



# wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 10:18 AM UTC

PDB ID : 8FLC / pdb\_00008flc  
EMDB ID : EMD-29274  
Title : Human nuclear pre-60S ribosomal subunit (State K3)  
Authors : Vanden Broeck, A.; Klinge, S.  
Deposited on : 2022-12-21  
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

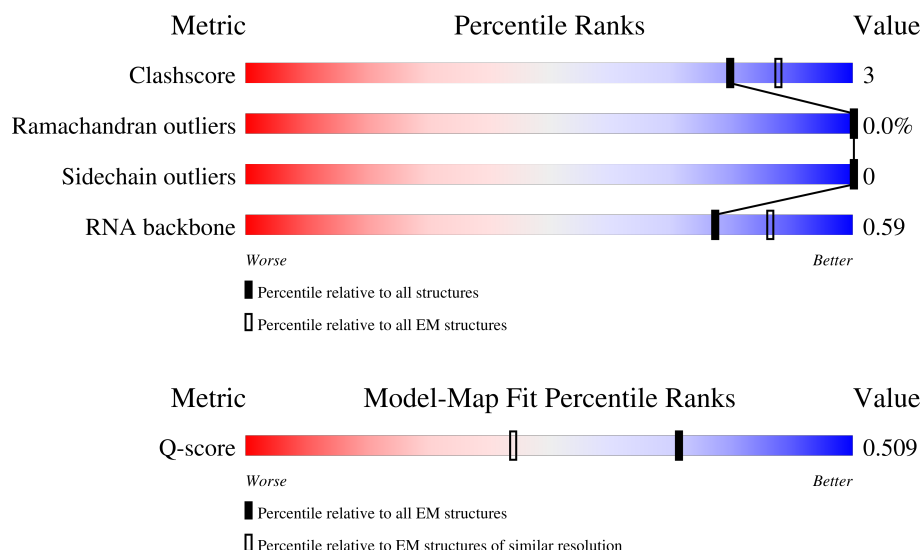
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.76 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.





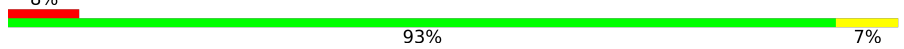
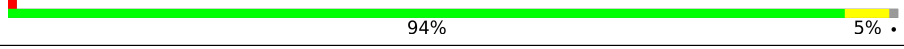

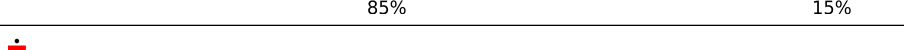
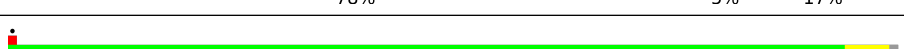
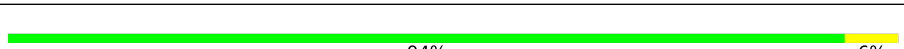

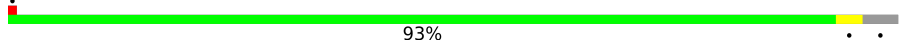

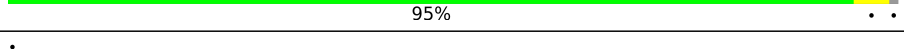


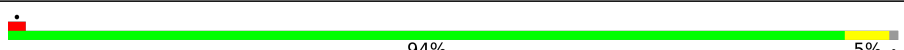

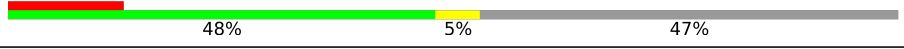








| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| RNA backbone          | 8273                        | 3508                        | -  |
| Q-score               | -                           | 25397                       | 10642 ( 2.26 - 3.26 )                                    |

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   | BA    | 165    | <div> <div>35%</div> <div>55%</div> <div>45%</div> </div>                           |
| 2   | L1    | 157    | <div> <div>6%</div> <div>76%</div> <div>19%</div> <div>••</div> </div>              |
| 3   | L3    | 5070   | <div> <div>•</div> <div>51%</div> <div>14%</div> <div>•</div> <div>33%</div> </div> |



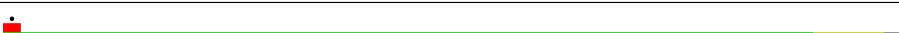
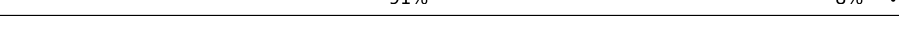





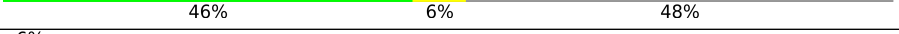












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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | L4    | 121    |    |
| 5   | L5    | 178    |    |
| 6   | L6    | 211    |    |
| 7   | L7    | 203    |    |
| 8   | L8    | 215    |    |
| 9   | L9    | 204    |    |
| 10  | LA    | 184    |    |
| 11  | LB    | 188    |    |
| 12  | LC    | 176    |    |
| 13  | LD    | 196    |    |
| 14  | LE    | 160    |   |
| 15  | LF    | 128    |  |
| 16  | LG    | 140    |  |
| 17  | LH    | 156    |  |
| 18  | LI    | 145    |  |
| 19  | LJ    | 136    |  |
| 20  | LK    | 148    |  |
| 21  | LL    | 137    |  |
| 22  | LM    | 159    |  |
| 23  | LN    | 403    |  |
| 24  | LO    | 115    |  |
| 25  | LP    | 125    |  |
| 26  | LQ    | 135    |  |
| 27  | LR    | 117    |  |
| 28  | LS    | 123    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 29  | LT    | 110    |    |
| 30  | LU    | 105    |    |
| 31  | LV    | 106    |    |
| 32  | LW    | 97     |    |
| 33  | LX    | 92     |    |
| 34  | LY    | 70     |    |
| 35  | LZ    | 51     |    |
| 36  | NK    | 129    |    |
| 37  | NP    | 134    |    |
| 38  | NR    | 203    |    |
| 39  | SA    | 427    |    |
| 40  | SB    | 297    |    |
| 41  | SC    | 288    |    |
| 42  | SD    | 248    |    |
| 43  | SE    | 266    |   |
| 44  | SF    | 257    |  |
| 45  | SG    | 192    |  |
| 46  | SK    | 245    |  |
| 47  | SQ    | 239    |  |
| 48  | SR    | 634    |  |
| 49  | SV    | 163    |  |
| 50  | VB    | 99     |  |

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 139595 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | BA    | 91       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 449   | 267 | 91 | 91 |         |       |

- Molecule 2 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 2   | L1    | 154      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3278  | 1463 | 581 | 1080 | 154 |         |       |

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3   | L3    | 3373     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 72412 | 32273 | 13268 | 23498 | 3373 |         |       |

- Molecule 4 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4   | L4    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2561  | 1141 | 456 | 844 | 120 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | L5    | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1349  | 853 | 251 | 239 | 6 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | L6    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1064 | 352 | 281 | 4 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | L7    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1063 | 321 | 261 | 5 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | L8    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 713 | 213 | 178 | 7 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | L9    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | LA    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | LB    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1512  | 944 | 314 | 249 | 5 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12  | LC    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1461  | 930 | 284 | 236 | 11 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | LD    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1289  | 805 | 277 | 198 | 9 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | LE    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1264  | 803 | 246 | 210 | 5 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | LF    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 842   | 538 | 148 | 154 | 2 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | LG    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 648 | 199 | 182 | 5 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | LH    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 612 | 179 | 166 | 1 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | LI    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LJ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | LK    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | LL    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | LM    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 699   | 437 | 152 | 107 | 3 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | LN    | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3239  | 2061 | 608 | 556 | 14 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LO    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 468 | 131 | 133 | 6 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LP    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 879   | 555 | 170 | 152 | 2 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LQ    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LR    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 555 | 183 | 144 | 6 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L35.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LS    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | LT    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | LU    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | LV    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 851   | 533 | 174 | 138 | 6 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | LW    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | LX    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 34  | LY    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | LZ    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 36 is a protein called Protein LLP homolog.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36  | NK    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 581   | 363 | 128 | 88 | 2 |         |       |

- Molecule 37 is a protein called Zinc finger protein 593.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | NP    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 847   | 520 | 178 | 145 | 4 |         |       |

- Molecule 38 is a protein called Translation machinery-associated protein 16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | NR    | 152      | Total | C   | N   | O   | P | S       |       |
|     |       |          | 1299  | 809 | 249 | 235 | 1 | 5       | 0     |

- Molecule 39 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39  | SA    | 358      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2853  | 1797 | 570 | 473 | 13 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40  | SB    | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2243  | 1419 | 406 | 404 | 14 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | SC    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1747  | 1124 | 332 | 287 | 4 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42  | SD    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43  | SE    | 231      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1869  | 1191 | 361 | 313 | 4 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44  | SF    | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1876  | 1177 | 383 | 310 | 6 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | SG    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 46 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46  | SK    | 244      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1852  | 1149 | 318 | 372 | 13 |         |       |

- Molecule 47 is a protein called mRNA turnover protein 4 homolog.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 47  | SQ    | 127      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 650   | 388 | 132 | 130 |  |         |       |

- Molecule 48 is a protein called GTP-binding protein 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | SR    | 601      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4932  | 3105 | 899 | 902 | 26 |         |       |

- Molecule 49 is a protein called Probable ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 49  | SV    | 139      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1184  | 754 | 229 | 191 | 10 |         |       |

- Molecule 50 is a protein called Leydig cell tumor 10 kDa protein homolog.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | VB    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 285 | 95 | 74 | 1 |         |       |

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 51  | L1    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |
| 51  | L3    | 74       | Total | Mg | 0       |
|     |       |          | 74    | 74 |         |
| 51  | L4    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |
| 51  | LG    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 51  | LN    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 51  | LQ    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 51  | LR    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 51  | LT    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 51  | LW    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 51  | SF    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 51  | SR    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

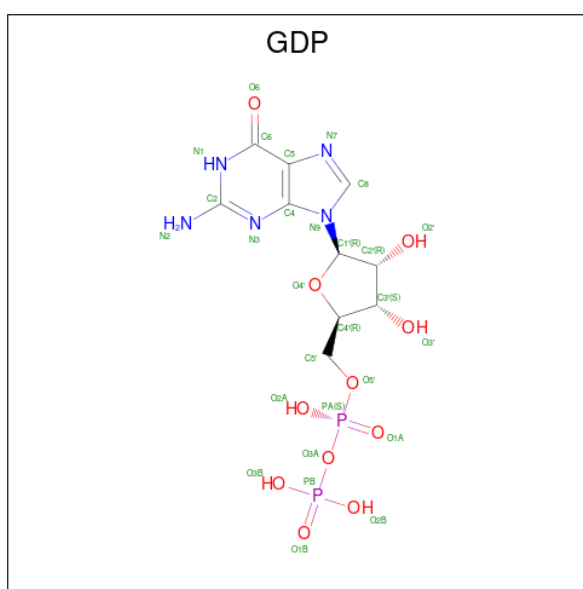
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 52  | LR    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 52  | LV    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 52  | LW    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 52  | LX    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 52  | NP    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 52  | SV    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 53 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 53  | SR    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

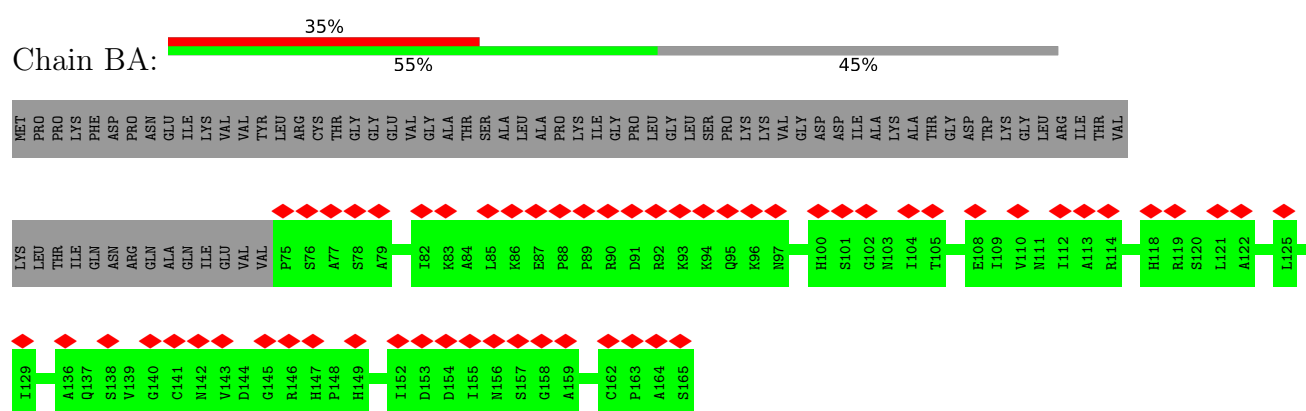
- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 54  | SR    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

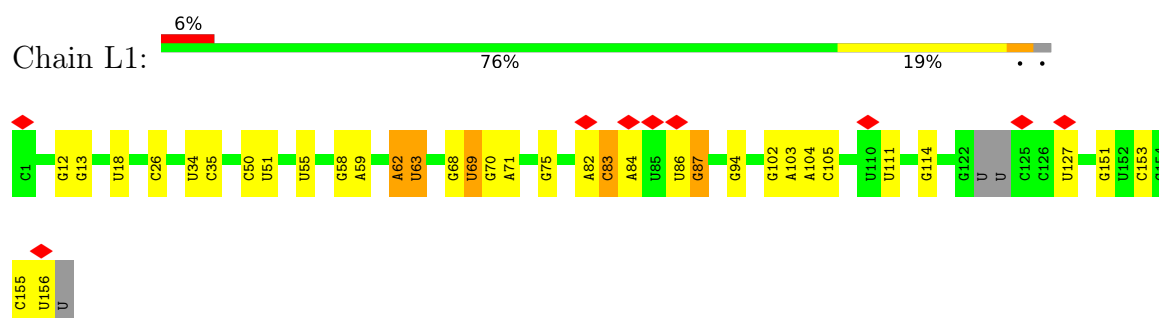
### 3 Residue-property plots

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

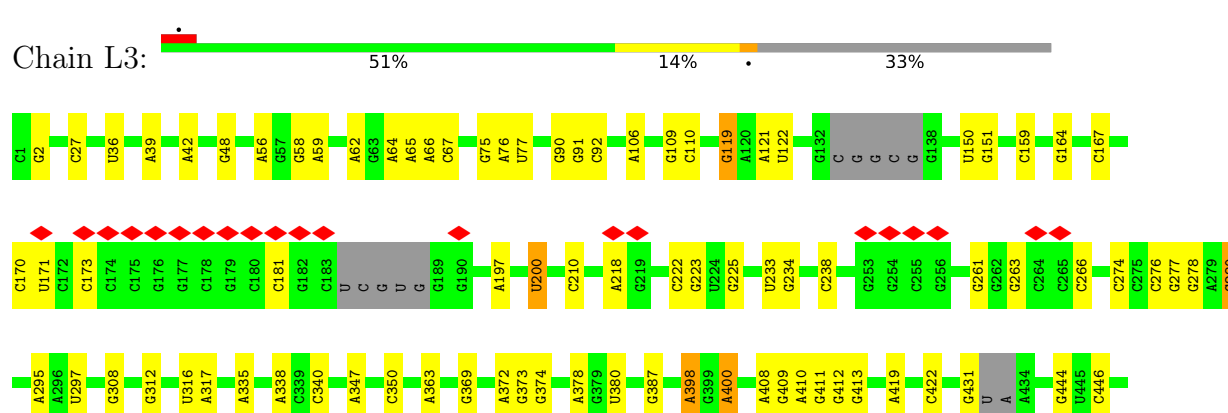
#### • Molecule 1: 60S ribosomal protein L12



#### • Molecule 2: 5.8S rRNA



#### • Molecule 3: 28S rRNA








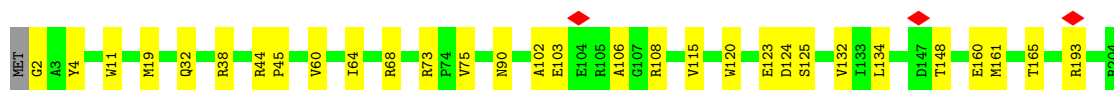







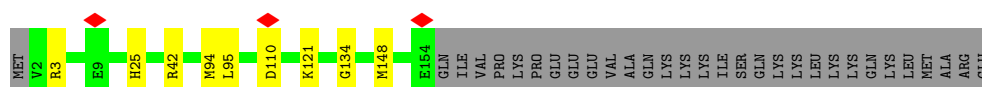
- Molecule 9: 60S ribosomal protein L15

Chain L9:  85% 15%



- Molecule 10: 60S ribosomal protein L17

Chain LA:  78% 5% 17%



- Molecule 11: 60S ribosomal protein L18

Chain LB:  94% 5%




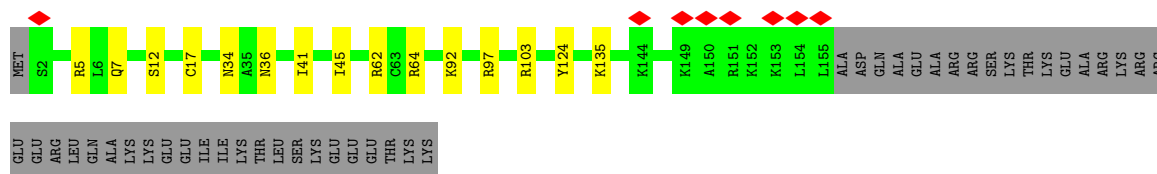
- Molecule 12: 60S ribosomal protein L18a

Chain LC:  94% 6%



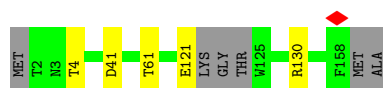
- Molecule 13: 60S ribosomal protein L19

Chain LD:  71% 8% 21%




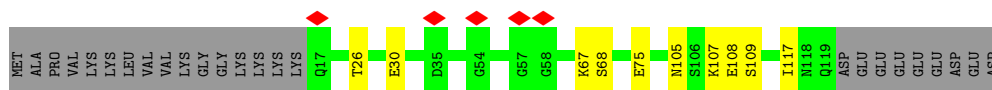
- Molecule 14: 60S ribosomal protein L21

Chain LE:  93%



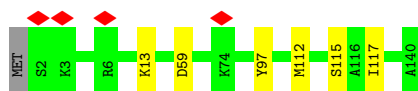
- Molecule 15: 60S ribosomal protein L22

Chain LF:  73% 8% 20%



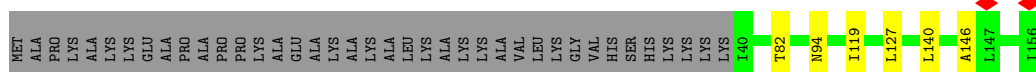
- Molecule 16: 60S ribosomal protein L23

Chain LG: 95%



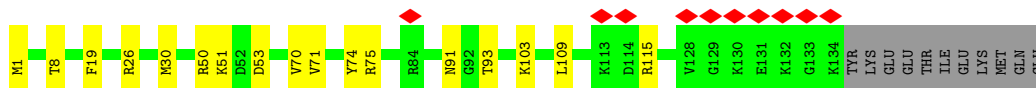
- Molecule 17: 60S ribosomal protein L23a

Chain LH: 71% 25%



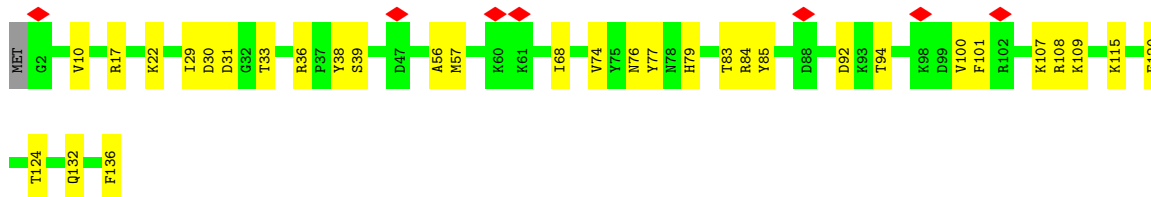
- Molecule 18: 60S ribosomal protein L26

Chain LI: 7% 81% 12% 8%



- Molecule 19: 60S ribosomal protein L27

Chain LJ: 5% 76% 24%



- Molecule 20: 60S ribosomal protein L27a

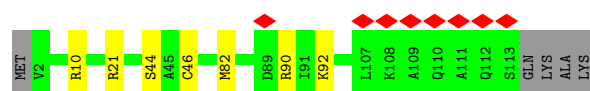
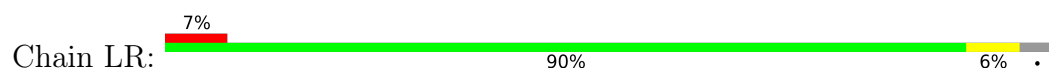
Chain LK: 94% 5%



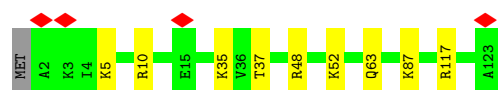
- Molecule 21: 60S ribosomal protein L28

Chain LL: 6% 88% 9%





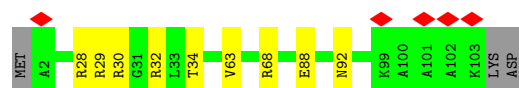
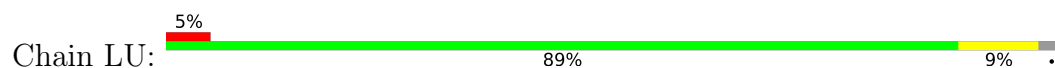
- Molecule 28: 60S ribosomal protein L35



- Molecule 29: 60S ribosomal protein L35a



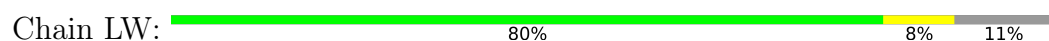
- Molecule 30: 60S ribosomal protein L36



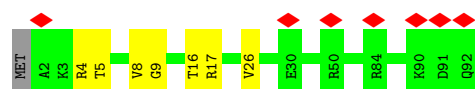
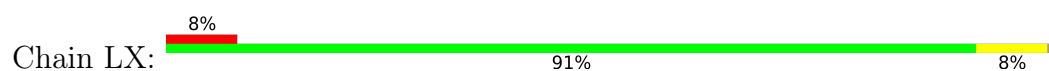
- Molecule 31: 60S ribosomal protein L36a



- Molecule 32: 60S ribosomal protein L37

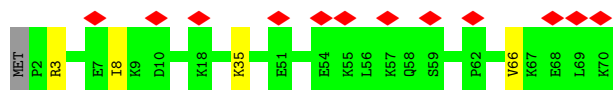


- Molecule 33: 60S ribosomal protein L37a




- Molecule 34: 60S ribosomal protein L38

Chain LY: 



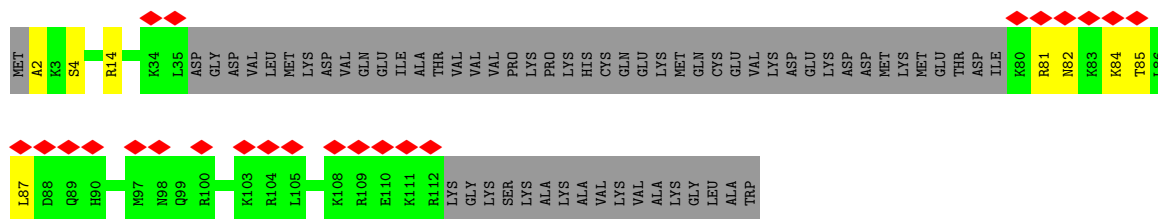
- Molecule 35: 60S ribosomal protein L39

Chain LZ: 




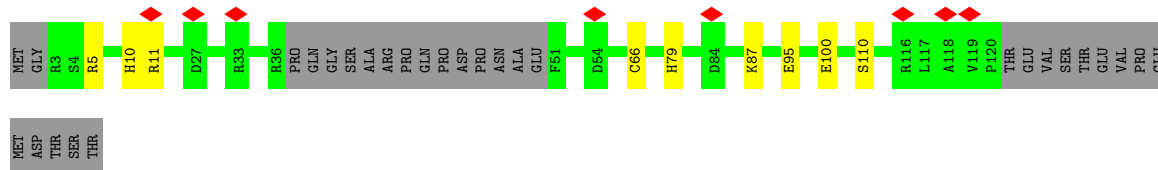
- Molecule 36: Protein LLP homolog

Chain NK: 



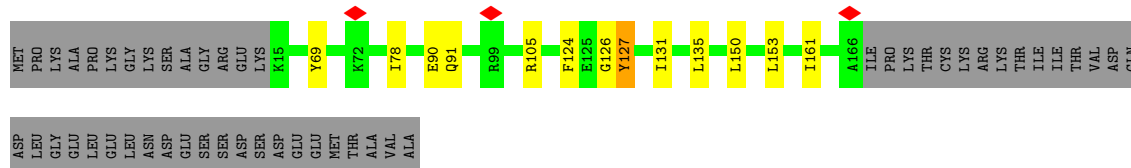
- Molecule 37: Zinc finger protein 593

Chain NP: 




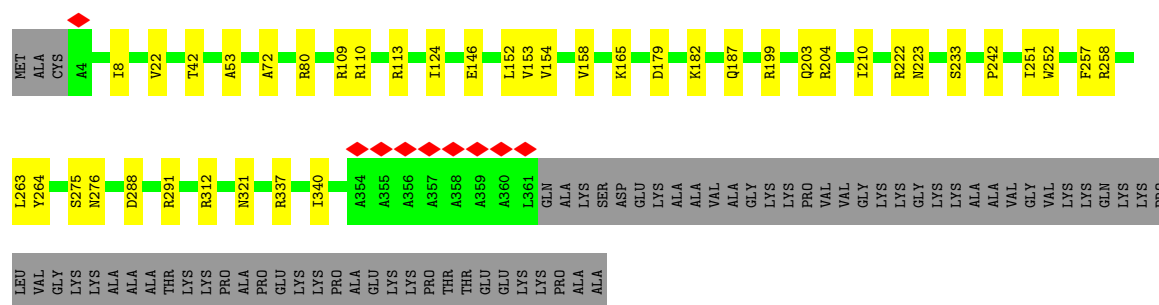
- Molecule 38: Translation machinery-associated protein 16

Chain NR: 

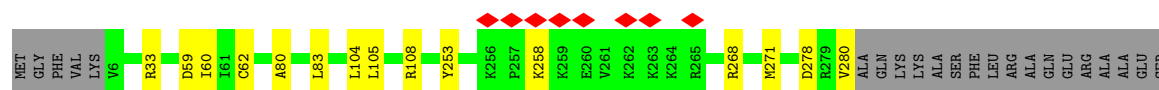


- Molecule 39: 60S ribosomal protein L4

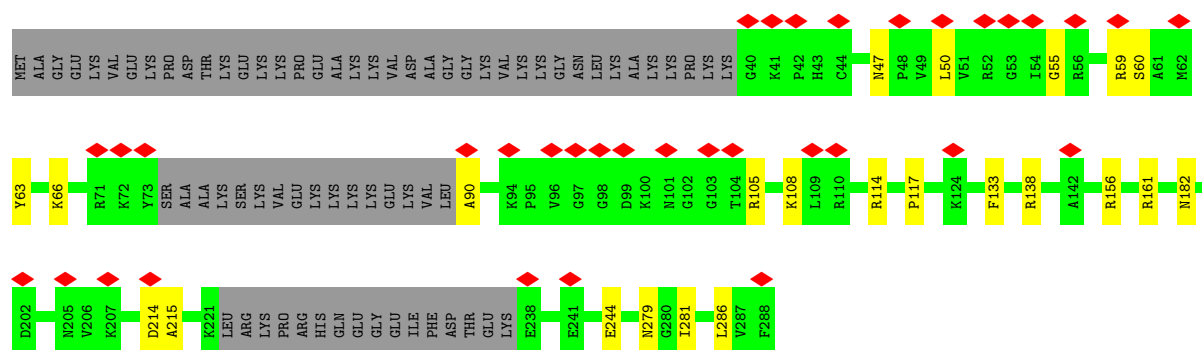
Chain SA: 



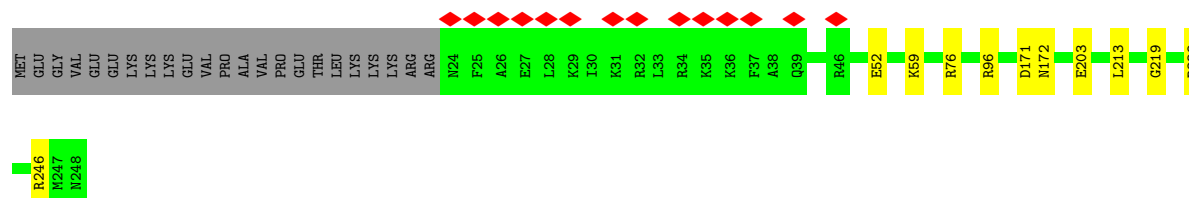
- Molecule 40: 60S ribosomal protein L5



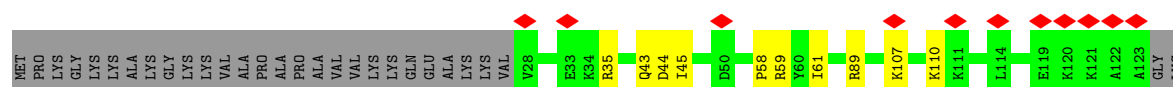
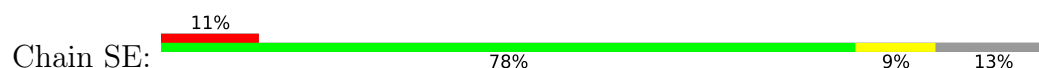
- Molecule 41: 60S ribosomal protein L6



- Molecule 42: 60S ribosomal protein L7



- Molecule 43: 60S ribosomal protein L7a







- Molecule 44: 60S ribosomal protein L8

Chain SF: 89% 7% 5%



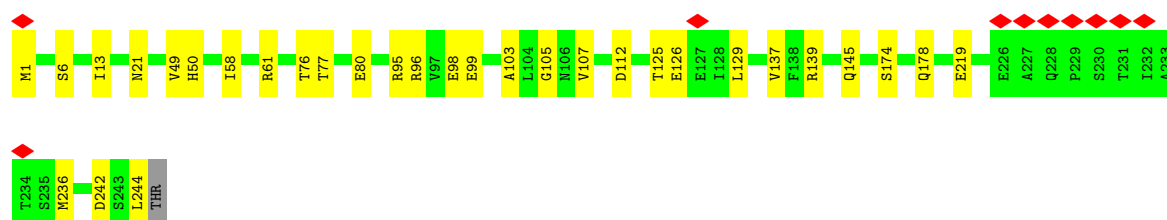
- Molecule 45: 60S ribosomal protein L9

Chain SG: 87% 12% .



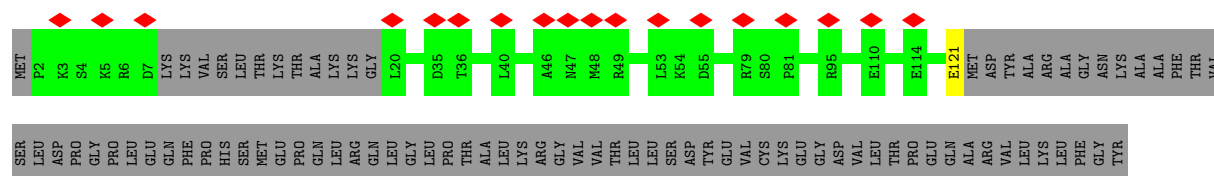
- Molecule 46: Eukaryotic translation initiation factor 6

Chain SK: 87% 13%



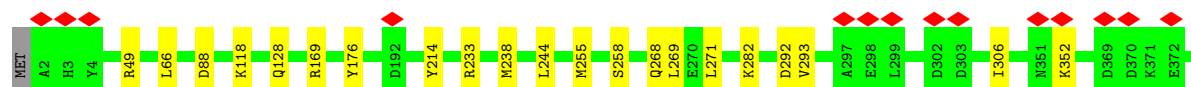
- Molecule 47: mRNA turnover protein 4 homolog

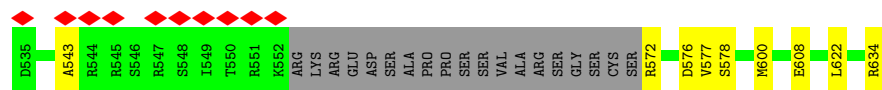
Chain SQ: 9% 52% 47%



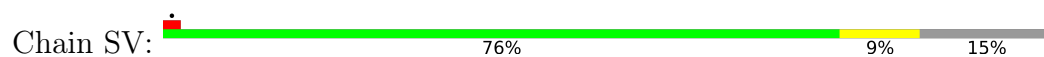
- Molecule 48: GTP-binding protein 4

Chain SR: 7% 89% 6% 5%

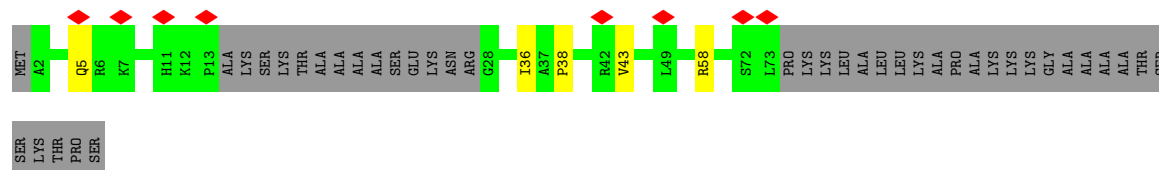




- Molecule 49: Probable ribosome biogenesis protein RLP24



- Molecule 50: Leydig cell tumor 10 kDa protein homolog



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 20809                                   | 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                    | 10.151                                  | Depositor |
| Minimum map value                    | -1.391                                  | Depositor |
| Average map value                    | 0.052                                   | Depositor |
| Map value standard deviation         | 0.177                                   | Depositor |
| Recommended contour level            | 0.85                                    | Depositor |
| Map size (Å)                         | 514.56, 514.56, 514.56                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 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: HIC, OMU, PTR, GDP, OMG, 1MA, UR3, MG, PSU, K, A2M, 6MZ, OMC, ZN

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   | BA    | 0.09         | 0/448       | 0.25        | 0/622       |
| 2   | L1    | 0.10         | 0/3589      | 0.23        | 0/5589      |
| 3   | L3    | 0.14         | 0/78513     | 0.26        | 0/122457    |
| 4   | L4    | 0.14         | 0/2861      | 0.26        | 0/4459      |
| 5   | L5    | 0.13         | 0/1372      | 0.31        | 0/1836      |
| 6   | L6    | 0.12         | 0/1732      | 0.28        | 0/2315      |
| 7   | L7    | 0.13         | 0/1682      | 0.29        | 0/2250      |
| 8   | L8    | 0.13         | 0/1133      | 0.26        | 0/1516      |
| 9   | L9    | 0.11         | 0/1746      | 0.25        | 0/2338      |
| 10  | LA    | 0.12         | 0/1268      | 0.29        | 0/1701      |
| 11  | LB    | 0.11         | 0/1536      | 0.28        | 0/2052      |
| 12  | LC    | 0.14         | 0/1501      | 0.29        | 0/2013      |
| 13  | LD    | 0.10         | 0/1305      | 0.25        | 0/1727      |
| 14  | LE    | 0.14         | 0/1291      | 0.34        | 0/1724      |
| 15  | LF    | 0.14         | 0/856       | 0.30        | 0/1149      |
| 16  | LG    | 0.13         | 0/1048      | 0.33        | 0/1402      |
| 17  | LH    | 0.10         | 0/975       | 0.26        | 0/1312      |
| 18  | LI    | 0.11         | 0/1132      | 0.26        | 0/1504      |
| 19  | LJ    | 0.11         | 0/1130      | 0.27        | 0/1507      |
| 20  | LK    | 0.12         | 0/1191      | 0.28        | 0/1591      |
| 21  | LL    | 0.09         | 0/1017      | 0.26        | 0/1364      |
| 22  | LM    | 0.13         | 0/710       | 0.29        | 0/935       |
| 23  | LN    | 0.11         | 0/3294      | 0.28        | 0/4406      |
| 24  | LO    | 0.12         | 0/748       | 0.28        | 0/1004      |
| 25  | LP    | 0.12         | 0/894       | 0.27        | 0/1204      |
| 26  | LQ    | 0.11         | 0/1071      | 0.29        | 0/1429      |
| 27  | LR    | 0.10         | 0/898       | 0.27        | 0/1197      |
| 28  | LS    | 0.09         | 0/1023      | 0.23        | 0/1351      |
| 29  | LT    | 0.11         | 0/895       | 0.28        | 0/1198      |
| 30  | LU    | 0.10         | 0/843       | 0.23        | 0/1115      |
| 31  | LV    | 0.13         | 0/864       | 0.29        | 0/1140      |
| 32  | LW    | 0.11         | 0/720       | 0.30        | 0/952       |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 33  | LX    | 0.10         | 0/718    | 0.27        | 0/953    |
| 34  | LY    | 0.10         | 0/575    | 0.27        | 0/761    |
| 35  | LZ    | 0.11         | 0/454    | 0.25        | 0/599    |
| 36  | NK    | 0.20         | 0/587    | 0.36        | 0/767    |
| 37  | NP    | 0.12         | 0/864    | 0.27        | 0/1154   |
| 38  | NR    | 0.11         | 0/1306   | 0.27        | 0/1740   |
| 39  | SA    | 0.12         | 0/2907   | 0.28        | 0/3905   |
| 40  | SB    | 0.13         | 0/2287   | 0.29        | 0/3065   |
| 41  | SC    | 0.12         | 0/1781   | 0.28        | 0/2388   |
| 42  | SD    | 0.11         | 0/1905   | 0.27        | 0/2539   |
| 43  | SE    | 0.11         | 0/1903   | 0.28        | 0/2559   |
| 44  | SF    | 0.13         | 0/1914   | 0.31        | 0/2567   |
| 45  | SG    | 0.13         | 0/1537   | 0.27        | 0/2066   |
| 46  | SK    | 0.12         | 0/1877   | 0.31        | 0/2554   |
| 47  | SQ    | 0.09         | 0/648    | 0.25        | 0/894    |
| 48  | SR    | 0.11         | 0/5014   | 0.26        | 0/6727   |
| 49  | SV    | 0.12         | 0/1207   | 0.27        | 0/1600   |
| 50  | VB    | 0.09         | 0/459    | 0.24        | 0/605    |
| All | All   | 0.13         | 0/147229 | 0.27        | 0/215802 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | BA    | 449   | 0        | 207      | 0       | 0            |
| 2   | L1    | 3278  | 0        | 1665     | 19      | 0            |
| 3   | L3    | 72412 | 0        | 36680    | 349     | 0            |
| 4   | L4    | 2561  | 0        | 1295     | 7       | 0            |
| 5   | L5    | 1349  | 0        | 1383     | 7       | 0            |
| 6   | L6    | 1701  | 0        | 1818     | 13      | 0            |
| 7   | L7    | 1650  | 0        | 1794     | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | L8    | 1111  | 0        | 1174     | 5       | 0            |
| 9   | L9    | 1701  | 0        | 1749     | 23      | 0            |
| 10  | LA    | 1242  | 0        | 1269     | 8       | 0            |
| 11  | LB    | 1512  | 0        | 1628     | 9       | 0            |
| 12  | LC    | 1461  | 0        | 1502     | 11      | 0            |
| 13  | LD    | 1289  | 0        | 1429     | 13      | 0            |
| 14  | LE    | 1264  | 0        | 1328     | 4       | 0            |
| 15  | LF    | 842   | 0        | 864      | 7       | 0            |
| 16  | LG    | 1034  | 0        | 1097     | 4       | 0            |
| 17  | LH    | 958   | 0        | 1027     | 4       | 0            |
| 18  | LI    | 1115  | 0        | 1205     | 12      | 0            |
| 19  | LJ    | 1107  | 0        | 1182     | 22      | 0            |
| 20  | LK    | 1162  | 0        | 1213     | 7       | 0            |
| 21  | LL    | 1002  | 0        | 1068     | 5       | 0            |
| 22  | LM    | 699   | 0        | 758      | 7       | 0            |
| 23  | LN    | 3239  | 0        | 3377     | 32      | 0            |
| 24  | LO    | 738   | 0        | 774      | 3       | 0            |
| 25  | LP    | 879   | 0        | 924      | 6       | 0            |
| 26  | LQ    | 1053  | 0        | 1147     | 12      | 0            |
| 27  | LR    | 888   | 0        | 977      | 6       | 0            |
| 28  | LS    | 1015  | 0        | 1148     | 8       | 0            |
| 29  | LT    | 876   | 0        | 912      | 6       | 0            |
| 30  | LU    | 832   | 0        | 917      | 7       | 0            |
| 31  | LV    | 851   | 0        | 920      | 6       | 0            |
| 32  | LW    | 705   | 0        | 737      | 7       | 0            |
| 33  | LX    | 708   | 0        | 756      | 6       | 0            |
| 34  | LY    | 569   | 0        | 637      | 5       | 0            |
| 35  | LZ    | 444   | 0        | 483      | 4       | 0            |
| 36  | NK    | 581   | 0        | 656      | 9       | 0            |
| 37  | NP    | 847   | 0        | 854      | 8       | 0            |
| 38  | NR    | 1299  | 0        | 1318     | 8       | 0            |
| 39  | SA    | 2853  | 0        | 3028     | 32      | 0            |
| 40  | SB    | 2243  | 0        | 2268     | 11      | 0            |
| 41  | SC    | 1747  | 0        | 1897     | 20      | 0            |
| 42  | SD    | 1870  | 0        | 1996     | 9       | 0            |
| 43  | SE    | 1869  | 0        | 2014     | 18      | 0            |
| 44  | SF    | 1876  | 0        | 1970     | 15      | 0            |
| 45  | SG    | 1518  | 0        | 1601     | 15      | 0            |
| 46  | SK    | 1852  | 0        | 1828     | 19      | 0            |
| 47  | SQ    | 650   | 0        | 308      | 1       | 0            |
| 48  | SR    | 4932  | 0        | 5072     | 30      | 0            |
| 49  | SV    | 1184  | 0        | 1248     | 12      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 50  | VB    | 455    | 0        | 504      | 4       | 0            |
| 51  | L1    | 3      | 0        | 0        | 0       | 0            |
| 51  | L3    | 74     | 0        | 0        | 0       | 0            |
| 51  | L4    | 3      | 0        | 0        | 0       | 0            |
| 51  | LG    | 1      | 0        | 0        | 0       | 0            |
| 51  | LN    | 1      | 0        | 0        | 0       | 0            |
| 51  | LQ    | 1      | 0        | 0        | 0       | 0            |
| 51  | LR    | 1      | 0        | 0        | 0       | 0            |
| 51  | LT    | 1      | 0        | 0        | 0       | 0            |
| 51  | LW    | 1      | 0        | 0        | 0       | 0            |
| 51  | SF    | 1      | 0        | 0        | 0       | 0            |
| 51  | SR    | 1      | 0        | 0        | 0       | 0            |
| 52  | LR    | 1      | 0        | 0        | 0       | 0            |
| 52  | LV    | 1      | 0        | 0        | 0       | 0            |
| 52  | LW    | 1      | 0        | 0        | 0       | 0            |
| 52  | LX    | 1      | 0        | 0        | 0       | 0            |
| 52  | NP    | 1      | 0        | 0        | 0       | 0            |
| 52  | SV    | 1      | 0        | 0        | 0       | 0            |
| 53  | SR    | 28     | 0        | 12       | 0       | 0            |
| 54  | SR    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 139595 | 0        | 103618   | 643     | 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 3.

The worst 5 of 643 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) |
|------------------|------------------|--------------------------|-------------------|
| 36:NK:81:ARG:NH2 | 36:NK:85:THR:OG1 | 2.02                     | 0.93              |
| 9:L9:64:ILE:HD11 | 9:L9:106:ALA:HB2 | 1.49                     | 0.93              |
| 3:L3:4903:G:OP1  | 36:NK:82:ASN:ND2 | 2.04                     | 0.90              |
| 6:L6:60:ARG:NH2  | 6:L6:67:HIS:O    | 2.10                     | 0.85              |
| 3:L3:2520:C:O2   | 3:L3:2640:G:N2   | 2.11                     | 0.83              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | BA    | 89/165 (54%)  | 89 (100%)  | 0       | 0        | 100         | 100 |
| 5   | L5    | 166/178 (93%) | 164 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 6   | L6    | 208/211 (99%) | 204 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 7   | L7    | 199/203 (98%) | 195 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 8   | L8    | 133/215 (62%) | 132 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 9   | L9    | 201/204 (98%) | 199 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 10  | LA    | 151/184 (82%) | 148 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 11  | LB    | 185/188 (98%) | 183 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 12  | LC    | 174/176 (99%) | 171 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 13  | LD    | 152/196 (78%) | 152 (100%) | 0       | 0        | 100         | 100 |
| 14  | LE    | 150/160 (94%) | 146 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 15  | LF    | 101/128 (79%) | 99 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 16  | LG    | 137/140 (98%) | 134 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 17  | LH    | 115/156 (74%) | 114 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 18  | LI    | 132/145 (91%) | 131 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 19  | LJ    | 133/136 (98%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 20  | LK    | 145/148 (98%) | 143 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 21  | LL    | 123/137 (90%) | 122 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 22  | LM    | 81/159 (51%)  | 80 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 23  | LN    | 399/403 (99%) | 390 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 24  | LO    | 93/115 (81%)  | 92 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 25  | LP    | 104/125 (83%) | 104 (100%) | 0       | 0        | 100         | 100 |
| 26  | LQ    | 126/135 (93%) | 124 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 27  | LR    | 110/117 (94%) | 108 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 28  | LS    | 120/123 (98%) | 120 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 29  | LT    | 107/110 (97%)   | 107 (100%) | 0        | 0        | 100         | 100 |
| 30  | LU    | 100/105 (95%)   | 99 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 31  | LV    | 102/106 (96%)   | 101 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 32  | LW    | 84/97 (87%)     | 83 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 33  | LX    | 89/92 (97%)     | 87 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 34  | LY    | 67/70 (96%)     | 67 (100%)  | 0        | 0        | 100         | 100 |
| 35  | LZ    | 48/51 (94%)     | 48 (100%)  | 0        | 0        | 100         | 100 |
| 36  | NK    | 63/129 (49%)    | 61 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 37  | NP    | 100/134 (75%)   | 100 (100%) | 0        | 0        | 100         | 100 |
| 38  | NR    | 150/203 (74%)   | 147 (98%)  | 2 (1%)   | 1 (1%)   | 18          | 34  |
| 39  | SA    | 356/427 (83%)   | 349 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 40  | SB    | 273/297 (92%)   | 265 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 41  | SC    | 211/288 (73%)   | 204 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 42  | SD    | 223/248 (90%)   | 219 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 43  | SE    | 228/266 (86%)   | 227 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 44  | SF    | 243/257 (95%)   | 236 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 45  | SG    | 188/192 (98%)   | 186 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 46  | SK    | 242/245 (99%)   | 235 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 47  | SQ    | 121/239 (51%)   | 121 (100%) | 0        | 0        | 100         | 100 |
| 48  | SR    | 595/634 (94%)   | 589 (99%)  | 5 (1%)   | 1 (0%)   | 43          | 64  |
| 49  | SV    | 137/163 (84%)   | 137 (100%) | 0        | 0        | 100         | 100 |
| 50  | VB    | 54/99 (54%)     | 54 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 7508/8699 (86%) | 7397 (98%) | 109 (2%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | NR    | 126 | GLY  |
| 48  | SR    | 88  | ASP  |

### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 5   | L5    | 142/149 (95%)  | 142 (100%) | 0        | 100         | 100 |
| 6   | L6    | 176/177 (99%)  | 176 (100%) | 0        | 100         | 100 |
| 7   | L7    | 173/174 (99%)  | 173 (100%) | 0        | 100         | 100 |
| 8   | L8    | 115/161 (71%)  | 115 (100%) | 0        | 100         | 100 |
| 9   | L9    | 171/172 (99%)  | 171 (100%) | 0        | 100         | 100 |
| 10  | LA    | 134/163 (82%)  | 134 (100%) | 0        | 100         | 100 |
| 11  | LB    | 164/165 (99%)  | 164 (100%) | 0        | 100         | 100 |
| 12  | LC    | 157/157 (100%) | 157 (100%) | 0        | 100         | 100 |
| 13  | LD    | 138/175 (79%)  | 138 (100%) | 0        | 100         | 100 |
| 14  | LE    | 136/140 (97%)  | 136 (100%) | 0        | 100         | 100 |
| 15  | LF    | 93/115 (81%)   | 93 (100%)  | 0        | 100         | 100 |
| 16  | LG    | 106/107 (99%)  | 106 (100%) | 0        | 100         | 100 |
| 17  | LH    | 105/133 (79%)  | 105 (100%) | 0        | 100         | 100 |
| 18  | LI    | 124/135 (92%)  | 124 (100%) | 0        | 100         | 100 |
| 19  | LJ    | 117/118 (99%)  | 117 (100%) | 0        | 100         | 100 |
| 20  | LK    | 120/121 (99%)  | 120 (100%) | 0        | 100         | 100 |
| 21  | LL    | 109/121 (90%)  | 109 (100%) | 0        | 100         | 100 |
| 22  | LM    | 71/126 (56%)   | 71 (100%)  | 0        | 100         | 100 |
| 23  | LN    | 347/348 (100%) | 347 (100%) | 0        | 100         | 100 |
| 24  | LO    | 80/97 (82%)    | 80 (100%)  | 0        | 100         | 100 |
| 25  | LP    | 97/110 (88%)   | 97 (100%)  | 0        | 100         | 100 |
| 26  | LQ    | 114/121 (94%)  | 114 (100%) | 0        | 100         | 100 |
| 27  | LR    | 96/100 (96%)   | 96 (100%)  | 0        | 100         | 100 |
| 28  | LS    | 109/110 (99%)  | 109 (100%) | 0        | 100         | 100 |
| 29  | LT    | 88/89 (99%)    | 88 (100%)  | 0        | 100         | 100 |
| 30  | LU    | 86/89 (97%)    | 86 (100%)  | 0        | 100         | 100 |
| 31  | LV    | 92/94 (98%)    | 92 (100%)  | 0        | 100         | 100 |
| 32  | LW    | 73/80 (91%)    | 73 (100%)  | 0        | 100         | 100 |
| 33  | LX    | 74/75 (99%)    | 74 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 34  | LY    | 64/65 (98%)     | 64 (100%)   | 0        | 100         | 100 |
| 35  | LZ    | 47/48 (98%)     | 47 (100%)   | 0        | 100         | 100 |
| 36  | NK    | 61/115 (53%)    | 61 (100%)   | 0        | 100         | 100 |
| 37  | NP    | 88/114 (77%)    | 88 (100%)   | 0        | 100         | 100 |
| 38  | NR    | 140/183 (76%)   | 140 (100%)  | 0        | 100         | 100 |
| 39  | SA    | 298/348 (86%)   | 298 (100%)  | 0        | 100         | 100 |
| 40  | SB    | 234/250 (94%)   | 234 (100%)  | 0        | 100         | 100 |
| 41  | SC    | 192/252 (76%)   | 192 (100%)  | 0        | 100         | 100 |
| 42  | SD    | 194/215 (90%)   | 194 (100%)  | 0        | 100         | 100 |
| 43  | SE    | 198/223 (89%)   | 198 (100%)  | 0        | 100         | 100 |
| 44  | SF    | 188/199 (94%)   | 188 (100%)  | 0        | 100         | 100 |
| 45  | SG    | 169/171 (99%)   | 169 (100%)  | 0        | 100         | 100 |
| 46  | SK    | 212/213 (100%)  | 212 (100%)  | 0        | 100         | 100 |
| 47  | SQ    | 6/214 (3%)      | 6 (100%)    | 0        | 100         | 100 |
| 48  | SR    | 545/574 (95%)   | 545 (100%)  | 0        | 100         | 100 |
| 49  | SV    | 128/149 (86%)   | 128 (100%)  | 0        | 100         | 100 |
| 50  | VB    | 48/76 (63%)     | 48 (100%)   | 0        | 100         | 100 |
| All | All   | 6419/7331 (88%) | 6419 (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. 5 of 60 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | LO    | 72  | HIS  |
| 48  | SR    | 153 | GLN  |
| 32  | LW    | 13  | ASN  |
| 48  | SR    | 64  | GLN  |
| 49  | SV    | 17  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 2   | L1    | 152/157 (96%) | 17 (11%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 3   | L3    | 3344/5070 (65%) | 432 (12%)         | 10 (0%)         |
| 4   | L4    | 119/121 (98%)   | 10 (8%)           | 1 (0%)          |
| All | All   | 3615/5348 (67%) | 459 (12%)         | 11 (0%)         |

5 of 459 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L1    | 34  | U    |
| 2   | L1    | 35  | C    |
| 2   | L1    | 59  | A    |
| 2   | L1    | 62  | A    |
| 2   | L1    | 63  | U    |

5 of 11 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L3    | 2469 | C    |
| 3   | L3    | 2477 | A    |
| 4   | L4    | 109  | U    |
| 3   | L3    | 3616 | U    |
| 3   | L3    | 1633 | G    |

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

109 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 | $\# Z  > 2$ |
| 3   | PSU  | L3    | 3639 | 3    | 18,21,22     | 1.11 | 1 (5%)      | 21,30,33    | 1.95 | 5 (23%)     |
| 3   | OMC  | L3    | 2861 | 3    | 19,22,23     | 0.48 | 0           | 25,31,34    | 0.68 | 0           |
| 3   | A2M  | L3    | 4523 | 3    | 22,25,26     | 0.85 | 0           | 30,36,39    | 2.12 | 8 (26%)     |
| 3   | PSU  | L3    | 4361 | 3    | 18,21,22     | 1.06 | 1 (5%)      | 21,30,33    | 1.96 | 5 (23%)     |
| 3   | OMU  | L3    | 2415 | 3    | 19,22,23     | 2.07 | 7 (36%)     | 25,31,34    | 1.80 | 5 (20%)     |
| 3   | A2M  | L3    | 1524 | 3    | 22,25,26     | 0.86 | 0           | 30,36,39    | 2.11 | 8 (26%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMG  | L3    | 4499 | 3    | 23,26,27     | 0.44 | 0        | 32,38,41    | 0.47 | 0        |
| 3   | PSU  | L3    | 4293 | 3    | 18,21,22     | 1.05 | 1 (5%)   | 21,30,33    | 1.87 | 4 (19%)  |
| 3   | OMG  | L3    | 4618 | 3    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.51 | 0        |
| 3   | OMU  | L3    | 4620 | 3    | 19,22,23     | 2.03 | 6 (31%)  | 25,31,34    | 1.68 | 4 (16%)  |
| 3   | A2M  | L3    | 398  | 3    | 22,25,26     | 0.83 | 0        | 30,36,39    | 2.13 | 8 (26%)  |
| 3   | OMG  | L3    | 1316 | 3    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.47 | 0        |
| 3   | PSU  | L3    | 3844 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | OMC  | L3    | 2365 | 3    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.70 | 0        |
| 3   | PSU  | L3    | 4431 | 3    | 18,21,22     | 1.14 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | PSU  | L3    | 3715 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.94 | 6 (28%)  |
| 3   | OMC  | L3    | 3869 | 3    | 19,22,23     | 0.50 | 0        | 25,31,34    | 0.65 | 0        |
| 3   | A2M  | L3    | 2363 | 3,51 | 22,25,26     | 0.88 | 0        | 30,36,39    | 2.09 | 7 (23%)  |
| 3   | OMC  | L3    | 3701 | 3    | 19,22,23     | 0.47 | 0        | 25,31,34    | 0.66 | 0        |
| 3   | A2M  | L3    | 4571 | 3    | 22,25,26     | 0.85 | 0        | 30,36,39    | 2.04 | 7 (23%)  |
| 3   | PSU  | L3    | 4576 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.93 | 6 (28%)  |
| 2   | OMG  | L1    | 75   | 2    | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.46 | 0        |
| 3   | OMC  | L3    | 2804 | 3    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.70 | 0        |
| 3   | OMG  | L3    | 4637 | 3    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.46 | 0        |
| 3   | A2M  | L3    | 2787 | 3    | 22,25,26     | 0.86 | 0        | 30,36,39    | 2.11 | 7 (23%)  |
| 3   | PSU  | L3    | 3822 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | PSU  | L3    | 2632 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.85 | 4 (19%)  |
| 3   | OMG  | L3    | 1625 | 3    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.45 | 0        |
| 3   | OMC  | L3    | 2422 | 3,51 | 19,22,23     | 0.50 | 0        | 25,31,34    | 0.78 | 1 (4%)   |
| 23  | HIC  | LN    | 245  | 23   | 10,11,12     | 1.53 | 1 (10%)  | 9,14,16     | 1.21 | 1 (11%)  |
| 3   | OMG  | L3    | 3627 | 3    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.53 | 0        |
| 3   | PSU  | L3    | 4689 | 3    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.96 | 5 (23%)  |
| 2   | PSU  | L1    | 69   | 2    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | OMG  | L3    | 3744 | 3    | 23,26,27     | 0.44 | 0        | 32,38,41    | 0.48 | 0        |
| 3   | PSU  | L3    | 4457 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 3   | PSU  | L3    | 4299 | 3    | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 2.00 | 5 (23%)  |
| 2   | PSU  | L1    | 55   | 2    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.96 | 5 (23%)  |
| 3   | A2M  | L3    | 400  | 3    | 22,25,26     | 0.85 | 0        | 30,36,39    | 2.09 | 8 (26%)  |
| 3   | PSU  | L3    | 3730 | 3    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | PSU  | L3    | 1677 | 3    | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.90 | 5 (23%)  |
| 3   | PSU  | L3    | 4500 | 3    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 3   | PSU  | L3    | 5010 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.93 | 5 (23%)  |
| 3   | OMG  | L3    | 2364 | 3    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.46 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | L3    | 4403 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.97 | 6 (28%)  |
| 3   | PSU  | L3    | 3884 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 3   | A2M  | L3    | 3867 | 3    | 22,25,26     | 0.85 | 0        | 30,36,39    | 2.12 | 8 (26%)  |
| 3   | PSU  | L3    | 4972 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.94 | 5 (23%)  |
| 3   | A2M  | L3    | 3830 | 3    | 22,25,26     | 0.83 | 0        | 30,36,39    | 2.08 | 7 (23%)  |
| 3   | PSU  | L3    | 3637 | 3    | 18,21,22     | 1.11 | 1 (5%)   | 21,30,33    | 2.12 | 5 (23%)  |
| 3   | A2M  | L3    | 1534 | 3,51 | 22,25,26     | 0.83 | 0        | 30,36,39    | 2.18 | 8 (26%)  |
| 3   | PSU  | L3    | 1792 | 3    | 18,21,22     | 1.11 | 1 (5%)   | 21,30,33    | 1.91 | 5 (23%)  |
| 3   | OMG  | L3    | 4370 | 3    | 23,26,27     | 0.49 | 0        | 32,38,41    | 0.53 | 0        |
| 3   | OMC  | L3    | 4456 | 3    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.65 | 0        |
| 3   | PSU  | L3    | 4296 | 3    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.99 | 5 (23%)  |
| 3   | PSU  | L3    | 4353 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.99 | 5 (23%)  |
| 3   | OMU  | L3    | 4498 | 3    | 19,22,23     | 2.10 | 7 (36%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 3   | OMC  | L3    | 4536 | 3    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.66 | 0        |
| 3   | PSU  | L3    | 4628 | 3    | 18,21,22     | 1.03 | 1 (5%)   | 21,30,33    | 1.92 | 6 (28%)  |
| 3   | OMC  | L3    | 2351 | 3,51 | 19,22,23     | 0.52 | 0        | 25,31,34    | 0.70 | 0        |
| 3   | PSU  | L3    | 2839 | 3    | 18,21,22     | 1.11 | 1 (5%)   | 21,30,33    | 1.96 | 5 (23%)  |
| 3   | OMU  | L3    | 4227 | 3    | 19,22,23     | 2.05 | 7 (36%)  | 25,31,34    | 1.85 | 4 (16%)  |
| 3   | OMG  | L3    | 4494 | 3    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.51 | 0        |
| 3   | OMG  | L3    | 4392 | 3    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.48 | 0        |
| 3   | PSU  | L3    | 1582 | 3    | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.92 | 4 (19%)  |
| 3   | PSU  | L3    | 1860 | 3    | 18,21,22     | 1.11 | 1 (5%)   | 21,30,33    | 1.93 | 5 (23%)  |
| 3   | PSU  | L3    | 2508 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.91 | 5 (23%)  |
| 3   | A2M  | L3    | 3724 | 3    | 22,25,26     | 0.86 | 0        | 30,36,39    | 2.05 | 7 (23%)  |
| 3   | PSU  | L3    | 3851 | 3    | 18,21,22     | 1.14 | 1 (5%)   | 21,30,33    | 1.95 | 6 (28%)  |
| 3   | OMG  | L3    | 2424 | 3    | 23,26,27     | 0.47 | 0        | 32,38,41    | 0.46 | 0        |
| 3   | PSU  | L3    | 3853 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.86 | 4 (19%)  |
| 3   | PSU  | L3    | 4471 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | A2M  | L3    | 1871 | 3    | 22,25,26     | 0.84 | 0        | 30,36,39    | 2.17 | 8 (26%)  |
| 3   | OMG  | L3    | 4623 | 3    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.53 | 0        |
| 3   | PSU  | L3    | 4493 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | A2M  | L3    | 2815 | 3    | 22,25,26     | 0.86 | 0        | 30,36,39    | 2.13 | 8 (26%)  |
| 3   | 6MZ  | L3    | 4220 | 3    | 22,25,26     | 1.14 | 1 (4%)   | 29,36,39    | 2.17 | 9 (31%)  |
| 3   | A2M  | L3    | 1326 | 3    | 22,25,26     | 0.86 | 0        | 30,36,39    | 2.08 | 7 (23%)  |
| 3   | A2M  | L3    | 4590 | 3    | 22,25,26     | 0.87 | 0        | 30,36,39    | 2.05 | 8 (26%)  |
| 3   | OMC  | L3    | 1340 | 3    | 19,22,23     | 0.52 | 0        | 25,31,34    | 0.64 | 0        |
| 3   | OMC  | L3    | 3841 | 3    | 19,22,23     | 0.49 | 0        | 25,31,34    | 0.63 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | L3    | 4579 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.93 | 4 (19%)  |
| 3   | PSU  | L3    | 4636 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 2.00 | 5 (23%)  |
| 3   | PSU  | L3    | 1536 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.96 | 5 (23%)  |
| 3   | A2M  | L3    | 3825 | 3    | 22,25,26     | 0.84 | 0        | 30,36,39    | 2.08 | 7 (23%)  |
| 3   | PSU  | L3    | 3920 | 3,51 | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.94 | 6 (28%)  |
| 3   | OMC  | L3    | 3887 | 3    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.68 | 0        |
| 3   | OMG  | L3    | 4228 | 3    | 23,26,27     | 0.48 | 0        | 32,38,41    | 0.54 | 0        |
| 38  | PTR  | NR    | 127  | 38   | 15,16,17     | 1.28 | 1 (6%)   | 17,22,24    | 0.65 | 0        |
| 3   | 1MA  | L3    | 1322 | 3    | 21,25,26     | 0.47 | 0        | 30,37,40    | 0.84 | 1 (3%)   |
| 3   | OMG  | L3    | 2876 | 3    | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.46 | 0        |
| 3   | PSU  | L3    | 1683 | 3    | 18,21,22     | 1.11 | 1 (5%)   | 21,30,33    | 1.93 | 5 (23%)  |
| 3   | OMU  | L3    | 2837 | 3    | 19,22,23     | 2.07 | 7 (36%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 3   | A2M  | L3    | 3718 | 3    | 22,25,26     | 0.85 | 0        | 30,36,39    | 2.11 | 8 (26%)  |
| 3   | PSU  | L3    | 4312 | 3    | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.99 | 5 (23%)  |
| 3   | UR3  | L3    | 4530 | 3    | 19,22,23     | 1.07 | 3 (15%)  | 26,32,35    | 1.52 | 2 (7%)   |
| 3   | PSU  | L3    | 3734 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.91 | 5 (23%)  |
| 3   | OMC  | L3    | 2824 | 3    | 19,22,23     | 0.49 | 0        | 25,31,34    | 0.62 | 0        |
| 3   | PSU  | L3    | 4532 | 3    | 18,21,22     | 1.11 | 1 (5%)   | 21,30,33    | 1.97 | 5 (23%)  |
| 3   | PSU  | L3    | 4552 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.92 | 5 (23%)  |
| 3   | PSU  | L3    | 1862 | 3    | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.99 | 6 (28%)  |
| 3   | PSU  | L3    | 4521 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.91 | 5 (23%)  |
| 3   | OMU  | L3    | 3925 | 3    | 19,22,23     | 2.06 | 7 (36%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 3   | PSU  | L3    | 4673 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.94 | 5 (23%)  |
| 3   | A2M  | L3    | 2401 | 3    | 22,25,26     | 0.85 | 0        | 30,36,39    | 2.13 | 8 (26%)  |
| 3   | PSU  | L3    | 5001 | 3    | 18,21,22     | 1.14 | 1 (5%)   | 21,30,33    | 1.94 | 6 (28%)  |
| 3   | PSU  | L3    | 3695 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.96 | 5 (23%)  |
| 3   | OMG  | L3    | 1522 | 3    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.47 | 0        |
| 3   | OMG  | L3    | 3899 | 3    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.54 | 0        |
| 3   | OMU  | L3    | 4306 | 3    | 19,22,23     | 2.04 | 6 (31%)  | 25,31,34    | 1.79 | 5 (20%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | PSU  | L3    | 3639 | 3    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | OMC  | L3    | 2861 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L3    | 4523 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4361 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 2415 | 3    | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L3    | 1524 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L3    | 4499 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4293 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 4618 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | OMU  | L3    | 4620 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L3    | 398  | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L3    | 1316 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3844 | 3    | -       | 1/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L3    | 2365 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 4431 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 3715 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L3    | 3869 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L3    | 2363 | 3,51 | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 3701 | 3    | -       | 7/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L3    | 4571 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4576 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | OMG  | L1    | 75   | 2    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 2804 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | OMG  | L3    | 4637 | 3    | -       | 3/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L3    | 2787 | 3    | -       | 5/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3822 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 2632 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 1625 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 2422 | 3,51 | -       | 2/9/27/28 | 0/2/2/2 |
| 23  | HIC  | LN    | 245  | 23   | -       | 2/5/6/8   | 0/1/1/1 |
| 3   | OMG  | L3    | 3627 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4689 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | PSU  | L1    | 69   | 2    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 3744 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4457 | 3    | -       | 1/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4299 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | PSU  | L1    | 55   | 2    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 400  | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3730 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 1677 | 3    | -       | 4/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4500 | 3    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | PSU  | L3    | 5010 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 2364 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4403 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 3884 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 3867 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4972 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 3830 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3637 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 1534 | 3,51 | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 1792 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 4370 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 4456 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 4296 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4353 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 4498 | 3    | -       | 4/9/27/28 | 0/2/2/2 |
| 3   | OMC  | L3    | 4536 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 4628 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L3    | 2351 | 3,51 | -       | 3/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 2839 | 3    | -       | 1/7/25/26 | 0/2/2/2 |
| 3   | OMU  | L3    | 4227 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | OMG  | L3    | 4494 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L3    | 4392 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 1582 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 1860 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 2508 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 3724 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3851 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L3    | 2424 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 3853 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L3    | 4471 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 1871 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L3    | 4623 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L3    | 4493 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L3    | 2815 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | 6MZ  | L3    | 4220 | 3    | -       | 3/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L3    | 1326 | 3    | -       | 4/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L3    | 4590 | 3    | -       | 4/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L3    | 1340 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | OMC  | L3    | 3841 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L3    | 4579 | 3    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | PSU  | L3    | 4636 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 1536 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L3    | 3825 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 3920 | 3,51 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L3    | 3887 | 3    | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | OMG  | L3    | 4228 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 38  | PTR  | NR    | 127  | 38   | -       | 0/10/11/13 | 0/1/1/1 |
| 3   | 1MA  | L3    | 1322 | 3    | -       | 0/7/25/26  | 0/3/3/3 |
| 3   | OMG  | L3    | 2876 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 1683 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | L3    | 2837 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L3    | 3718 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 4312 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | UR3  | L3    | 4530 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 3734 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L3    | 2824 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L3    | 4532 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 4552 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 1862 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 4521 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | OMU  | L3    | 3925 | 3    | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L3    | 4673 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L3    | 2401 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L3    | 5001 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L3    | 3695 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L3    | 1522 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L3    | 3899 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMU  | L3    | 4306 | 3    | -       | 1/9/27/28  | 0/2/2/2 |

The worst 5 of 101 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | L3    | 4498 | OMU  | C6-N1 | 4.87 | 1.49        | 1.38     |
| 3   | L3    | 2837 | OMU  | C6-N1 | 4.77 | 1.49        | 1.38     |
| 3   | L3    | 2415 | OMU  | C6-N1 | 4.76 | 1.49        | 1.38     |
| 3   | L3    | 4620 | OMU  | C6-N1 | 4.75 | 1.49        | 1.38     |
| 3   | L3    | 3925 | OMU  | C6-N1 | 4.73 | 1.49        | 1.38     |

The worst 5 of 424 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L3    | 4220 | 6MZ  | C5-C4-N3 | -5.81 | 118.71      | 126.72   |
| 3   | L3    | 1534 | A2M  | C5-C4-N3 | -5.71 | 118.86      | 126.72   |
| 3   | L3    | 2363 | A2M  | C5-C4-N3 | -5.66 | 118.93      | 126.72   |
| 3   | L3    | 4571 | A2M  | C5-C4-N3 | -5.62 | 118.98      | 126.72   |
| 3   | L3    | 4227 | OMU  | C4-N3-C2 | -5.60 | 119.66      | 126.61   |

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | L1    | 75   | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 398  | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 400  | A2M  | C1'-C2'-O2'-CM' |
| 3   | L3    | 1316 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | L3    | 1326 | A2M  | O4'-C4'-C5'-O5' |

There are no ring outliers.

63 monomers are involved in 90 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | L3    | 2861 | OMC  | 1       | 0            |
| 3   | L3    | 4361 | PSU  | 1       | 0            |
| 3   | L3    | 2415 | OMU  | 1       | 0            |
| 3   | L3    | 1524 | A2M  | 2       | 0            |
| 3   | L3    | 4618 | OMG  | 1       | 0            |
| 3   | L3    | 4620 | OMU  | 1       | 0            |
| 3   | L3    | 398  | A2M  | 1       | 0            |
| 3   | L3    | 3715 | PSU  | 1       | 0            |
| 3   | L3    | 3869 | OMC  | 1       | 0            |
| 3   | L3    | 2363 | A2M  | 1       | 0            |
| 3   | L3    | 4571 | A2M  | 2       | 0            |
| 2   | L1    | 75   | OMG  | 2       | 0            |
| 3   | L3    | 4637 | OMG  | 2       | 0            |
| 3   | L3    | 3822 | PSU  | 1       | 0            |
| 3   | L3    | 2632 | PSU  | 1       | 0            |
| 3   | L3    | 2422 | OMC  | 2       | 0            |
| 2   | L1    | 69   | PSU  | 2       | 0            |
| 3   | L3    | 3744 | OMG  | 3       | 0            |
| 3   | L3    | 4457 | PSU  | 2       | 0            |
| 3   | L3    | 4299 | PSU  | 1       | 0            |
| 3   | L3    | 400  | A2M  | 1       | 0            |
| 3   | L3    | 3730 | PSU  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | L3    | 1677 | PSU  | 2       | 0            |
| 3   | L3    | 4500 | PSU  | 1       | 0            |
| 3   | L3    | 2364 | OMG  | 2       | 0            |
| 3   | L3    | 3867 | A2M  | 1       | 0            |
| 3   | L3    | 3637 | PSU  | 1       | 0            |
| 3   | L3    | 4456 | OMC  | 1       | 0            |
| 3   | L3    | 4296 | PSU  | 1       | 0            |
| 3   | L3    | 4353 | PSU  | 1       | 0            |
| 3   | L3    | 4498 | OMU  | 1       | 0            |
| 3   | L3    | 4536 | OMC  | 1       | 0            |
| 3   | L3    | 2351 | OMC  | 2       | 0            |
| 3   | L3    | 4227 | OMU  | 1       | 0            |
| 3   | L3    | 4392 | OMG  | 1       | 0            |
| 3   | L3    | 3724 | A2M  | 2       | 0            |
| 3   | L3    | 2424 | OMG  | 1       | 0            |
| 3   | L3    | 4623 | OMG  | 1       | 0            |
| 3   | L3    | 4220 | 6MZ  | 3       | 0            |
| 3   | L3    | 1326 | A2M  | 2       | 0            |
| 3   | L3    | 4590 | A2M  | 1       | 0            |
| 3   | L3    | 1340 | OMC  | 2       | 0            |
| 3   | L3    | 3841 | OMC  | 1       | 0            |
| 3   | L3    | 4636 | PSU  | 2       | 0            |
| 3   | L3    | 3920 | PSU  | 1       | 0            |
| 3   | L3    | 3887 | OMC  | 1       | 0            |
| 38  | NR    | 127  | PTR  | 1       | 0            |
| 3   | L3    | 1322 | 1MA  | 2       | 0            |
| 3   | L3    | 2876 | OMG  | 2       | 0            |
| 3   | L3    | 1683 | PSU  | 2       | 0            |
| 3   | L3    | 2837 | OMU  | 1       | 0            |
| 3   | L3    | 3718 | A2M  | 2       | 0            |
| 3   | L3    | 4312 | PSU  | 1       | 0            |
| 3   | L3    | 4530 | UR3  | 2       | 0            |
| 3   | L3    | 3734 | PSU  | 1       | 0            |
| 3   | L3    | 2824 | OMC  | 2       | 0            |
| 3   | L3    | 4552 | PSU  | 2       | 0            |
| 3   | L3    | 3925 | OMU  | 2       | 0            |
| 3   | L3    | 4673 | PSU  | 2       | 0            |
| 3   | L3    | 5001 | PSU  | 1       | 0            |
| 3   | L3    | 1522 | OMG  | 1       | 0            |
| 3   | L3    | 3899 | OMG  | 1       | 0            |
| 3   | L3    | 4306 | OMU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 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 | $\# Z  > 2$ |
| 53  | GDP  | SR    | 1001 | 51,54 | 29,30,30     | 3.03 | 12 (41%)    | 45,47,47    | 2.69 | 16 (35%)    |

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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 53  | GDP  | SR    | 1001 | 51,54 | -       | 0/16/32/32 | 0/3/3/3 |

The worst 5 of 12 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 53  | SR    | 1001 | GDP  | O6-C6  | 8.81  | 1.40        | 1.23     |
| 53  | SR    | 1001 | GDP  | C5-N7  | 6.54  | 1.52        | 1.39     |
| 53  | SR    | 1001 | GDP  | PA-O3A | 5.20  | 1.65        | 1.59     |
| 53  | SR    | 1001 | GDP  | C2-N2  | 4.80  | 1.45        | 1.34     |
| 53  | SR    | 1001 | GDP  | C8-N9  | -3.96 | 1.28        | 1.37     |

The worst 5 of 16 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 53  | SR    | 1001 | GDP  | C8-N9-C4 | 7.70  | 120.47      | 106.03   |
| 53  | SR    | 1001 | GDP  | C5-C4-N3 | -6.71 | 117.71      | 128.39   |
| 53  | SR    | 1001 | GDP  | N9-C4-N3 | 6.62  | 139.19      | 125.95   |
| 53  | SR    | 1001 | GDP  | C2-N3-C4 | 5.38  | 121.56      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 53  | SR    | 1001 | GDP  | C6-C5-N7 | 4.84 | 139.11      | 130.29   |

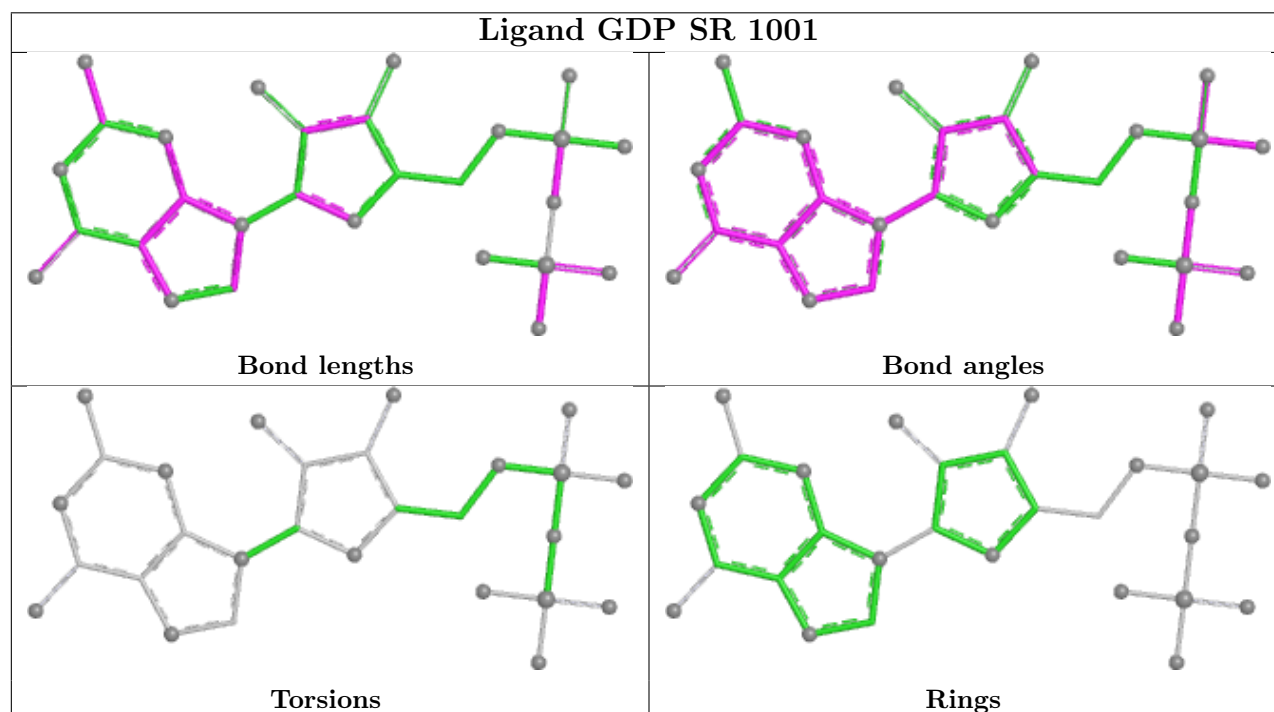
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

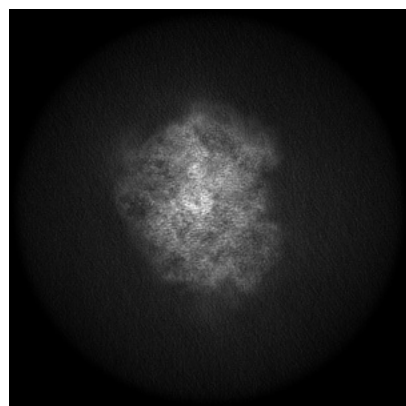
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29274. These allow visual inspection of the internal detail of the map and identification of artifacts.

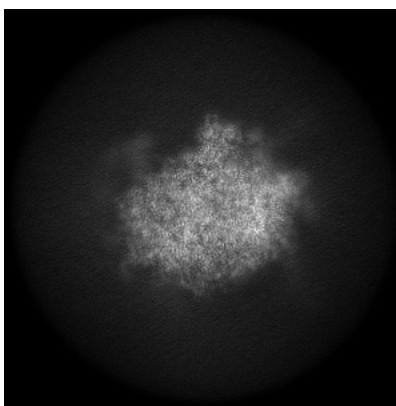
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

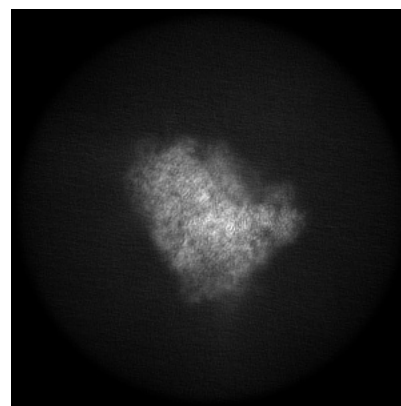
#### 6.1.1 Primary map



X

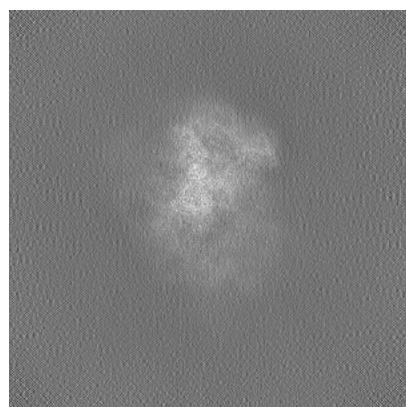


Y

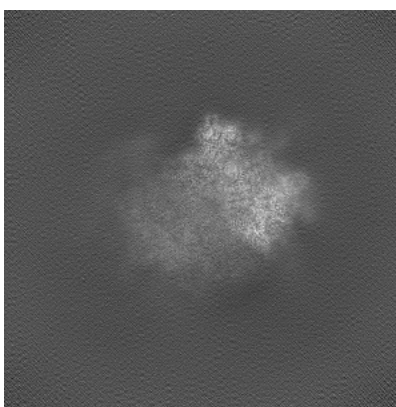


Z

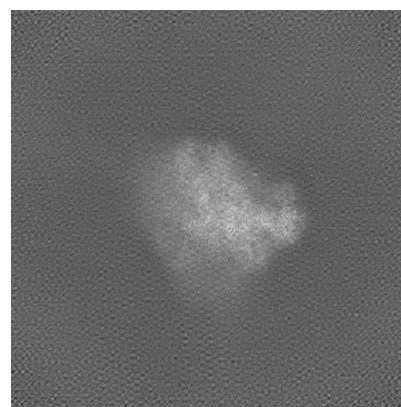
#### 6.1.2 Raw map



X



Y



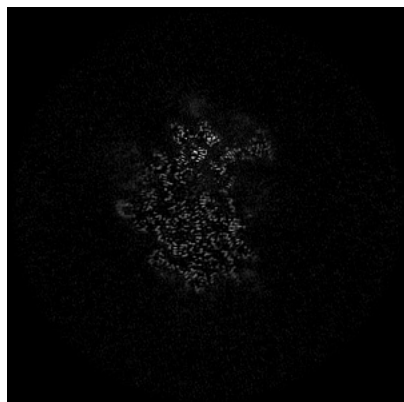
Z

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

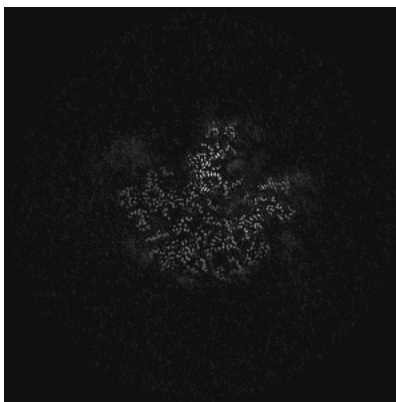


## 6.2 Central slices [i](#)

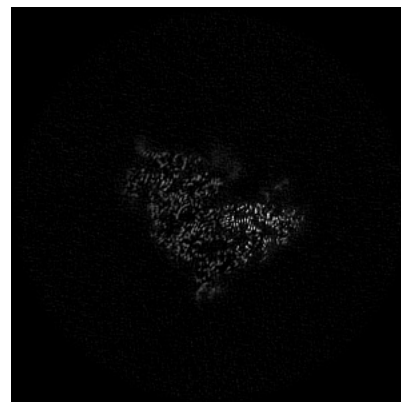
### 6.2.1 Primary map



X Index: 240

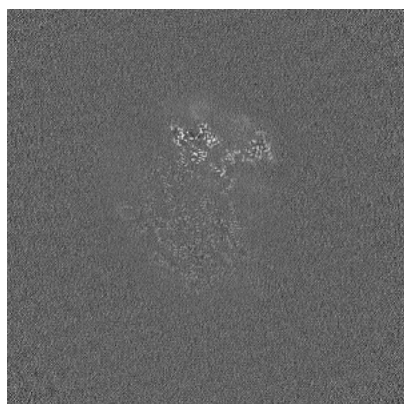


Y Index: 240

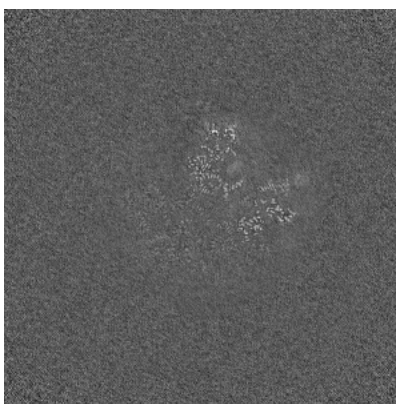


Z Index: 240

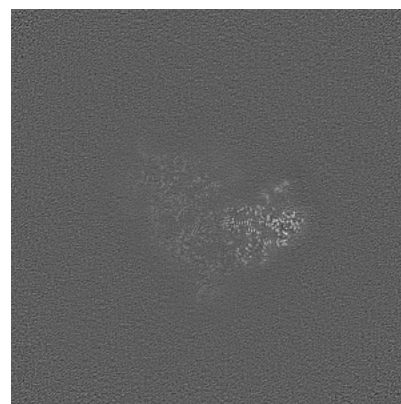
### 6.2.2 Raw map



X Index: 240



Y Index: 240

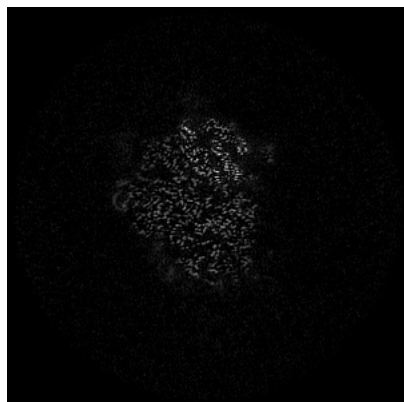


Z Index: 240

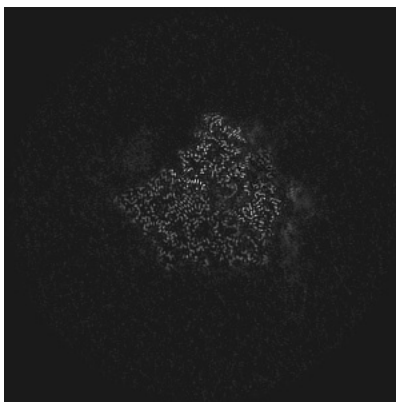
The images above show central slices of the map in three orthogonal directions.

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

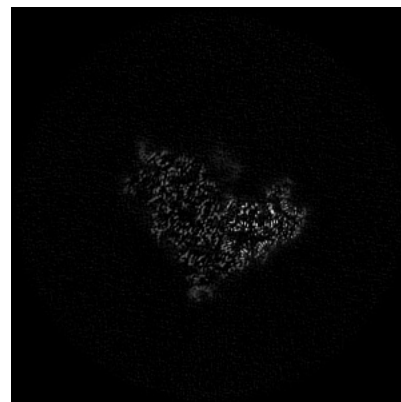
### 6.3.1 Primary map



X Index: 226

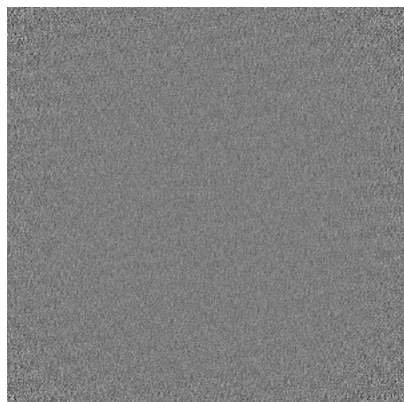


Y Index: 227

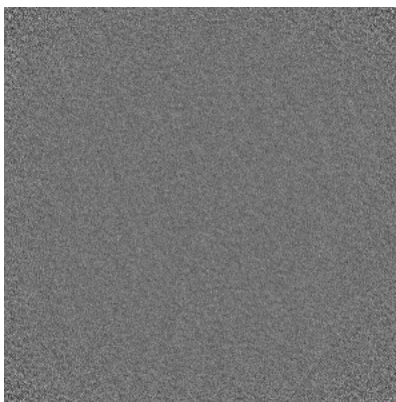


Z Index: 245

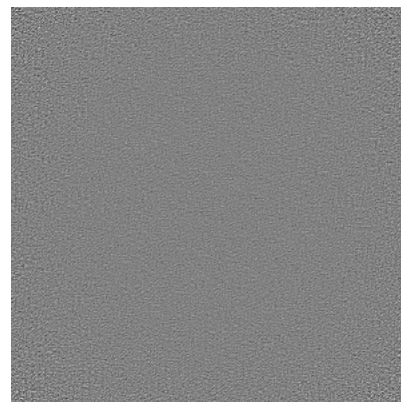
### 6.3.2 Raw map



X Index: 0



Y Index: 0

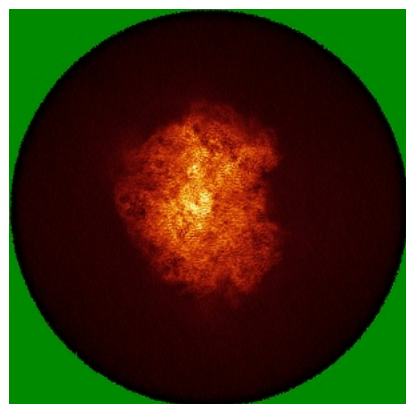


Z Index: 0

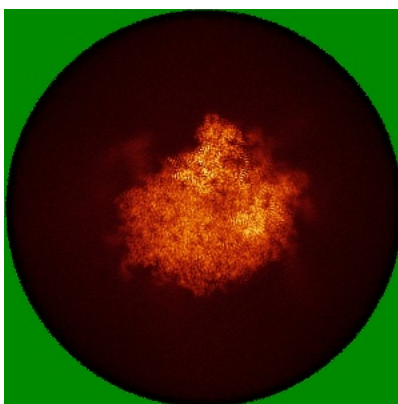
The images above show the largest variance slices of the map in three orthogonal directions.

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

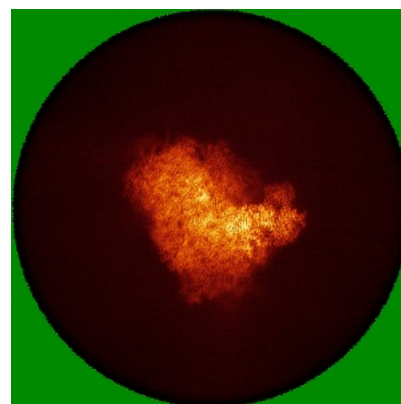
### 6.4.1 Primary map



X

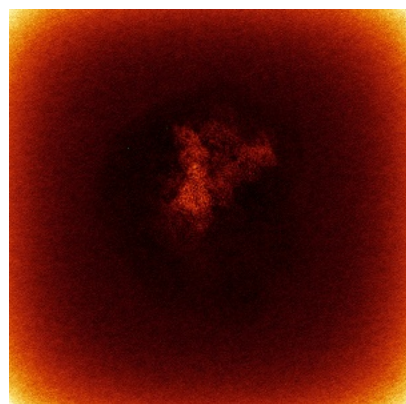


Y

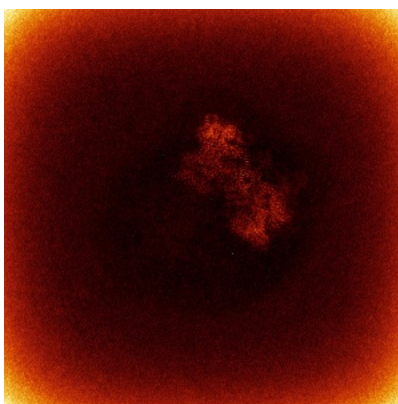


Z

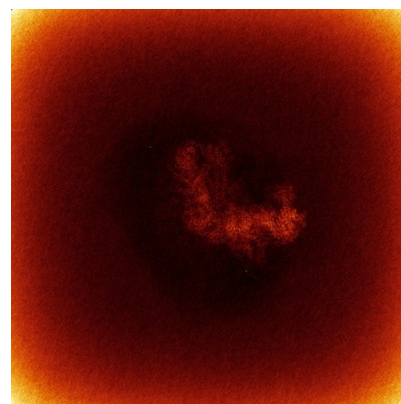
### 6.4.2 Raw map



X



Y

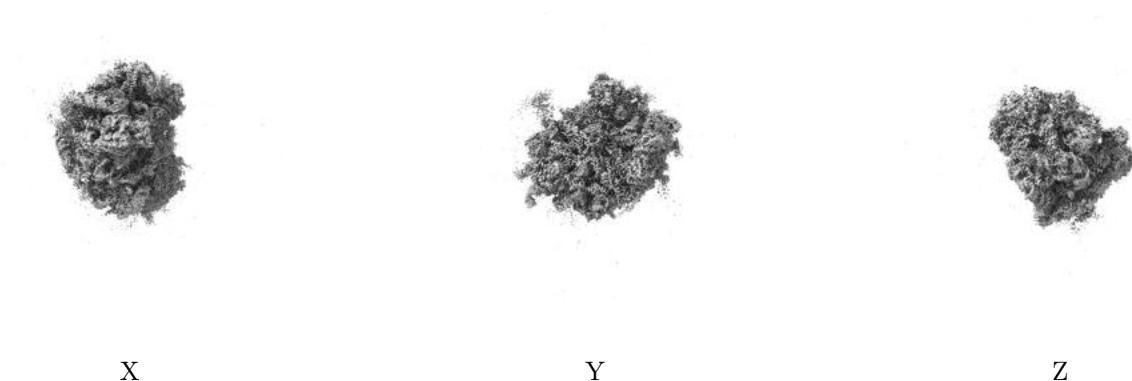


Z

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.

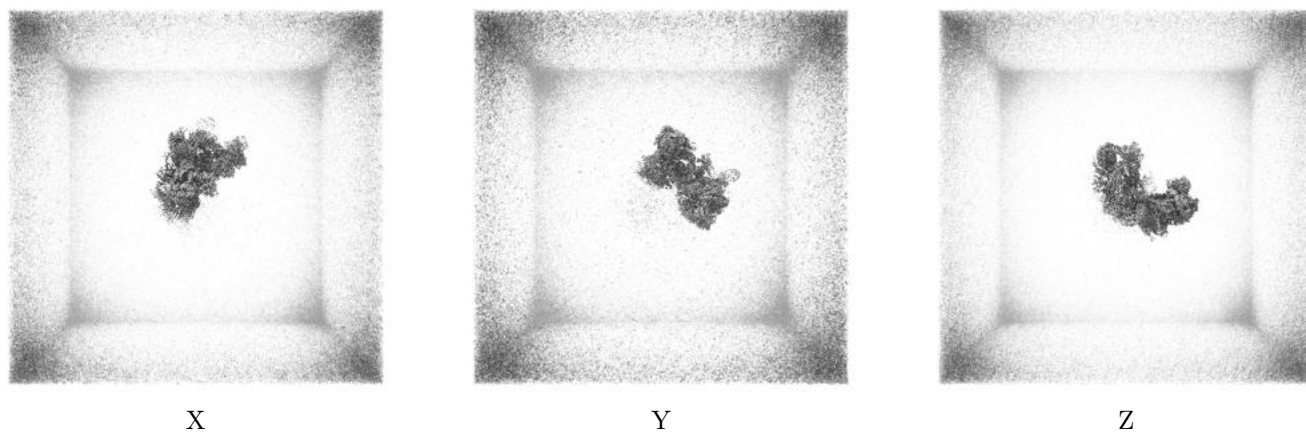
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. 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



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.



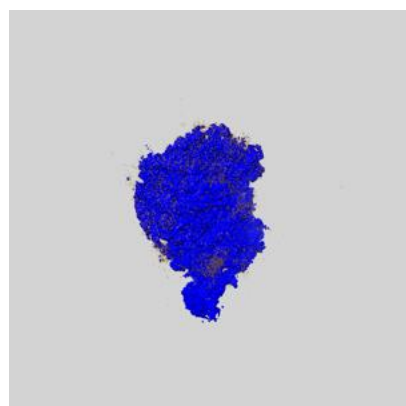
## 6.6 Mask visualisation [i](#)

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

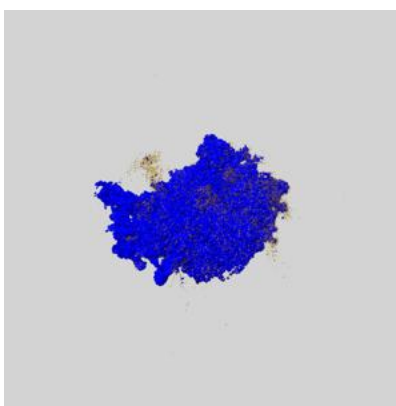
A mask typically either:

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

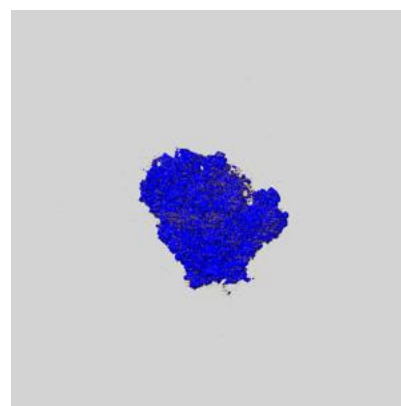
### 6.6.1 emd\_29274\_msk\_1.map [i](#)



X



Y

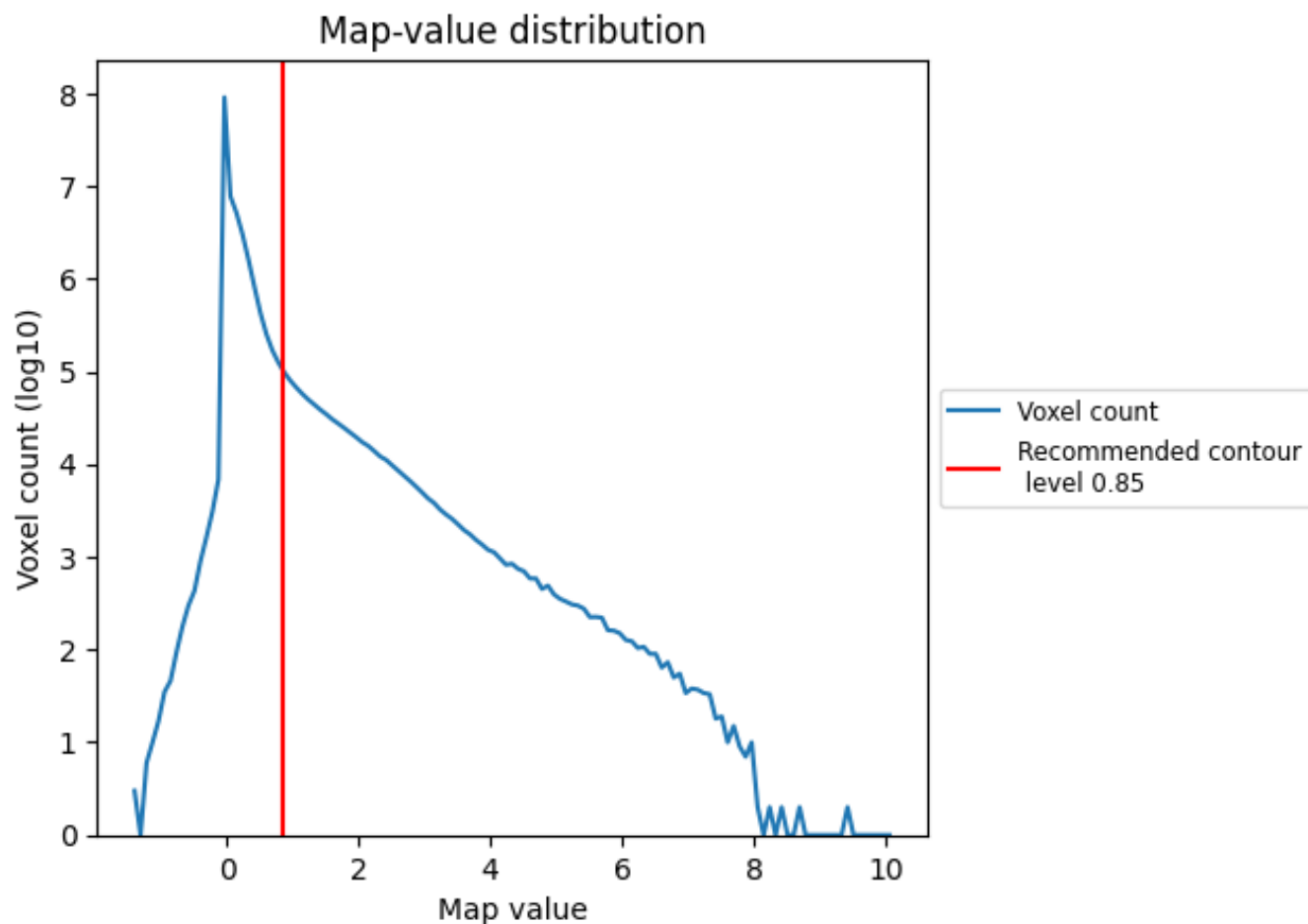


Z

## 7 Map analysis [i](#)

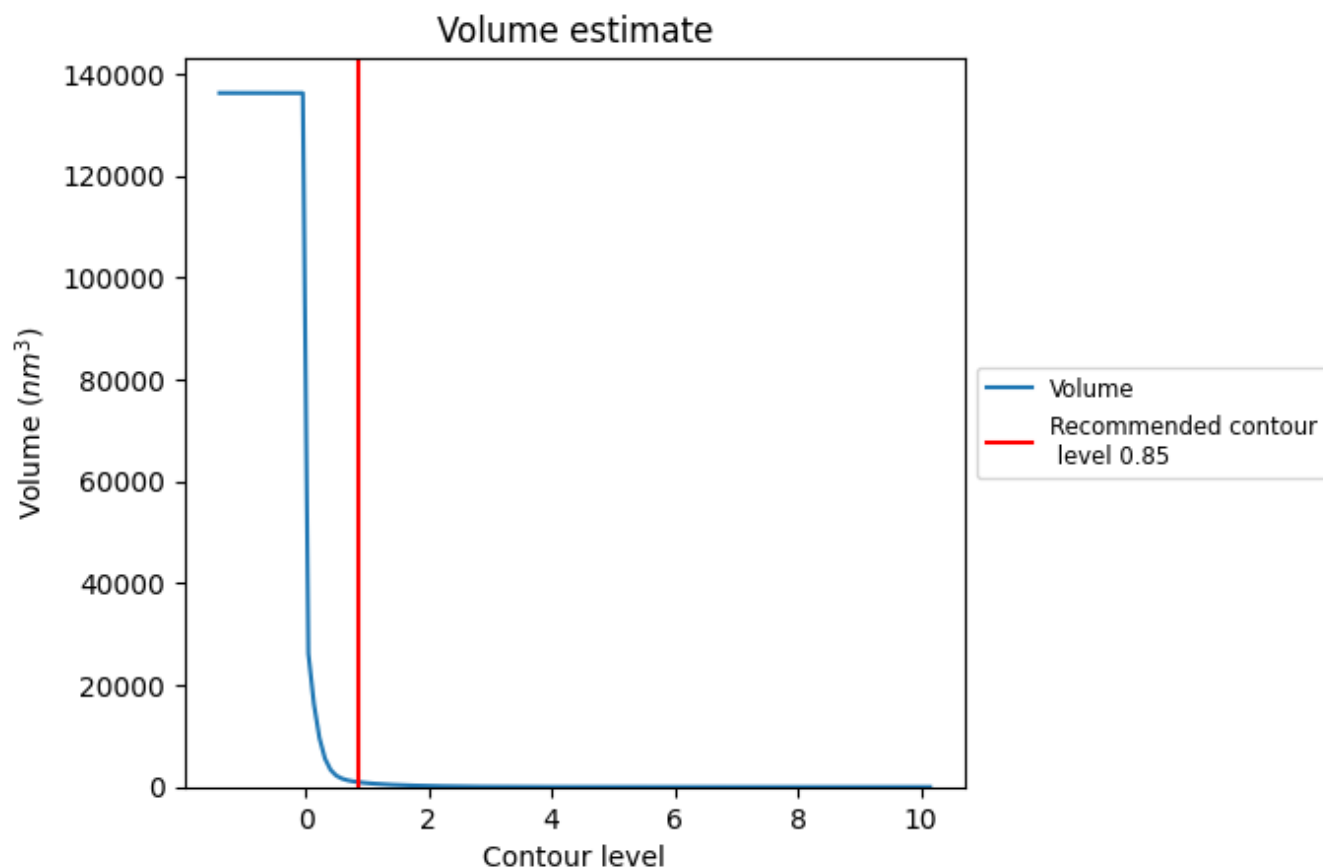
This section contains the results of statistical analysis of the map.

### 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.

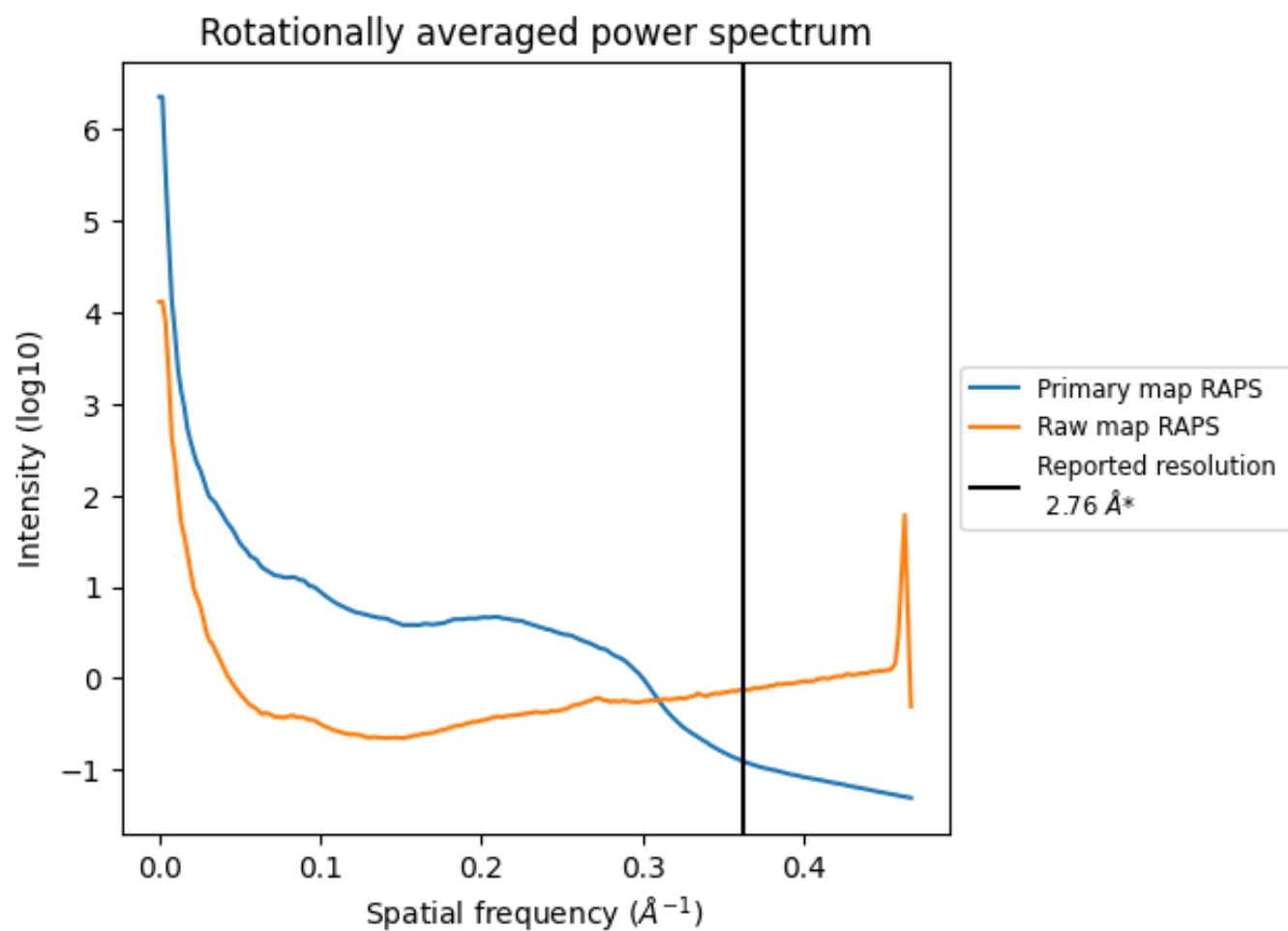
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 966  $\text{nm}^3$ ; this corresponds to an approximate mass of 873 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 ⓘ



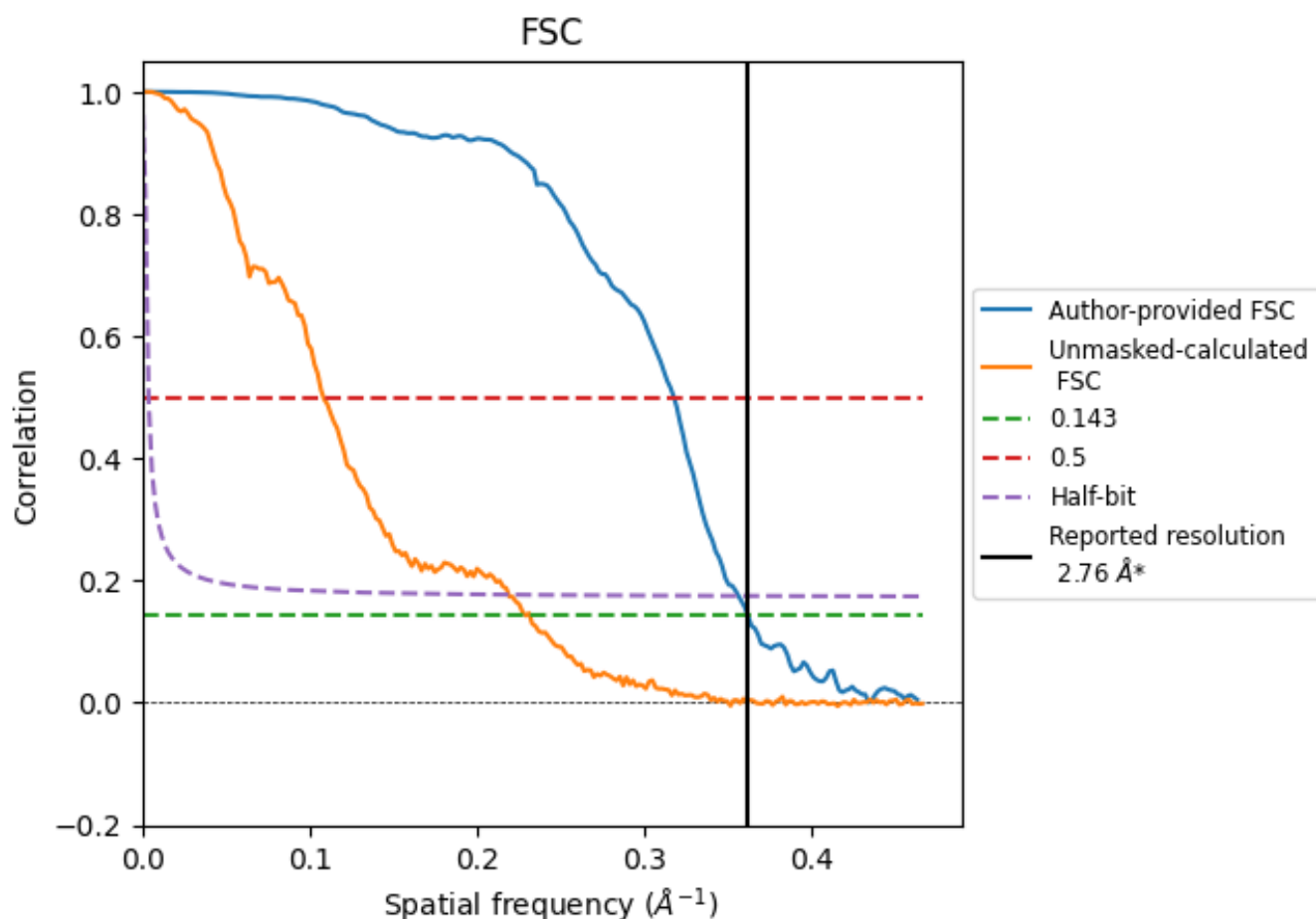
\*Reported resolution corresponds to spatial frequency of 0.362 Å<sup>-1</sup>



## 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 0.362 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

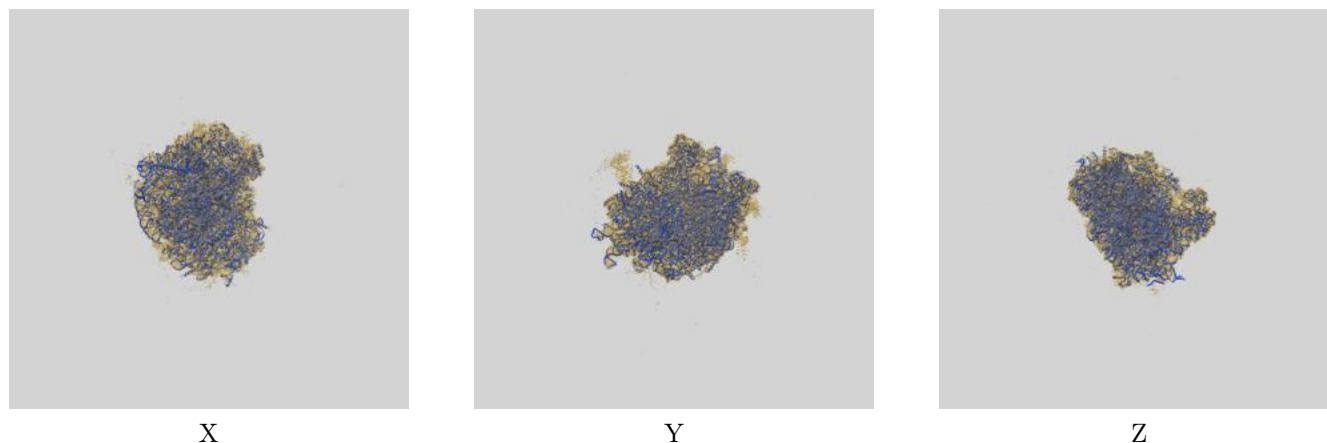
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.76                               | -    | -        |
| Author-provided FSC curve | 2.76                               | 3.14 | 2.80     |
| Unmasked-calculated*      | 4.36                               | 9.23 | 4.56     |

\*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 4.36 differs from the reported value 2.76 by more than 10 %

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

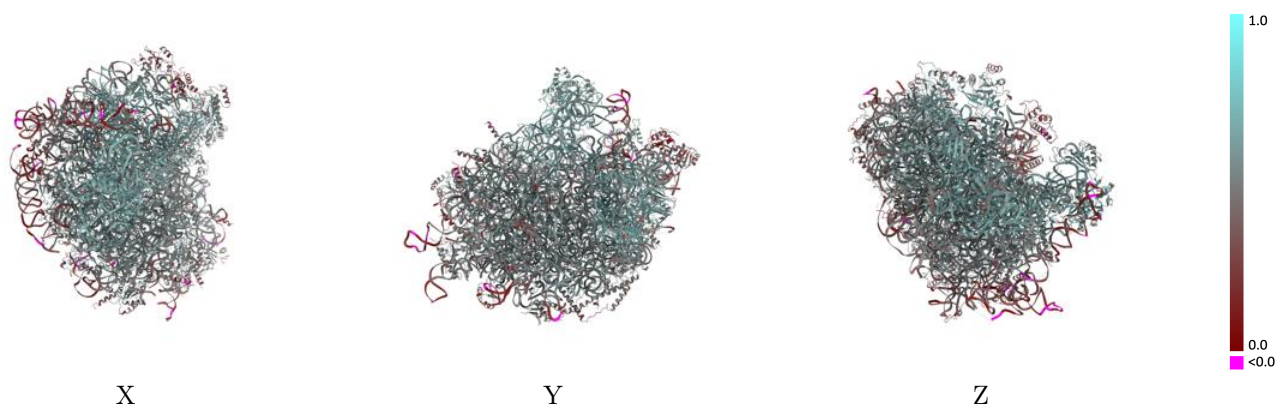
This section contains information regarding the fit between EMDB map EMD-29274 and PDB model 8FLC. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



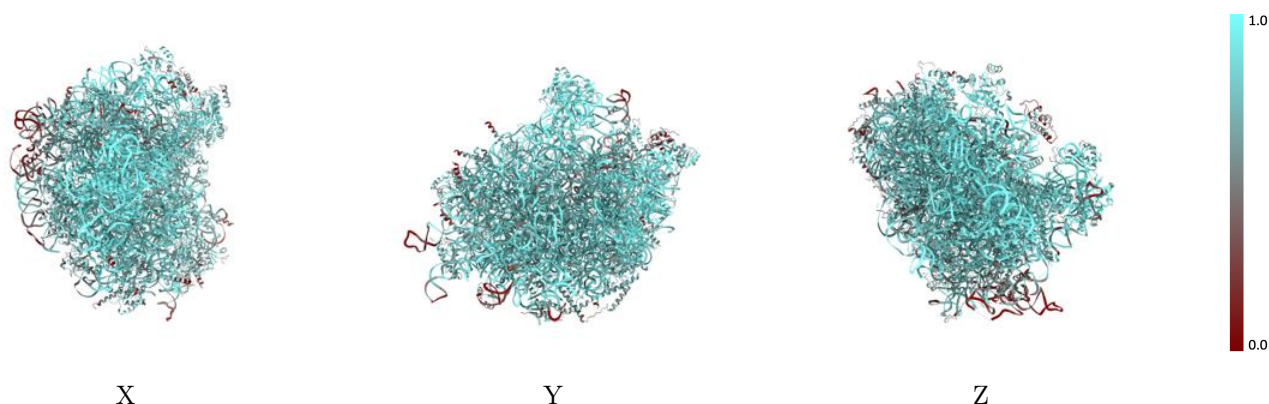
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



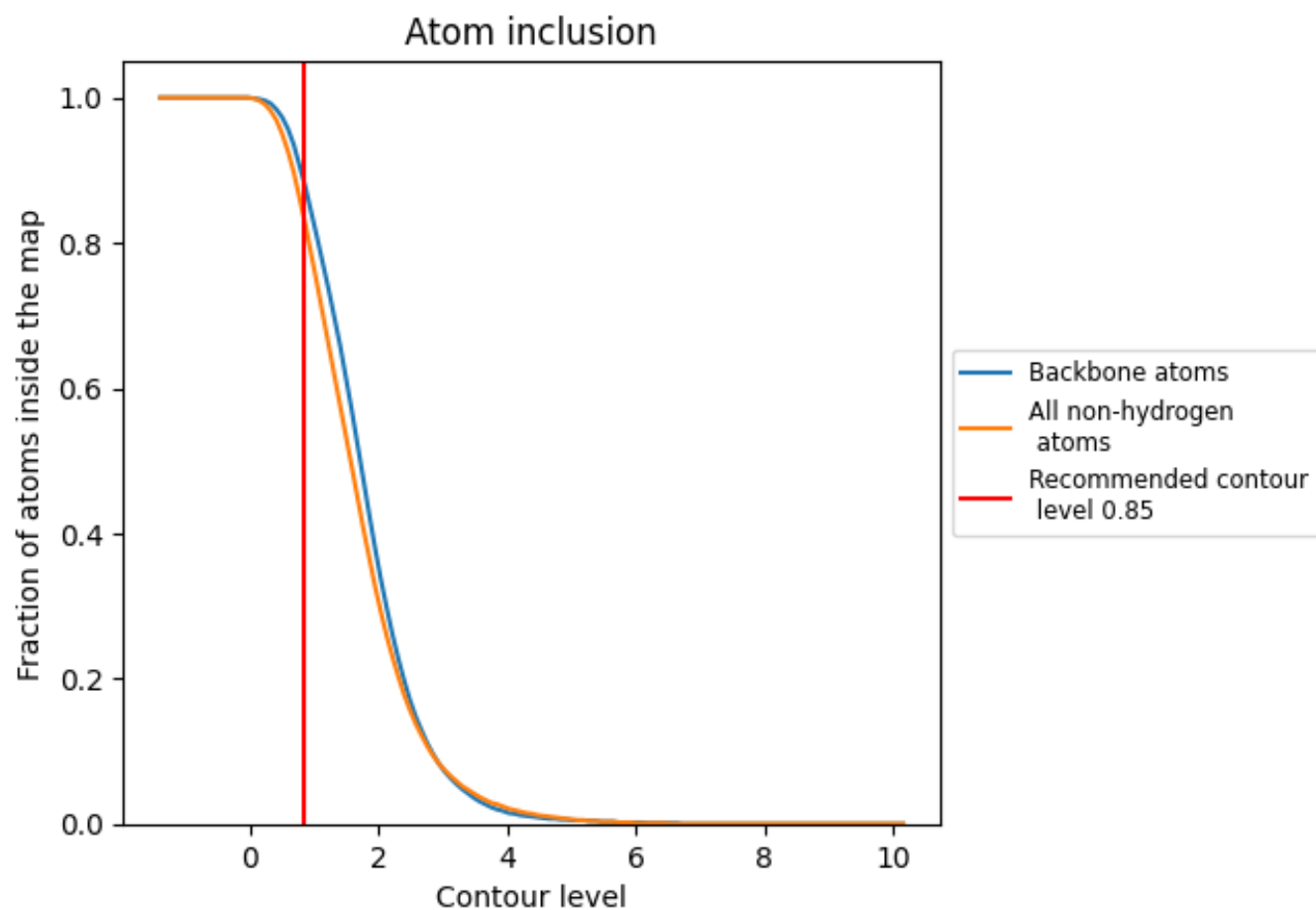
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8300   |  0.5090   |
| BA    |  0.3790   |  0.2720   |
| L1    |  0.8720   |  0.5000   |
| L3    |  0.8560   |  0.4900   |
| L4    |  0.9820   |  0.6130   |
| L5    |  0.8410   |  0.5550   |
| L6    |  0.7570   |  0.5030   |
| L7    |  0.8900   |  0.6050   |
| L8    |  0.8970   |  0.5880   |
| L9    |  0.8550   |  0.5550   |
| LA    |  0.7840   |  0.5220   |
| LB    |  0.8400   |  0.5570   |
| LC    |  0.9650   |  0.6500   |
| LD    |  0.7530   |  0.4990   |
| LE    |  0.9070  |  0.5930  |
| LF    |  0.7200 |  0.4790 |
| LG    |  0.8700 |  0.5890 |
| LH    |  0.7600 |  0.5050 |
| LI    |  0.7560 |  0.5010 |
| LJ    |  0.7070 |  0.4770 |
| LK    |  0.8560 |  0.5630 |
| LL    |  0.7580 |  0.5000 |
| LM    |  0.6970 |  0.5030 |
| LN    |  0.8310 |  0.5500 |
| LO    |  0.6860 |  0.4460 |
| LP    |  0.7380 |  0.5090 |
| LQ    |  0.7740 |  0.5360 |
| LR    |  0.7430 |  0.5010 |
| LS    |  0.7440 |  0.4920 |
| LT    |  0.8280 |  0.5480 |
| LU    |  0.7290 |  0.4960 |
| LV    |  0.8910 |  0.6010 |
| LW    |  0.8460 |  0.5490 |
| LX    |  0.7320 |  0.4910 |
| LY    |  0.6410 |  0.4340 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| LZ    |  0.8370 |  0.5480 |
| NK    |  0.5990 |  0.4310 |
| NP    |  0.7180 |  0.4880 |
| NR    |  0.7440 |  0.5330 |
| SA    |  0.7880 |  0.5240 |
| SB    |  0.8970 |  0.5930 |
| SC    |  0.6260 |  0.4410 |
| SD    |  0.8140 |  0.5350 |
| SE    |  0.6760 |  0.4500 |
| SF    |  0.8090 |  0.5320 |
| SG    |  0.9180 |  0.6090 |
| SK    |  0.8260 |  0.5500 |
| SQ    |  0.7150 |  0.3740 |
| SR    |  0.7680 |  0.5160 |
| SV    |  0.7590 |  0.5010 |
| VB    |  0.6670 |  0.5280 |