



## wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 12:59 PM UTC

PDB ID : 8K2D / pdb\_00008k2d  
EMDB ID : EMD-36839  
Title : Cryo-EM structure of the yeast 80S ribosome with tigecycline, eEF2, Stm1 and eIF5A  
Authors : Buschauer, R.; Beckmann, R.; Cheng, J.  
Deposited on : 2023-07-12  
Resolution : 3.20 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:

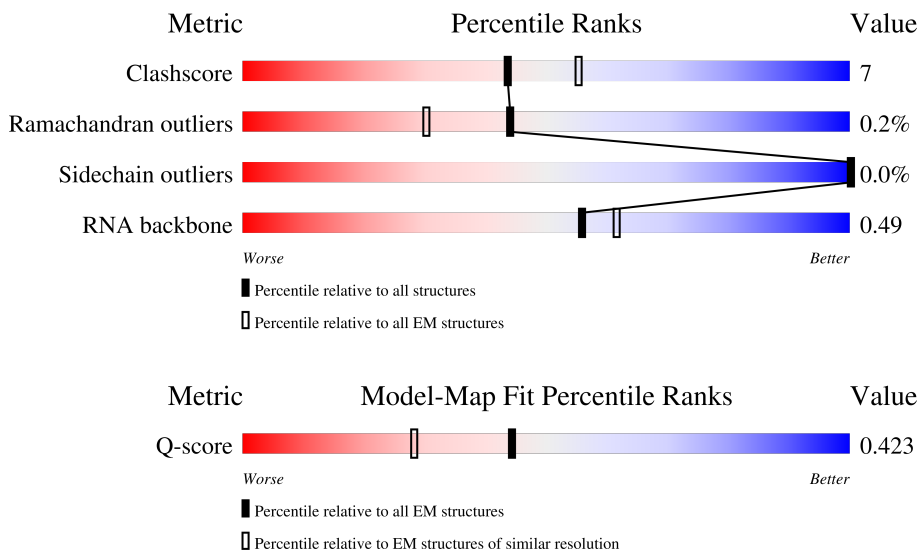
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.20 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.





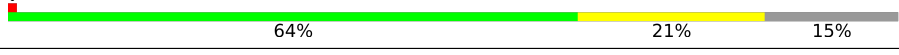


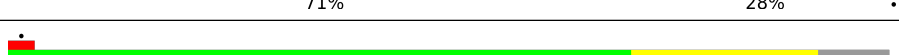
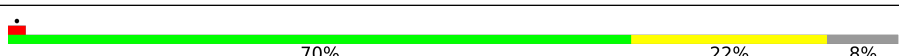



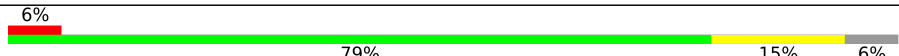



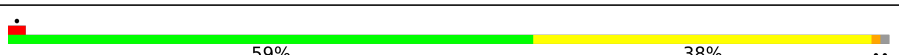









| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| RNA backbone          | 8273                        | 3508                        | -  |
| Q-score               | -                           | 25397                       | 15020 ( 2.70 - 3.70 )                                    |

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   | C2    | 1800   |                  |
| 2   | C1    | 3396   |                  |
| 3   | C4    | 121    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | C3    | 158    |  73% 22%           |
| 5   | SA    | 252    |  64% 17% 18%       |
| 6   | SB    | 255    |  64% 21% 15%       |
| 7   | SC    | 254    |  66% 19% 15%       |
| 8   | SD    | 240    |  69% 24% 7%        |
| 9   | SE    | 261    |  71% 28%           |
| 10  | SF    | 225    |  70% 21% 8%        |
| 11  | SG    | 236    |  70% 22% 8%        |
| 12  | SH    | 190    |  75% 22%           |
| 13  | SI    | 200    |  71% 23% 6%        |
| 14  | SJ    | 197    |  72% 22% 6%      |
| 15  | SK    | 105    |  51% 35% 12%     |
| 16  | SL    | 156    |  6% 79% 15% 6%   |
| 17  | SM    | 143    |  24% 64% 22% 13% |
| 18  | SN    | 151    |  83% 17%         |
| 19  | SO    | 137    |  77% 17% 7%      |
| 20  | SP    | 142    |  63% 20% 16%     |
| 21  | SQ    | 143    |  59% 38%         |
| 22  | SR    | 136    |  68% 16% 15%     |
| 23  | SS    | 146    |  69% 30%         |
| 24  | ST    | 144    |  80% 19%         |
| 25  | SU    | 121    |  63% 20% 17%     |
| 26  | SV    | 87     |  76% 24%         |
| 27  | SW    | 130    |  77% 22%         |
| 28  | SX    | 145    |  83% 17%         |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | SY    | 135    | 73% 25% ...      |
| 30  | SZ    | 108    | 45% 19% 36%      |
| 31  | Sa    | 119    | 65% 17% 18%      |
| 32  | Sb    | 82     | 84% 15% .        |
| 33  | Sc    | 67     | 6% 73% 21% 6%    |
| 34  | Sd    | 56     | 86% 9% 5%        |
| 35  | Se    | 63     | 14% 68% 25% 5%   |
| 36  | Sf    | 152    | 18% 78%          |
| 37  | Sg    | 319    | 69% 29% .        |
| 38  | LA    | 254    | 79% 20% .        |
| 39  | LB    | 387    | 80% 20%          |
| 40  | LC    | 362    | 80% 20%          |
| 41  | LD    | 297    | 85% 14% .        |
| 42  | LE    | 176    | 70% 19% 11%      |
| 43  | LF    | 244    | 78% 14% 9%       |
| 44  | LG    | 256    | 73% 18% 10%      |
| 45  | LH    | 191    | 86% 14% .        |
| 46  | LI    | 221    | 70% 25% 5%       |
| 47  | LJ    | 174    | 76% 20% ..       |
| 48  | LK    | 165    | 22% 76% 19% .    |
| 49  | LL    | 199    | 72% 23% ...      |
| 50  | LM    | 138    | 82% 17% .        |
| 51  | LN    | 204    | 78% 21%          |
| 52  | LO    | 199    | 81% 18% .        |
| 53  | LP    | 184    | 82% 14% 5%       |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 54  | LQ    | 186    |  82% 18%        |
| 55  | LR    | 189    |  84% 8% 8%      |
| 56  | LS    | 172    |  79% 21%        |
| 57  | LT    | 160    |  74% 24% ..     |
| 58  | LU    | 121    |  69% 12% 19%    |
| 59  | LV    | 137    |  79% 19% .      |
| 60  | LW    | 155    |  28% 12% 59%    |
| 61  | LX    | 142    |  75% 9% 15%     |
| 62  | LY    | 127    |  85% 13% .      |
| 63  | LZ    | 136    |  75% 24% ..     |
| 64  | La    | 149    |  77% 21% ..     |
| 65  | Lb    | 59     |  83% 14% ..    |
| 66  | Lc    | 105    |  80% 15% 5%   |
| 67  | Ld    | 113    |  6% 75% 21% . |
| 68  | Le    | 130    |  84% 14% .    |
| 69  | Lf    | 107    |  66% 33% .    |
| 70  | Lg    | 121    |  85% 7% 7%    |
| 71  | Lh    | 120    |  84% 15% .    |
| 72  | Li    | 100    |  82% 17% .    |
| 73  | Lj    | 88     |  76% 17% 7%   |
| 74  | Lk    | 78     |  71% 28% .    |
| 75  | Ll    | 51     |  78% 20% .    |
| 76  | Lm    | 128    |  33% 8% 59%   |
| 77  | Ln    | 25     |  16% 92% 8%   |
| 78  | Lo    | 106    |  81% 18% .    |

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| Mol | Chain | Length | Quality of chain       |
|-----|-------|--------|------------------------|
| 79  | Lp    | 92     | <p>78% 21%</p>         |
| 80  | CE    | 157    | <p>76% 17% 7%</p>      |
| 81  | L1    | 217    | <p>66% 33%</p>         |
| 82  | P0    | 312    | <p>17% 55% 10% 35%</p> |
| 83  | CD    | 842    | <p>43% 69% 27%</p>     |
| 84  | CS    | 273    | <p>37% 7% 55%</p>      |

## 2 Entry composition i

There are 88 unique types of molecules in this entry. The entry contains 210169 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
|     |       |          | Total | C     | N    | O     | P    |         |       |
| 1   | C2    | 1700     | 36234 | 16201 | 6426 | 11907 | 1700 | 0       | 0     |

- Molecule 2 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
|     |       |          | Total | C     | N     | O     | P    |         |       |
| 2   | C1    | 3188     | 68200 | 30463 | 12307 | 22242 | 3188 | 0       | 0     |

- Molecule 3 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
|     |       |          | Total | C    | N   | O   | P   |         |       |
| 3   | C4    | 121      | 2579  | 1152 | 461 | 845 | 121 | 0       | 0     |

- Molecule 4 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
|     |       |          | Total | C    | N   | O    | P   |         |       |
| 4   | C3    | 157      | 3333  | 1491 | 584 | 1101 | 157 | 0       | 0     |

- Molecule 5 is a protein called Small ribosomal subunit protein uS2A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 5   | SA    | 206      | 1583  | 1017 | 281 | 283 | 2 | 0       | 0     |

- Molecule 6 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 6   | SB    | 216      | 1722  | 1091 | 312 | 315 | 4 | 0       | 0     |

- Molecule 7 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 7   | SC    | 217      | 1635  | 1047 | 289 | 297 | 2 | 0       | 0     |

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 8   | SD    | 223      | 1734  | 1101 | 313 | 314 | 6 | 0       | 0     |

- Molecule 9 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 9   | SE    | 260      | 2068  | 1316 | 389 | 360 | 3 | 0       | 0     |

- Molecule 10 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 10  | SF    | 206      | 1609  | 1007 | 300 | 299 | 3 | 0       | 0     |

- Molecule 11 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 11  | SG    | 218      | 1755  | 1102 | 337 | 313 | 3 | 0       | 0     |

- Molecule 12 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 12  | SH    | 185      | 1486  | 954 | 266 | 266 | 0       | 0     |

- Molecule 13 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 13  | SI    | 188      | 1489  | 925 | 298 | 264 | 2 | 0       | 0     |

- Molecule 14 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | SJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein eS10A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | SK    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 478 | 121 | 140 | 2 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein uS17A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | SL    | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1168  | 747 | 221 | 197 | 3 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | SM    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 890   | 560 | 156 | 172 | 2 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | SN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | SO    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 949   | 582 | 188 | 176 | 3 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | SP    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 939   | 595 | 176 | 161 | 7 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein uS9A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 21  | SQ    | 141      | 1105  | 708 | 203 | 194 | 0       | 0     |

- Molecule 22 is a protein called Small ribosomal subunit protein eS17A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 22  | SR    | 115      | 896   | 557 | 172 | 165 | 2 | 0       | 0     |

- Molecule 23 is a protein called Small ribosomal subunit protein uS13A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 23  | SS    | 145      | 1192  | 743 | 237 | 210 | 2 | 0       | 0     |

- Molecule 24 is a protein called Small ribosomal subunit protein eS19A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 24  | ST    | 143      | 1112  | 694 | 208 | 208 | 2 | 0       | 0     |

- Molecule 25 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 25  | SU    | 101      | 805   | 512 | 145 | 147 | 1 | 0       | 0     |

- Molecule 26 is a protein called Small ribosomal subunit protein eS21A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 26  | SV    | 87       | 684   | 420 | 125 | 137 | 2 | 0       | 0     |

- Molecule 27 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 27  | SW    | 129      | 1021  | 650 | 188 | 180 | 3 | 0       | 0     |

- Molecule 28 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 28  | SX    | 144      | 1121  | 708 | 220 | 191 | 2 | 0       | 0     |

- Molecule 29 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 29  | SY    | 134      | 1073  | 676 | 208 | 189 |   | 0       | 0     |

- Molecule 30 is a protein called Small ribosomal subunit protein eS25A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 30  | SZ    | 69       | 558   | 357 | 103 | 98 |   | 0       | 0     |

- Molecule 31 is a protein called Small ribosomal subunit protein eS26B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 31  | Sa    | 97       | 769   | 475 | 160 | 129 | 5 | 0       | 0     |

- Molecule 32 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 32  | Sb    | 81       | 610   | 382 | 110 | 113 | 5 | 0       | 0     |

- Molecule 33 is a protein called Small ribosomal subunit protein eS28A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 33  | Sc    | 63       | 497   | 306 | 99 | 91 | 1 | 0       | 0     |

- Molecule 34 is a protein called Small ribosomal subunit protein uS14A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 34  | Sd    | 53       | 442   | 274 | 92 | 72 | 4 | 0       | 0     |

- Molecule 35 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | Se    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 475   | 299 | 98 | 77 | 1 |         |       |

- Molecule 36 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 36  | Sf    | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 248   | 153 | 46 | 45 | 4 |         |       |

- Molecule 37 is a protein called Small ribosomal subunit protein RACK1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | Sg    | 313      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2403  | 1521 | 411 | 463 | 8 |         |       |

- Molecule 38 is a protein called Large ribosomal subunit protein uL2A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | LA    | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1912  | 1190 | 388 | 333 | 1 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | LB    | 386      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein uL4A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | LC    | 361      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | LD    | 294      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2359  | 1489 | 412 | 456 | 2 |         |       |

- Molecule 42 is a protein called Large ribosomal subunit protein eL6A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 42  | LE    | 157      | 1248  | 806 | 224 | 217 | 1 | 0       | 0     |

- Molecule 43 is a protein called Large ribosomal subunit protein uL30A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 43  | LF    | 223      | 1791  | 1155 | 325 | 310 | 1 | 0       | 0     |

- Molecule 44 is a protein called Large ribosomal subunit protein eL8A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 44  | LG    | 231      | 1763  | 1130 | 316 | 314 | 3 | 0       | 0     |

- Molecule 45 is a protein called Large ribosomal subunit protein uL6A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 45  | LH    | 190      | 1510  | 957 | 273 | 276 | 4 | 0       | 0     |

- Molecule 46 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 46  | LI    | 209      | 1696  | 1077 | 321 | 293 | 5 | 0       | 0     |

- Molecule 47 is a protein called Large ribosomal subunit protein uL5A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 47  | LJ    | 169      | 1353  | 847 | 253 | 249 | 4 | 0       | 0     |

- Molecule 48 is a protein called Large ribosomal subunit protein uL11A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 48  | LK    | 158      | 1196  | 750 | 216 | 228 | 2 | 0       | 0     |

- Molecule 49 is a protein called Large ribosomal subunit protein eL13A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 49  | LL    | 194      | 1548  | 965 | 316 | 267 | 0       | 0     |

- Molecule 50 is a protein called Large ribosomal subunit protein eL14A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 50  | LM    | 137      | 1059  | 678 | 200 | 179 | 2 | 0       | 0     |

- Molecule 51 is a protein called Large ribosomal subunit protein eL15A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 51  | LN    | 203      | 1720  | 1077 | 361 | 281 | 1 | 0       | 0     |

- Molecule 52 is a protein called Large ribosomal subunit protein uL13A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 52  | LO    | 197      | 1555  | 1003 | 289 | 262 | 1 | 0       | 0     |

- Molecule 53 is a protein called Large ribosomal subunit protein uL22A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 53  | LP    | 175      | 1378  | 856 | 273 | 249 | 0       | 0     |

- Molecule 54 is a protein called Large ribosomal subunit protein eL18A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 54  | LQ    | 185      | 1441  | 908 | 290 | 241 | 2 | 0       | 0     |

- Molecule 55 is a protein called Large ribosomal subunit protein eL19A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 55  | LR    | 174      | 1365  | 843 | 286 | 236 | 0       | 0     |

- Molecule 56 is a protein called Large ribosomal subunit protein eL20A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 56  | LS    | 172      | 1445  | 930 | 267 | 244 | 4 | 0       | 0     |

- Molecule 57 is a protein called Large ribosomal subunit protein eL21A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 57  | LT    | 159      | 1276  | 805 | 246 | 221 | 4 | 0       | 0     |

- Molecule 58 is a protein called Large ribosomal subunit protein eL22A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 58  | LU    | 98       | 778   | 505 | 127 | 146 | 0       | 0     |

- Molecule 59 is a protein called Large ribosomal subunit protein uL14A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 59  | LV    | 134      | 993   | 623 | 187 | 176 | 7 | 0       | 0     |

- Molecule 60 is a protein called Large ribosomal subunit protein eL24A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 60  | LW    | 63       | 521   | 336 | 102 | 82 | 1 | 0       | 0     |

- Molecule 61 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 61  | LX    | 120      | 959   | 617 | 168 | 172 | 2 | 0       | 0     |

- Molecule 62 is a protein called Large ribosomal subunit protein uL24A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 62  | LY    | 124      | 976   | 614 | 190 | 172 | 0       | 0     |

- Molecule 63 is a protein called Large ribosomal subunit protein eL27A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 63  | LZ    | 135      | 1092  | 710 | 202 | 180 | 0       | 0     |

- Molecule 64 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 64  | La    | 148      | 1173  | 749 | 231 | 190 | 3 | 0       | 0     |

- Molecule 65 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O  |         |       |
| 65  | Lb    | 58       | 462   | 289 | 100 | 73 | 0       | 0     |

- Molecule 66 is a protein called Large ribosomal subunit protein eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 66  | Lc    | 100      | 767   | 492 | 128 | 146 | 1 | 0       | 0     |

- Molecule 67 is a protein called Large ribosomal subunit protein eL31A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 67  | Ld    | 109      | 883   | 559 | 167 | 156 | 1 | 0       | 0     |

- Molecule 68 is a protein called Large ribosomal subunit protein eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 68  | Le    | 127      | 1020  | 647 | 205 | 167 | 1 | 0       | 0     |

- Molecule 69 is a protein called Large ribosomal subunit protein eL33A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 69  | Lf    | 106      | 850   | 540 | 165 | 144 | 1 | 0       | 0     |

- Molecule 70 is a protein called Large ribosomal subunit protein eL34A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 70  | Lg    | 112      | 880   | 545 | 179 | 152 | 4 | 0       | 0     |

- Molecule 71 is a protein called Large ribosomal subunit protein uL29A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 71  | Lh    | 119      | 965   | 612 | 185 | 167 | 1 | 0       | 0     |

- Molecule 72 is a protein called Large ribosomal subunit protein eL36A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 72  | Li    | 99       | 770   | 481 | 156 | 131 | 2 | 0       | 0     |

- Molecule 73 is a protein called Large ribosomal subunit protein eL37A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 73  | Lj    | 82       | 650   | 396 | 142 | 107 | 5 | 0       | 0     |

- Molecule 74 is a protein called Large ribosomal subunit protein eL38.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 74  | Lk    | 77       | 608   | 388 | 114 | 106 | 0       | 0     |

- Molecule 75 is a protein called Large ribosomal subunit protein eL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 75  | Ll    | 50       | 436   | 272 | 97 | 65 | 2 | 0       | 0     |

- Molecule 76 is a protein called Ubiquitin-ribosomal protein eL40A fusion protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 76  | Lm    | 52       | 417   | 259 | 86 | 67 | 5 | 0       | 0     |

- Molecule 77 is a protein called Large ribosomal subunit protein eL41A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 77  | Ln    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |       |

- Molecule 78 is a protein called Large ribosomal subunit protein eL42A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | Lo    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |       |

- Molecule 79 is a protein called Large ribosomal subunit protein eL43A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |       |

- Molecule 80 is a protein called Eukaryotic translation initiation factor 5A-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | CE    | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1097  | 686 | 184 | 218 | 9 |         |       |

- Molecule 81 is a protein called Large ribosomal subunit protein uL1A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 81  | L1    | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1718  | 1097 | 299 | 312 | 10 |         |       |

- Molecule 82 is a protein called Large ribosomal subunit protein uL10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 82  | P0    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1571  | 1006 | 272 | 289 | 4 |         |       |

- Molecule 83 is a protein called Elongation factor 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 83  | CD    | 816      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6348  | 4042 | 1079 | 1197 | 30 |         |       |

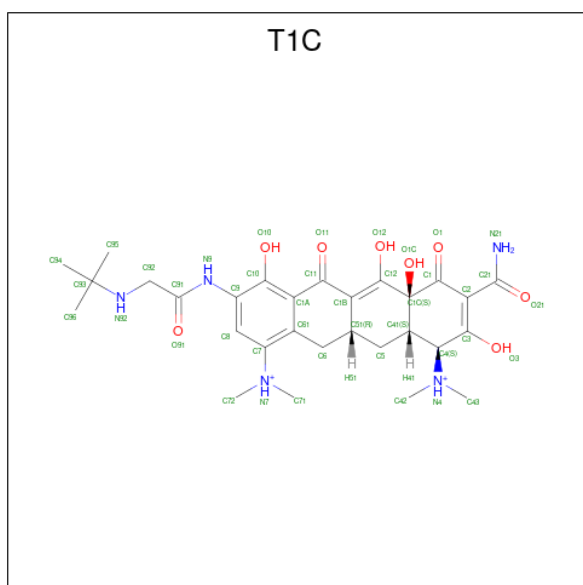
- Molecule 84 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms |     |     | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 84  | CS    | 122      | Total | C   | N   | O       | 0     | 0 |
|     |       |          | 919   | 541 | 184 | 194     |       |   |

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 85  | C2    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | SM    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Sa    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Sb    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lm    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lo    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lp    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 86 is TIGECYCLINE (CCD ID: T1C) (formula: C<sub>29</sub>H<sub>41</sub>N<sub>5</sub>O<sub>8</sub>).

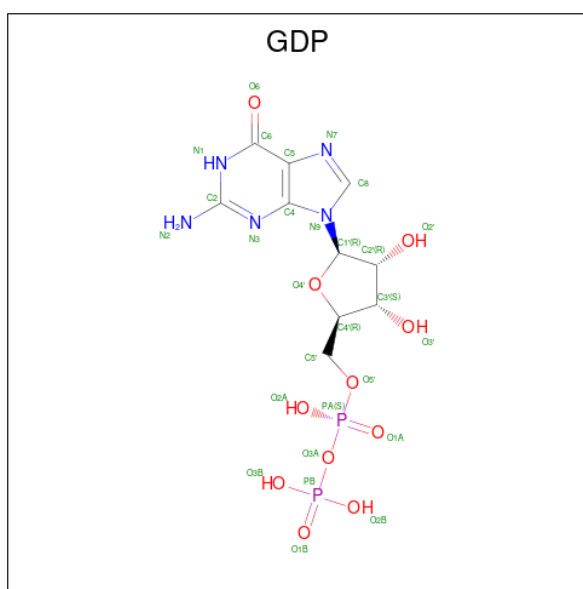


| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 86  | C1    | 1        | Total | C  | N | O | 0       |
|     |       |          | 42    | 29 | 5 | 8 |         |
| 86  | C1    | 1        | Total | C  | N | O | 0       |
|     |       |          | 42    | 29 | 5 | 8 |         |
| 86  | C1    | 1        | Total | C  | N | O | 0       |
|     |       |          | 42    | 29 | 5 | 8 |         |
| 86  | C1    | 1        | Total | C  | N | O | 0       |
|     |       |          | 42    | 29 | 5 | 8 |         |
| 86  | C1    | 1        | Total | C  | N | O | 0       |
|     |       |          | 42    | 29 | 5 | 8 |         |

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 87  | C1    | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 87  | C3    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 87  | CD    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 88  | CD    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

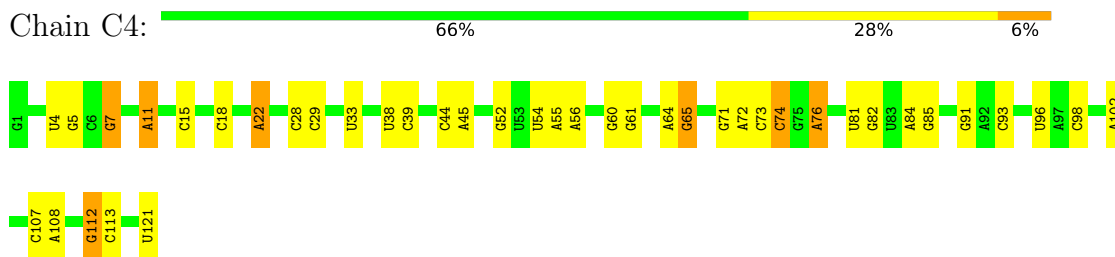




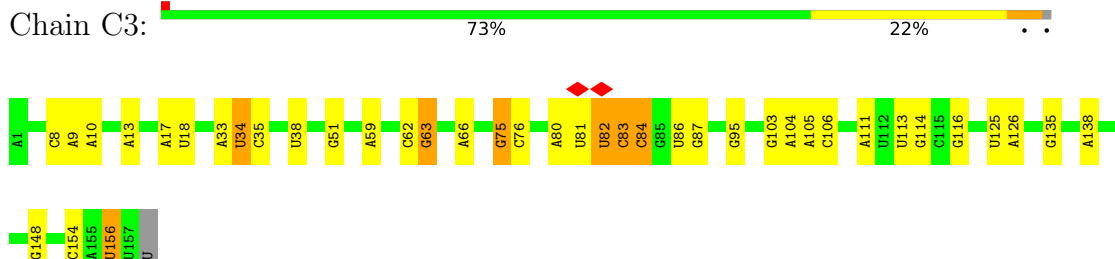




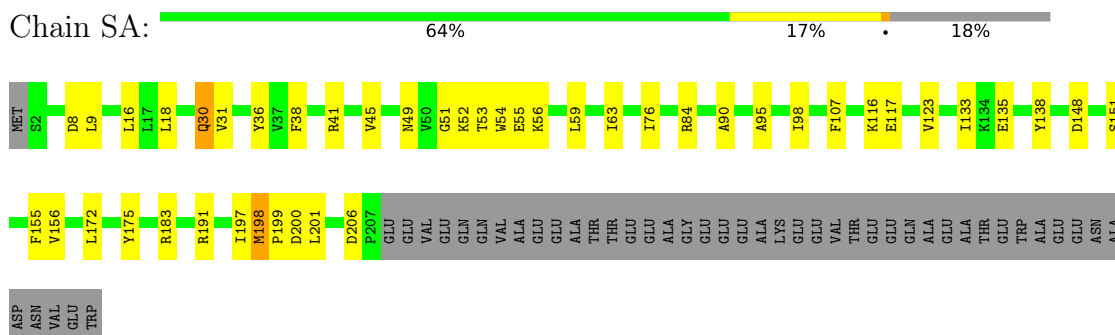
• Molecule 3: 5S rRNA



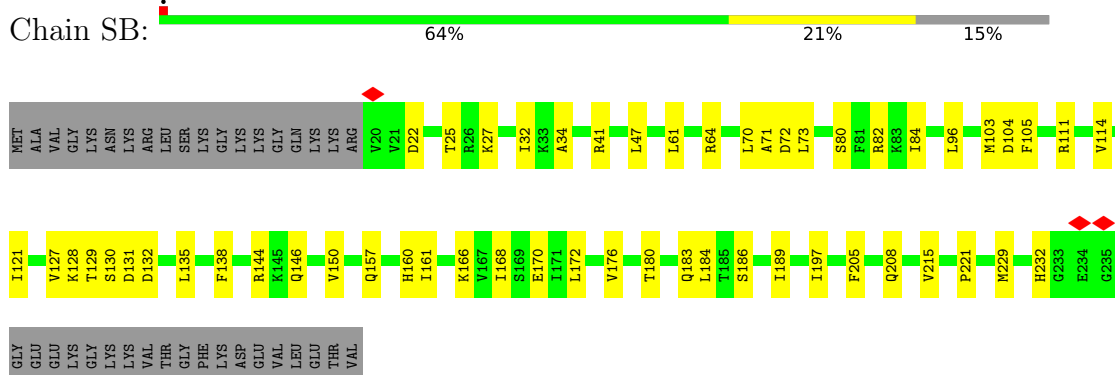
• Molecule 4: 5.8S rRNA



• Molecule 5: Small ribosomal subunit protein uS2A

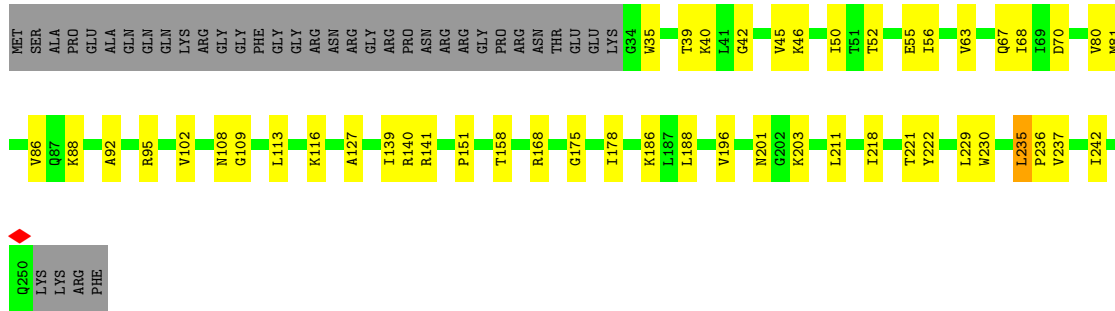


• Molecule 6: 40S ribosomal protein S1-A

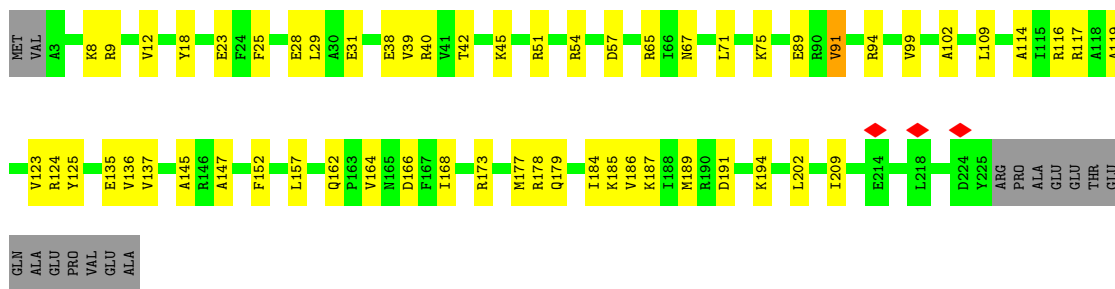


• Molecule 7: 40S ribosomal protein S2

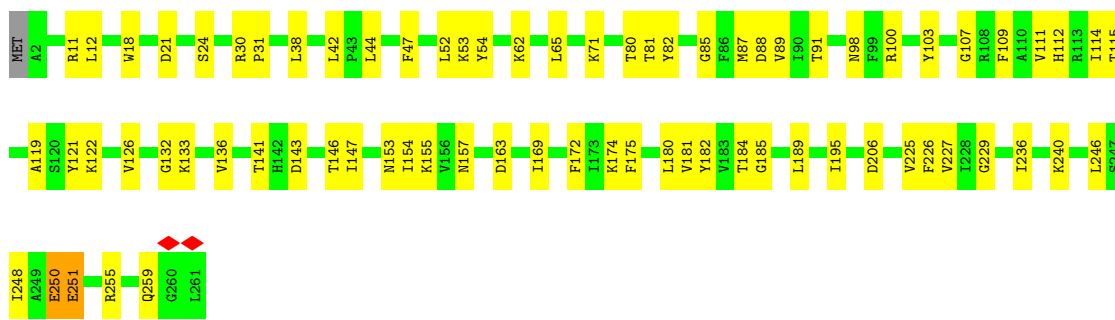




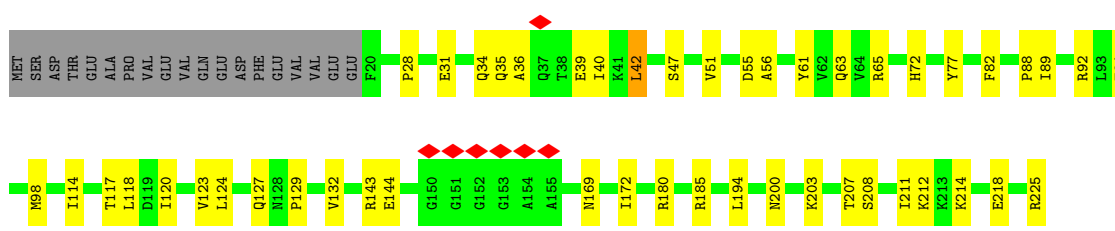
- Molecule 8: Small ribosomal subunit protein uS3



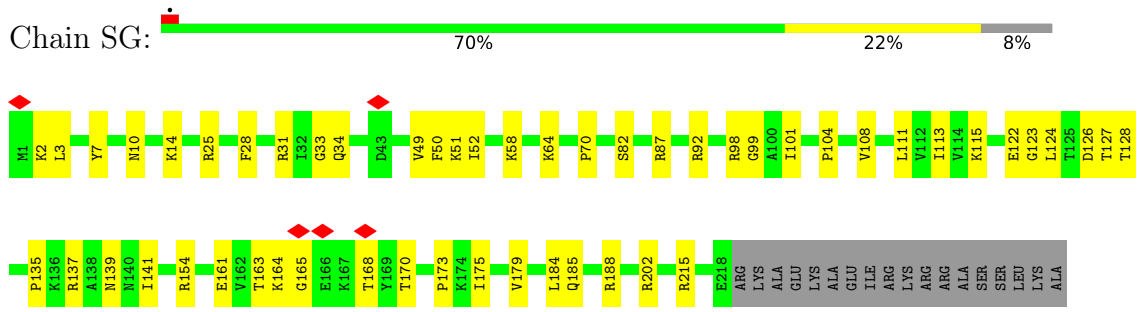
- Molecule 9: 40S ribosomal protein S4-A



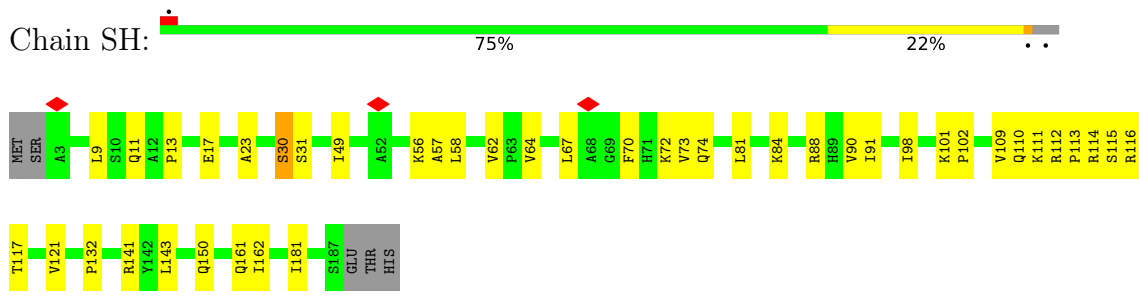
- Molecule 10: Small ribosomal subunit protein uS7



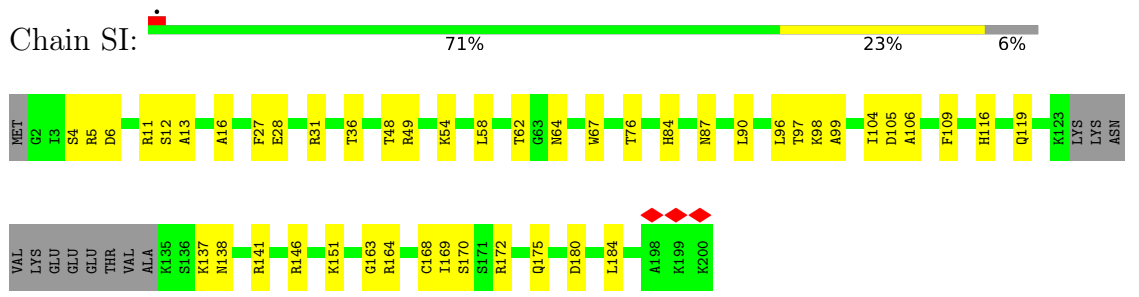
- Molecule 11: 40S ribosomal protein S6-A



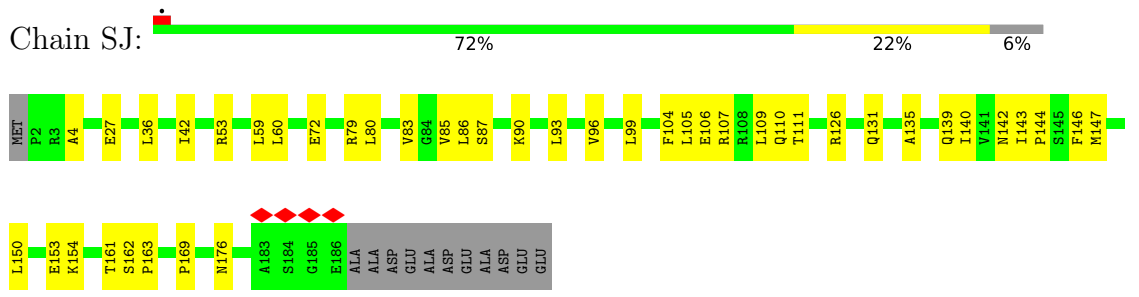
• Molecule 12: 40S ribosomal protein S7-A



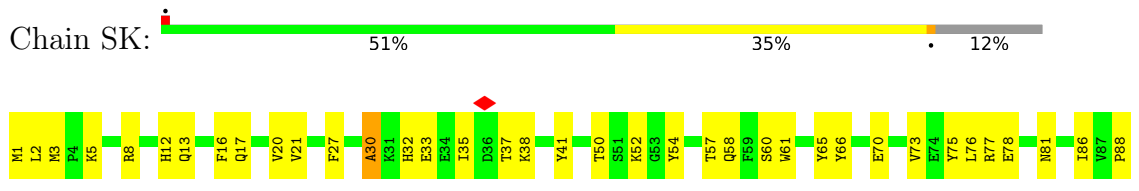
• Molecule 13: 40S ribosomal protein S8-A



• Molecule 14: 40S ribosomal protein S9-A

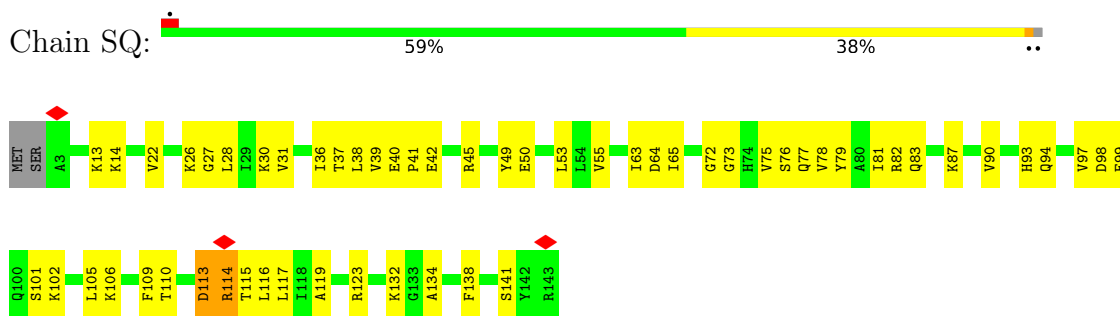


• Molecule 15: Small ribosomal subunit protein eS10A

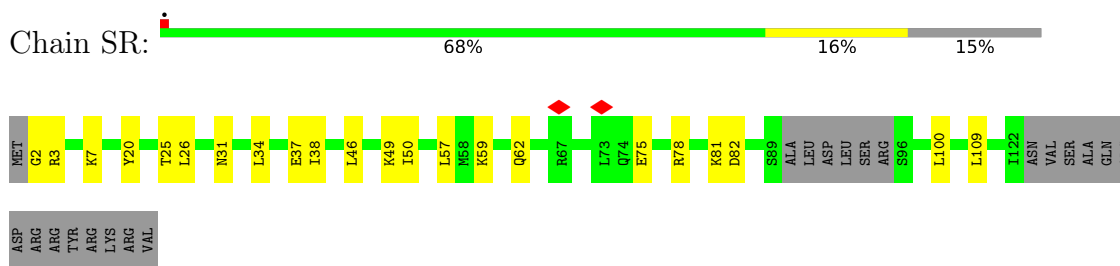




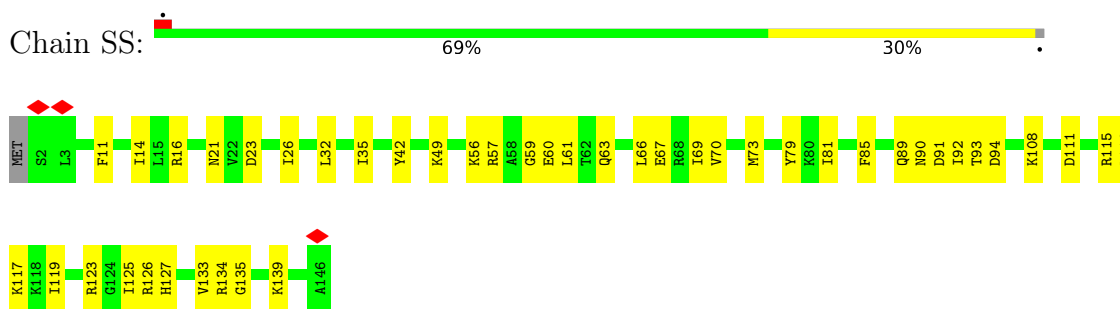
• Molecule 21: Small ribosomal subunit protein uS9A



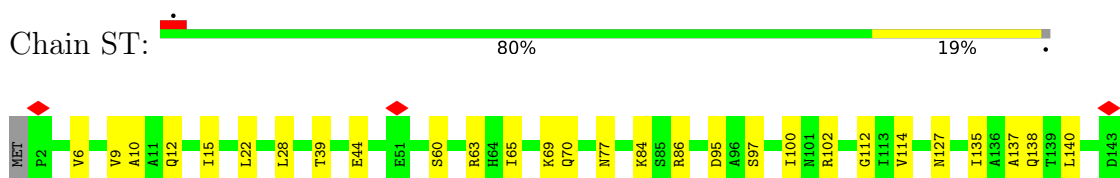
• Molecule 22: Small ribosomal subunit protein eS17A



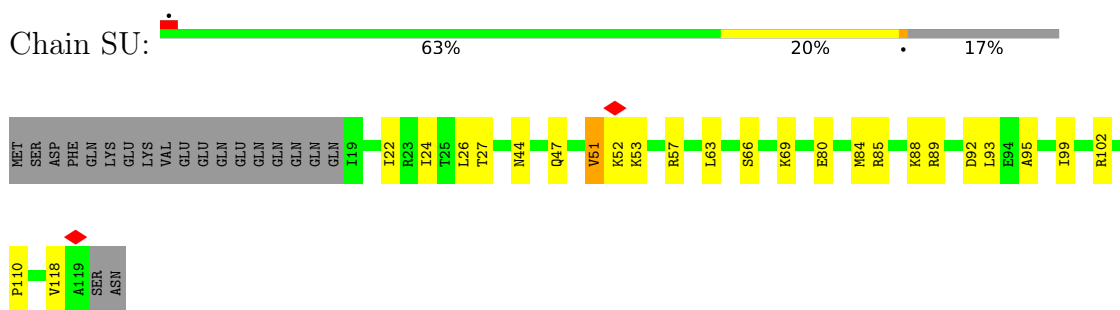
• Molecule 23: Small ribosomal subunit protein uS13A



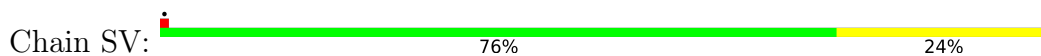
• Molecule 24: Small ribosomal subunit protein eS19A



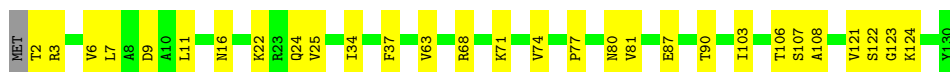
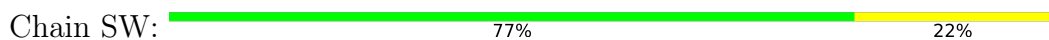
• Molecule 25: Small ribosomal subunit protein uS10



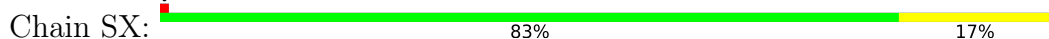
• Molecule 26: Small ribosomal subunit protein eS21A



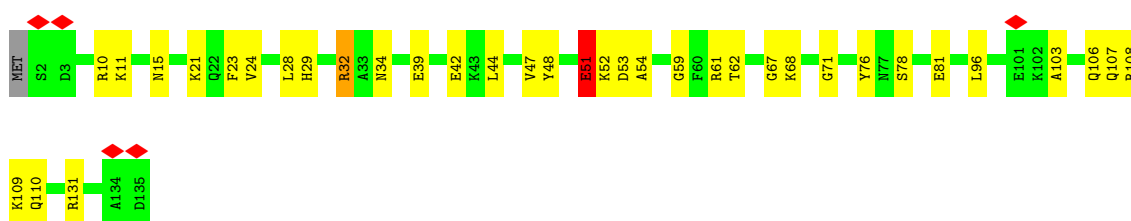
• Molecule 27: 40S ribosomal protein S22-A



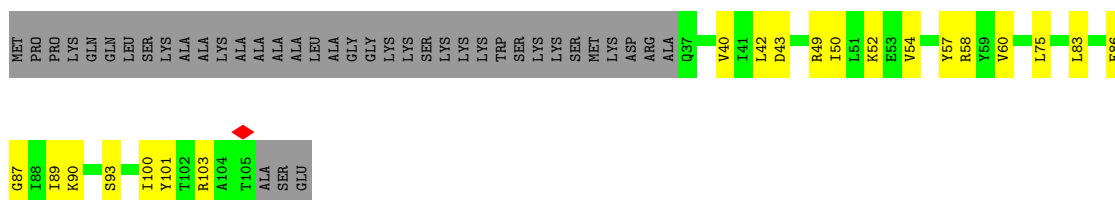
• Molecule 28: 40S ribosomal protein S23-A



• Molecule 29: 40S ribosomal protein S24-A



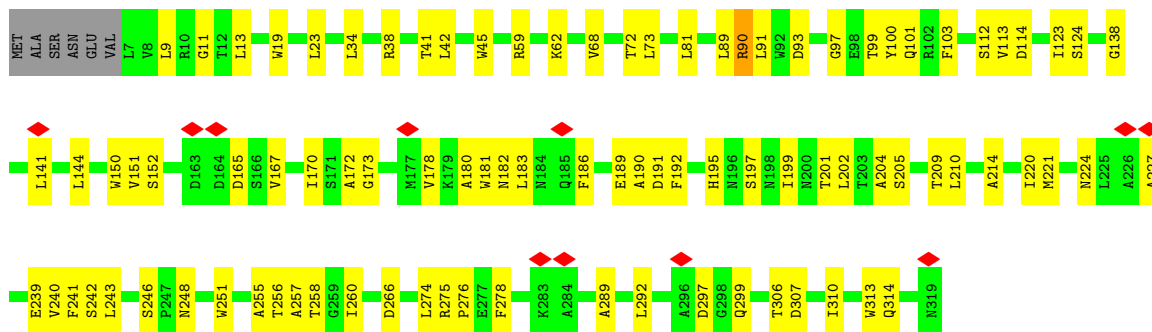
• Molecule 30: Small ribosomal subunit protein eS25A



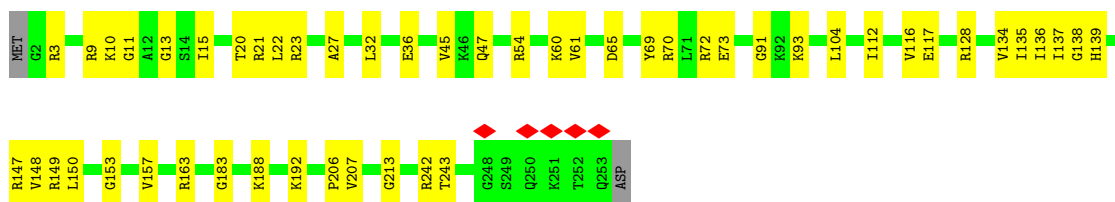
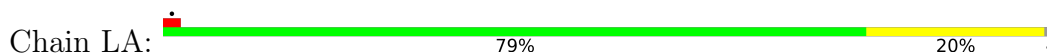
• Molecule 31: Small ribosomal subunit protein eS26B



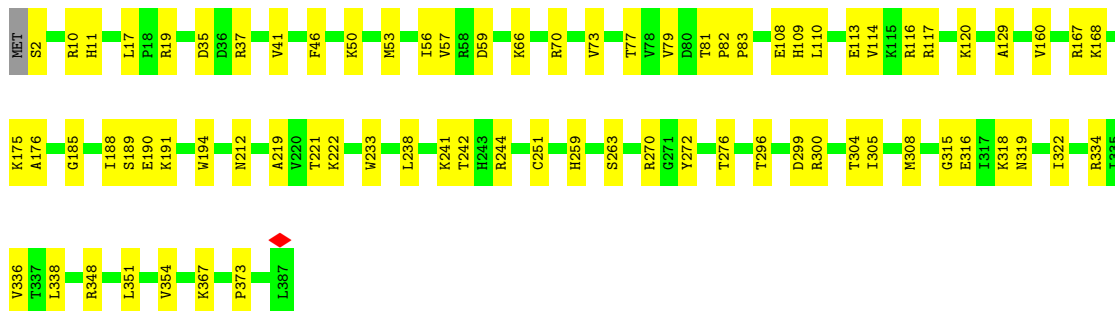
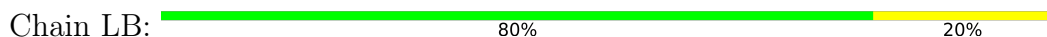




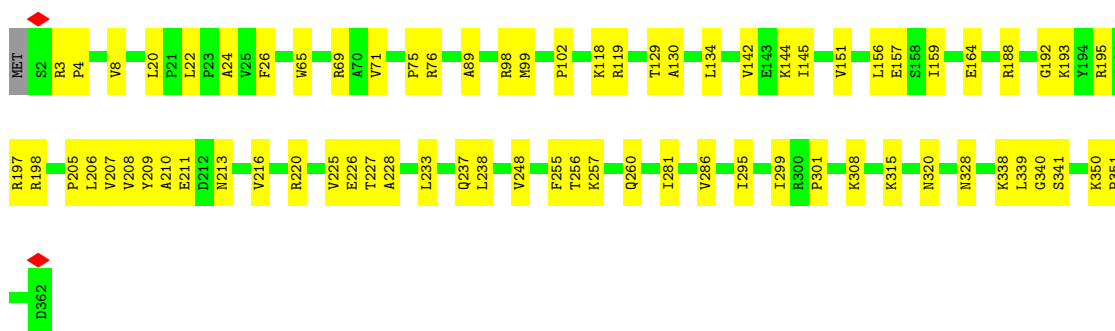
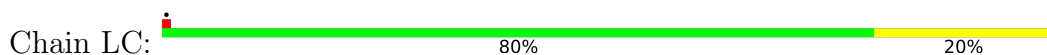
- Molecule 38: Large ribosomal subunit protein uL2A



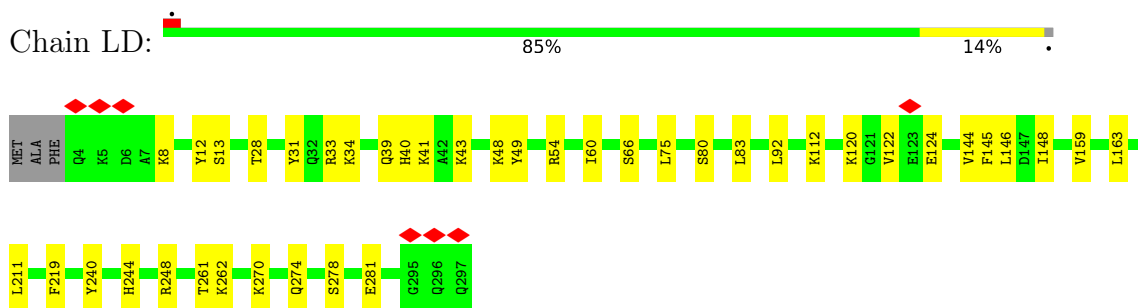
- Molecule 39: Large ribosomal subunit protein uL3



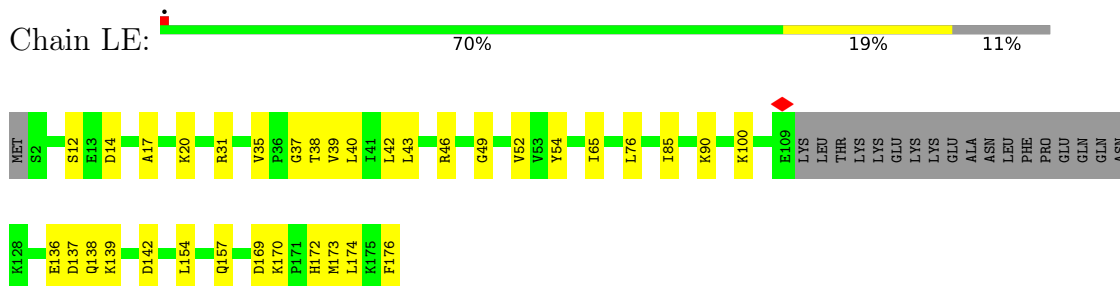
- Molecule 40: Large ribosomal subunit protein uL4A



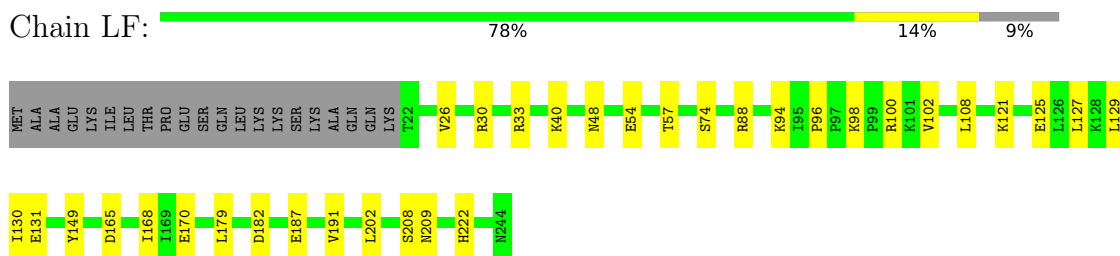
- Molecule 41: Large ribosomal subunit protein uL18



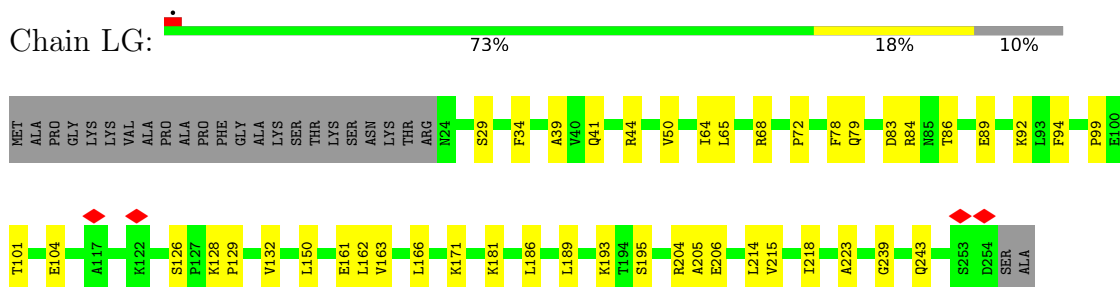
- Molecule 42: Large ribosomal subunit protein eL6A



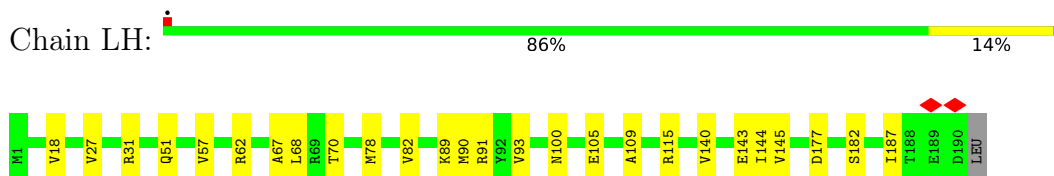
- Molecule 43: Large ribosomal subunit protein uL30A



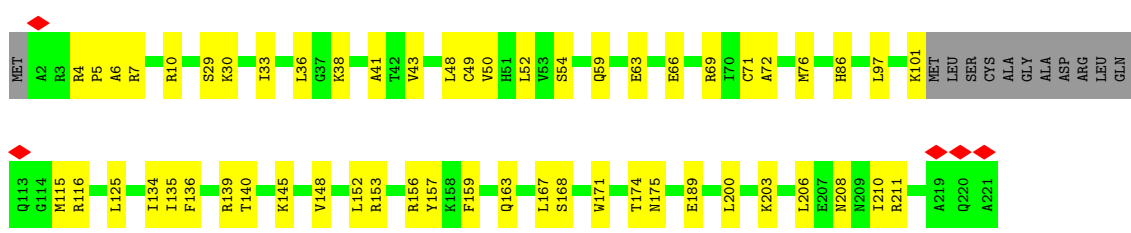
- Molecule 44: Large ribosomal subunit protein eL8A



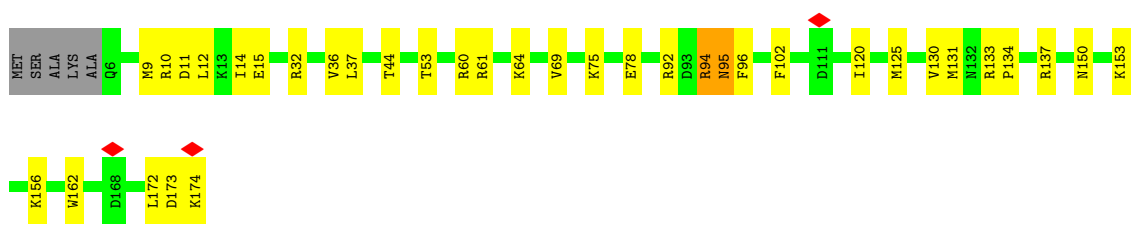
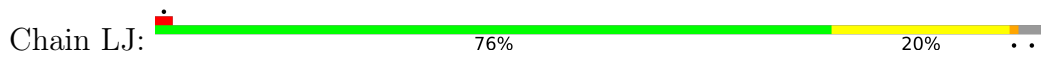
- Molecule 45: Large ribosomal subunit protein uL6A



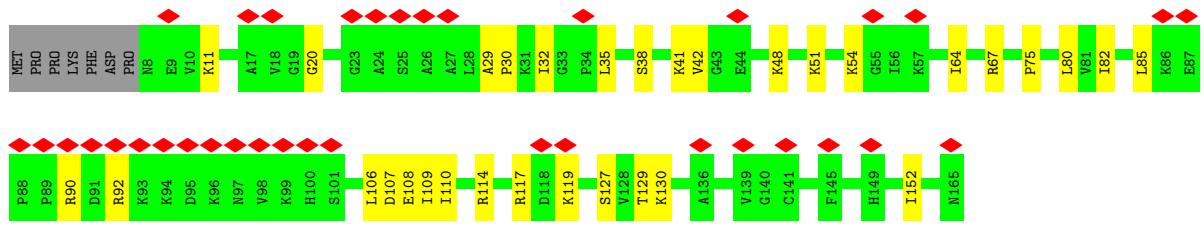
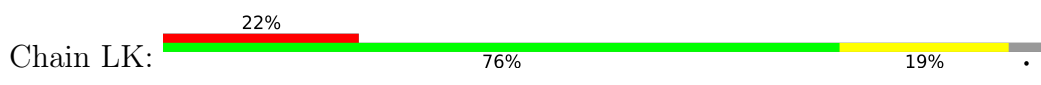
- Molecule 46: Large ribosomal subunit protein uL16



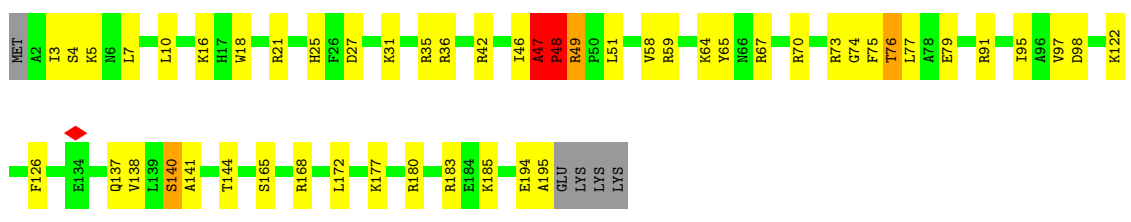
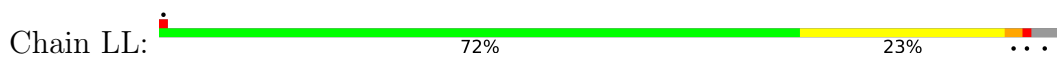
• Molecule 47: Large ribosomal subunit protein uL5A



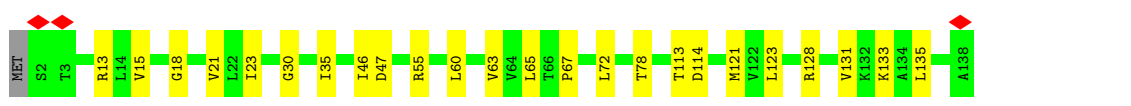
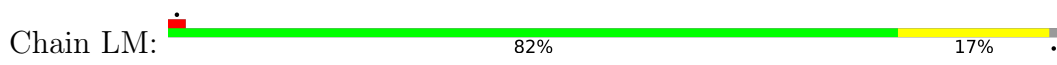
• Molecule 48: Large ribosomal subunit protein uL11A



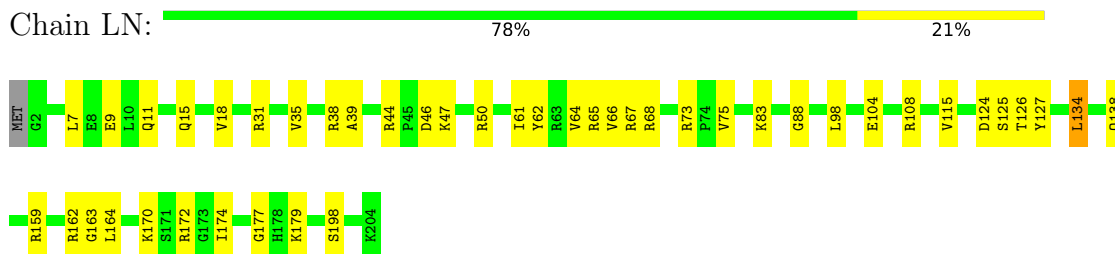
• Molecule 49: Large ribosomal subunit protein eL13A



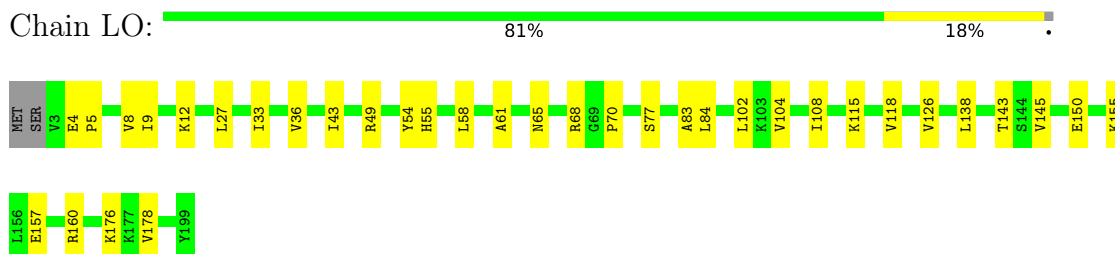
• Molecule 50: Large ribosomal subunit protein eL14A



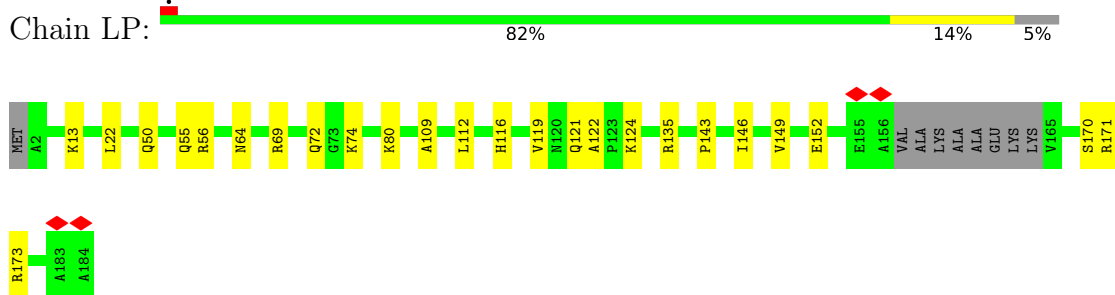
- Molecule 51: Large ribosomal subunit protein eL15A



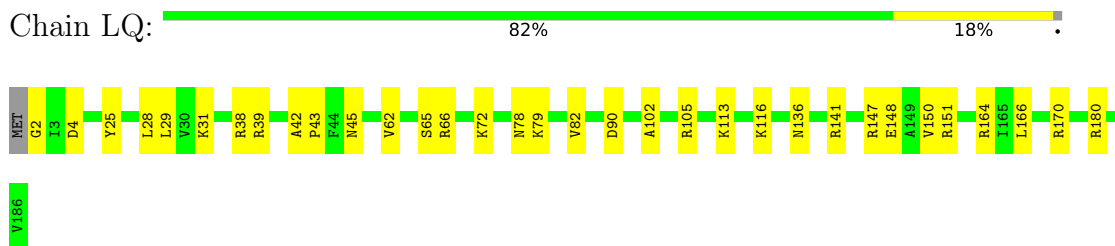
- Molecule 52: Large ribosomal subunit protein uL13A



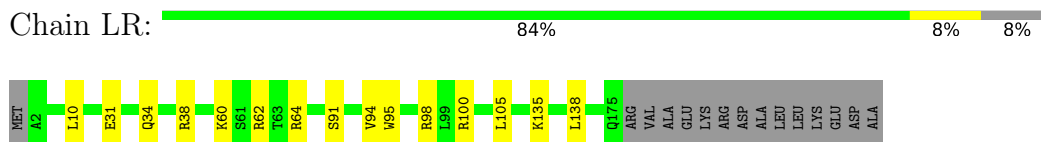
- Molecule 53: Large ribosomal subunit protein uL22A



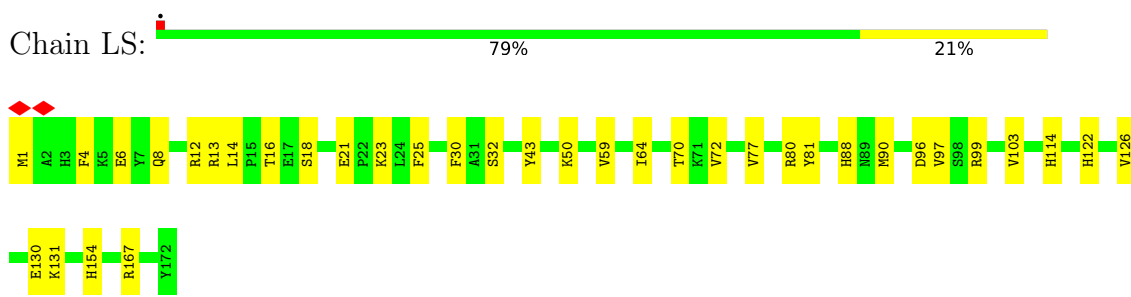
- Molecule 54: Large ribosomal subunit protein eL18A



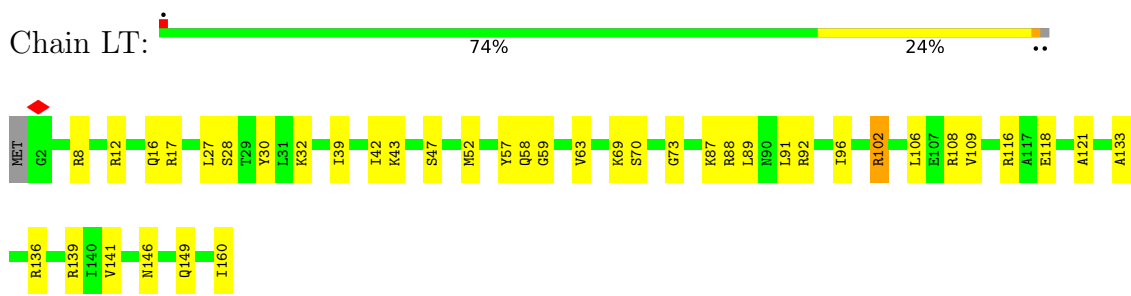
- Molecule 55: Large ribosomal subunit protein eL19A



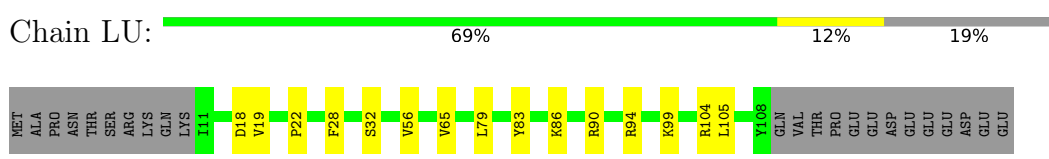
- Molecule 56: Large ribosomal subunit protein eL20A



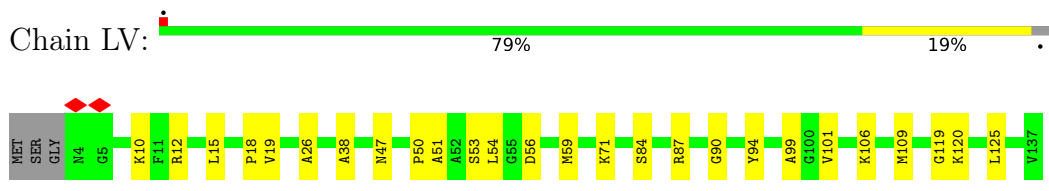
• Molecule 57: Large ribosomal subunit protein eL21A



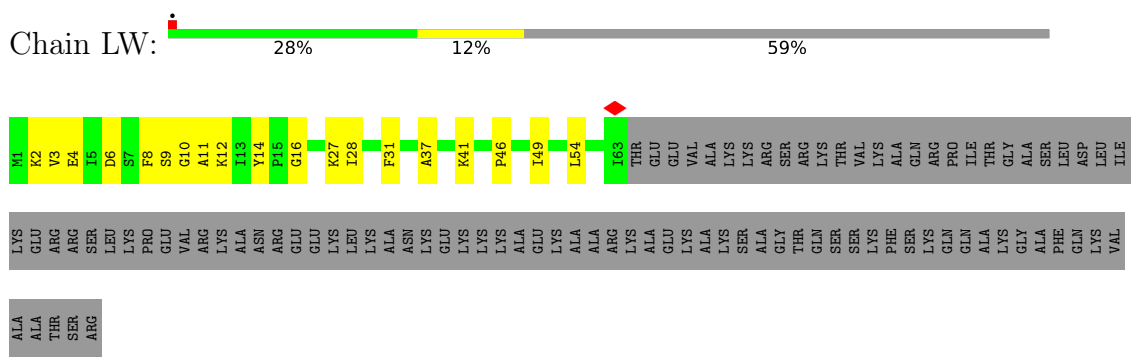
• Molecule 58: Large ribosomal subunit protein eL22A



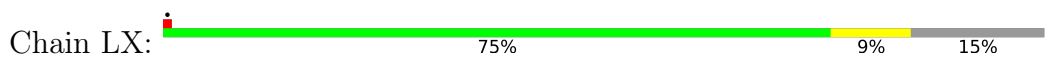
• Molecule 59: Large ribosomal subunit protein uL14A



• Molecule 60: Large ribosomal subunit protein eL24A

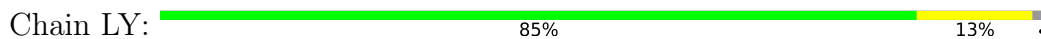


• Molecule 61: Large ribosomal subunit protein uL23

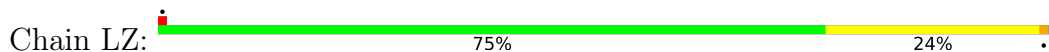




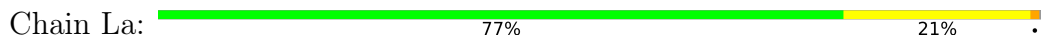
- Molecule 62: Large ribosomal subunit protein uL24A



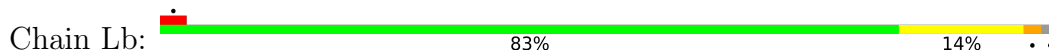
- Molecule 63: Large ribosomal subunit protein eL27A



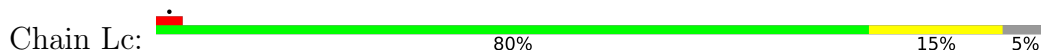
- Molecule 64: Large ribosomal subunit protein uL15



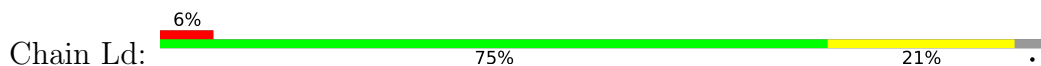
- Molecule 65: Large ribosomal subunit protein eL29




- Molecule 66: Large ribosomal subunit protein eL30



- Molecule 67: Large ribosomal subunit protein eL31A



- Molecule 68: Large ribosomal subunit protein eL32

Chain Le:  84% 14%




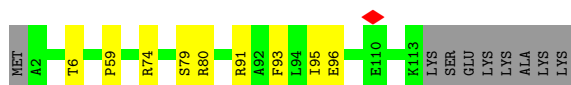
- Molecule 69: Large ribosomal subunit protein eL33A

Chain Lf:  66% 33%




- Molecule 70: Large ribosomal subunit protein eL34A

Chain Lg:  85% 7% 7%




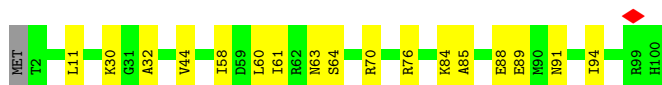
- Molecule 71: Large ribosomal subunit protein uL29A

Chain Lh:  84% 15%




- Molecule 72: Large ribosomal subunit protein eL36A

Chain Li:  82% 17%



- Molecule 73: Large ribosomal subunit protein eL37A

Chain Lj:  76% 17% 7%

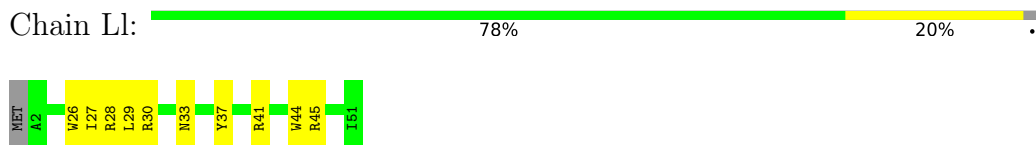


- Molecule 74: Large ribosomal subunit protein eL38

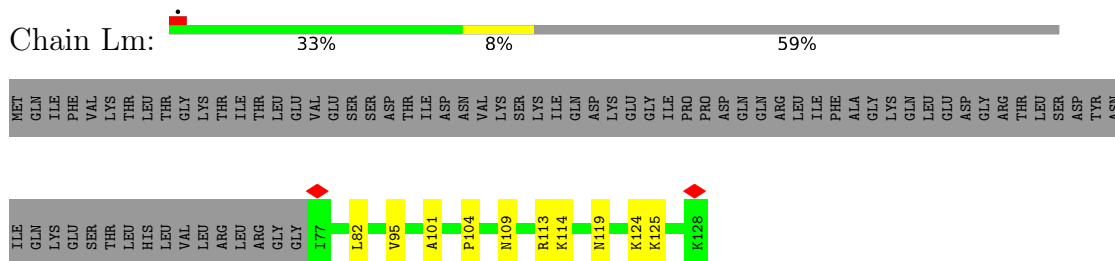
Chain Lk:  71% 28%



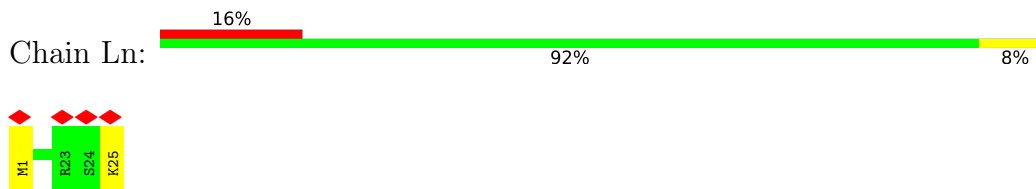
- Molecule 75: Large ribosomal subunit protein eL39



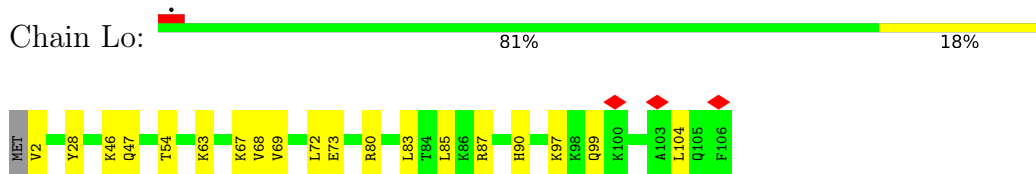
- Molecule 76: Ubiquitin-ribosomal protein eL40A fusion protein



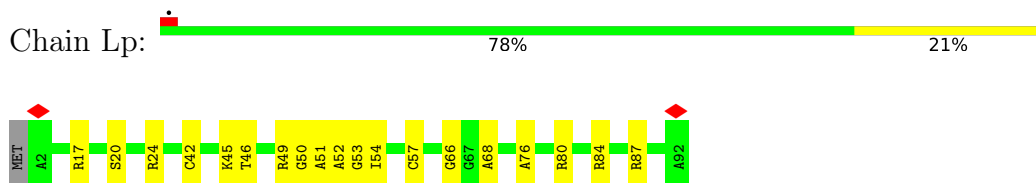
- Molecule 77: Large ribosomal subunit protein eL41A



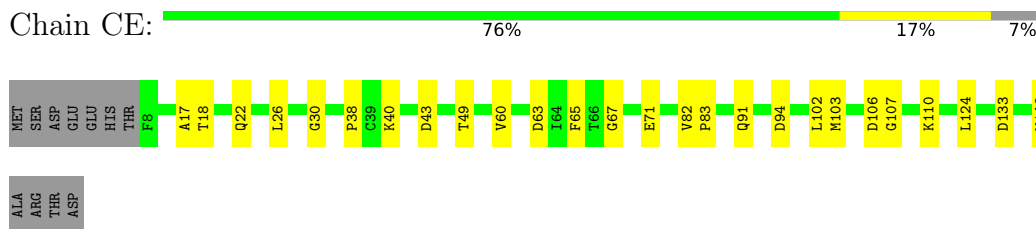
- Molecule 78: Large ribosomal subunit protein eL42A



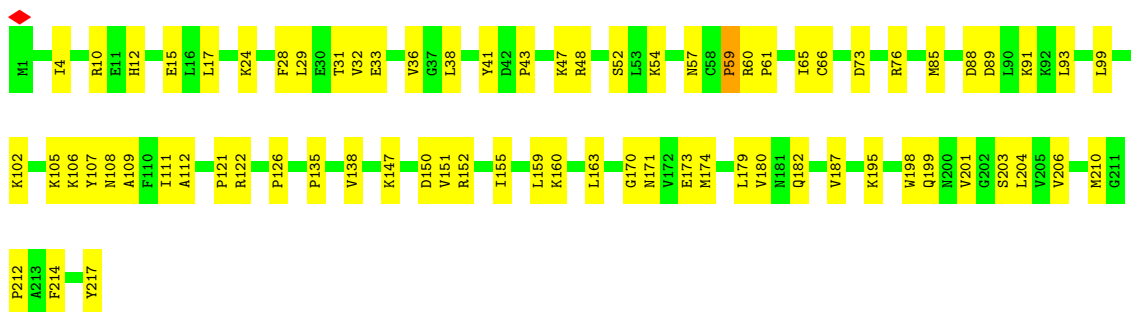
- Molecule 79: Large ribosomal subunit protein eL43A



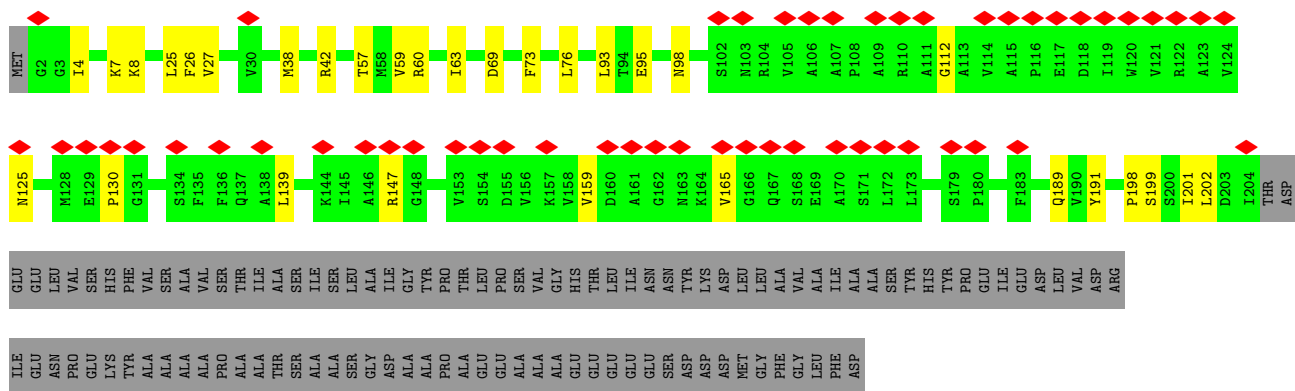
- Molecule 80: Eukaryotic translation initiation factor 5A-1



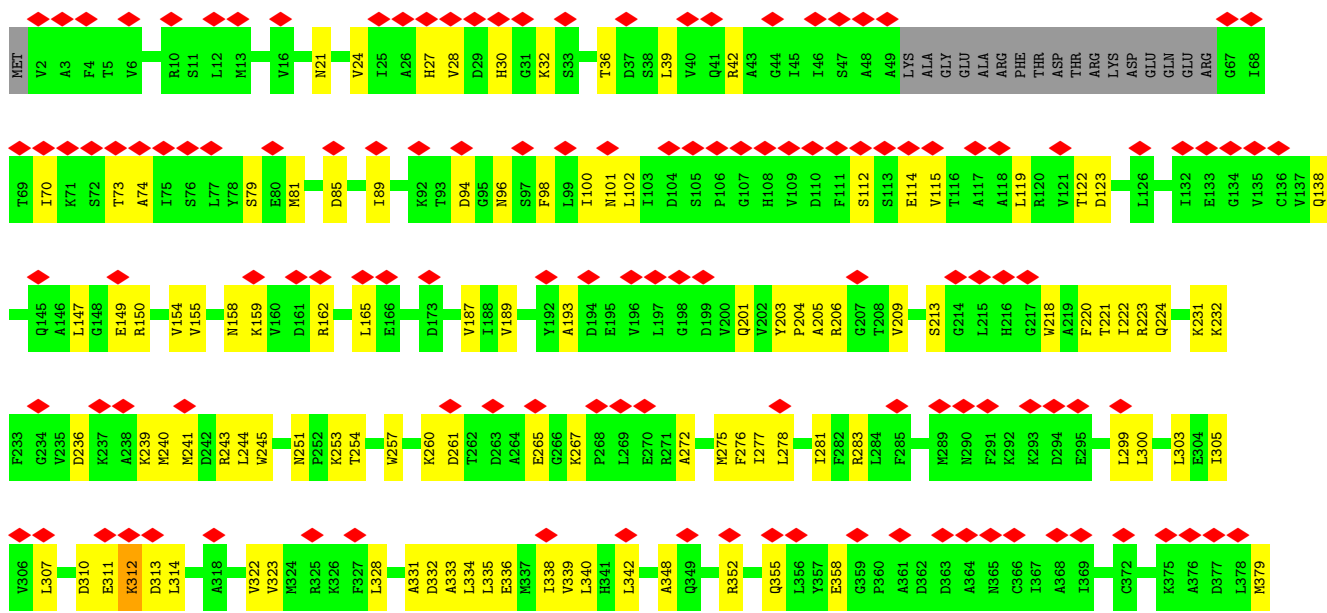
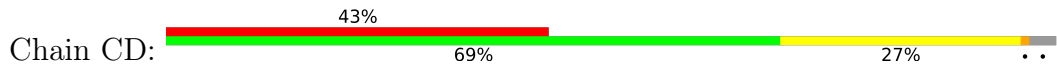
- Molecule 81: Large ribosomal subunit protein uL1A



• Molecule 82: Large ribosomal subunit protein uL10



• Molecule 83: Elongation factor 2





## 4 Experimental information

| Property                             | Value   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                 | Depositor |
| Imposed symmetry                     | POINT, Not provided                             |           |
| Number of particles used             | 105095  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                               | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion | Depositor |
| Microscope                           | FEI TITAN KRIOS                                 | Depositor |
| Voltage (kV)                         | 300   | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 44  | Depositor |
| Minimum defocus (nm)                 | 1000  | Depositor |
| Maximum defocus (nm)                 | 3500  | Depositor |
| Magnification                        | Not provided                                    |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)                       | Depositor |
| Maximum map value                    | 2.447   | Depositor |
| Minimum map value                    | -0.053  | Depositor |
| Average map value                    | 0.008   | Depositor |
| Map value standard deviation         | 0.069   | Depositor |
| Recommended contour level            | 0.02  | Depositor |
| Map size (Å)                         | 406.56, 406.56, 406.56                          | wwPDB     |
| Map dimensions                       | 480, 480, 480                                   | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                | wwPDB     |
| Pixel spacing (Å)                    | 0.847, 0.847, 0.847                             | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: T1C, 5CT, MG, ZN, GDP

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   | C2    | 0.23         | 0/40528 | 0.36        | 0/63141         |
| 2   | C1    | 0.33         | 0/76341 | 0.37        | 1/119019 (0.0%) |
| 3   | C4    | 0.25         | 0/2883  | 0.30        | 0/4491          |
| 4   | C3    | 0.31         | 0/3724  | 0.35        | 0/5798          |
| 5   | SA    | 0.29         | 0/1623  | 0.69        | 1/2222 (0.0%)   |
| 6   | SB    | 0.31         | 0/1748  | 0.67        | 0/2352          |
| 7   | SC    | 0.32         | 0/1665  | 0.63        | 0/2263          |
| 8   | SD    | 0.31         | 0/1759  | 0.73        | 2/2368 (0.1%)   |
| 9   | SE    | 0.29         | 0/2109  | 0.67        | 3/2839 (0.1%)   |
| 10  | SF    | 0.28         | 0/1629  | 0.64        | 0/2202          |
| 11  | SG    | 0.23         | 0/1779  | 0.53        | 0/2379          |
| 12  | SH    | 0.30         | 0/1511  | 0.68        | 2/2036 (0.1%)   |
| 13  | SI    | 0.29         | 0/1514  | 0.57        | 0/2021          |
| 14  | SJ    | 0.31         | 0/1519  | 0.66        | 1/2035 (0.0%)   |
| 15  | SK    | 0.38         | 0/757   | 0.83        | 0/1022          |
| 16  | SL    | 0.26         | 0/1194  | 0.47        | 0/1610          |
| 17  | SM    | 0.34         | 0/898   | 0.86        | 0/1220          |
| 18  | SN    | 0.30         | 0/1215  | 0.65        | 1/1638 (0.1%)   |
| 19  | SO    | 0.27         | 0/960   | 0.56        | 0/1290          |
| 20  | SP    | 0.27         | 0/959   | 0.69        | 0/1288          |
| 21  | SQ    | 0.30         | 0/1125  | 0.71        | 2/1510 (0.1%)   |
| 22  | SR    | 0.34         | 0/904   | 0.78        | 1/1210 (0.1%)   |
| 23  | SS    | 0.32         | 0/1211  | 0.76        | 0/1628          |
| 24  | ST    | 0.24         | 0/1130  | 0.53        | 0/1517          |
| 25  | SU    | 0.30         | 0/815   | 0.72        | 0/1102          |
| 26  | SV    | 0.30         | 0/693   | 0.71        | 0/935           |
| 27  | SW    | 0.28         | 0/1038  | 0.56        | 0/1395          |
| 28  | SX    | 0.28         | 0/1139  | 0.56        | 0/1518          |
| 29  | SY    | 0.28         | 0/1087  | 0.82        | 3/1449 (0.2%)   |
| 30  | SZ    | 0.32         | 0/566   | 0.74        | 2/761 (0.3%)    |
| 31  | Sa    | 0.28         | 0/782   | 0.54        | 0/1047          |
| 32  | Sb    | 0.22         | 0/620   | 0.69        | 0/838           |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 33  | Sc    | 0.30         | 0/499         | 0.75        | 0/670         |
| 34  | Sd    | 0.25         | 0/452         | 0.55        | 0/600         |
| 35  | Se    | 0.40         | 0/483         | 0.71        | 1/643 (0.2%)  |
| 36  | Sf    | 0.23         | 0/253         | 0.64        | 0/340         |
| 37  | Sg    | 0.25         | 0/2456        | 0.71        | 0/3343        |
| 38  | LA    | 0.39         | 0/1946        | 0.69        | 2/2614 (0.1%) |
| 39  | LB    | 0.33         | 0/3146        | 0.54        | 0/4228        |
| 40  | LC    | 0.33         | 0/2800        | 0.59        | 0/3790        |
| 41  | LD    | 0.26         | 0/2408        | 0.55        | 0/3248        |
| 42  | LE    | 0.29         | 0/1269        | 0.57        | 0/1705        |
| 43  | LF    | 0.31         | 0/1828        | 0.59        | 0/2461        |
| 44  | LG    | 0.32         | 0/1795        | 0.66        | 0/2429        |
| 45  | LH    | 0.33         | 0/1531        | 0.63        | 0/2062        |
| 46  | LI    | 0.30         | 0/1732        | 0.57        | 1/2323 (0.0%) |
| 47  | LJ    | 0.27         | 0/1374        | 0.69        | 0/1842        |
| 48  | LK    | 0.22         | 0/1210        | 0.51        | 0/1627        |
| 49  | LL    | 0.32         | 0/1573        | 0.73        | 3/2113 (0.1%) |
| 50  | LM    | 0.30         | 0/1074        | 0.53        | 0/1446        |
| 51  | LN    | 0.39         | 1/1757 (0.1%) | 0.52        | 0/2354        |
| 52  | LO    | 0.37         | 0/1585        | 0.57        | 0/2128        |
| 53  | LP    | 0.30         | 0/1400        | 0.48        | 0/1882        |
| 54  | LQ    | 0.28         | 0/1465        | 0.50        | 0/1965        |
| 55  | LR    | 0.31         | 0/1382        | 0.53        | 0/1849        |
| 56  | LS    | 0.33         | 0/1481        | 0.57        | 0/1990        |
| 57  | LT    | 0.31         | 0/1300        | 0.58        | 0/1743        |
| 58  | LU    | 0.27         | 0/794         | 0.57        | 0/1076        |
| 59  | LV    | 0.32         | 0/1008        | 0.56        | 0/1356        |
| 60  | LW    | 0.32         | 0/533         | 0.60        | 0/707         |
| 61  | LX    | 0.37         | 0/974         | 0.65        | 0/1314        |
| 62  | LY    | 0.25         | 0/987         | 0.48        | 0/1318        |
| 63  | LZ    | 0.33         | 0/1118        | 0.69        | 1/1497 (0.1%) |
| 64  | La    | 0.35         | 0/1204        | 0.69        | 2/1612 (0.1%) |
| 65  | Lb    | 0.29         | 0/473         | 0.69        | 0/629         |
| 66  | Lc    | 0.24         | 0/775         | 0.52        | 0/1040        |
| 67  | Ld    | 0.30         | 0/897         | 0.53        | 0/1205        |
| 68  | Le    | 0.37         | 0/1041        | 0.67        | 0/1394        |
| 69  | Lf    | 0.36         | 0/868         | 0.55        | 0/1168        |
| 70  | Lg    | 0.30         | 0/890         | 0.47        | 0/1189        |
| 71  | Lh    | 0.31         | 0/974         | 0.58        | 0/1297        |
| 72  | Li    | 0.29         | 0/777         | 0.55        | 0/1033        |
| 73  | Lj    | 0.37         | 0/665         | 0.48        | 0/882         |
| 74  | Lk    | 0.25         | 0/614         | 0.55        | 0/822         |
| 75  | Ll    | 0.39         | 0/443         | 0.64        | 0/588         |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 76  | Lm    | 0.27         | 0/423           | 0.54        | 0/562            |
| 77  | Ln    | 0.25         | 0/234           | 0.45        | 0/300            |
| 78  | Lo    | 0.29         | 0/860           | 0.49        | 0/1136           |
| 79  | Lp    | 0.33         | 0/701           | 0.68        | 0/934            |
| 80  | CE    | 0.34         | 0/1097          | 0.74        | 0/1476           |
| 81  | L1    | 0.35         | 0/1745          | 0.75        | 0/2342           |
| 82  | P0    | 0.23         | 0/1598          | 0.58        | 0/2161           |
| 83  | CD    | 0.33         | 0/6469          | 0.73        | 8/8760 (0.1%)    |
| 84  | CS    | 0.31         | 0/929           | 0.60        | 1/1245 (0.1%)    |
| All | All   | 0.30         | 1/224715 (0.0%) | 0.49        | 38/328582 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | SA    | 0                   | 1                   |
| 10  | SF    | 0                   | 1                   |
| 12  | SH    | 0                   | 3                   |
| 16  | SL    | 0                   | 1                   |
| 17  | SM    | 0                   | 1                   |
| 21  | SQ    | 0                   | 2                   |
| 23  | SS    | 0                   | 2                   |
| 25  | SU    | 0                   | 1                   |
| 29  | SY    | 0                   | 1                   |
| 32  | Sb    | 0                   | 1                   |
| 35  | Se    | 0                   | 1                   |
| 37  | Sg    | 0                   | 1                   |
| 38  | LA    | 0                   | 1                   |
| 40  | LC    | 0                   | 1                   |
| 47  | LJ    | 0                   | 1                   |
| 49  | LL    | 0                   | 2                   |
| 57  | LT    | 0                   | 1                   |
| 64  | La    | 0                   | 1                   |
| 65  | Lb    | 0                   | 1                   |
| 72  | Li    | 0                   | 1                   |
| 79  | Lp    | 0                   | 1                   |
| 83  | CD    | 0                   | 2                   |
| All | All   | 0                   | 28                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 51  | LN    | 134 | LEU  | CG-CD2 | -5.04 | 1.35        | 1.52     |

The worst 5 of 38 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 83  | CD    | 606 | ILE  | CA-C-N | 9.07 | 133.90      | 121.20   |
| 83  | CD    | 606 | ILE  | C-N-CA | 9.07 | 133.90      | 121.20   |
| 64  | La    | 47  | LYS  | CA-C-N | 8.76 | 138.27      | 121.54   |
| 64  | La    | 47  | LYS  | C-N-CA | 8.76 | 138.27      | 121.54   |
| 49  | LL    | 140 | SER  | CA-C-N | 7.56 | 135.97      | 121.54   |

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 5   | SA    | 206 | ASP  | Peptide |
| 10  | SF    | 42  | LEU  | Peptide |
| 12  | SH    | 111 | LYS  | Peptide |
| 12  | SH    | 30  | SER  | Peptide |
| 12  | SH    | 31  | SER  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C2    | 36234 | 0        | 18231    | 331     | 0            |
| 2   | C1    | 68200 | 0        | 34275    | 476     | 0            |
| 3   | C4    | 2579  | 0        | 1304     | 24      | 0            |
| 4   | C3    | 3333  | 0        | 1685     | 23      | 0            |
| 5   | SA    | 1583  | 0        | 1578     | 31      | 0            |
| 6   | SB    | 1722  | 0        | 1793     | 39      | 0            |
| 7   | SC    | 1635  | 0        | 1723     | 36      | 0            |
| 8   | SD    | 1734  | 0        | 1817     | 43      | 0            |
| 9   | SE    | 2068  | 0        | 2154     | 55      | 0            |
| 10  | SF    | 1609  | 0        | 1675     | 37      | 0            |
| 11  | SG    | 1755  | 0        | 1846     | 37      | 0            |
| 12  | SH    | 1486  | 0        | 1576     | 27      | 0            |
| 13  | SI    | 1489  | 0        | 1525     | 35      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | SJ    | 1494  | 0        | 1573     | 28      | 0            |
| 15  | SK    | 741   | 0        | 691      | 22      | 0            |
| 16  | SL    | 1168  | 0        | 1233     | 16      | 0            |
| 17  | SM    | 890   | 0        | 887      | 22      | 0            |
| 18  | SN    | 1192  | 0        | 1255     | 18      | 0            |
| 19  | SO    | 949   | 0        | 985      | 16      | 0            |
| 20  | SP    | 939   | 0        | 968      | 23      | 0            |
| 21  | SQ    | 1105  | 0        | 1166     | 44      | 0            |
| 22  | SR    | 896   | 0        | 902      | 17      | 0            |
| 23  | SS    | 1192  | 0        | 1222     | 31      | 0            |
| 24  | ST    | 1112  | 0        | 1124     | 20      | 0            |
| 25  | SU    | 805   | 0        | 874      | 18      | 0            |
| 26  | SV    | 684   | 0        | 672      | 19      | 0            |
| 27  | SW    | 1021  | 0        | 1060     | 22      | 0            |
| 28  | SX    | 1121  | 0        | 1196     | 19      | 0            |
| 29  | SY    | 1073  | 0        | 1132     | 32      | 0            |
| 30  | SZ    | 558   | 0        | 598      | 13      | 0            |
| 31  | Sa    | 769   | 0        | 814      | 17      | 0            |
| 32  | Sb    | 610   | 0        | 633      | 7       | 0            |
| 33  | Sc    | 497   | 0        | 535      | 11      | 0            |
| 34  | Sd    | 442   | 0        | 432      | 5       | 0            |
| 35  | Se    | 475   | 0        | 525      | 15      | 0            |
| 36  | Sf    | 248   | 0        | 237      | 4       | 0            |
| 37  | Sg    | 2403  | 0        | 2350     | 65      | 0            |
| 38  | LA    | 1912  | 0        | 1976     | 40      | 0            |
| 39  | LB    | 3075  | 0        | 3142     | 50      | 0            |
| 40  | LC    | 2748  | 0        | 2859     | 48      | 0            |
| 41  | LD    | 2359  | 0        | 2311     | 29      | 0            |
| 42  | LE    | 1248  | 0        | 1339     | 27      | 0            |
| 43  | LF    | 1791  | 0        | 1869     | 24      | 0            |
| 44  | LG    | 1763  | 0        | 1819     | 35      | 0            |
| 45  | LH    | 1510  | 0        | 1576     | 17      | 0            |
| 46  | LI    | 1696  | 0        | 1731     | 39      | 0            |
| 47  | LJ    | 1353  | 0        | 1383     | 30      | 0            |
| 48  | LK    | 1196  | 0        | 1257     | 19      | 0            |
| 49  | LL    | 1548  | 0        | 1613     | 44      | 0            |
| 50  | LM    | 1059  | 0        | 1154     | 16      | 0            |
| 51  | LN    | 1720  | 0        | 1779     | 39      | 0            |
| 52  | LO    | 1555  | 0        | 1659     | 24      | 0            |
| 53  | LP    | 1378  | 0        | 1404     | 16      | 0            |
| 54  | LQ    | 1441  | 0        | 1543     | 30      | 0            |
| 55  | LR    | 1365  | 0        | 1414     | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | LS    | 1445  | 0        | 1487     | 26      | 0            |
| 57  | LT    | 1276  | 0        | 1323     | 36      | 0            |
| 58  | LU    | 778   | 0        | 791      | 10      | 0            |
| 59  | LV    | 993   | 0        | 1040     | 19      | 0            |
| 60  | LW    | 521   | 0        | 551      | 13      | 0            |
| 61  | LX    | 959   | 0        | 1023     | 8       | 0            |
| 62  | LY    | 976   | 0        | 1064     | 12      | 0            |
| 63  | LZ    | 1092  | 0        | 1155     | 22      | 0            |
| 64  | La    | 1173  | 0        | 1215     | 22      | 0            |
| 65  | Lb    | 462   | 0        | 491      | 5       | 0            |
| 66  | Lc    | 767   | 0        | 816      | 9       | 0            |
| 67  | Ld    | 883   | 0        | 918      | 20      | 0            |
| 68  | Le    | 1020  | 0        | 1090     | 13      | 0            |
| 69  | Lf    | 850   | 0        | 880      | 27      | 0            |
| 70  | Lg    | 880   | 0        | 942      | 8       | 0            |
| 71  | Lh    | 965   | 0        | 1067     | 16      | 0            |
| 72  | Li    | 770   | 0        | 846      | 14      | 0            |
| 73  | Lj    | 650   | 0        | 650      | 10      | 0            |
| 74  | Lk    | 608   | 0        | 671      | 15      | 0            |
| 75  | Ll    | 436   | 0        | 475      | 7       | 0            |
| 76  | Lm    | 417   | 0        | 455      | 9       | 0            |
| 77  | Ln    | 233   | 0        | 284      | 2       | 0            |
| 78  | Lo    | 847   | 0        | 915      | 14      | 0            |
| 79  | Lp    | 694   | 0        | 734      | 13      | 0            |
| 80  | CE    | 1097  | 0        | 1078     | 22      | 0            |
| 81  | L1    | 1718  | 0        | 1811     | 51      | 0            |
| 82  | P0    | 1571  | 0        | 1614     | 21      | 0            |
| 83  | CD    | 6348  | 0        | 6422     | 159     | 0            |
| 84  | CS    | 919   | 0        | 913      | 17      | 0            |
| 85  | C2    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lg    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lj    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lm    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lo    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lp    | 1     | 0        | 0        | 0       | 0            |
| 85  | SM    | 1     | 0        | 0        | 0       | 0            |
| 85  | Sa    | 1     | 0        | 0        | 0       | 0            |
| 85  | Sb    | 1     | 0        | 0        | 0       | 0            |
| 86  | C1    | 252   | 0        | 228      | 4       | 0            |
| 87  | C1    | 2     | 0        | 0        | 0       | 0            |
| 87  | C3    | 1     | 0        | 0        | 0       | 0            |
| 87  | CD    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 88  | CD    | 28     | 0        | 12       | 0       | 0            |
| All | All   | 210169 | 0        | 159035   | 2365    | 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 7.

The worst 5 of 2365 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) |
|------------------|------------------|--------------------------|-------------------|
| 60:LW:4:GLU:O    | 60:LW:12:LYS:HA  | 1.36                     | 1.22              |
| 47:LJ:92:ARG:O   | 47:LJ:95:ASN:HB2 | 1.42                     | 1.20              |
| 79:Lp:53:GLY:HA2 | 79:Lp:66:GLY:O   | 1.55                     | 1.07              |
| 2:C1:3165:A:N6   | 2:C1:3285:C:H42  | 1.54                     | 1.04              |
| 1:C2:1588:G:H1   | 1:C2:1608:U:H3   | 1.02                     | 1.01              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 5   | SA    | 204/252 (81%) | 175 (86%) | 28 (14%) | 1 (0%)   | 24 59       |
| 6   | SB    | 214/255 (84%) | 196 (92%) | 18 (8%)  | 0        | 100 100     |
| 7   | SC    | 215/254 (85%) | 201 (94%) | 13 (6%)  | 1 (0%)   | 24 59       |
| 8   | SD    | 221/240 (92%) | 195 (88%) | 25 (11%) | 1 (0%)   | 24 59       |
| 9   | SE    | 258/261 (99%) | 234 (91%) | 24 (9%)  | 0        | 100 100     |
| 10  | SF    | 204/225 (91%) | 176 (86%) | 28 (14%) | 0        | 100 100     |
| 11  | SG    | 216/236 (92%) | 202 (94%) | 14 (6%)  | 0        | 100 100     |
| 12  | SH    | 183/190 (96%) | 161 (88%) | 22 (12%) | 0        | 100 100     |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 13  | SI    | 184/200 (92%) | 175 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 14  | SJ    | 183/197 (93%) | 168 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 15  | SK    | 90/105 (86%)  | 76 (84%)  | 9 (10%)  | 5 (6%)   | 1           | 11  |
| 16  | SL    | 144/156 (92%) | 134 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 17  | SM    | 122/143 (85%) | 85 (70%)  | 36 (30%) | 1 (1%)   | 16          | 50  |
| 18  | SN    | 148/151 (98%) | 138 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 19  | SO    | 126/137 (92%) | 106 (84%) | 20 (16%) | 0        | 100         | 100 |
| 20  | SP    | 117/142 (82%) | 105 (90%) | 11 (9%)  | 1 (1%)   | 14          | 47  |
| 21  | SQ    | 139/143 (97%) | 123 (88%) | 15 (11%) | 1 (1%)   | 18          | 52  |
| 22  | SR    | 111/136 (82%) | 102 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 23  | SS    | 143/146 (98%) | 127 (89%) | 15 (10%) | 1 (1%)   | 18          | 52  |
| 24  | ST    | 141/144 (98%) | 132 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 25  | SU    | 99/121 (82%)  | 94 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 26  | SV    | 85/87 (98%)   | 78 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 27  | SW    | 127/130 (98%) | 120 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 28  | SX    | 142/145 (98%) | 135 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 29  | SY    | 132/135 (98%) | 117 (89%) | 13 (10%) | 2 (2%)   | 8           | 37  |
| 30  | SZ    | 67/108 (62%)  | 65 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 31  | Sa    | 95/119 (80%)  | 81 (85%)  | 14 (15%) | 0        | 100         | 100 |
| 32  | Sb    | 79/82 (96%)   | 67 (85%)  | 12 (15%) | 0        | 100         | 100 |
| 33  | Sc    | 61/67 (91%)   | 54 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 34  | Sd    | 51/56 (91%)   | 49 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 35  | Se    | 58/63 (92%)   | 50 (86%)  | 8 (14%)  | 0        | 100         | 100 |
| 36  | Sf    | 31/152 (20%)  | 27 (87%)  | 4 (13%)  | 0        | 100         | 100 |
| 37  | Sg    | 311/319 (98%) | 277 (89%) | 34 (11%) | 0        | 100         | 100 |
| 38  | LA    | 250/254 (98%) | 225 (90%) | 25 (10%) | 0        | 100         | 100 |
| 39  | LB    | 384/387 (99%) | 366 (95%) | 18 (5%)  | 0        | 100         | 100 |
| 40  | LC    | 359/362 (99%) | 325 (90%) | 33 (9%)  | 1 (0%)   | 36          | 68  |
| 41  | LD    | 292/297 (98%) | 277 (95%) | 15 (5%)  | 0        | 100         | 100 |
| 42  | LE    | 153/176 (87%) | 140 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 43  | LF    | 221/244 (91%) | 218 (99%) | 3 (1%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 44  | LG    | 229/256 (90%) | 206 (90%) | 23 (10%) | 0        | 100         | 100 |
| 45  | LH    | 188/191 (98%) | 182 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 46  | LI    | 205/221 (93%) | 196 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 47  | LJ    | 167/174 (96%) | 141 (84%) | 25 (15%) | 1 (1%)   | 21          | 56  |
| 48  | LK    | 156/165 (94%) | 152 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 49  | LL    | 192/199 (96%) | 171 (89%) | 17 (9%)  | 4 (2%)   | 5           | 31  |
| 50  | LM    | 135/138 (98%) | 131 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 51  | LN    | 201/204 (98%) | 193 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 52  | LO    | 195/199 (98%) | 192 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 53  | LP    | 171/184 (93%) | 167 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 54  | LQ    | 183/186 (98%) | 177 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 55  | LR    | 172/189 (91%) | 169 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 56  | LS    | 170/172 (99%) | 167 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 57  | LT    | 157/160 (98%) | 153 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 58  | LU    | 96/121 (79%)  | 93 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 59  | LV    | 132/137 (96%) | 127 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 60  | LW    | 61/155 (39%)  | 59 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 61  | LX    | 118/142 (83%) | 107 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 62  | LY    | 122/127 (96%) | 117 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 63  | LZ    | 133/136 (98%) | 118 (89%) | 12 (9%)  | 3 (2%)   | 5           | 29  |
| 64  | La    | 146/149 (98%) | 124 (85%) | 20 (14%) | 2 (1%)   | 9           | 39  |
| 65  | Lb    | 56/59 (95%)   | 46 (82%)  | 10 (18%) | 0        | 100         | 100 |
| 66  | Lc    | 98/105 (93%)  | 93 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 67  | Ld    | 107/113 (95%) | 101 (94%) | 6 (6%)   | 0        | 100         | 100 |
| 68  | Le    | 125/130 (96%) | 116 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 69  | Lf    | 104/107 (97%) | 97 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 70  | Lg    | 110/121 (91%) | 108 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 71  | Lh    | 117/120 (98%) | 108 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 72  | Li    | 97/100 (97%)  | 92 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 73  | Lj    | 80/88 (91%)   | 76 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 74  | Lk    | 75/78 (96%)   | 70 (93%)  | 4 (5%)   | 1 (1%)   | 9           | 40  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 75  | Ll    | 48/51 (94%)       | 45 (94%)    | 3 (6%)   | 0        | 100         | 100 |
| 76  | Lm    | 50/128 (39%)      | 50 (100%)   | 0        | 0        | 100         | 100 |
| 77  | Ln    | 23/25 (92%)       | 22 (96%)    | 1 (4%)   | 0        | 100         | 100 |
| 78  | Lo    | 103/106 (97%)     | 100 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 79  | Lp    | 89/92 (97%)       | 84 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 80  | CE    | 143/157 (91%)     | 130 (91%)   | 12 (8%)  | 1 (1%)   | 18          | 52  |
| 81  | L1    | 215/217 (99%)     | 190 (88%)   | 24 (11%) | 1 (0%)   | 24          | 59  |
| 82  | P0    | 201/312 (64%)     | 194 (96%)   | 7 (4%)   | 0        | 100         | 100 |
| 83  | CD    | 810/842 (96%)     | 749 (92%)   | 58 (7%)  | 3 (0%)   | 30          | 62  |
| 84  | CS    | 120/273 (44%)     | 113 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| All | All   | 12460/13846 (90%) | 11502 (92%) | 927 (7%) | 31 (0%)  | 44          | 73  |

5 of 31 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | SK    | 81  | ASN  |
| 29  | SY    | 32  | ARG  |
| 47  | LJ    | 95  | ASN  |
| 49  | LL    | 48  | PRO  |
| 80  | CE    | 110 | LYS  |

### 5.3.2 Protein sidechains [i](#)

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   | SA    | 165/210 (79%)  | 165 (100%) | 0        | 100         | 100 |
| 6   | SB    | 192/224 (86%)  | 192 (100%) | 0        | 100         | 100 |
| 7   | SC    | 176/205 (86%)  | 176 (100%) | 0        | 100         | 100 |
| 8   | SD    | 182/195 (93%)  | 182 (100%) | 0        | 100         | 100 |
| 9   | SE    | 221/222 (100%) | 221 (100%) | 0        | 100         | 100 |
| 10  | SF    | 173/191 (91%)  | 173 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 11  | SG    | 187/201 (93%)  | 187 (100%) | 0        | 100         | 100 |
| 12  | SH    | 165/170 (97%)  | 165 (100%) | 0        | 100         | 100 |
| 13  | SI    | 150/161 (93%)  | 150 (100%) | 0        | 100         | 100 |
| 14  | SJ    | 158/166 (95%)  | 158 (100%) | 0        | 100         | 100 |
| 15  | SK    | 73/98 (74%)    | 73 (100%)  | 0        | 100         | 100 |
| 16  | SL    | 129/137 (94%)  | 129 (100%) | 0        | 100         | 100 |
| 17  | SM    | 88/119 (74%)   | 88 (100%)  | 0        | 100         | 100 |
| 18  | SN    | 127/128 (99%)  | 127 (100%) | 0        | 100         | 100 |
| 19  | SO    | 97/105 (92%)   | 97 (100%)  | 0        | 100         | 100 |
| 20  | SP    | 98/118 (83%)   | 98 (100%)  | 0        | 100         | 100 |
| 21  | SQ    | 117/119 (98%)  | 117 (100%) | 0        | 100         | 100 |
| 22  | SR    | 92/124 (74%)   | 92 (100%)  | 0        | 100         | 100 |
| 23  | SS    | 128/129 (99%)  | 128 (100%) | 0        | 100         | 100 |
| 24  | ST    | 115/116 (99%)  | 115 (100%) | 0        | 100         | 100 |
| 25  | SU    | 94/114 (82%)   | 94 (100%)  | 0        | 100         | 100 |
| 26  | SV    | 74/74 (100%)   | 74 (100%)  | 0        | 100         | 100 |
| 27  | SW    | 110/111 (99%)  | 110 (100%) | 0        | 100         | 100 |
| 28  | SX    | 119/120 (99%)  | 119 (100%) | 0        | 100         | 100 |
| 29  | SY    | 112/113 (99%)  | 112 (100%) | 0        | 100         | 100 |
| 30  | SZ    | 61/89 (68%)    | 61 (100%)  | 0        | 100         | 100 |
| 31  | Sa    | 83/100 (83%)   | 83 (100%)  | 0        | 100         | 100 |
| 32  | Sb    | 70/71 (99%)    | 70 (100%)  | 0        | 100         | 100 |
| 33  | Sc    | 56/60 (93%)    | 56 (100%)  | 0        | 100         | 100 |
| 34  | Sd    | 47/49 (96%)    | 47 (100%)  | 0        | 100         | 100 |
| 35  | Se    | 51/54 (94%)    | 51 (100%)  | 0        | 100         | 100 |
| 36  | Sf    | 27/135 (20%)   | 27 (100%)  | 0        | 100         | 100 |
| 37  | Sg    | 255/262 (97%)  | 255 (100%) | 0        | 100         | 100 |
| 38  | LA    | 192/196 (98%)  | 192 (100%) | 0        | 100         | 100 |
| 39  | LB    | 318/323 (98%)  | 318 (100%) | 0        | 100         | 100 |
| 40  | LC    | 288/289 (100%) | 288 (100%) | 0        | 100         | 100 |
| 41  | LD    | 243/245 (99%)  | 242 (100%) | 1 (0%)   | 84          | 86  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 42  | LE    | 135/153 (88%)  | 135 (100%) | 0        | 100         | 100 |
| 43  | LF    | 187/205 (91%)  | 187 (100%) | 0        | 100         | 100 |
| 44  | LG    | 177/208 (85%)  | 177 (100%) | 0        | 100         | 100 |
| 45  | LH    | 170/171 (99%)  | 170 (100%) | 0        | 100         | 100 |
| 46  | LI    | 177/187 (95%)  | 177 (100%) | 0        | 100         | 100 |
| 47  | LJ    | 147/150 (98%)  | 147 (100%) | 0        | 100         | 100 |
| 48  | LK    | 129/136 (95%)  | 129 (100%) | 0        | 100         | 100 |
| 49  | LL    | 154/159 (97%)  | 154 (100%) | 0        | 100         | 100 |
| 50  | LM    | 108/109 (99%)  | 108 (100%) | 0        | 100         | 100 |
| 51  | LN    | 175/176 (99%)  | 175 (100%) | 0        | 100         | 100 |
| 52  | LO    | 160/162 (99%)  | 160 (100%) | 0        | 100         | 100 |
| 53  | LP    | 139/146 (95%)  | 139 (100%) | 0        | 100         | 100 |
| 54  | LQ    | 150/151 (99%)  | 150 (100%) | 0        | 100         | 100 |
| 55  | LR    | 133/154 (86%)  | 133 (100%) | 0        | 100         | 100 |
| 56  | LS    | 156/156 (100%) | 156 (100%) | 0        | 100         | 100 |
| 57  | LT    | 136/137 (99%)  | 136 (100%) | 0        | 100         | 100 |
| 58  | LU    | 85/107 (79%)   | 85 (100%)  | 0        | 100         | 100 |
| 59  | LV    | 103/105 (98%)  | 103 (100%) | 0        | 100         | 100 |
| 60  | LW    | 55/129 (43%)   | 55 (100%)  | 0        | 100         | 100 |
| 61  | LX    | 104/118 (88%)  | 104 (100%) | 0        | 100         | 100 |
| 62  | LY    | 107/110 (97%)  | 107 (100%) | 0        | 100         | 100 |
| 63  | LZ    | 115/116 (99%)  | 115 (100%) | 0        | 100         | 100 |
| 64  | La    | 118/119 (99%)  | 118 (100%) | 0        | 100         | 100 |
| 65  | Lb    | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 66  | Lc    | 84/88 (96%)    | 84 (100%)  | 0        | 100         | 100 |
| 67  | Ld    | 94/97 (97%)    | 94 (100%)  | 0        | 100         | 100 |
| 68  | Le    | 109/111 (98%)  | 109 (100%) | 0        | 100         | 100 |
| 69  | Lf    | 90/91 (99%)    | 90 (100%)  | 0        | 100         | 100 |
| 70  | Lg    | 95/103 (92%)   | 95 (100%)  | 0        | 100         | 100 |
| 71  | Lh    | 103/105 (98%)  | 103 (100%) | 0        | 100         | 100 |
| 72  | Li    | 80/82 (98%)    | 80 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 73  | Lj    | 67/71 (94%)       | 67 (100%)    | 0        | 100         | 100 |
| 74  | Lk    | 67/69 (97%)       | 67 (100%)    | 0        | 100         | 100 |
| 75  | Ll    | 45/46 (98%)       | 44 (98%)     | 1 (2%)   | 45          | 71  |
| 76  | Lm    | 47/116 (40%)      | 47 (100%)    | 0        | 100         | 100 |
| 77  | Ln    | 23/23 (100%)      | 23 (100%)    | 0        | 100         | 100 |
| 78  | Lo    | 90/91 (99%)       | 90 (100%)    | 0        | 100         | 100 |
| 79  | Lp    | 71/72 (99%)       | 71 (100%)    | 0        | 100         | 100 |
| 80  | CE    | 116/132 (88%)     | 116 (100%)   | 0        | 100         | 100 |
| 81  | L1    | 198/198 (100%)    | 198 (100%)   | 0        | 100         | 100 |
| 82  | P0    | 171/254 (67%)     | 171 (100%)   | 0        | 100         | 100 |
| 83  | CD    | 695/715 (97%)     | 695 (100%)   | 0        | 100         | 100 |
| 84  | CS    | 97/228 (42%)      | 97 (100%)    | 0        | 100         | 100 |
| All | All   | 10541/11646 (90%) | 10539 (100%) | 2 (0%)   | 100         | 100 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | LD    | 274 | GLN  |
| 75  | Ll    | 45  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | LQ    | 5   | HIS  |
| 69  | Lf    | 24  | ASN  |
| 56  | LS    | 157 | GLN  |
| 63  | LZ    | 29  | HIS  |
| 75  | Ll    | 33  | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | C2    | 1693/1800 (94%) | 389 (22%)         | 20 (1%)         |
| 2   | C1    | 3182/3396 (93%) | 605 (19%)         | 29 (0%)         |
| 3   | C4    | 120/121 (99%)   | 19 (15%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 4   | C3    | 156/158 (98%)   | 24 (15%)          | 1 (0%)          |
| All | All   | 5151/5475 (94%) | 1037 (20%)        | 50 (0%)         |

5 of 1037 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C2    | 4   | C    |
| 1   | C2    | 17  | C    |
| 1   | C2    | 25  | C    |
| 1   | C2    | 26  | A    |
| 1   | C2    | 27  | U    |

5 of 50 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C1    | 1216 | C    |
| 2   | C1    | 1841 | A    |
| 4   | C3    | 80   | A    |
| 2   | C1    | 1307 | G    |
| 2   | C1    | 1716 | U    |

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 80  | 5CT  | CE    | 51  | 80   | 13,14,15     | 0.77 | 0           | 8,15,17     | 1.01 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 80  | 5CT  | CE    | 51  | 80   | -       | 7/13/14/16 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 80  | CE    | 51  | 5CT  | C1-C2-C3-C4 |
| 80  | CE    | 51  | 5CT  | O1-C2-C3-C4 |
| 80  | CE    | 51  | 5CT  | C-CA-CB-CG  |
| 80  | CE    | 51  | 5CT  | O-C-CA-CB   |
| 80  | CE    | 51  | 5CT  | CG-CD-CE-NZ |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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 | $\# Z  > 2$ |
| 86  | T1C  | C1    | 3401 | -    | 45,45,45     | 1.14 | 4 (8%)      | 56,72,72    | 1.44 | 9 (16%)     |
| 86  | T1C  | C1    | 3403 | -    | 45,45,45     | 1.12 | 3 (6%)      | 56,72,72    | 0.98 | 2 (3%)      |
| 86  | T1C  | C1    | 3404 | 87   | 45,45,45     | 1.16 | 4 (8%)      | 56,72,72    | 1.05 | 5 (8%)      |
| 86  | T1C  | C1    | 3402 | -    | 45,45,45     | 1.17 | 4 (8%)      | 56,72,72    | 1.14 | 4 (7%)      |
| 88  | GDP  | CD    | 902  | 87   | 29,30,30     | 1.16 | 3 (10%)     | 45,47,47    | 1.79 | 7 (15%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | T1C  | C1    | 3406 | 87   | 45,45,45     | 1.14 | 4 (8%)   | 56,72,72    | 1.14 | 5 (8%)   |
| 86  | T1C  | C1    | 3405 | -    | 45,45,45     | 1.17 | 4 (8%)   | 56,72,72    | 1.44 | 7 (12%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 86  | T1C  | C1    | 3401 | -    | -       | 11/22/80/80 | 0/4/4/4 |
| 86  | T1C  | C1    | 3403 | -    | -       | 9/22/80/80  | 0/4/4/4 |
| 86  | T1C  | C1    | 3404 | 87   | -       | 13/22/80/80 | 0/4/4/4 |
| 86  | T1C  | C1    | 3402 | -    | -       | 13/22/80/80 | 0/4/4/4 |
| 88  | GDP  | CD    | 902  | 87   | -       | 3/16/32/32  | 0/3/3/3 |
| 86  | T1C  | C1    | 3406 | 87   | -       | 13/22/80/80 | 0/4/4/4 |
| 86  | T1C  | C1    | 3405 | -    | -       | 14/22/80/80 | 0/4/4/4 |

The worst 5 of 26 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 86  | C1    | 3402 | T1C  | C21-N21 | 5.07 | 1.48        | 1.33     |
| 86  | C1    | 3401 | T1C  | C21-N21 | 5.05 | 1.48        | 1.33     |
| 86  | C1    | 3405 | T1C  | C21-N21 | 5.02 | 1.47        | 1.33     |
| 86  | C1    | 3403 | T1C  | C21-N21 | 5.01 | 1.47        | 1.33     |
| 86  | C1    | 3406 | T1C  | C21-N21 | 5.00 | 1.47        | 1.33     |

The worst 5 of 39 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 88  | CD    | 902  | GDP  | C5-C4-N3    | -6.23 | 118.47      | 128.39   |
| 88  | CD    | 902  | GDP  | C2-N3-C4    | 5.12  | 121.12      | 112.30   |
| 86  | C1    | 3405 | T1C  | C1-C1C-C12  | 4.92  | 115.64      | 109.88   |
| 88  | CD    | 902  | GDP  | N9-C4-N3    | 4.67  | 135.29      | 125.95   |
| 86  | C1    | 3401 | T1C  | C11-C1B-C12 | 4.63  | 122.47      | 118.80   |

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

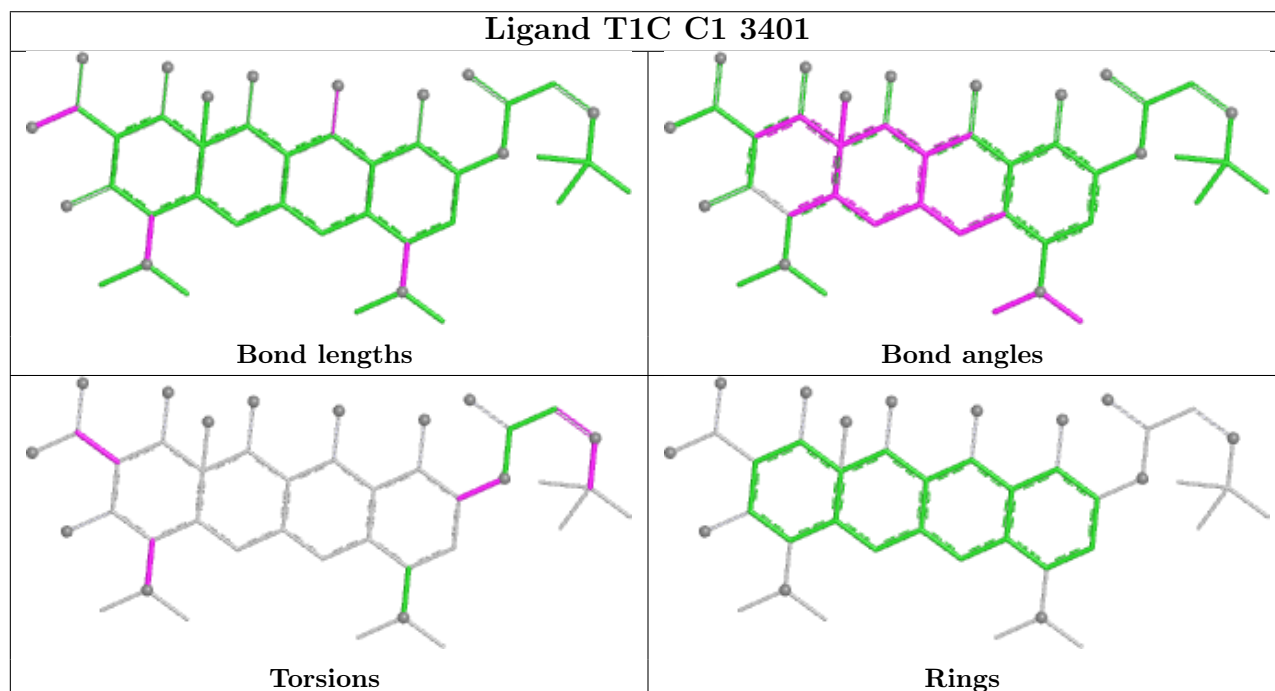
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 86  | C1    | 3401 | T1C  | C94-C93-N92-C92 |
| 86  | C1    | 3401 | T1C  | C95-C93-N92-C92 |
| 86  | C1    | 3401 | T1C  | C96-C93-N92-C92 |
| 86  | C1    | 3401 | T1C  | C41-C4-N4-C43   |
| 86  | C1    | 3401 | T1C  | C1-C2-C21-O21   |

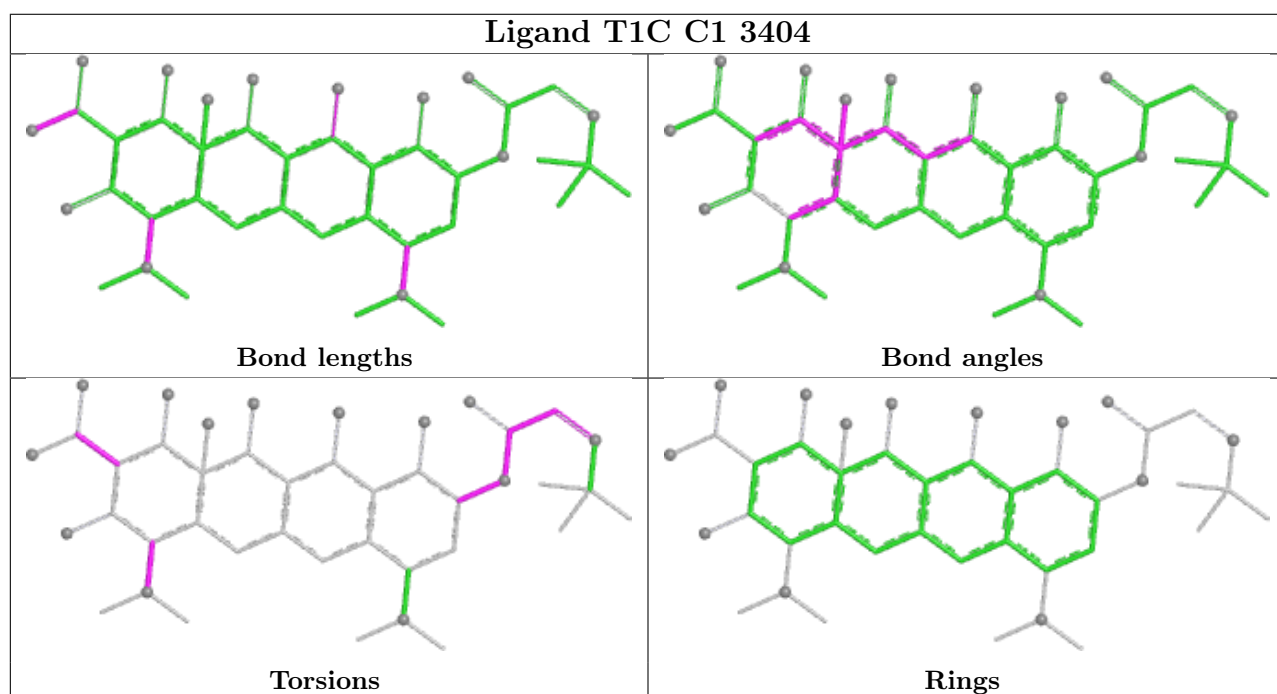
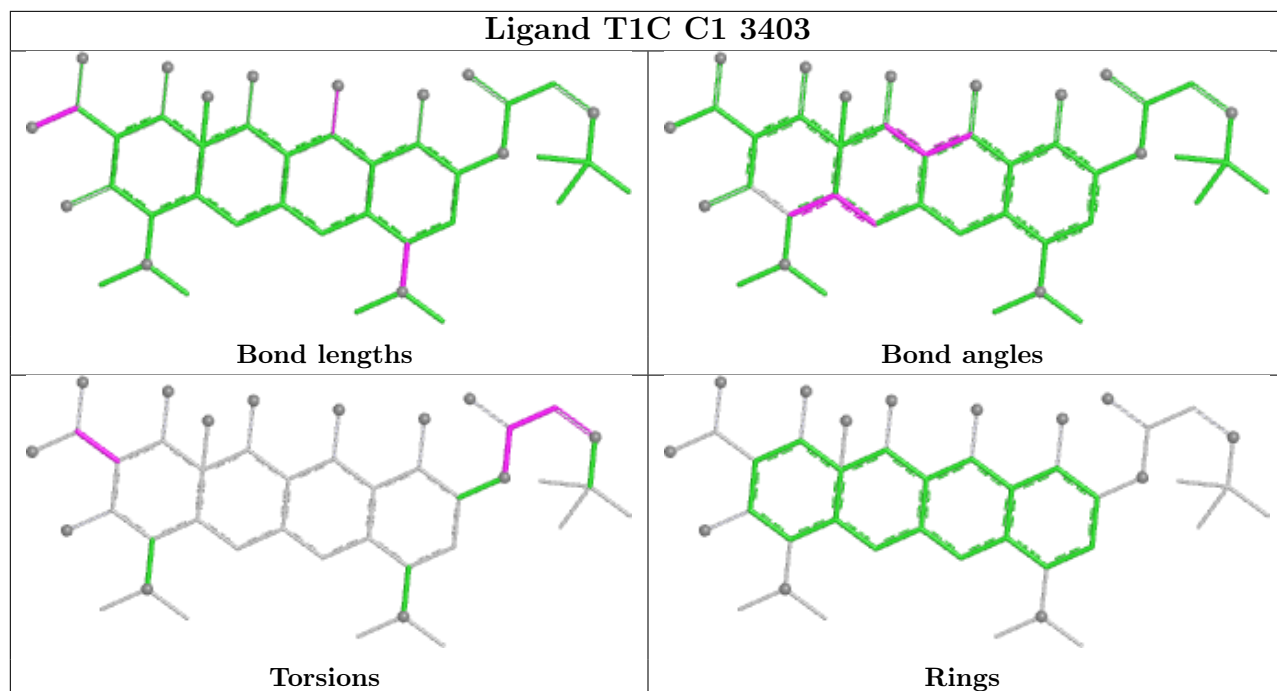
There are no ring outliers.

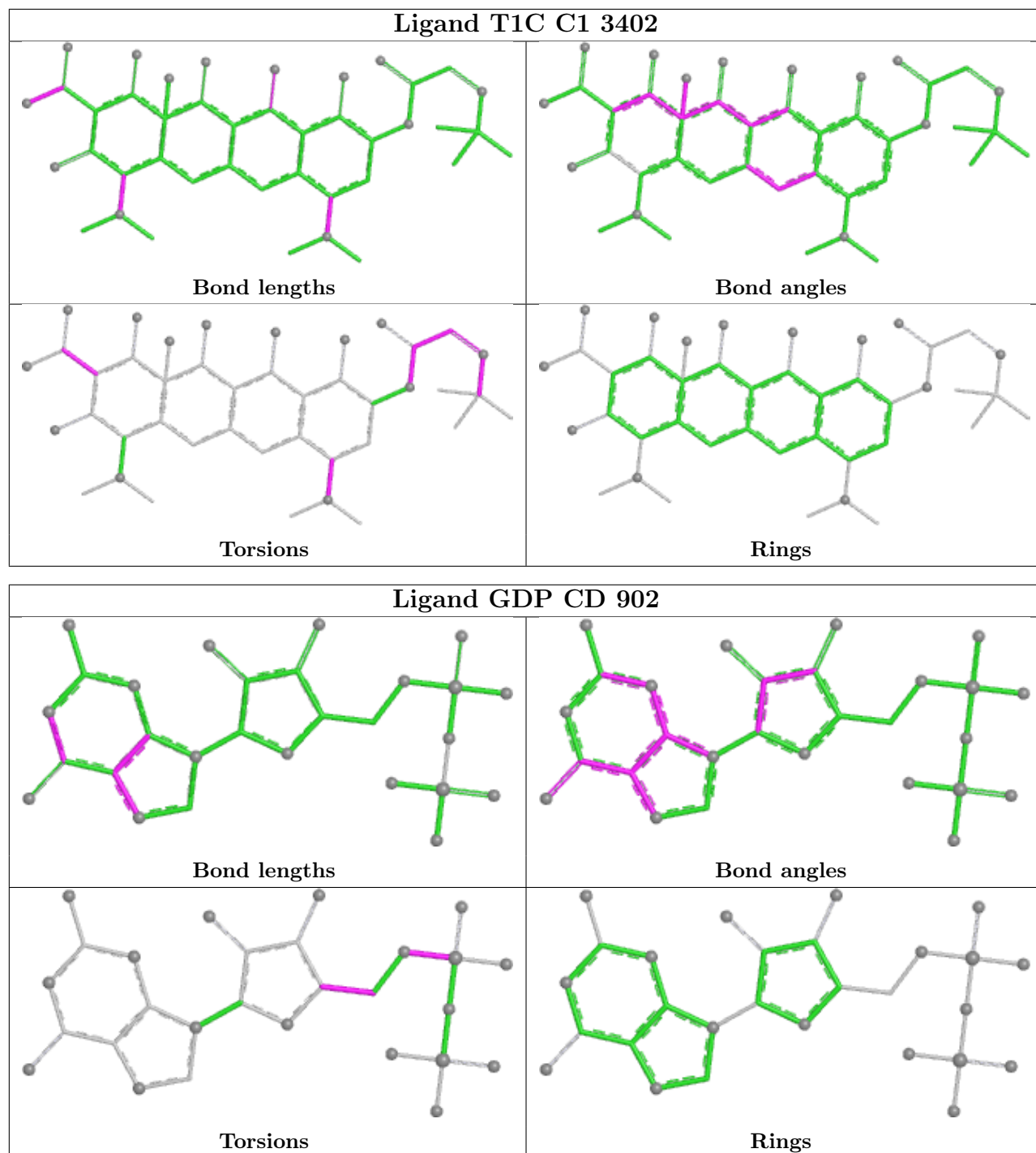
2 monomers are involved in 4 short contacts:

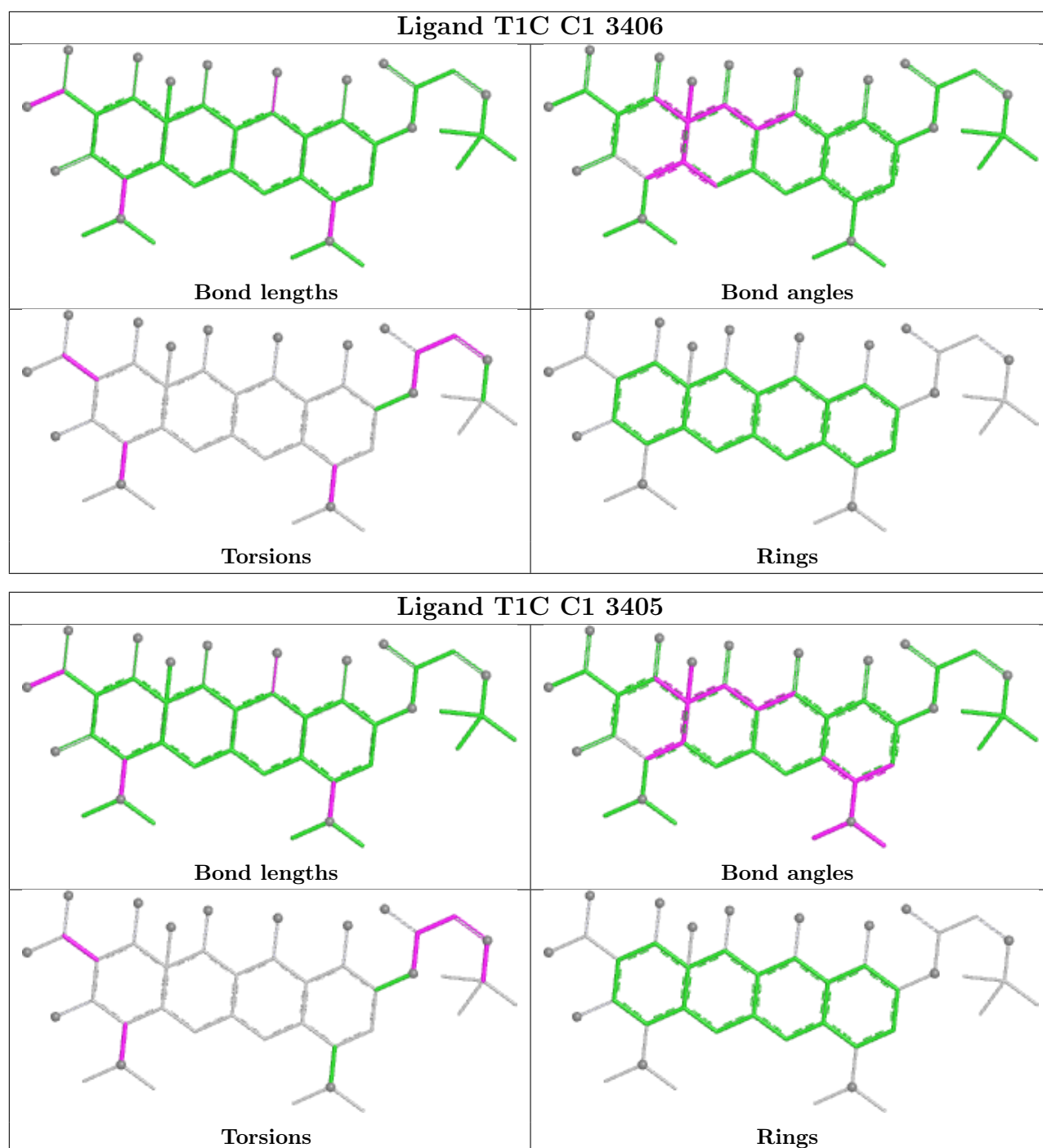
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | C1    | 3401 | T1C  | 2       | 0            |
| 86  | C1    | 3406 | T1C  | 2       | 0            |

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









## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

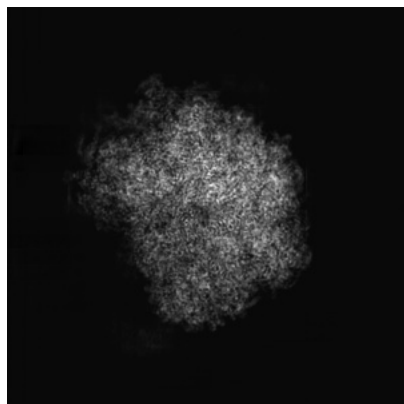
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36839. These allow visual inspection of the internal detail of the map and identification of artifacts.

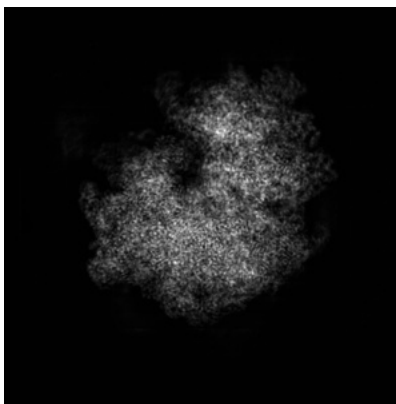
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

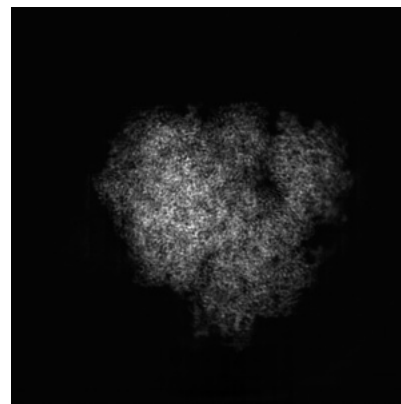
#### 6.1.1 Primary map



X

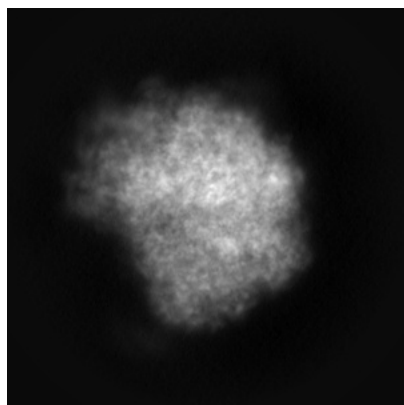


Y

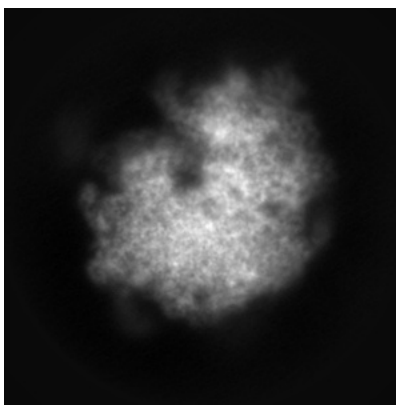


Z

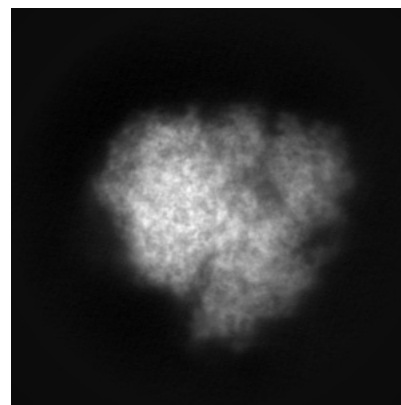
#### 6.1.2 Raw map



X



Y

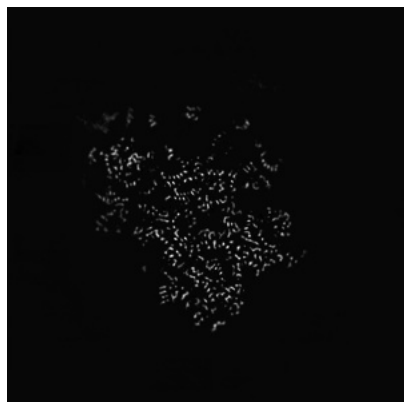


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 240

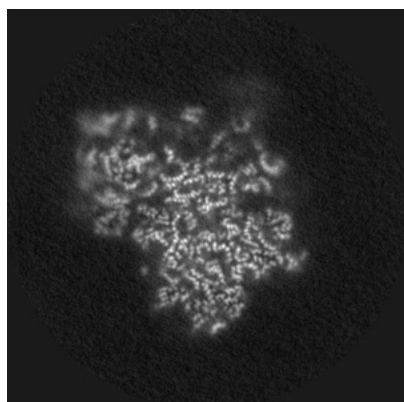


Y Index: 240

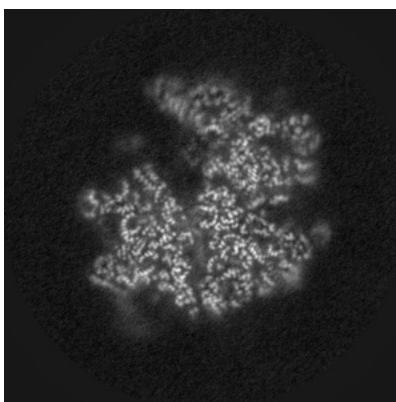


Z Index: 240

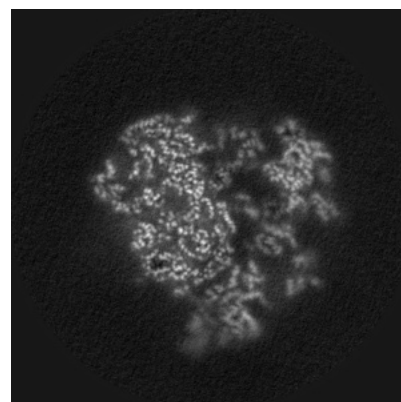
### 6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

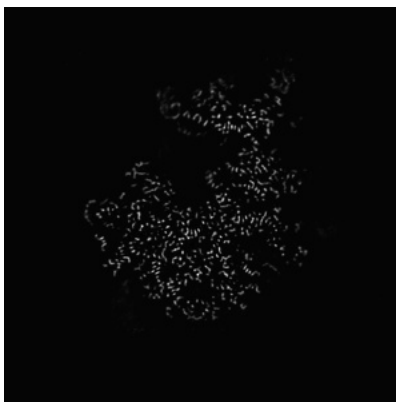
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 215

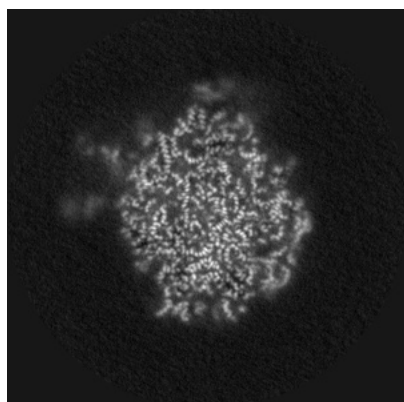


Y Index: 257

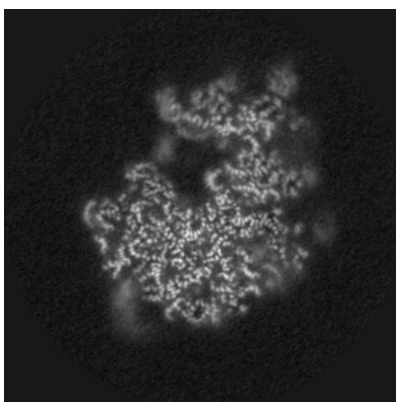


Z Index: 273

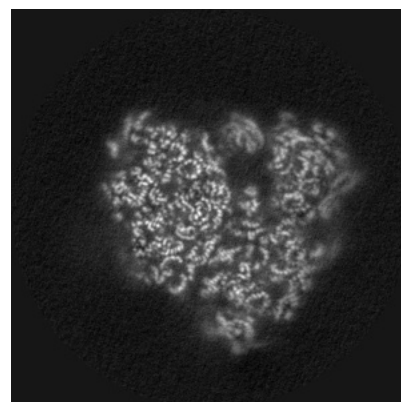
### 6.3.2 Raw map



X Index: 214



Y Index: 257

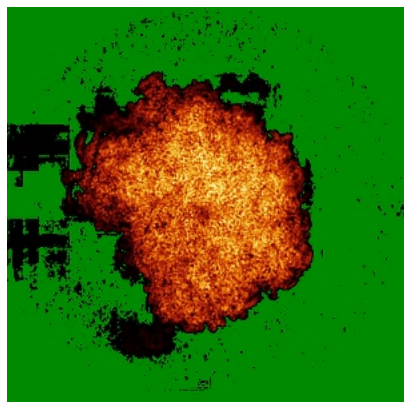


Z Index: 268

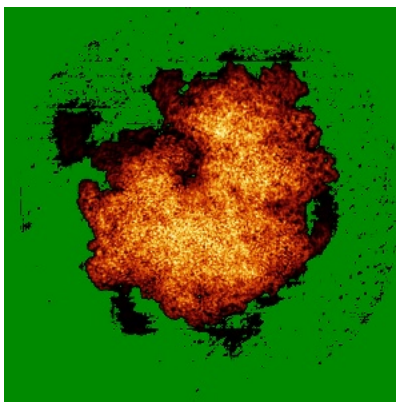
The images above show the largest variance slices of the map in three orthogonal directions.

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

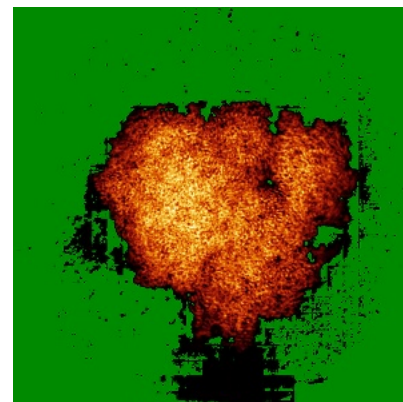
### 6.4.1 Primary map



X

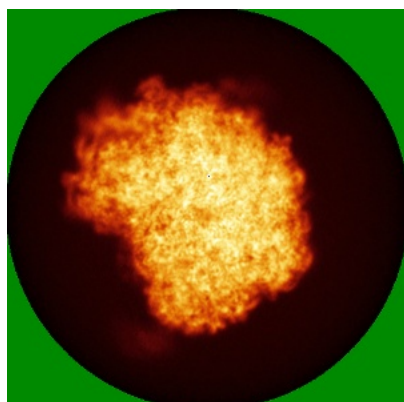


Y

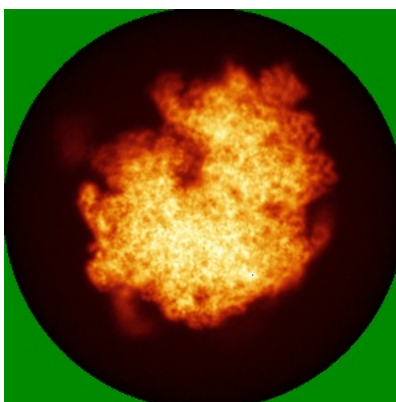


Z

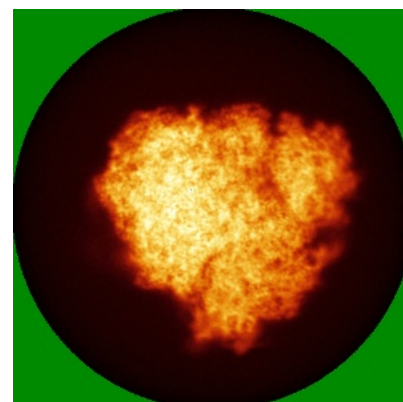
### 6.4.2 Raw map



X



Y

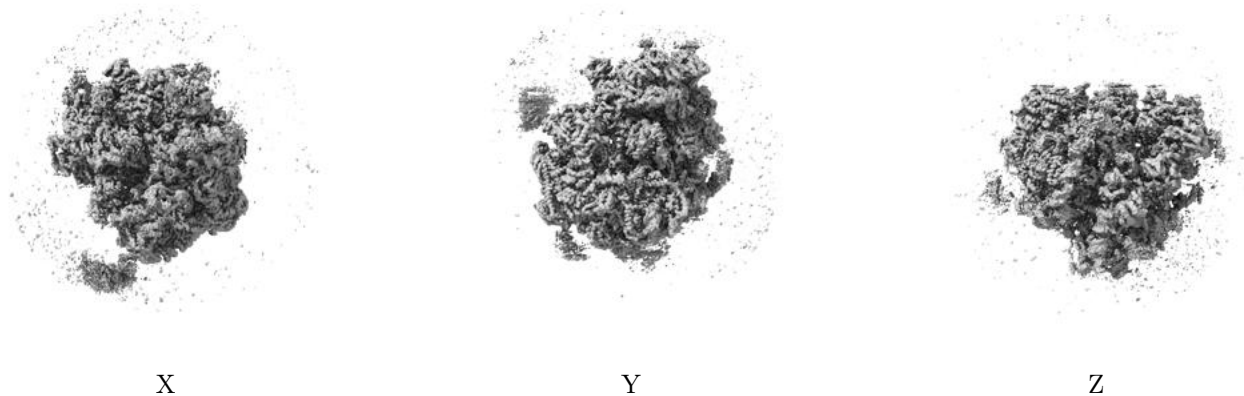


Z

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.

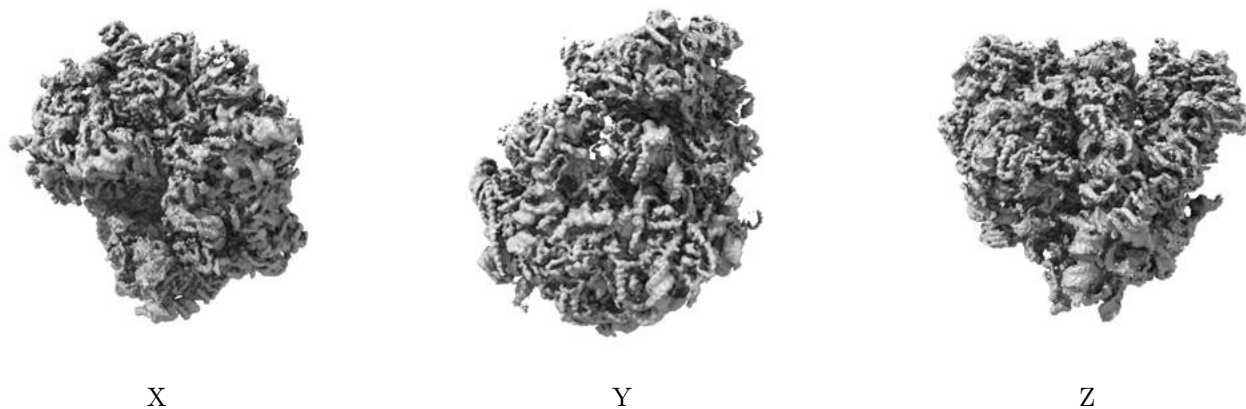
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

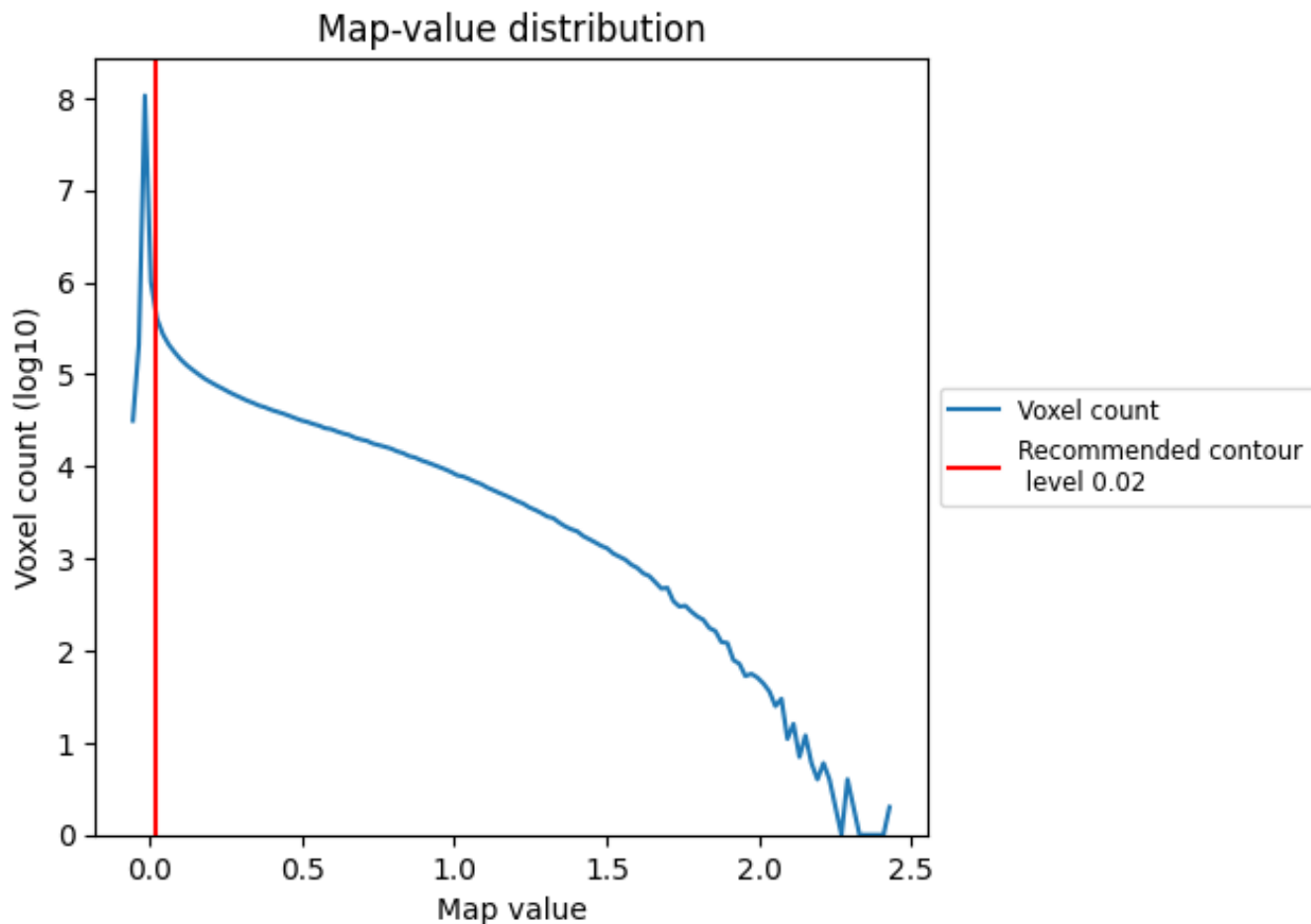
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

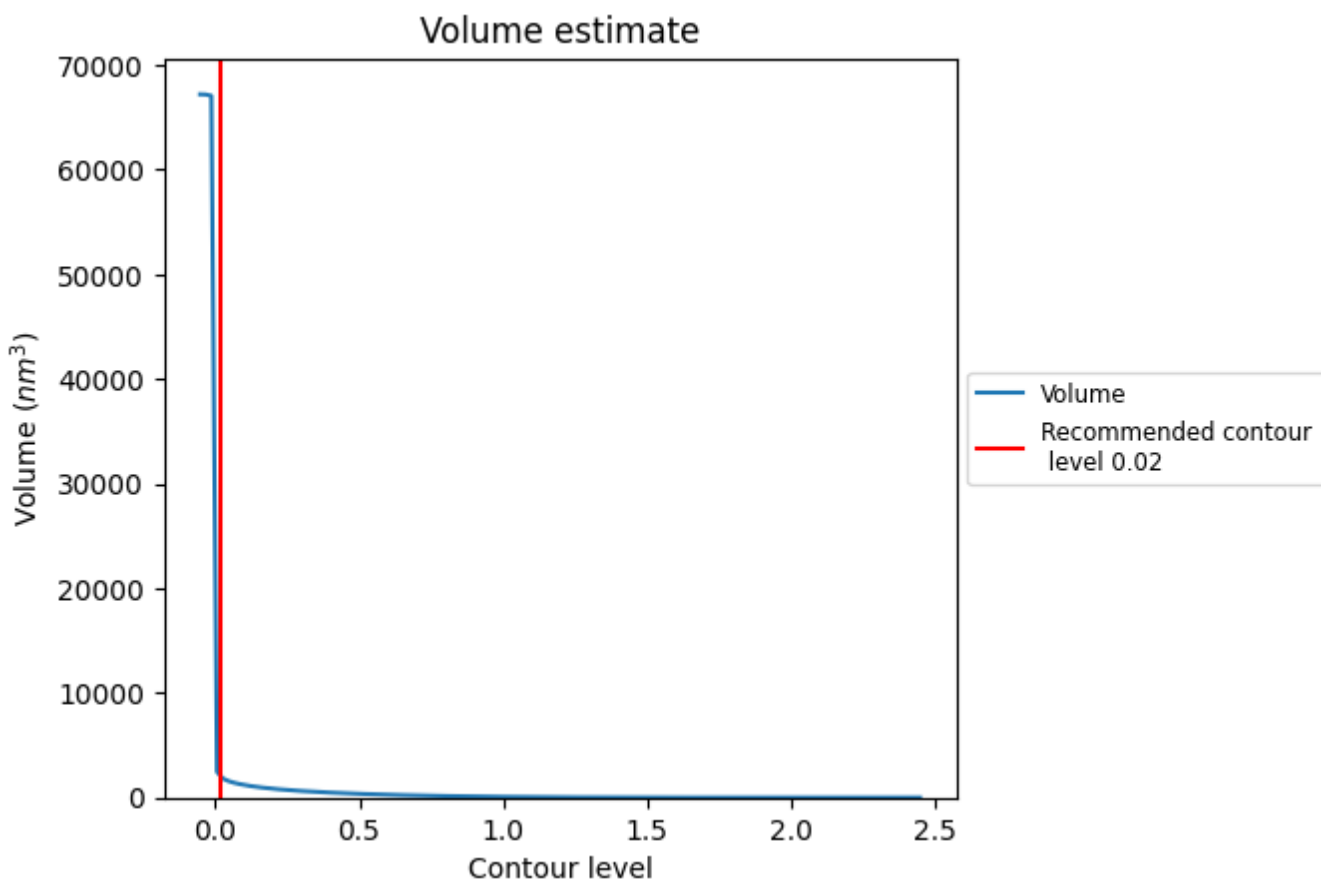
This section contains the results of statistical analysis of the map.

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



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

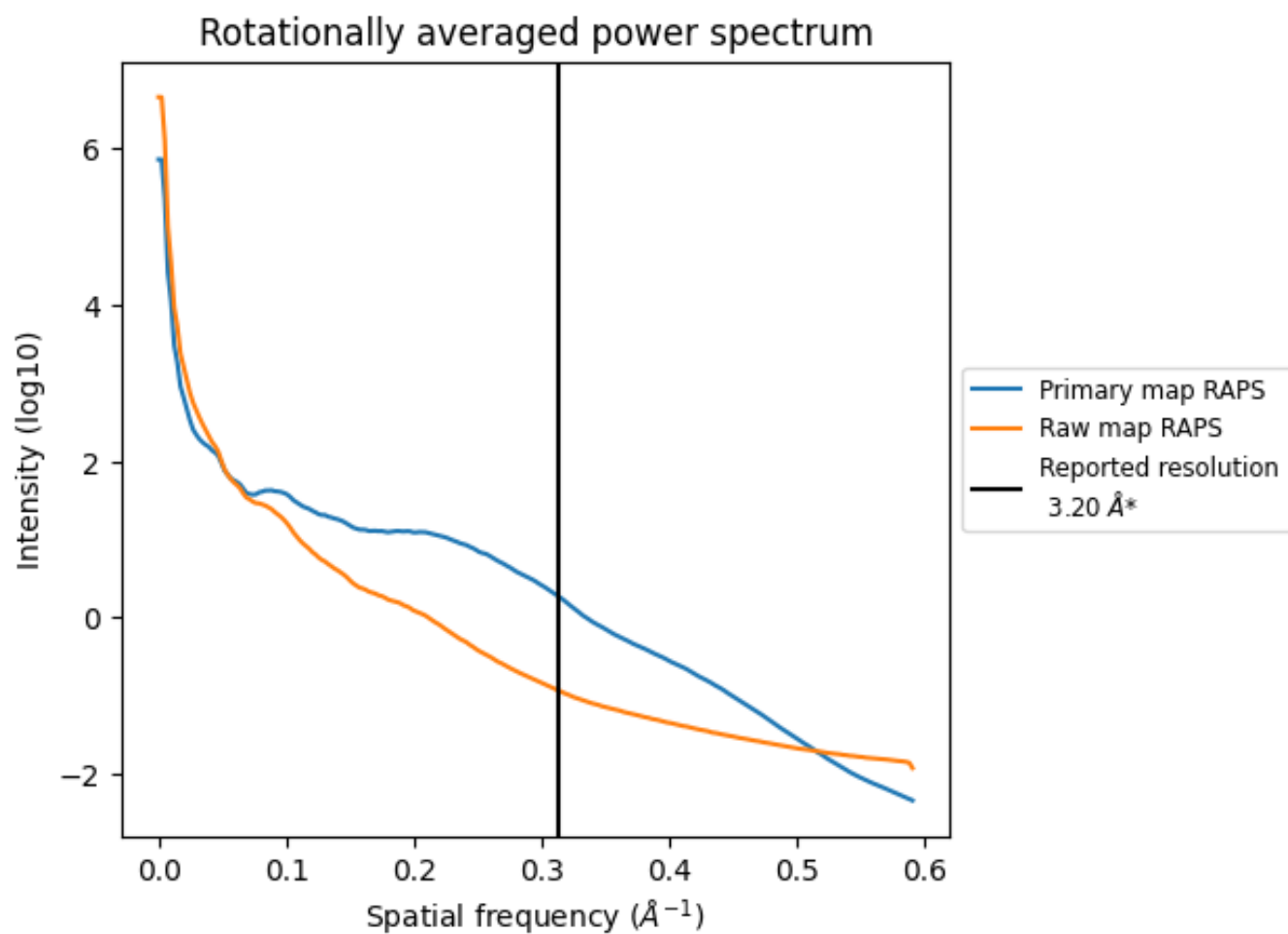
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2009  $\text{nm}^3$ ; this corresponds to an approximate mass of 1814 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 [i](#)

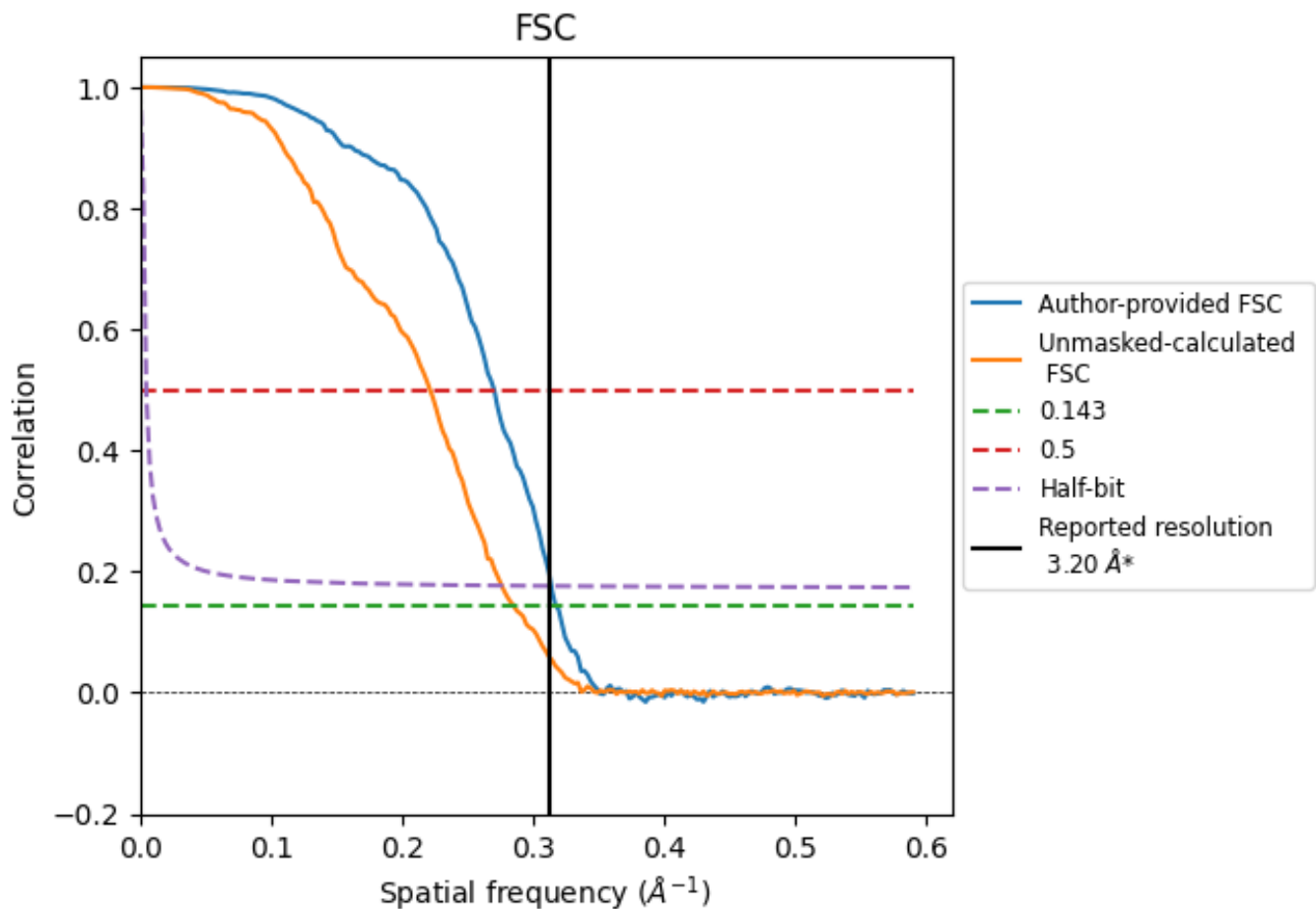


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

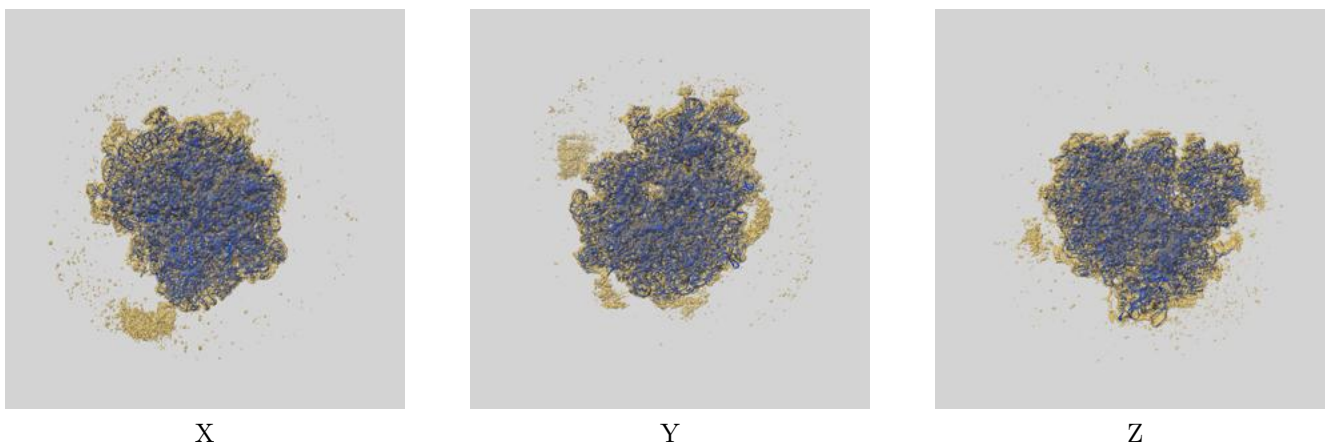
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.20                               | -    | -        |
| Author-provided FSC curve | 3.15                               | 3.70 | 3.18     |
| Unmasked-calculated*      | 3.50                               | 4.51 | 3.62     |

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

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

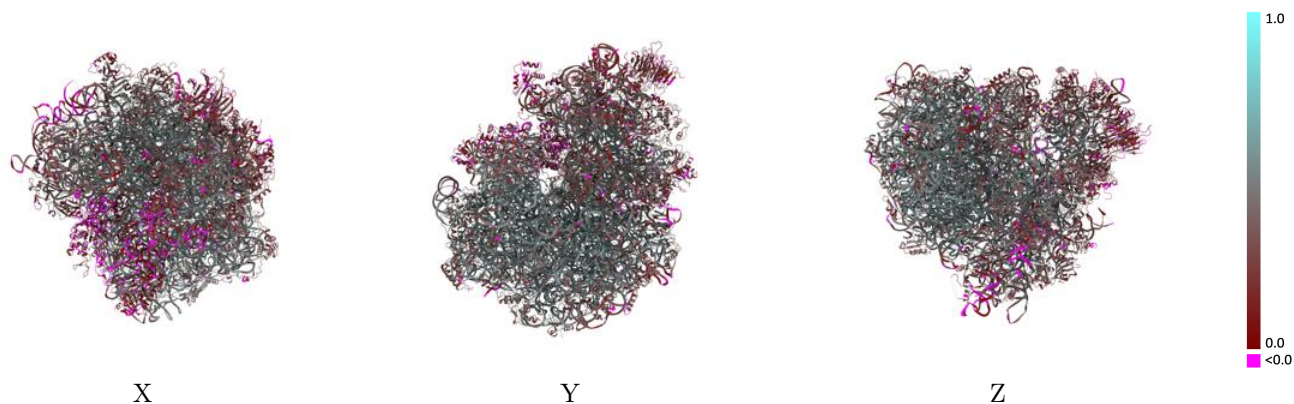
This section contains information regarding the fit between EMDB map EMD-36839 and PDB model 8K2D. Per-residue inclusion information can be found in section 3 on page 21.

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



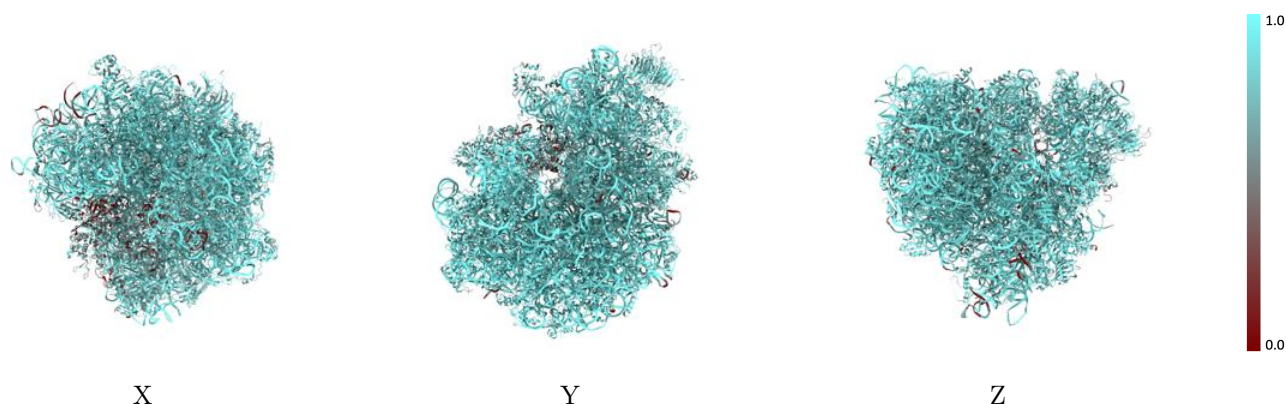
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



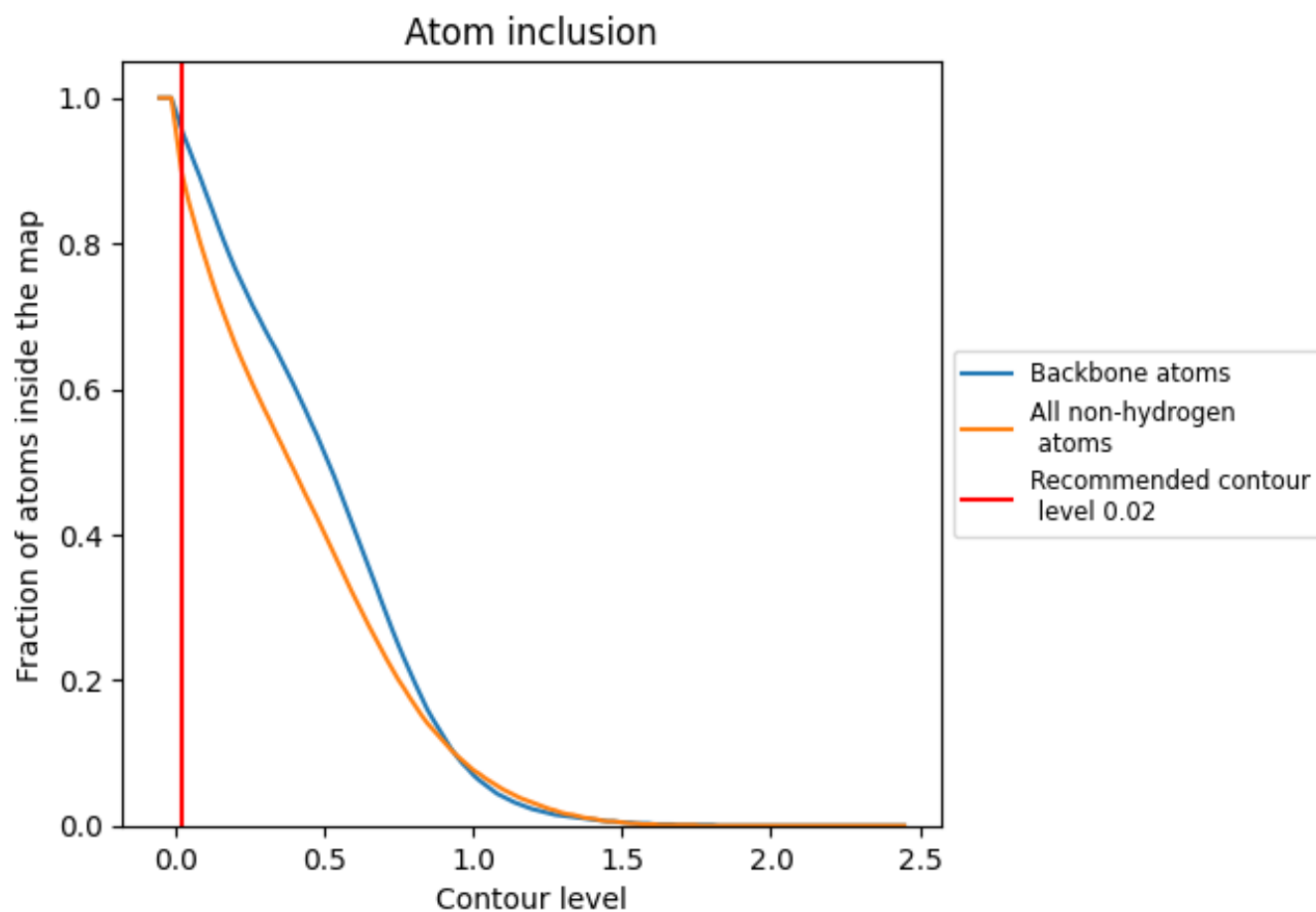
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9000   |  0.4230   |
| C1    |  0.9620   |  0.5020   |
| C2    |  0.9420   |  0.4350   |
| C3    |  0.9710   |  0.5150   |
| C4    |  0.9860   |  0.5090   |
| CD    |  0.4440   |  0.0840   |
| CE    |  0.8360   |  0.3830   |
| CS    |  0.7520   |  0.2870   |
| L1    |  0.8120   |  0.3130   |
| LA    |  0.9230   |  0.4870   |
| LB    |  0.9210   |  0.4770   |
| LC    |  0.9180   |  0.4430   |
| LD    |  0.8600   |  0.3730   |
| LE    |  0.8800   |  0.4040   |
| LF    |  0.9230  |  0.4680  |
| LG    |  0.8900 |  0.3810 |
| LH    |  0.8950 |  0.4250 |
| LI    |  0.8790 |  0.4210 |
| LJ    |  0.8710 |  0.3800 |
| LK    |  0.5530 |  0.0950 |
| LL    |  0.8960 |  0.4120 |
| LM    |  0.9060 |  0.4350 |
| LN    |  0.9420 |  0.5080 |
| LO    |  0.9290 |  0.4850 |
| LP    |  0.9130 |  0.4790 |
| LQ    |  0.9180 |  0.4610 |
| LR    |  0.9230 |  0.4750 |
| LS    |  0.9190 |  0.4660 |
| LT    |  0.9040 |  0.4640 |
| LU    |  0.8670 |  0.3870 |
| LV    |  0.9040 |  0.4670 |
| LW    |  0.9010 |  0.4500 |
| LX    |  0.8910 |  0.4410 |
| LY    |  0.8850 |  0.4330 |
| LZ    |  0.8970 |  0.4020 |



















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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| La    |  0.9290   |  0.4640   |
| Lb    |  0.8580   |  0.4070   |
| Lc    |  0.8600   |  0.4080   |
| Ld    |  0.8540   |  0.4350   |
| Le    |  0.9000   |  0.4730   |
| Lf    |  0.9430   |  0.5020   |
| Lg    |  0.9100   |  0.4730   |
| Lh    |  0.8680   |  0.4160   |
| Li    |  0.8590   |  0.3880   |
| Lj    |  0.9540   |  0.5330   |
| Lk    |  0.8590   |  0.3490   |
| Ll    |  0.9160   |  0.4700   |
| Lm    |  0.8810   |  0.4510   |
| Ln    |  0.6840   |  0.3370   |
| Lo    |  0.8720   |  0.4510   |
| Lp    |  0.9060   |  0.4630   |
| P0    |  0.5980   |  0.1070   |
| SA    |  0.9010  |  0.3580  |
| SB    |  0.8390 |  0.3260 |
| SC    |  0.8940 |  0.4070 |
| SD    |  0.8300 |  0.3090 |
| SE    |  0.8760 |  0.3740 |
| SF    |  0.8050 |  0.2530 |
| SG    |  0.7980 |  0.2840 |
| SH    |  0.8310 |  0.2840 |
| SI    |  0.8710 |  0.3860 |
| SJ    |  0.8450 |  0.3470 |
| SK    |  0.8350 |  0.2590 |
| SL    |  0.8710 |  0.4210 |
| SM    |  0.6440 |  0.0520 |
| SN    |  0.8800 |  0.3890 |
| SO    |  0.8720 |  0.3790 |
| SP    |  0.8410 |  0.2920 |
| SQ    |  0.8480 |  0.2960 |
| SR    |  0.8280 |  0.2760 |
| SS    |  0.8530 |  0.2990 |
| ST    |  0.8320 |  0.2860 |
| SU    |  0.8430 |  0.2770 |
| SV    |  0.8780 |  0.3650 |
| SW    |  0.9220 |  0.4620 |
| SX    |  0.8850 |  0.4200 |
| SY    |  0.8000 |  0.3060 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| SZ    |  0.8080 |  0.2260 |
| Sa    |  0.9040 |  0.4240 |
| Sb    |  0.8990 |  0.3820 |
| Sc    |  0.7900 |  0.2750 |
| Sd    |  0.9050 |  0.4130 |
| Se    |  0.7230 |  0.2750 |
| Sf    |  0.6430 |  0.0470 |
| Sg    |  0.8050 |  0.1970 |