclusion information can be found in section 3 on page 13.

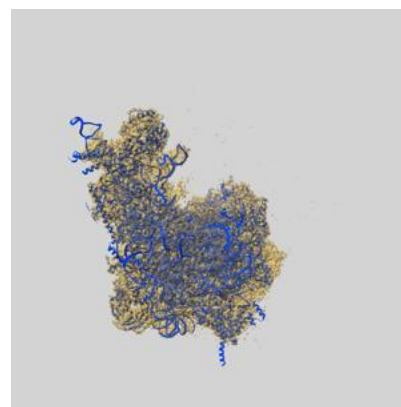
### 9.1 Map-model overlay [i](#)



X



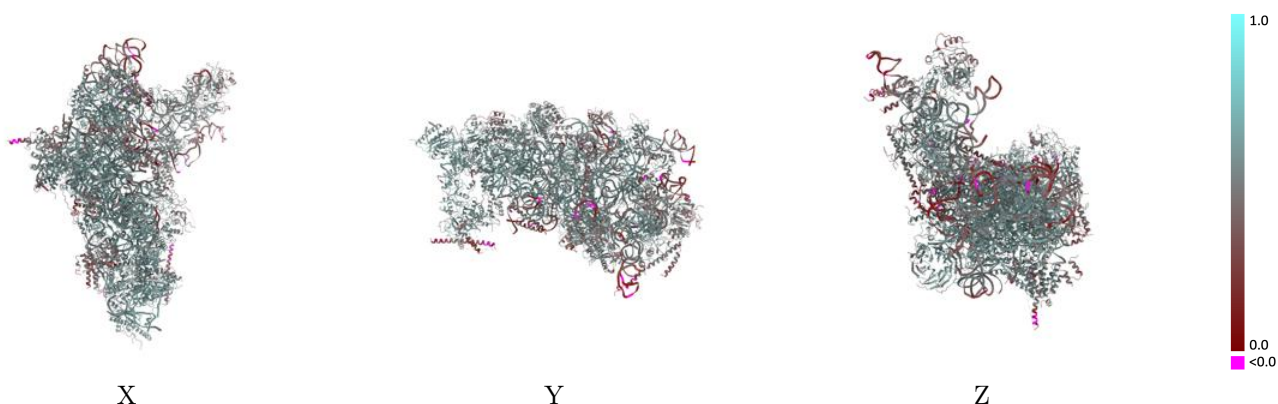
Y



Z

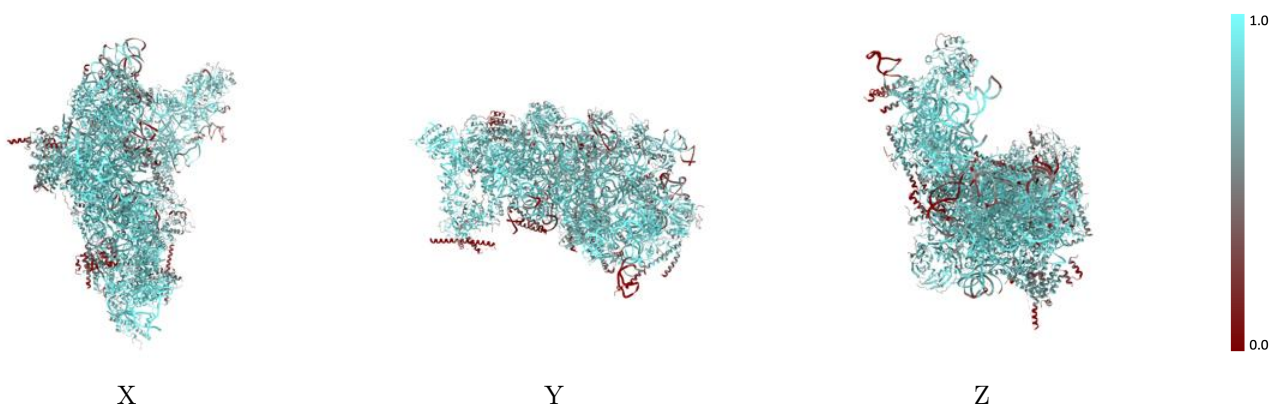
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



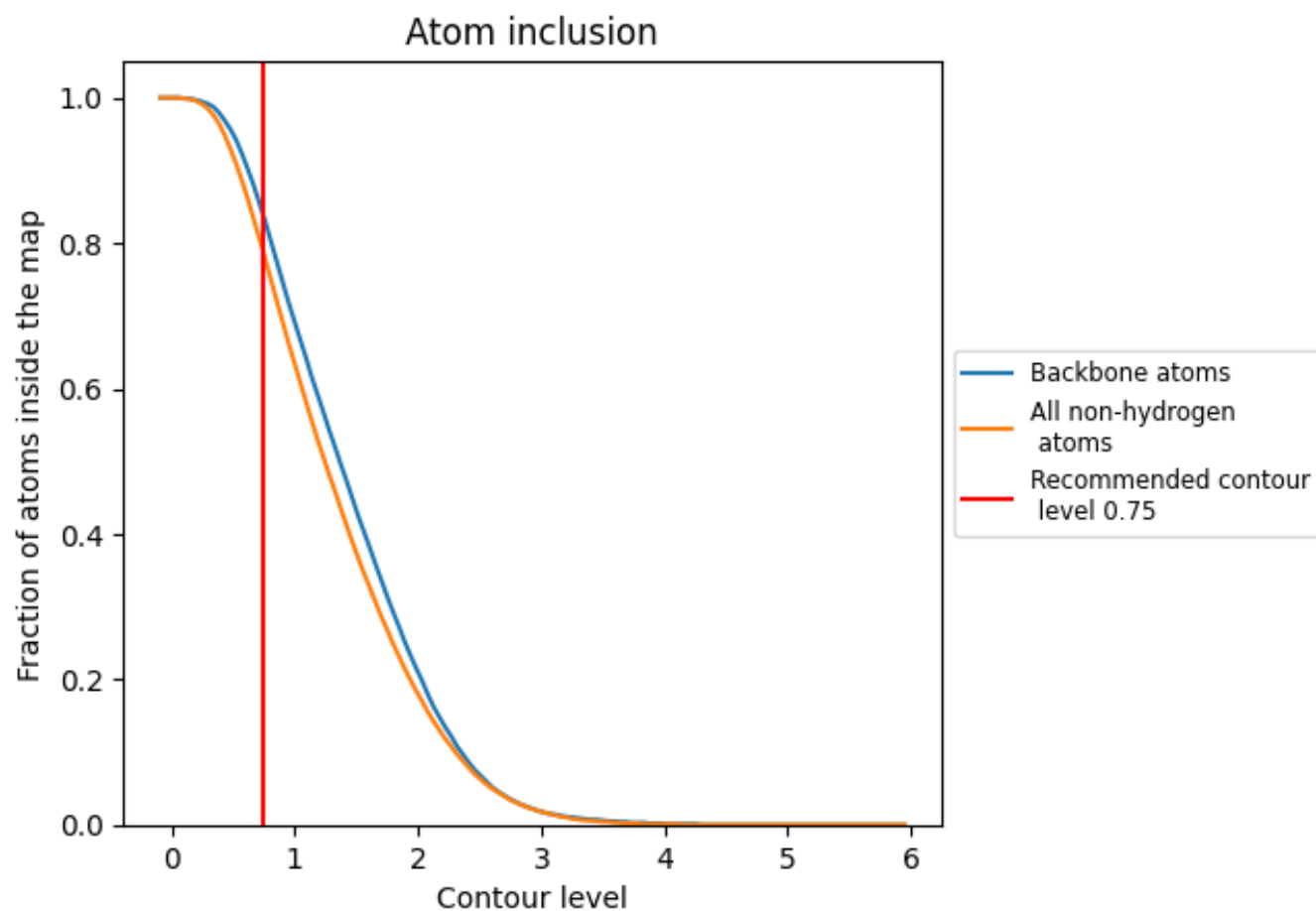
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.75) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7850   |  0.5210   |
| L1    |  0.6870   |  0.4690   |
| L2    |  0.9420   |  0.5730   |
| L3    |  0.8430   |  0.5100   |
| L6    |  0.9290   |  0.5970   |
| L7    |  0.7300   |  0.5000   |
| L8    |  0.7170   |  0.5030   |
| L9    |  0.9330   |  0.6090   |
| LA    |  0.6360   |  0.4950   |
| LB    |  0.9260   |  0.6010   |
| LC    |  0.6930   |  0.5140   |
| LE    |  0.5030   |  0.4160   |
| LG    |  0.7450   |  0.4930   |
| LH    |  0.4790   |  0.5160   |
| LI    |  0.8440  |  0.5840  |
| LK    |  0.7970 |  0.4360 |
| LN    |  0.8600 |  0.5490 |
| LQ    |  0.9020 |  0.6020 |
| LS    |  0.5390 |  0.4600 |
| LT    |  0.9240 |  0.6090 |
| LU    |  0.7820 |  0.5600 |
| LW    |  0.5850 |  0.5180 |
| NB    |  0.1980 |  0.3840 |
| NE    |  0.6460 |  0.4130 |
| NG    |  0.4660 |  0.3970 |
| NM    |  0.8390 |  0.5810 |
| NN    |  0.8450 |  0.5150 |
| NO    |  0.6770 |  0.5150 |
| NQ    |  0.7730 |  0.5540 |
| NS    |  0.7850 |  0.5650 |
| SA    |  0.8830 |  0.5900 |
| SC    |  0.7560 |  0.5490 |
| SD    |  0.8510 |  0.5740 |
| SE    |  0.9040 |  0.5840 |
| SH    |  0.8660 |  0.5770 |



*Continued on next page...*

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| SI    |  0.8180 |  0.5770 |
| SJ    |  0.5700 |  0.4960 |
| SK    |  0.7450 |  0.4590 |
| SL    |  0.8320 |  0.5630 |
| SM    |  0.6990 |  0.5030 |
| SN    |  0.6670 |  0.4780 |
| SO    |  0.7810 |  0.5360 |
| SR    |  0.5710 |  0.3990 |
| SS    |  0.6790 |  0.5050 |
| ST    |  0.5100 |  0.4710 |
| SV    |  0.6570 |  0.4430 |
| SW    |  0.5790 |  0.4790 |
| SZ    |  0.8110 |  0.5460 |