# wwPDB EM Validation Summary Report

Jul 16, 2023 – 08:44 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 8FLB |
| EMDB ID | : | EMD-29273 |
| Title | : | Human nuclear pre-60S ribosomal subunit (State K2) |
| Authors | : | Vanden Broeck, A.; Klinge, S. |
| Deposited on | : | 2022-12-21 |
| Resolution | : | 2.55 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*
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.

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

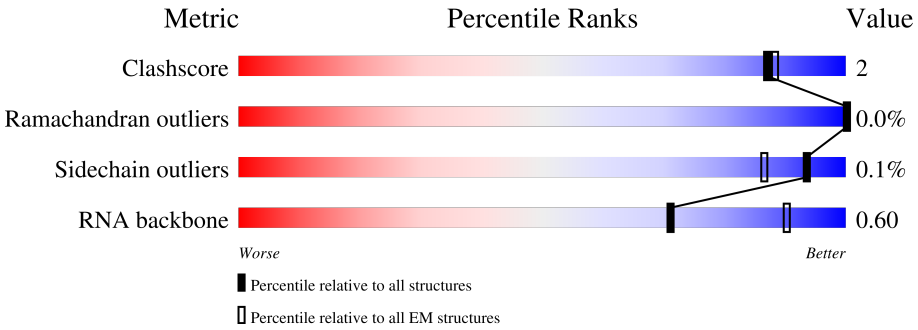
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev50 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.34 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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 (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | BA | 165 | 39% 55% 45% |
| 2 | L1 | 157 | 80% 15% |
| 3 | L3 | 5070 | 53% 12% 33% |
| 4 | L4 | 121 | 85% 13% |
| 5 | L5 | 178 | 90% 6% |
| 6 | L6 | 211 | 8% 95% 5% |
| 7 | L7 | 203 | 95% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | L8 | 215 | 60% 37% |
| 9 | L9 | 204 | 93% 6% |
| 10 | LA | 184 | 78% 5% 17% |
| 11 | LB | 188 | 95% 5% |
| 12 | LC | 176 | 94% 6% |
| 13 | LD | 196 | 74% 21% |
| 14 | LE | 160 | 92% |
| 15 | LF | 128 | 74% 6% 20% |
| 16 | LG | 140 | 98% |
| 17 | LH | 156 | 89% 8% |
| 18 | LI | 145 | 86% 6% 8% |
| 19 | LJ | 136 | 89% 10% |
| 20 | LK | 148 | 93% 6% |
| 21 | LL | 137 | 86% 5% 9% |
| 22 | LM | 159 | 9% 53% 43% |
| 23 | LN | 403 | 92% 7% |
| 24 | LO | 115 | 6% 81% 17% |
| 25 | LP | 125 | 82% 15% |
| 26 | LQ | 135 | 90% 5% 5% |
| 27 | LR | 117 | 91% |
| 28 | LS | 123 | 96% |
| 29 | LT | 110 | 97% |
| 30 | LU | 105 | 7% 90% 7% |
| 31 | LV | 106 | 97% |
| 32 | LW | 97 | 81% 7% 11% |

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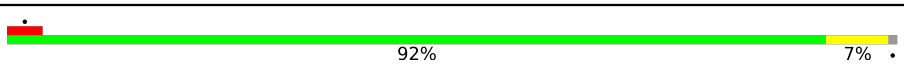
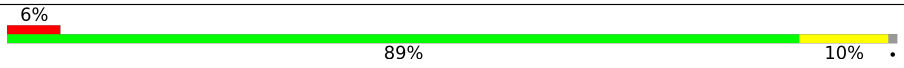
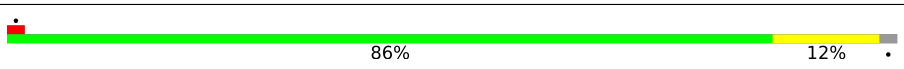
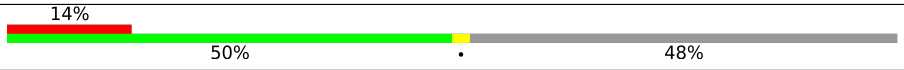
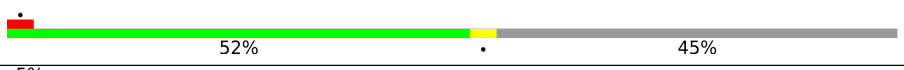
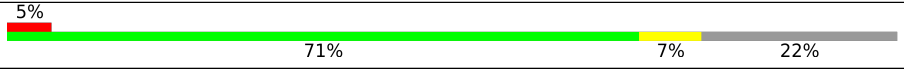
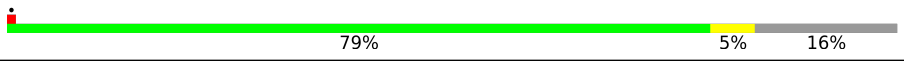
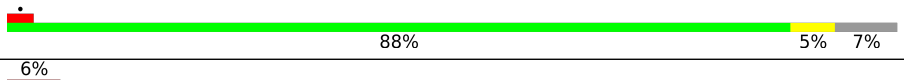
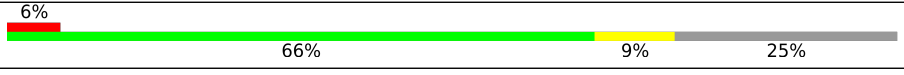
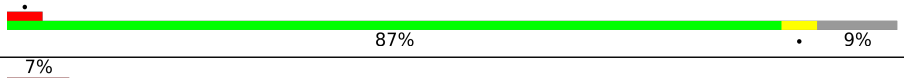
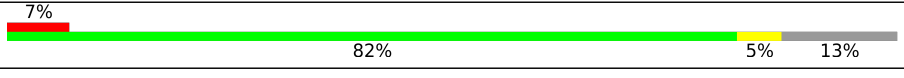
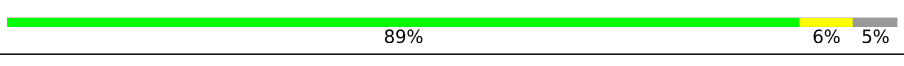
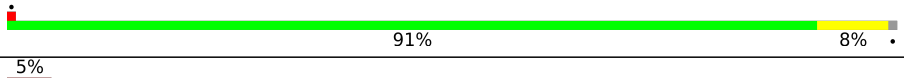
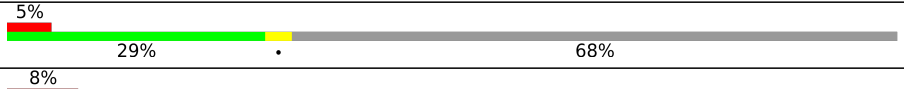
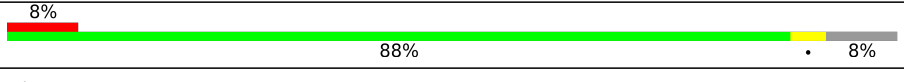
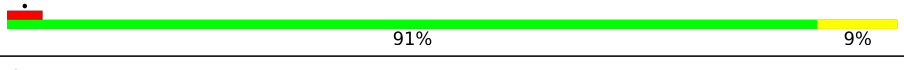
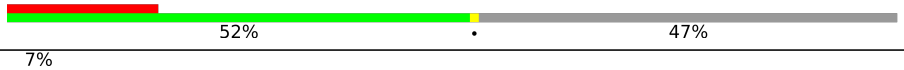
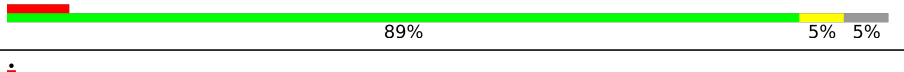
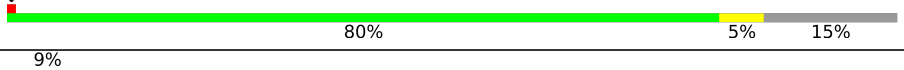
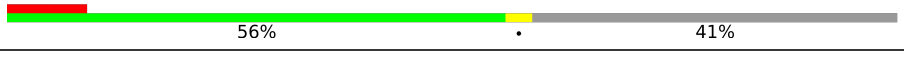
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | LX | 92 |   |
| 34 | LY | 70 |   |
| 35 | LZ | 51 |   |
| 36 | NK | 129 |   |
| 37 | NL | 478 |   |
| 38 | NP | 134 |   |
| 39 | NR | 203 |   |
| 40 | SA | 427 |   |
| 41 | SB | 297 |   |
| 42 | SC | 288 |   |
| 43 | SD | 248 |   |
| 44 | SE | 266 |   |
| 45 | SF | 257 |   |
| 46 | SG | 192 |   |
| 47 | SH | 293 |   |
| 48 | SI | 255 |   |
| 49 | SK | 245 |   |
| 50 | SM | 588 |   |
| 51 | SQ | 239 |   |
| 52 | SR | 634 |   |
| 53 | SV | 163 |   |
| 54 | VB | 99 |   |

# 2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 149034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | L3 | 3420 | Total | C | N | O | P | 0 | 0 |
| | | | 73423 | 32721 | 13453 | 23829 | 3420 | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | LH | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1156 | 740 | 220 | 195 | 1 | | |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | LM | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 751 | 469 | 165 | 113 | 4 | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 36 is a protein called Protein LLP homolog.

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

- Molecule 37 is a protein called Ribosome biogenesis protein NOP53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | NL | 263 | Total | C | N | O | S | 0 | 0 |
| | | | 2175 | 1347 | 433 | 393 | 2 | | |

- Molecule 38 is a protein called Zinc finger protein 593.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | NP | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 847 | 520 | 178 | 145 | 4 | | |

- Molecule 39 is a protein called Translation machinery-associated protein 16.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | NR | 152 | Total | C | N | O | P | S | 1 | 0 |
| | | | 1299 | 809 | 249 | 235 | 1 | 5 | | |

- Molecule 40 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | SA | 358 | Total | C | N | O | S | 0 | 0 |
| | | | 2853 | 1797 | 570 | 473 | 13 | | |

- Molecule 41 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | SB | 275 | Total | C | N | O | S | 0 | 0 |
| | | | 2243 | 1419 | 406 | 404 | 14 | | |

- Molecule 42 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | SC | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1747 | 1124 | 332 | 287 | 4 | | |

- Molecule 43 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | SD | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1870 | 1202 | 358 | 301 | 9 | | |

- Molecule 44 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | SE | 231 | Total | C | N | O | S | 1 | 0 |
| | | | 1869 | 1191 | 361 | 313 | 4 | | |

- Molecule 45 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | SF | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 1876 | 1177 | 383 | 310 | 6 | | |

- Molecule 46 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | SG | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1518 | 956 | 284 | 272 | 6 | | |

- Molecule 47 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | SH | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 773 | 501 | 130 | 139 | 3 | | |

- Molecule 48 is a protein called 60S ribosomal protein L7-like 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | SI | 234 | Total | C | N | O | S | 3 | 0 |
| | | | 1952 | 1267 | 365 | 316 | 4 | | |

- Molecule 49 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | SK | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1852 | 1149 | 318 | 372 | 13 | | |

- Molecule 50 is a protein called Pescadillo homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | SM | 399 | Total | C | N | O | S | 0 | 0 |
| | | | 3278 | 2120 | 576 | 571 | 11 | | |

- Molecule 51 is a protein called mRNA turnover protein 4 homolog.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 51 | SQ | 127 | Total | C | N | O | 0 | 0 |
| | | | 650 | 388 | 132 | 130 | | |

- Molecule 52 is a protein called GTP-binding protein 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | SR | 601 | Total | C | N | O | S | 0 | 0 |
| | | | 4932 | 3105 | 899 | 902 | 26 | | |

- Molecule 53 is a protein called Probable ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | SV | 139 | Total | C | N | O | S | 0 | 0 |
| | | | 1184 | 754 | 229 | 191 | 10 | | |

- Molecule 54 is a protein called Leydig cell tumor 10 kDa protein homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | VB | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 455 | 285 | 95 | 74 | 1 | | |

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 55 | L1 | 4 | Total | Mg | 0 |
| | | | 4 | 4 | |
| 55 | L3 | 74 | Total | Mg | 0 |
| | | | 74 | 74 | |
| 55 | L4 | 3 | Total | Mg | 0 |
| | | | 3 | 3 | |

*Continued on next page...*

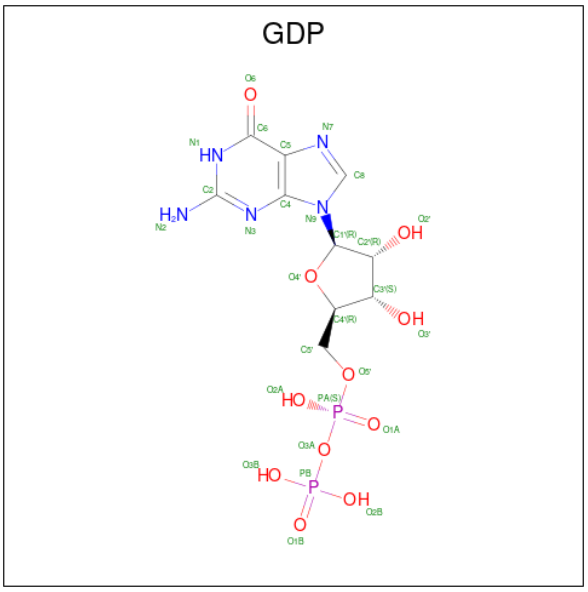
*Continued from previous page...*

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 55 | LG | 1 | Total Mg<br>1 1 | 0 |
| 55 | LN | 1 | Total Mg<br>1 1 | 0 |
| 55 | LQ | 1 | Total Mg<br>1 1 | 0 |
| 55 | LR | 1 | Total Mg<br>1 1 | 0 |
| 55 | LT | 1 | Total Mg<br>1 1 | 0 |
| 55 | SF | 1 | Total Mg<br>1 1 | 0 |
| 55 | SR | 1 | Total Mg<br>1 1 | 0 |

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 56 | LR | 1 | Total Zn<br>1 1 | 0 |
| 56 | LV | 1 | Total Zn<br>1 1 | 0 |
| 56 | LW | 1 | Total Zn<br>1 1 | 0 |
| 56 | LX | 1 | Total Zn<br>1 1 | 0 |
| 56 | NP | 1 | Total Zn<br>1 1 | 0 |
| 56 | SV | 1 | Total Zn<br>1 1 | 0 |

- Molecule 57 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 57 | SR | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

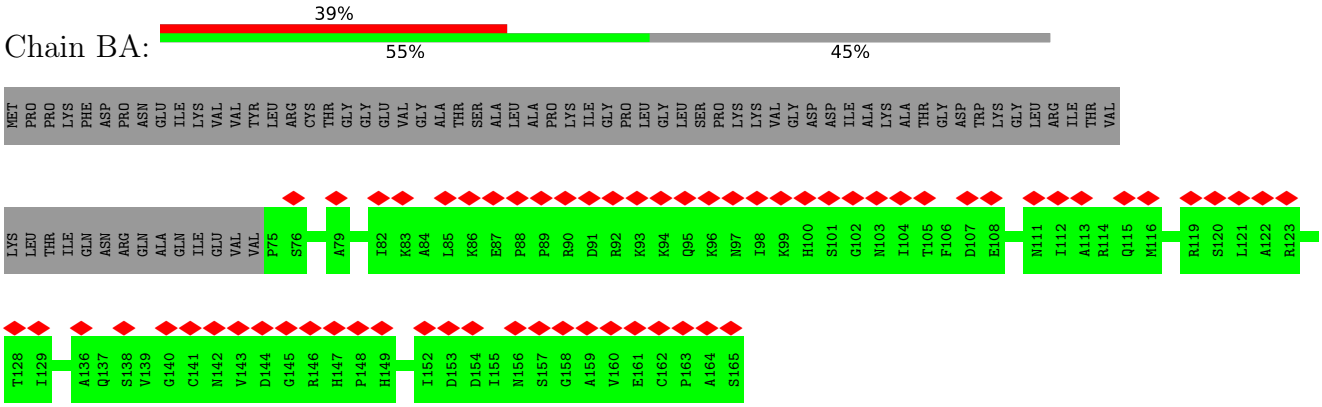
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 58 | SR | 1 | Total | K | 0 |
| | | | 1 | 1 | |

# 3 Residue-property plots (i)

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

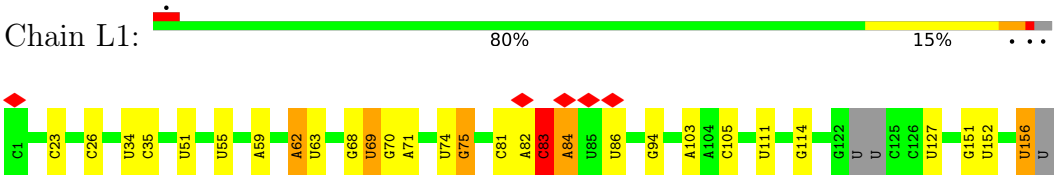
- Molecule 1: 60S ribosomal protein L12

Chain BA:



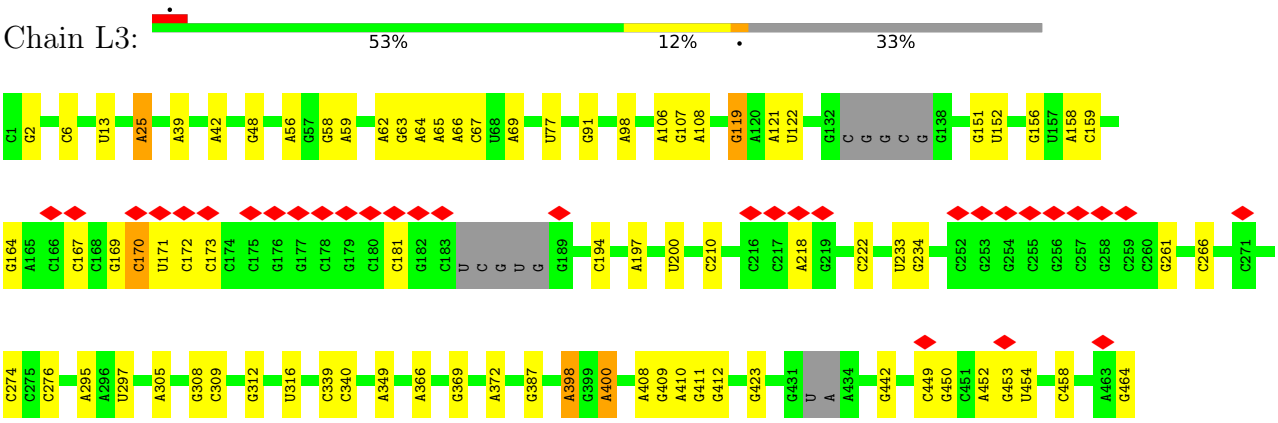

- Molecule 2: 5.8S rRNA

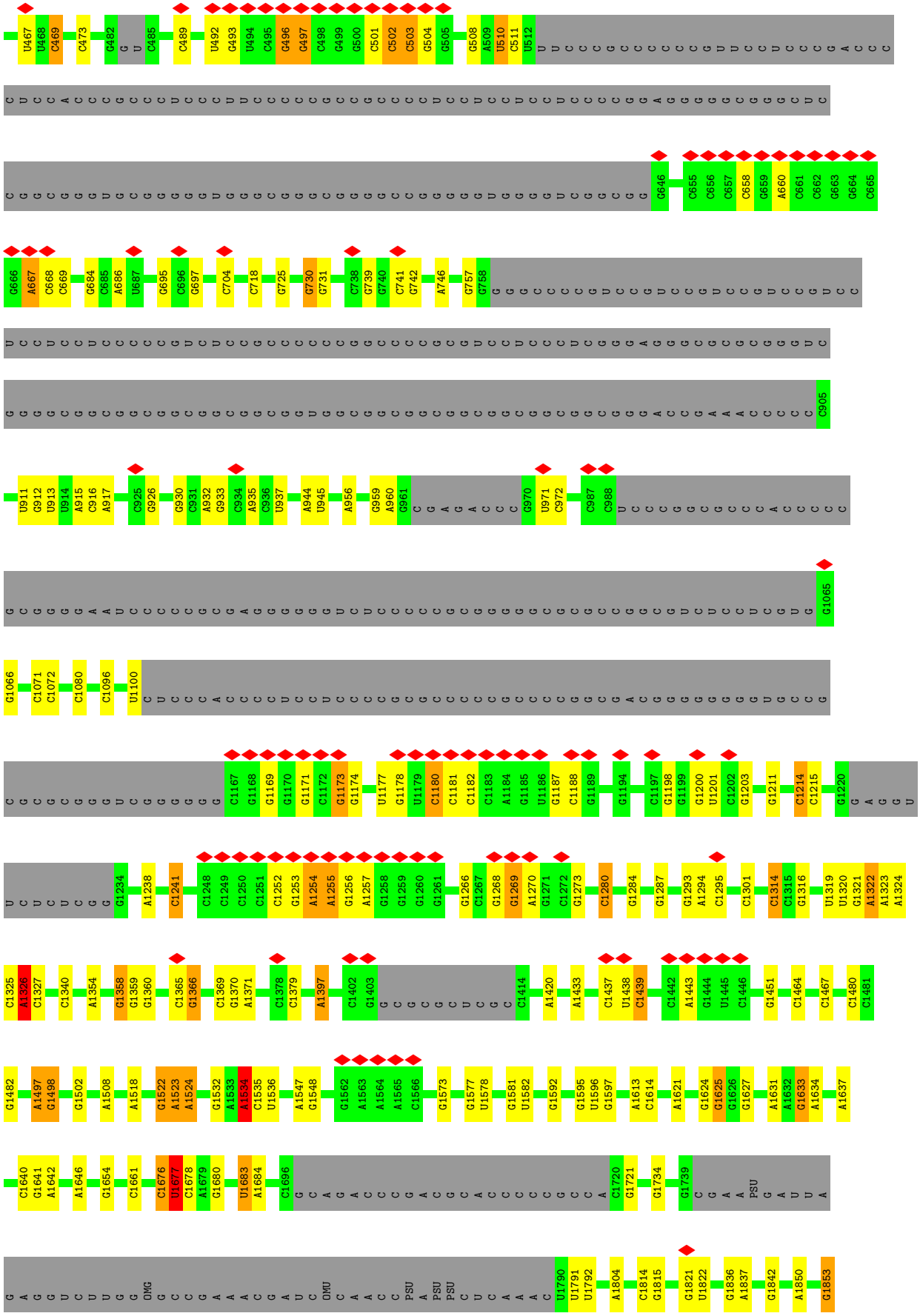
Chain L1:

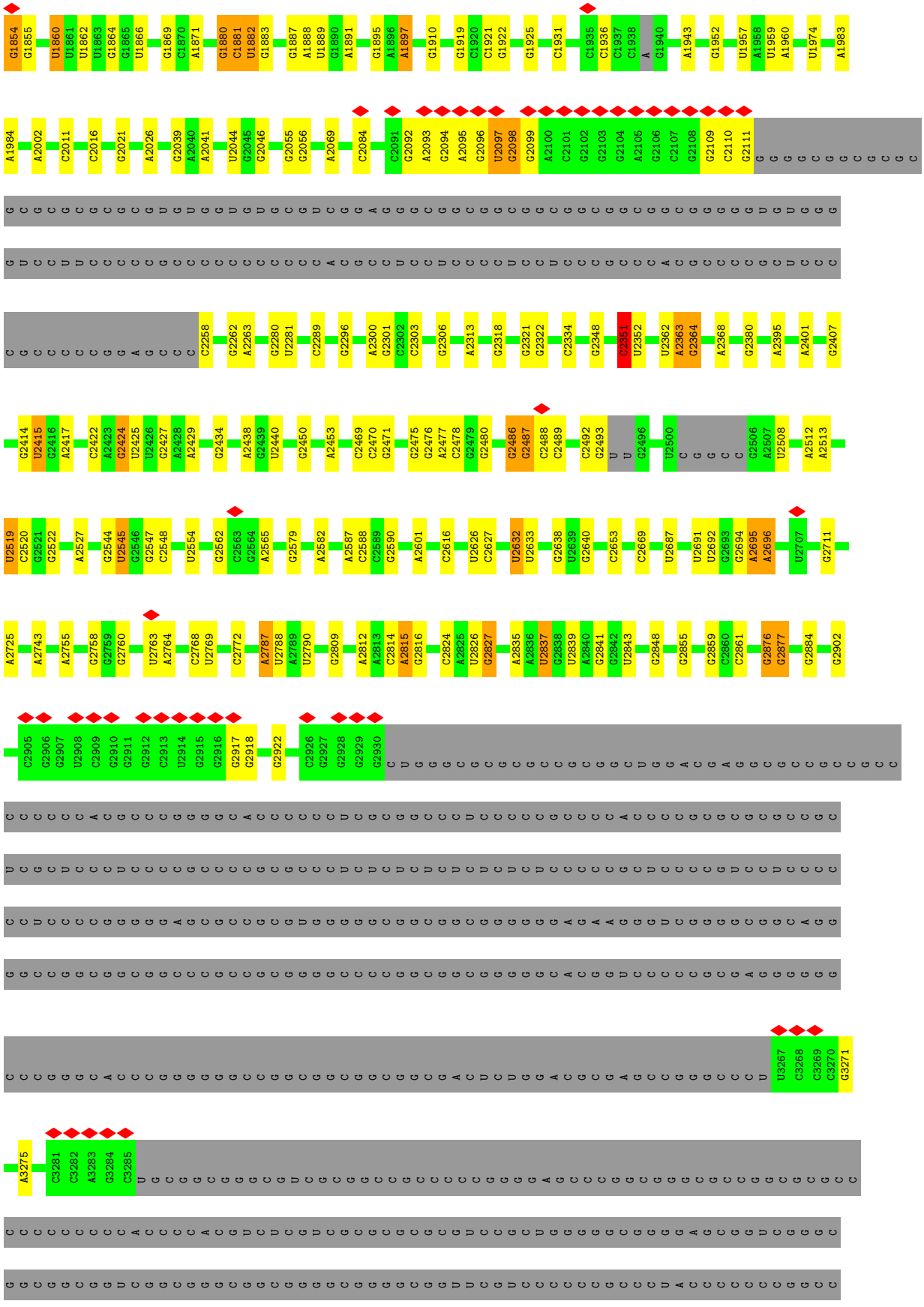


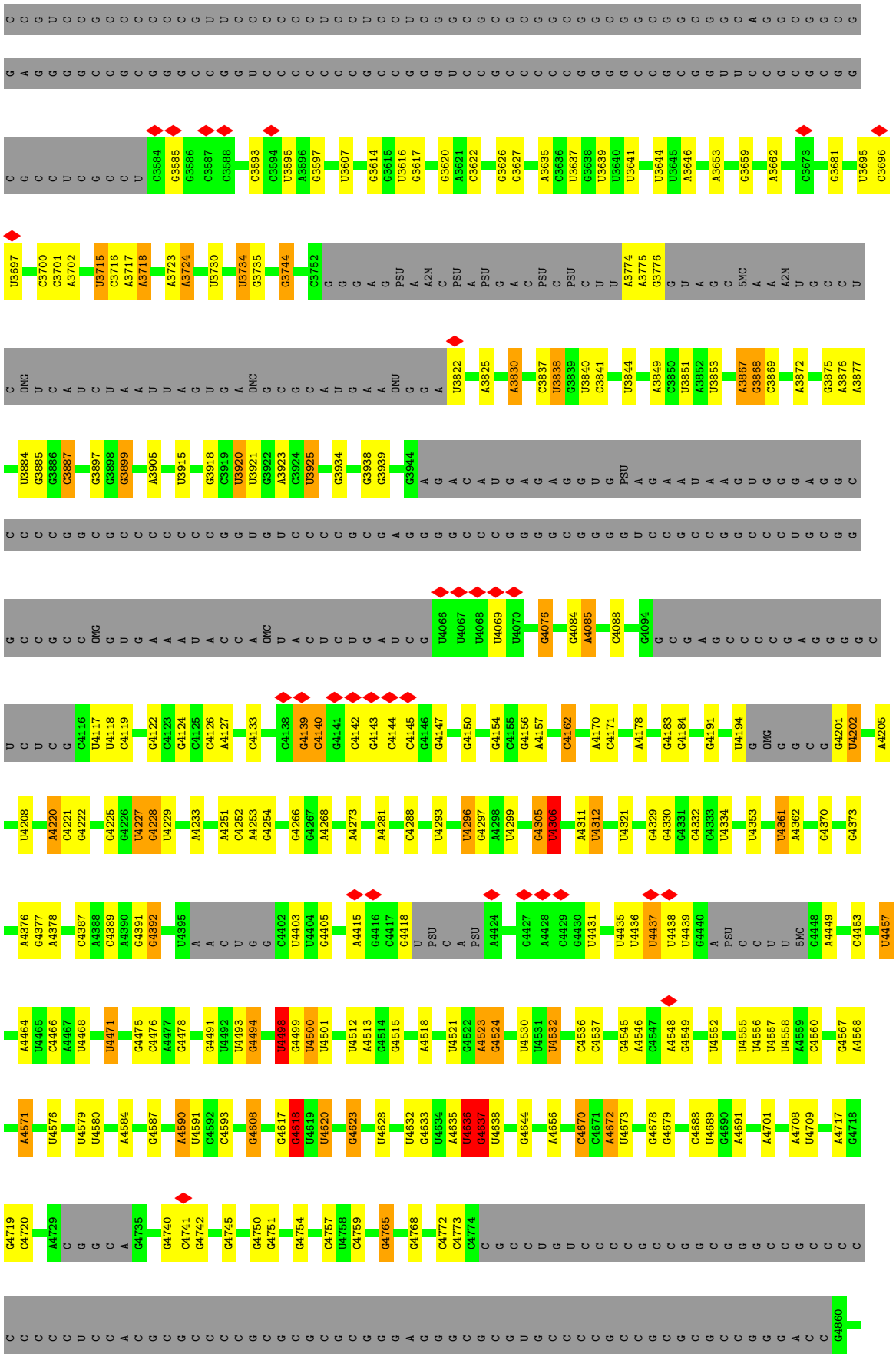

- Molecule 3: 28S rRNA

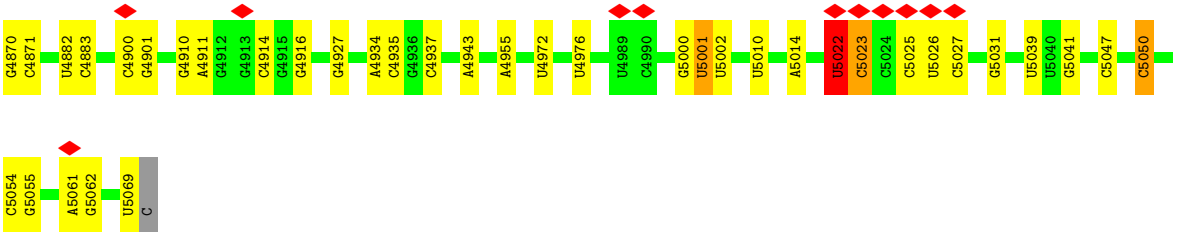
Chain L3:





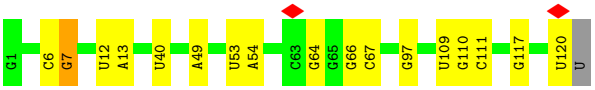






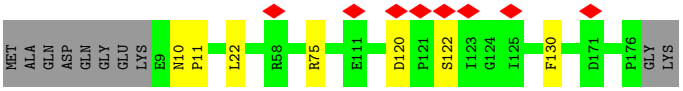

• Molecule 4: 5S rRNA

Chain L4:

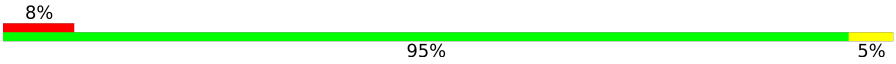

• Molecule 5: 60S ribosomal protein L11

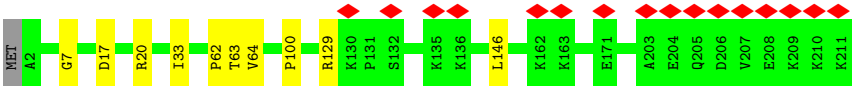
Chain L5:


• Molecule 6: 60S ribosomal protein L13

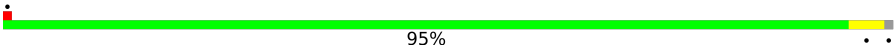
Chain L6:

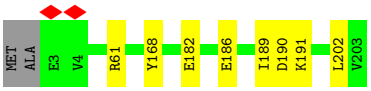



• Molecule 7: 60S ribosomal protein L13a

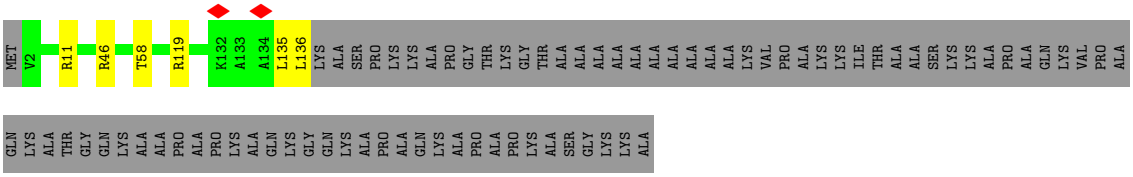
Chain L7:



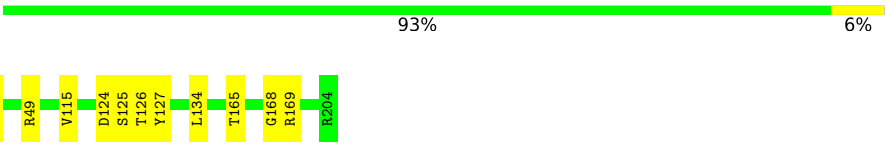

• Molecule 8: 60S ribosomal protein L14

Chain L8:

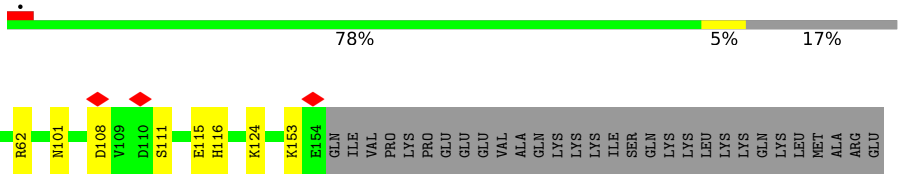

• Molecule 9: 60S ribosomal protein L15

Chain L9:



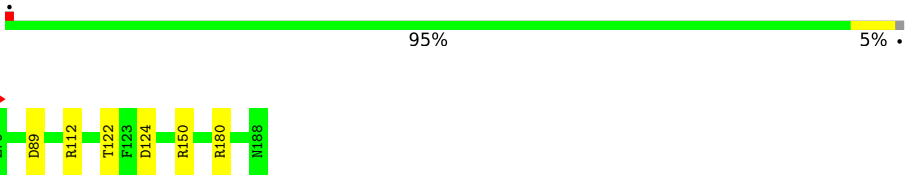

• Molecule 10: 60S ribosomal protein L17

Chain LA:



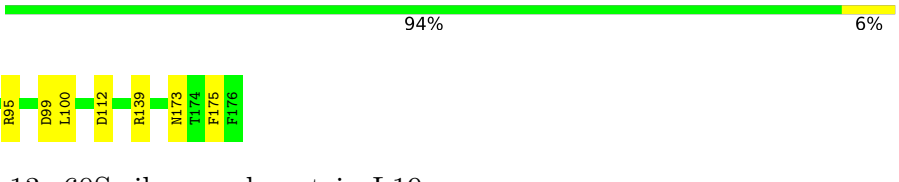

• Molecule 11: 60S ribosomal protein L18

Chain LB:



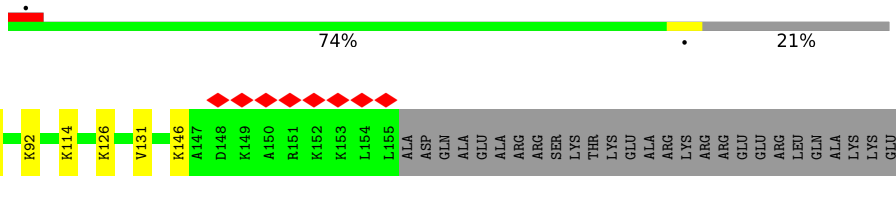

• Molecule 12: 60S ribosomal protein L18a

Chain LC:



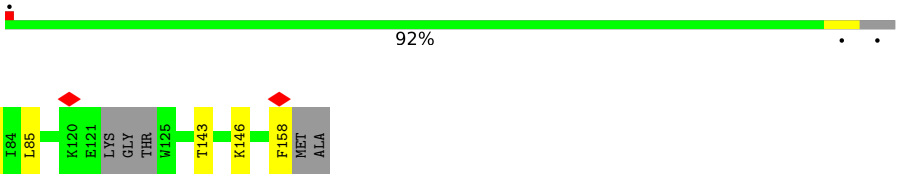

• Molecule 13: 60S ribosomal protein L19

Chain LD:



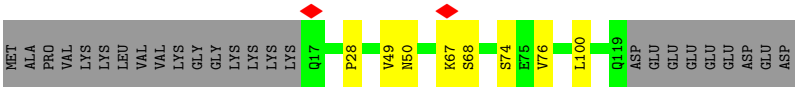

• Molecule 14: 60S ribosomal protein L21

Chain LE:



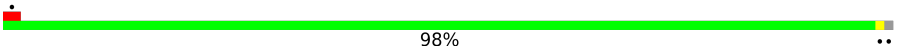

• Molecule 15: 60S ribosomal protein L22

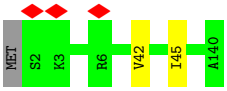
Chain LF:




• Molecule 16: 60S ribosomal protein L23

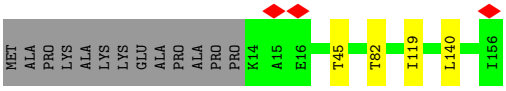
Chain LG:



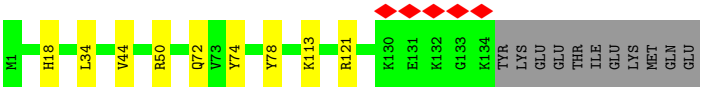

• Molecule 17: 60S ribosomal protein L23a

Chain LH:


• Molecule 18: 60S ribosomal protein L26

Chain LI:

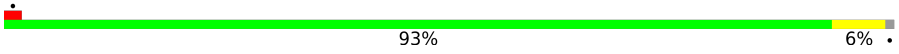

• Molecule 19: 60S ribosomal protein L27

Chain LJ:



• Molecule 20: 60S ribosomal protein L27a

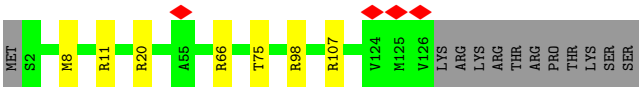
Chain LK:





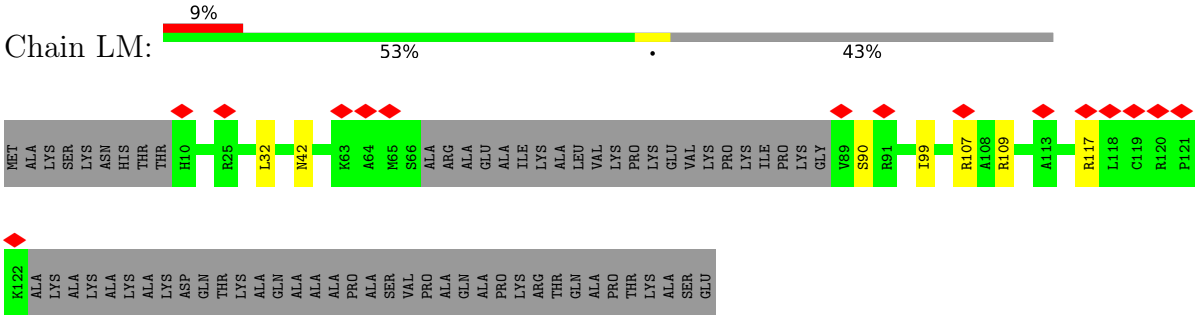
• Molecule 21: 60S ribosomal protein L28

Chain LL:

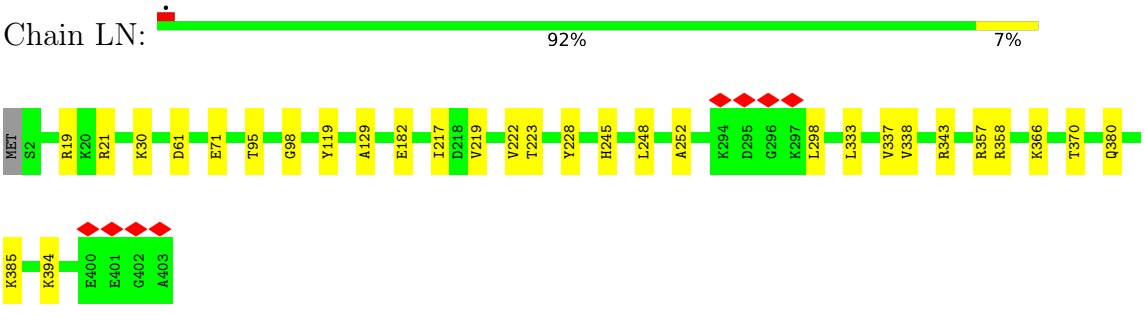

• Molecule 22: 60S ribosomal protein L29

Chain LM:



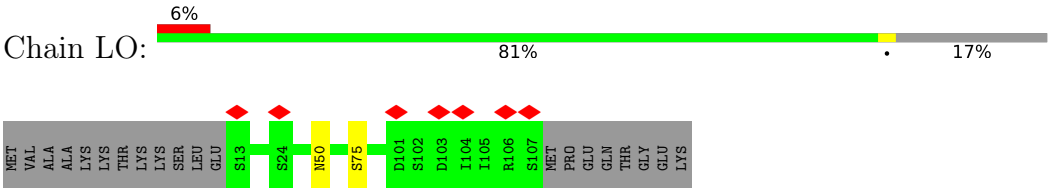

• Molecule 23: 60S ribosomal protein L3

Chain LN:



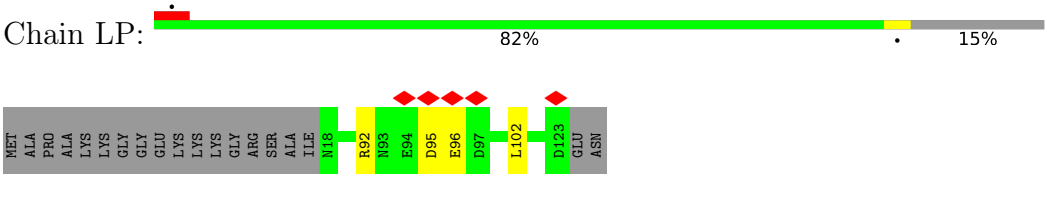

• Molecule 24: 60S ribosomal protein L30

Chain LO:



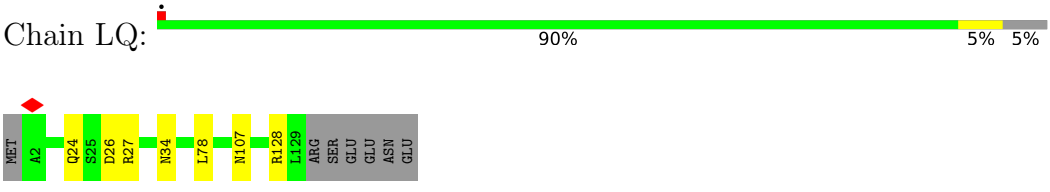

• Molecule 25: 60S ribosomal protein L31

Chain LP:



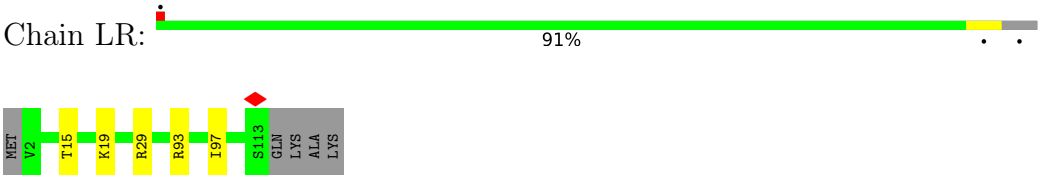

• Molecule 26: 60S ribosomal protein L32

Chain LQ:



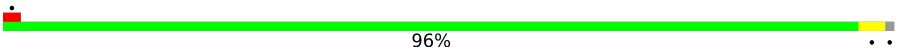

• Molecule 27: 60S ribosomal protein L34

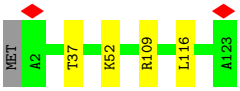
Chain LR:



• Molecule 28: 60S ribosomal protein L35

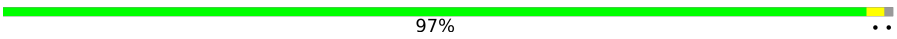
Chain LS:

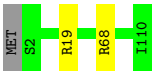



• Molecule 29: 60S ribosomal protein L35a

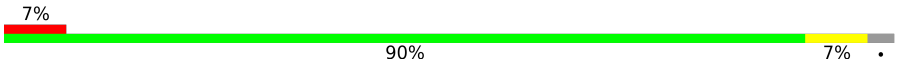
Chain LT:

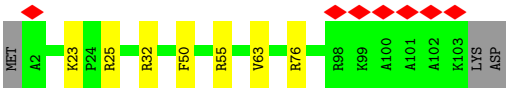



• Molecule 30: 60S ribosomal protein L36

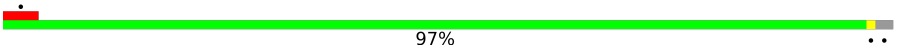
Chain LU:

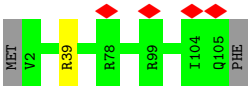



• Molecule 31: 60S ribosomal protein L36a

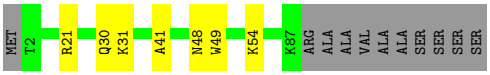
Chain LV:



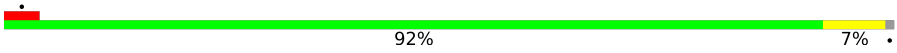

• Molecule 32: 60S ribosomal protein L37

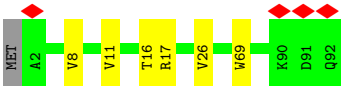
Chain LW:


• Molecule 33: 60S ribosomal protein L37a

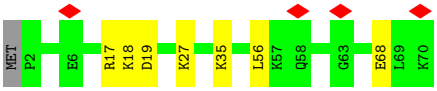
Chain LX:



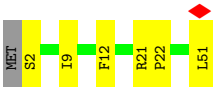

• Molecule 34: 60S ribosomal protein L38

Chain LY:



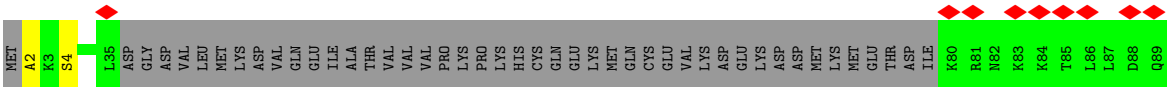

• Molecule 35: 60S ribosomal protein L39

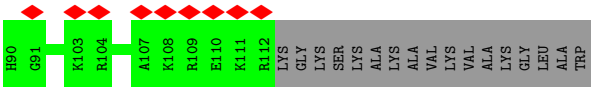
Chain LZ:


• Molecule 36: Protein LLP homolog

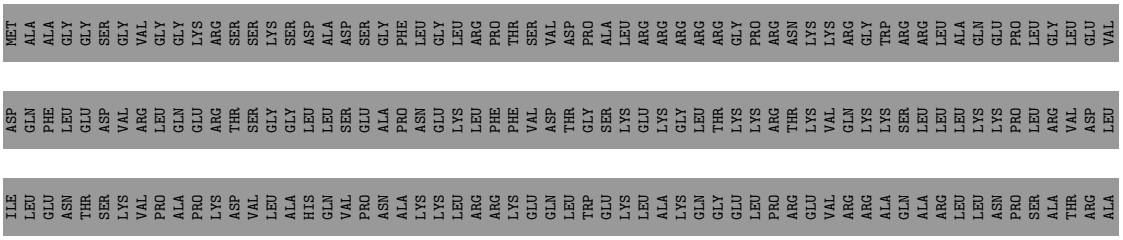
Chain NK:

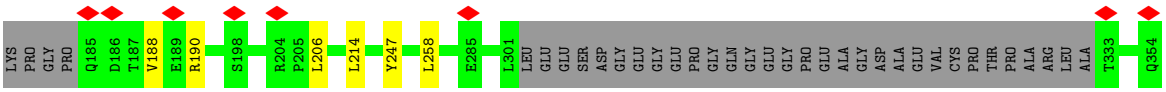



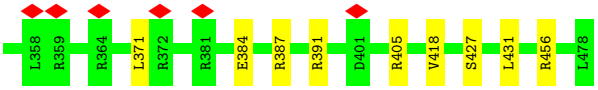




• Molecule 37: Ribosome biogenesis protein NOP53

Chain NL:

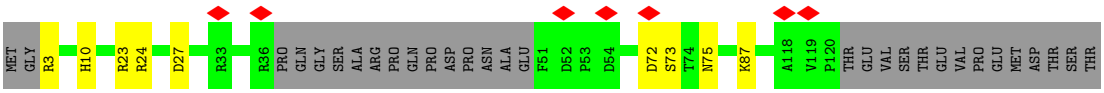



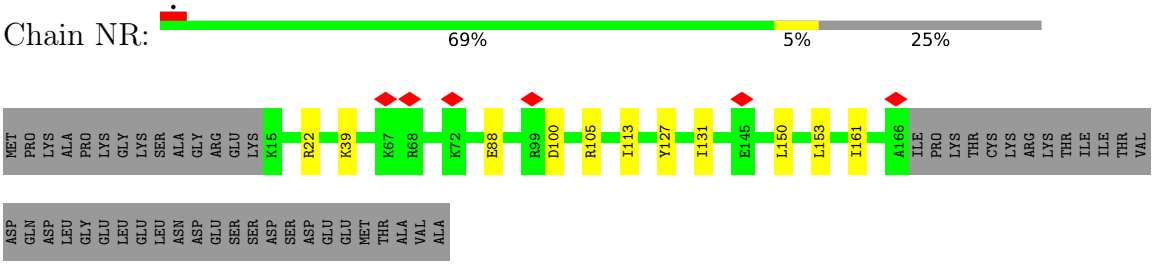

• Molecule 38: Zinc finger protein 593

Chain NP:

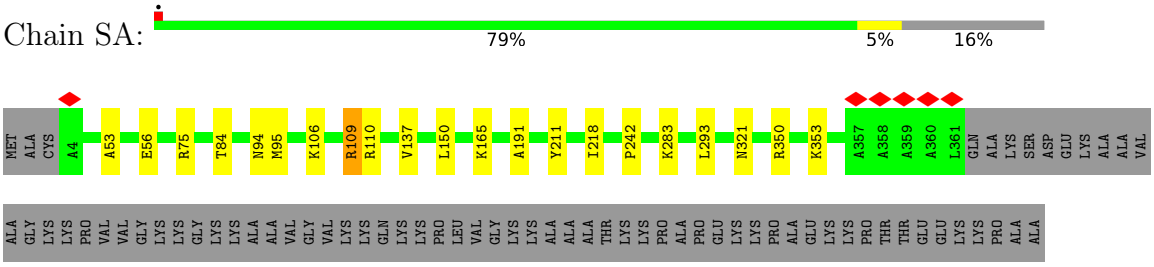

• Molecule 39: Translation machinery-associated protein 16

Chain NR:



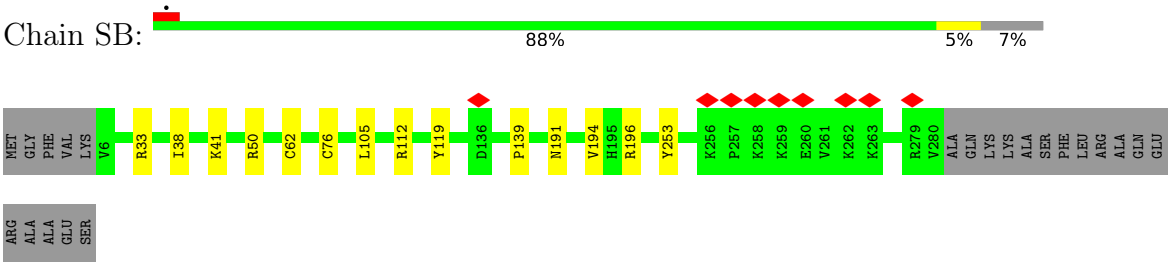

• Molecule 40: 60S ribosomal protein L4

Chain SA:



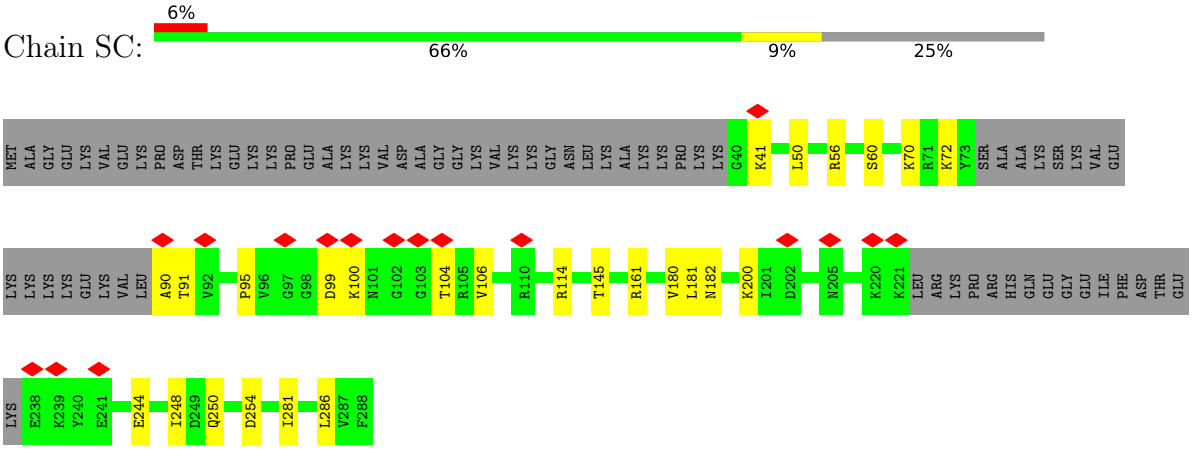

• Molecule 41: 60S ribosomal protein L5

Chain SB:



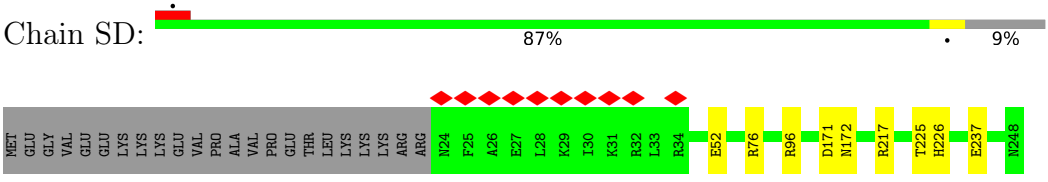

• Molecule 42: 60S ribosomal protein L6

Chain SC:



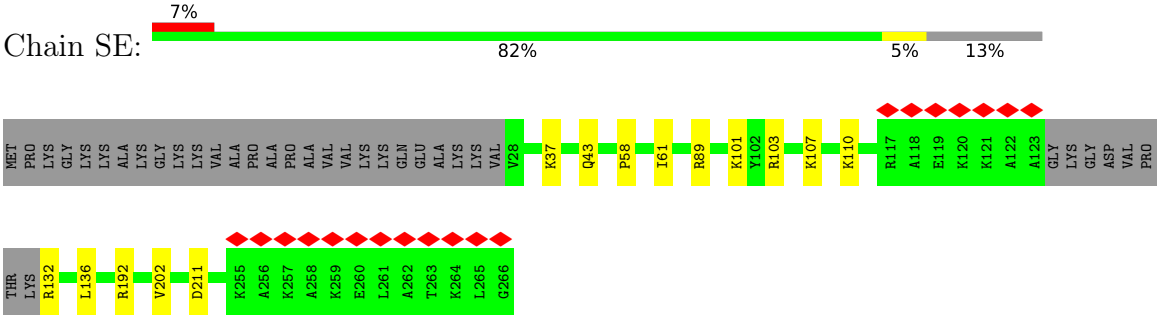

• Molecule 43: 60S ribosomal protein L7

Chain SD:



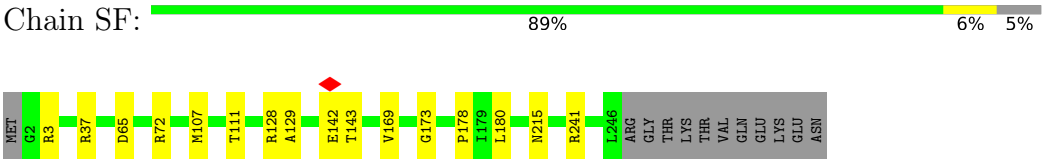
• Molecule 44: 60S ribosomal protein L7a

Chain SE:



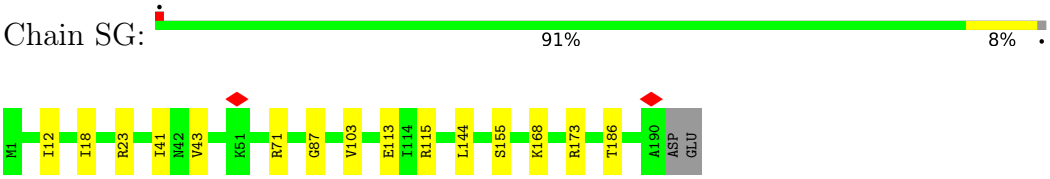

• Molecule 45: 60S ribosomal protein L8

Chain SF:



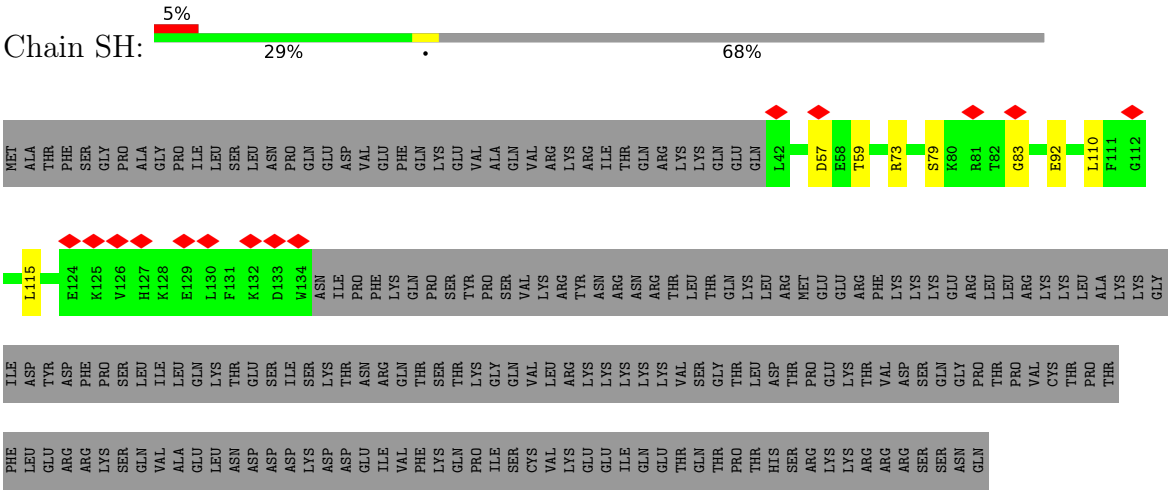

• Molecule 46: 60S ribosomal protein L9

Chain SG:



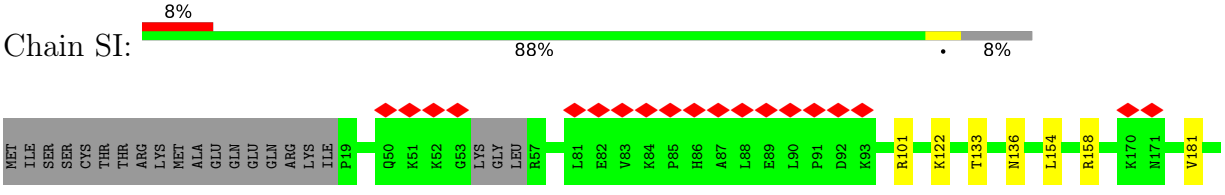

• Molecule 47: MKI67 FHA domain-interacting nucleolar phosphoprotein

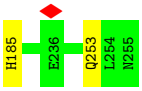
Chain SH:




• Molecule 48: 60S ribosomal protein L7-like 1

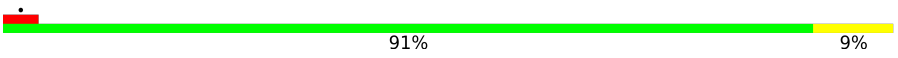
Chain SI:

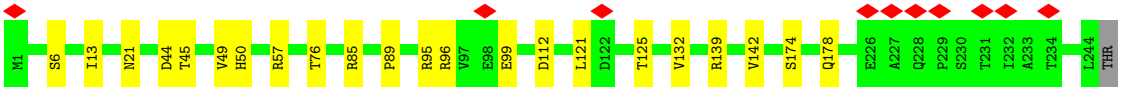





• Molecule 49: Eukaryotic translation initiation factor 6

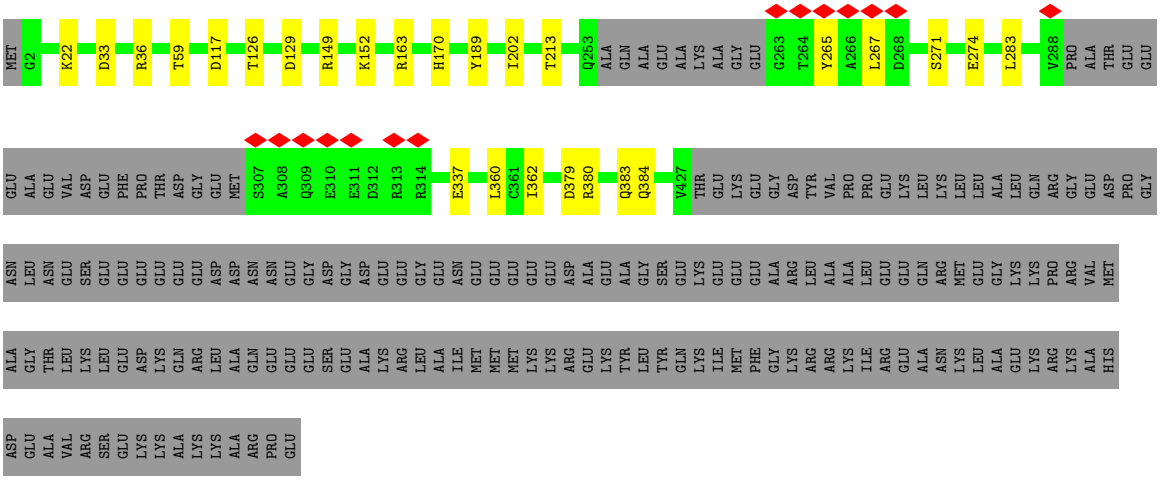
Chain SK:



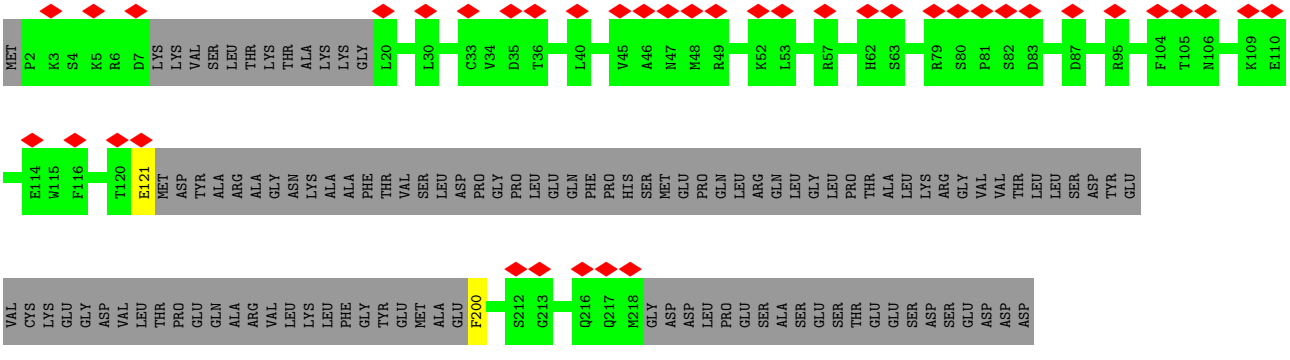

• Molecule 50: Pescadillo homolog

Chain SM:

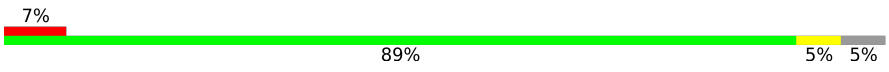

• Molecule 51: mRNA turnover protein 4 homolog

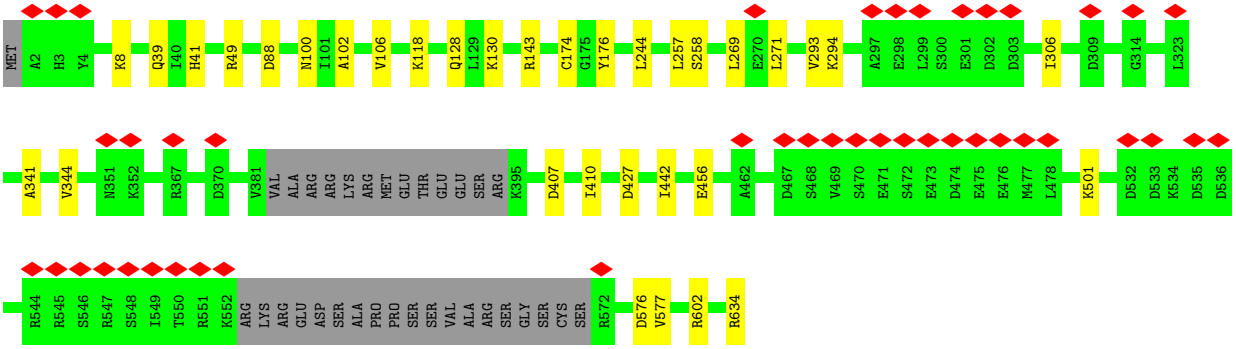
Chain SQ:


• Molecule 52: GTP-binding protein 4

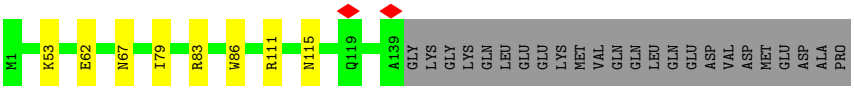
Chain SR:





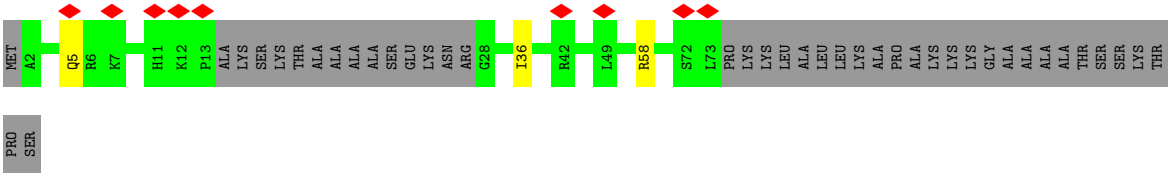

• Molecule 53: Probable ribosome biogenesis protein RLP24

Chain SV:


• Molecule 54: Leydig cell tumor 10 kDa protein homolog

Chain VB:

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 66157 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | 64000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 10.877 | Depositor |
| Minimum map value | -0.003 | Depositor |
| Average map value | 0.055 | Depositor |
| Map value standard deviation | 0.194 | Depositor |
| Recommended contour level | 0.85 | Depositor |
| Map size (Å) | 514.56, 514.56, 514.56 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.072, 1.072, 1.072 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, 1MA, OMU, PSU, OMC, A2M, K, HIC, OMG, ZN, UR3, 6MZ, PTR

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | BA | 0.23 | 0/448 | 0.41 | 0/622 |
| 2 | L1 | 0.44 | 0/3589 | 0.75 | 1/5589 (0.0%) |
| 3 | L3 | 0.40 | 0/79642 | 0.78 | 6/124218 (0.0%) |
| 4 | L4 | 0.52 | 0/2861 | 0.81 | 0/4459 |
| 5 | L5 | 0.27 | 0/1372 | 0.58 | 0/1836 |
| 6 | L6 | 0.26 | 0/1732 | 0.60 | 0/2315 |
| 7 | L7 | 0.28 | 0/1682 | 0.57 | 0/2250 |
| 8 | L8 | 0.27 | 0/1133 | 0.53 | 0/1516 |
| 9 | L9 | 0.29 | 0/1746 | 0.64 | 0/2338 |
| 10 | LA | 0.26 | 0/1268 | 0.54 | 0/1701 |
| 11 | LB | 0.28 | 0/1536 | 0.65 | 0/2052 |
| 12 | LC | 0.30 | 0/1501 | 0.60 | 0/2013 |
| 13 | LD | 0.24 | 0/1305 | 0.59 | 0/1727 |
| 14 | LE | 0.31 | 0/1291 | 0.56 | 0/1724 |
| 15 | LF | 0.27 | 0/856 | 0.51 | 0/1149 |
| 16 | LG | 0.28 | 0/1048 | 0.58 | 0/1402 |
| 17 | LH | 0.26 | 0/1175 | 0.52 | 0/1572 |
| 18 | LI | 0.28 | 0/1132 | 0.57 | 0/1504 |
| 19 | LJ | 0.29 | 0/1130 | 0.55 | 0/1507 |
| 20 | LK | 0.27 | 0/1191 | 0.55 | 0/1591 |
| 21 | LL | 0.26 | 0/1017 | 0.60 | 0/1364 |
| 22 | LM | 0.26 | 0/763 | 0.56 | 0/1005 |
| 23 | LN | 0.27 | 0/3294 | 0.55 | 0/4406 |
| 24 | LO | 0.26 | 0/748 | 0.48 | 0/1004 |
| 25 | LP | 0.28 | 0/894 | 0.59 | 0/1204 |
| 26 | LQ | 0.27 | 0/1071 | 0.58 | 0/1429 |
| 27 | LR | 0.27 | 0/898 | 0.62 | 0/1197 |
| 28 | LS | 0.25 | 0/1023 | 0.57 | 0/1351 |
| 29 | LT | 0.27 | 0/895 | 0.61 | 0/1198 |
| 30 | LU | 0.25 | 0/843 | 0.59 | 0/1115 |
| 31 | LV | 0.30 | 0/864 | 0.61 | 0/1140 |
| 32 | LW | 0.28 | 0/720 | 0.65 | 0/952 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | LX | 0.26 | 0/718 | 0.55 | 0/953 |
| 34 | LY | 0.26 | 0/575 | 0.51 | 0/761 |
| 35 | LZ | 0.25 | 0/454 | 0.61 | 0/599 |
| 36 | NK | 0.24 | 0/587 | 0.59 | 0/767 |
| 37 | NL | 0.25 | 0/2207 | 0.59 | 0/2955 |
| 38 | NP | 0.25 | 0/864 | 0.61 | 0/1154 |
| 39 | NR | 0.24 | 0/1306 | 0.54 | 0/1740 |
| 40 | SA | 0.27 | 0/2907 | 0.57 | 0/3905 |
| 41 | SB | 0.30 | 0/2287 | 0.55 | 0/3065 |
| 42 | SC | 0.26 | 0/1781 | 0.56 | 0/2388 |
| 43 | SD | 0.28 | 0/1905 | 0.56 | 0/2539 |
| 44 | SE | 0.27 | 0/1903 | 0.55 | 0/2559 |
| 45 | SF | 0.27 | 0/1914 | 0.60 | 0/2567 |
| 46 | SG | 0.26 | 0/1537 | 0.54 | 0/2066 |
| 47 | SH | 0.26 | 0/794 | 0.48 | 0/1071 |
| 48 | SI | 0.25 | 0/2003 | 0.52 | 0/2688 |
| 49 | SK | 0.26 | 0/1877 | 0.53 | 0/2554 |
| 50 | SM | 0.27 | 0/3357 | 0.51 | 0/4529 |
| 51 | SQ | 0.22 | 0/648 | 0.45 | 0/894 |
| 52 | SR | 0.25 | 0/5014 | 0.52 | 0/6727 |
| 53 | SV | 0.29 | 0/1207 | 0.54 | 0/1600 |
| 54 | VB | 0.24 | 0/459 | 0.51 | 0/605 |
| All | All | 0.35 | 0/156972 | 0.70 | 7/229136 (0.0%) |

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | L3 | 2469 | C | C2-N1-C1' | 6.33 | 125.76 | 118.80 |
| 3 | L3 | 2486 | G | N1-C6-O6 | -6.22 | 116.17 | 119.90 |
| 3 | L3 | 170 | C | C6-N1-C2 | -6.16 | 117.84 | 120.30 |
| 3 | L3 | 5022 | U | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 3 | L3 | 2486 | G | C5-C6-O6 | 5.64 | 131.99 | 128.60 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | BA | 449 | 0 | 207 | 0 | 0 |
| 2 | L1 | 3278 | 0 | 1665 | 14 | 0 |
| 3 | L3 | 73423 | 0 | 37192 | 275 | 0 |
| 4 | L4 | 2561 | 0 | 1295 | 7 | 0 |
| 5 | L5 | 1349 | 0 | 1383 | 4 | 0 |
| 6 | L6 | 1701 | 0 | 1818 | 10 | 0 |
| 7 | L7 | 1650 | 0 | 1794 | 7 | 0 |
| 8 | L8 | 1111 | 0 | 1174 | 7 | 0 |
| 9 | L9 | 1701 | 0 | 1749 | 10 | 0 |
| 10 | LA | 1242 | 0 | 1269 | 7 | 0 |
| 11 | LB | 1512 | 0 | 1628 | 7 | 0 |
| 12 | LC | 1461 | 0 | 1502 | 6 | 0 |
| 13 | LD | 1289 | 0 | 1429 | 7 | 0 |
| 14 | LE | 1264 | 0 | 1328 | 6 | 0 |
| 15 | LF | 842 | 0 | 864 | 4 | 0 |
| 16 | LG | 1034 | 0 | 1097 | 3 | 0 |
| 17 | LH | 1156 | 0 | 1268 | 5 | 0 |
| 18 | LI | 1115 | 0 | 1205 | 8 | 0 |
| 19 | LJ | 1107 | 0 | 1182 | 7 | 0 |
| 20 | LK | 1162 | 0 | 1213 | 7 | 0 |
| 21 | LL | 1002 | 0 | 1068 | 5 | 0 |
| 22 | LM | 751 | 0 | 820 | 6 | 0 |
| 23 | LN | 3239 | 0 | 3377 | 24 | 0 |
| 24 | LO | 738 | 0 | 774 | 1 | 0 |
| 25 | LP | 879 | 0 | 924 | 2 | 0 |
| 26 | LQ | 1053 | 0 | 1147 | 6 | 0 |
| 27 | LR | 888 | 0 | 977 | 3 | 0 |
| 28 | LS | 1015 | 0 | 1148 | 4 | 0 |
| 29 | LT | 876 | 0 | 912 | 2 | 0 |
| 30 | LU | 832 | 0 | 917 | 5 | 0 |
| 31 | LV | 851 | 0 | 920 | 1 | 0 |
| 32 | LW | 705 | 0 | 737 | 5 | 0 |
| 33 | LX | 708 | 0 | 756 | 6 | 0 |
| 34 | LY | 569 | 0 | 637 | 5 | 0 |
| 35 | LZ | 444 | 0 | 483 | 5 | 0 |
| 36 | NK | 581 | 0 | 656 | 3 | 0 |
| 37 | NL | 2175 | 0 | 2235 | 12 | 0 |
| 38 | NP | 847 | 0 | 854 | 7 | 0 |
| 39 | NR | 1299 | 0 | 1318 | 7 | 0 |
| 40 | SA | 2853 | 0 | 3028 | 19 | 0 |
| 41 | SB | 2243 | 0 | 2268 | 9 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 42 | SC | 1747 | 0 | 1897 | 15 | 0 |
| 43 | SD | 1870 | 0 | 1996 | 7 | 0 |
| 44 | SE | 1869 | 0 | 2014 | 11 | 0 |
| 45 | SF | 1876 | 0 | 1970 | 12 | 0 |
| 46 | SG | 1518 | 0 | 1601 | 10 | 0 |
| 47 | SH | 773 | 0 | 755 | 4 | 0 |
| 48 | SI | 1952 | 0 | 2086 | 6 | 0 |
| 49 | SK | 1852 | 0 | 1828 | 11 | 0 |
| 50 | SM | 3278 | 0 | 3332 | 19 | 0 |
| 51 | SQ | 650 | 0 | 308 | 1 | 0 |
| 52 | SR | 4932 | 0 | 5071 | 23 | 0 |
| 53 | SV | 1184 | 0 | 1248 | 7 | 0 |
| 54 | VB | 455 | 0 | 504 | 3 | 0 |
| 55 | L1 | 4 | 0 | 0 | 0 | 0 |
| 55 | L3 | 74 | 0 | 0 | 0 | 0 |
| 55 | L4 | 3 | 0 | 0 | 0 | 0 |
| 55 | LG | 1 | 0 | 0 | 0 | 0 |
| 55 | LN | 1 | 0 | 0 | 0 | 0 |
| 55 | LQ | 1 | 0 | 0 | 0 | 0 |
| 55 | LR | 1 | 0 | 0 | 0 | 0 |
| 55 | LT | 1 | 0 | 0 | 0 | 0 |
| 55 | SF | 1 | 0 | 0 | 0 | 0 |
| 55 | SR | 1 | 0 | 0 | 0 | 0 |
| 56 | LR | 1 | 0 | 0 | 0 | 0 |
| 56 | LV | 1 | 0 | 0 | 0 | 0 |
| 56 | LW | 1 | 0 | 0 | 0 | 0 |
| 56 | LX | 1 | 0 | 0 | 0 | 0 |
| 56 | NP | 1 | 0 | 0 | 0 | 0 |
| 56 | SV | 1 | 0 | 0 | 0 | 0 |
| 57 | SR | 28 | 0 | 12 | 0 | 0 |
| 58 | SR | 1 | 0 | 0 | 0 | 0 |
| All | All | 149034 | 0 | 112840 | 498 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 498 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) |
|---|---|---|---|
| 40:SA:109:ARG:O | 40:SA:109:ARG:HG2 | 1.76 | 0.86 |
| 3:L3:4156:G:OP2 | 3:L3:4157:A:O2' | 1.97 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L3:1322:1MA:O2' | 3:L3:1323:A:O4' | 1.94 | 0.82 |
| 3:L3:1480:C:O2' | 3:L3:1482:G:OP2 | 1.98 | 0.81 |
| 4:L4:40:U:O2 | 5:L5:75:ARG:NH1 | 2.13 | 0.81 |

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 | |
|---|---|---|---|---|---|---|---|
| 1 | BA | 89/165 (54%) | 89 (100%) | 0 | 0 | 100 | 100 |
| 5 | L5 | 166/178 (93%) | 165 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | L6 | 208/211 (99%) | 203 (98%) | 5 (2%) | 0 | 100 | 100 |
| 7 | L7 | 199/203 (98%) | 196 (98%) | 3 (2%) | 0 | 100 | 100 |
| 8 | L8 | 133/215 (62%) | 130 (98%) | 3 (2%) | 0 | 100 | 100 |
| 9 | L9 | 201/204 (98%) | 198 (98%) | 3 (2%) | 0 | 100 | 100 |
| 10 | LA | 151/184 (82%) | 147 (97%) | 4 (3%) | 0 | 100 | 100 |
| 11 | LB | 185/188 (98%) | 180 (97%) | 5 (3%) | 0 | 100 | 100 |
| 12 | LC | 174/176 (99%) | 172 (99%) | 2 (1%) | 0 | 100 | 100 |
| 13 | LD | 152/196 (78%) | 150 (99%) | 2 (1%) | 0 | 100 | 100 |
| 14 | LE | 150/160 (94%) | 145 (97%) | 5 (3%) | 0 | 100 | 100 |
| 15 | LF | 101/128 (79%) | 99 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | LG | 137/140 (98%) | 135 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | LH | 141/156 (90%) | 141 (100%) | 0 | 0 | 100 | 100 |
| 18 | LI | 132/145 (91%) | 130 (98%) | 2 (2%) | 0 | 100 | 100 |
| 19 | LJ | 133/136 (98%) | 131 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | LK | 145/148 (98%) | 143 (99%) | 2 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 21 | LL | 123/137 (90%) | 122 (99%) | 1 (1%) | 0 | 100 | 100 |
| 22 | LM | 87/159 (55%) | 86 (99%) | 1 (1%) | 0 | 100 | 100 |
| 23 | LN | 399/403 (99%) | 391 (98%) | 8 (2%) | 0 | 100 | 100 |
| 24 | LO | 93/115 (81%) | 93 (100%) | 0 | 0 | 100 | 100 |
| 25 | LP | 104/125 (83%) | 102 (98%) | 2 (2%) | 0 | 100 | 100 |
| 26 | LQ | 126/135 (93%) | 125 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | LR | 110/117 (94%) | 110 (100%) | 0 | 0 | 100 | 100 |
| 28 | LS | 120/123 (98%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 29 | LT | 107/110 (97%) | 106 (99%) | 1 (1%) | 0 | 100 | 100 |
| 30 | LU | 100/105 (95%) | 100 (100%) | 0 | 0 | 100 | 100 |
| 31 | LV | 102/106 (96%) | 100 (98%) | 2 (2%) | 0 | 100 | 100 |
| 32 | LW | 84/97 (87%) | 83 (99%) | 1 (1%) | 0 | 100 | 100 |
| 33 | LX | 89/92 (97%) | 86 (97%) | 3 (3%) | 0 | 100 | 100 |
| 34 | LY | 67/70 (96%) | 67 (100%) | 0 | 0 | 100 | 100 |
| 35 | LZ | 48/51 (94%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 36 | NK | 63/129 (49%) | 62 (98%) | 1 (2%) | 0 | 100 | 100 |
| 37 | NL | 259/478 (54%) | 258 (100%) | 1 (0%) | 0 | 100 | 100 |
| 38 | NP | 100/134 (75%) | 100 (100%) | 0 | 0 | 100 | 100 |
| 39 | NR | 150/203 (74%) | 147 (98%) | 3 (2%) | 0 | 100 | 100 |
| 40 | SA | 356/427 (83%) | 352 (99%) | 4 (1%) | 0 | 100 | 100 |
| 41 | SB | 273/297 (92%) | 269 (98%) | 4 (2%) | 0 | 100 | 100 |
| 42 | SC | 211/288 (73%) | 204 (97%) | 7 (3%) | 0 | 100 | 100 |
| 43 | SD | 223/248 (90%) | 218 (98%) | 5 (2%) | 0 | 100 | 100 |
| 44 | SE | 228/266 (86%) | 226 (99%) | 2 (1%) | 0 | 100 | 100 |
| 45 | SF | 243/257 (95%) | 236 (97%) | 7 (3%) | 0 | 100 | 100 |
| 46 | SG | 188/192 (98%) | 187 (100%) | 1 (0%) | 0 | 100 | 100 |
| 47 | SH | 91/293 (31%) | 90 (99%) | 1 (1%) | 0 | 100 | 100 |
| 48 | SI | 233/255 (91%) | 230 (99%) | 3 (1%) | 0 | 100 | 100 |
| 49 | SK | 242/245 (99%) | 237 (98%) | 5 (2%) | 0 | 100 | 100 |
| 50 | SM | 393/588 (67%) | 388 (99%) | 5 (1%) | 0 | 100 | 100 |
| 51 | SQ | 121/239 (51%) | 119 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 52 | SR | 595/634 (94%) | 587 (99%) | 7 (1%) | 1 (0%) | 47 | 60 |
| 53 | SV | 137/163 (84%) | 136 (99%) | 1 (1%) | 0 | 100 | 100 |
| 54 | VB | 54/99 (54%) | 54 (100%) | 0 | 0 | 100 | 100 |
| All | All | 8516/10313 (83%) | 8390 (98%) | 125 (2%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | SR | 88 | ASP |

### 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 | L5 | 142/149 (95%) | 142 (100%) | 0 | 100 | 100 |
| 6 | L6 | 176/177 (99%) | 176 (100%) | 0 | 100 | 100 |
| 7 | L7 | 173/174 (99%) | 173 (100%) | 0 | 100 | 100 |
| 8 | L8 | 115/161 (71%) | 115 (100%) | 0 | 100 | 100 |
| 9 | L9 | 171/172 (99%) | 171 (100%) | 0 | 100 | 100 |
| 10 | LA | 134/163 (82%) | 134 (100%) | 0 | 100 | 100 |
| 11 | LB | 164/165 (99%) | 164 (100%) | 0 | 100 | 100 |
| 12 | LC | 157/157 (100%) | 157 (100%) | 0 | 100 | 100 |
| 13 | LD | 138/175 (79%) | 138 (100%) | 0 | 100 | 100 |
| 14 | LE | 136/140 (97%) | 136 (100%) | 0 | 100 | 100 |
| 15 | LF | 93/115 (81%) | 93 (100%) | 0 | 100 | 100 |
| 16 | LG | 106/107 (99%) | 106 (100%) | 0 | 100 | 100 |
| 17 | LH | 124/133 (93%) | 124 (100%) | 0 | 100 | 100 |
| 18 | LI | 124/135 (92%) | 124 (100%) | 0 | 100 | 100 |
| 19 | LJ | 117/118 (99%) | 117 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 20 | LK | 120/121 (99%) | 120 (100%) | 0 | 100 100 |
| 21 | LL | 109/121 (90%) | 109 (100%) | 0 | 100 100 |
| 22 | LM | 77/126 (61%) | 76 (99%) | 1 (1%) | 69 80 |
| 23 | LN | 347/348 (100%) | 347 (100%) | 0 | 100 100 |
| 24 | LO | 80/97 (82%) | 80 (100%) | 0 | 100 100 |
| 25 | LP | 97/110 (88%) | 97 (100%) | 0 | 100 100 |
| 26 | LQ | 114/121 (94%) | 114 (100%) | 0 | 100 100 |
| 27 | LR | 96/100 (96%) | 96 (100%) | 0 | 100 100 |
| 28 | LS | 109/110 (99%) | 109 (100%) | 0 | 100 100 |
| 29 | LT | 88/89 (99%) | 88 (100%) | 0 | 100 100 |
| 30 | LU | 86/89 (97%) | 85 (99%) | 1 (1%) | 71 81 |
| 31 | LV | 92/94 (98%) | 92 (100%) | 0 | 100 100 |
| 32 | LW | 73/80 (91%) | 73 (100%) | 0 | 100 100 |
| 33 | LX | 74/75 (99%) | 74 (100%) | 0 | 100 100 |
| 34 | LY | 64/65 (98%) | 63 (98%) | 1 (2%) | 62 77 |
| 35 | LZ | 47/48 (98%) | 47 (100%) | 0 | 100 100 |
| 36 | NK | 61/115 (53%) | 61 (100%) | 0 | 100 100 |
| 37 | NL | 227/402 (56%) | 227 (100%) | 0 | 100 100 |
| 38 | NP | 88/114 (77%) | 88 (100%) | 0 | 100 100 |
| 39 | NR | 140/183 (76%) | 140 (100%) | 0 | 100 100 |
| 40 | SA | 298/348 (86%) | 297 (100%) | 1 (0%) | 92 96 |
| 41 | SB | 234/250 (94%) | 233 (100%) | 1 (0%) | 91 95 |
| 42 | SC | 192/252 (76%) | 190 (99%) | 2 (1%) | 76 84 |
| 43 | SD | 194/215 (90%) | 194 (100%) | 0 | 100 100 |
| 44 | SE | 198/223 (89%) | 198 (100%) | 0 | 100 100 |
| 45 | SF | 188/199 (94%) | 188 (100%) | 0 | 100 100 |
| 46 | SG | 169/171 (99%) | 169 (100%) | 0 | 100 100 |
| 47 | SH | 85/274 (31%) | 85 (100%) | 0 | 100 100 |
| 48 | SI | 212/228 (93%) | 212 (100%) | 0 | 100 100 |
| 49 | SK | 212/213 (100%) | 211 (100%) | 1 (0%) | 88 93 |
| 50 | SM | 354/509 (70%) | 354 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 51 | SQ | 6/214 (3%) | 6 (100%) | 0 | 100 100 |
| 52 | SR | 545/574 (95%) | 543 (100%) | 2 (0%) | 91 95 |
| 53 | SV | 128/149 (86%) | 128 (100%) | 0 | 100 100 |
| 54 | VB | 48/76 (63%) | 48 (100%) | 0 | 100 100 |
| All | All | 7322/8744 (84%) | 7312 (100%) | 10 (0%) | 93 97 |

5 of 10 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | SK | 57 | ARG |
| 52 | SR | 8 | LYS |
| 52 | SR | 100 | ASN |
| 40 | SA | 109 | ARG |
| 41 | SB | 196 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 42 | SC | 190 | HIS |
| 46 | SG | 40 | HIS |
| 52 | SR | 209 | HIS |
| 52 | SR | 100 | ASN |
| 52 | SR | 157 | HIS |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 2 | L1 | 152/157 (96%) | 18 (11%) | 0 |
| 3 | L3 | 3389/5070 (66%) | 431 (12%) | 8 (0%) |
| 4 | L4 | 119/121 (98%) | 10 (8%) | 0 |
| All | All | 3660/5348 (68%) | 459 (12%) | 8 (0%) |

5 of 459 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L1 | 23 | C |
| 2 | L1 | 34 | U |
| 2 | L1 | 35 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L1 | 59 | A |
| 2 | L1 | 62 | A |

5 of 8 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | L3 | 3616 | U |
| 3 | L3 | 2095 | A |
| 3 | L3 | 1625 | OMG |
| 3 | L3 | 1324 | A |
| 3 | L3 | 1853 | G |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | PSU | L3 | 3730 | 3 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.79 | 4 (18%) |
| 3 | PSU | L3 | 4500 | 3 | 18,21,22 | 1.00 | 1 (5%) | 22,30,33 | 1.84 | 4 (18%) |
| 3 | A2M | L3 | 2787 | 3 | 18,25,26 | 1.23 | 2 (11%) | 18,36,39 | 1.36 | 2 (11%) |
| 3 | OMC | L3 | 2351 | 3,55 | 19,22,23 | 0.65 | 0 | 26,31,34 | 0.87 | 1 (3%) |
| 3 | PSU | L3 | 3853 | 3 | 18,21,22 | 1.01 | 1 (5%) | 22,30,33 | 1.74 | 4 (18%) |
| 3 | A2M | L3 | 1534 | 3,55 | 18,25,26 | 1.24 | 3 (16%) | 18,36,39 | 1.35 | 2 (11%) |
| 3 | 6MZ | L3 | 4220 | 3 | 18,25,26 | 1.08 | 2 (11%) | 16,36,39 | 1.94 | 4 (25%) |
| 3 | PSU | L3 | 1862 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.84 | 5 (22%) |
| 3 | A2M | L3 | 3718 | 3 | 18,25,26 | 1.26 | 3 (16%) | 18,36,39 | 1.17 | 1 (5%) |
| 3 | OMU | L3 | 4620 | 3 | 19,22,23 | 1.93 | 6 (31%) | 26,31,34 | 1.56 | 4 (15%) |
| 2 | OMG | L1 | 75 | 2 | 18,26,27 | 1.19 | 2 (11%) | 19,38,41 | 0.86 | 1 (5%) |
| 3 | OMC | L3 | 2804 | 3 | 19,22,23 | 0.60 | 0 | 26,31,34 | 0.65 | 0 |
| 3 | OMU | L3 | 2837 | 3 | 19,22,23 | 2.03 | 6 (31%) | 26,31,34 | 1.78 | 5 (19%) |
| 23 | HIC | LN | 245 | 23 | 8,11,12 | 1.63 | 2 (25%) | 6,14,16 | 1.13 | 1 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | A2M | L3 | 2815 | 3 | 18,25,26 | 1.23 | 3 (16%) | 18,36,39 | 1.24 | 2 (11%) |
| 3 | PSU | L3 | 2508 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 3 | PSU | L3 | 3920 | 3,55 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.77 | 5 (22%) |
| 3 | PSU | L3 | 4299 | 3 | 18,21,22 | 1.00 | 1 (5%) | 22,30,33 | 1.89 | 5 (22%) |
| 3 | A2M | L3 | 2363 | 3,55 | 18,25,26 | 1.23 | 2 (11%) | 18,36,39 | 1.25 | 2 (11%) |
| 3 | OMC | L3 | 2824 | 3 | 19,22,23 | 0.58 | 0 | 26,31,34 | 0.70 | 0 |
| 3 | A2M | L3 | 3825 | 3 | 18,25,26 | 1.22 | 3 (16%) | 18,36,39 | 1.22 | 1 (5%) |
| 3 | PSU | L3 | 4579 | 3 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 3 | OMG | L3 | 3899 | 3 | 18,26,27 | 1.23 | 3 (16%) | 19,38,41 | 0.88 | 1 (5%) |
| 3 | A2M | L3 | 3867 | 3 | 18,25,26 | 1.19 | 2 (11%) | 18,36,39 | 1.27 | 1 (5%) |
| 3 | PSU | L3 | 4552 | 3 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 3 | A2M | L3 | 3724 | 3 | 18,25,26 | 1.22 | 2 (11%) | 18,36,39 | 1.32 | 2 (11%) |
| 3 | PSU | L3 | 3695 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.80 | 5 (22%) |
| 3 | PSU | L3 | 4457 | 3 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 1.77 | 4 (18%) |
| 3 | A2M | L3 | 1524 | 3 | 18,25,26 | 1.18 | 3 (16%) | 18,36,39 | 1.34 | 2 (11%) |
| 3 | OMC | L3 | 3887 | 3 | 19,22,23 | 0.58 | 0 | 26,31,34 | 0.66 | 0 |
| 2 | PSU | L1 | 55 | 2 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.79 | 5 (22%) |
| 3 | A2M | L3 | 4590 | 3 | 18,25,26 | 1.23 | 3 (16%) | 18,36,39 | 1.42 | 3 (16%) |
| 3 | PSU | L3 | 4296 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.83 | 5 (22%) |
| 3 | OMG | L3 | 3627 | 3 | 18,26,27 | 1.18 | 2 (11%) | 19,38,41 | 0.90 | 1 (5%) |
| 3 | A2M | L3 | 400 | 3 | 18,25,26 | 1.20 | 2 (11%) | 18,36,39 | 1.31 | 2 (11%) |
| 3 | PSU | L3 | 5010 | 3 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.78 | 5 (22%) |
| 3 | PSU | L3 | 1860 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.83 | 5 (22%) |
| 2 | PSU | L1 | 69 | 2 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.86 | 6 (27%) |
| 3 | PSU | L3 | 3734 | 3 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.82 | 6 (27%) |
| 3 | A2M | L3 | 4523 | 3 | 18,25,26 | 1.20 | 2 (11%) | 18,36,39 | 1.25 | 2 (11%) |
| 3 | PSU | L3 | 3715 | 3 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 1.83 | 6 (27%) |
| 3 | OMC | L3 | 4456 | 3 | 19,22,23 | 0.56 | 0 | 26,31,34 | 0.66 | 0 |
| 3 | OMG | L3 | 4499 | 3 | 18,26,27 | 1.13 | 2 (11%) | 19,38,41 | 0.82 | 1 (5%) |
| 3 | PSU | L3 | 3822 | 3 | 18,21,22 | 1.10 | 1 (5%) | 22,30,33 | 1.80 | 5 (22%) |
| 3 | PSU | L3 | 4972 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 3 | OMC | L3 | 1340 | 3 | 19,22,23 | 0.61 | 0 | 26,31,34 | 0.74 | 0 |
| 3 | PSU | L3 | 4689 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.83 | 5 (22%) |
| 3 | PSU | L3 | 4673 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 3 | OMU | L3 | 2415 | 3 | 19,22,23 | 2.02 | 6 (31%) | 26,31,34 | 1.73 | 5 (19%) |
| 3 | OMC | L3 | 3841 | 3 | 19,22,23 | 0.57 | 0 | 26,31,34 | 0.64 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | OMC | L3 | 2365 | 3 | 19,22,23 | 0.57 | 0 | 26,31,34 | 0.71 | 0 |
| 3 | PSU | L3 | 2839 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.75 | 4 (18%) |
| 3 | OMG | L3 | 2364 | 3 | 18,26,27 | 1.18 | 2 (11%) | 19,38,41 | 0.91 | 1 (5%) |
| 3 | OMG | L3 | 4618 | 3 | 18,26,27 | 1.21 | 3 (16%) | 19,38,41 | 0.88 | 1 (5%) |
| 3 | 1MA | L3 | 1322 | 3 | 16,25,26 | 0.92 | 2 (12%) | 18,37,40 | 1.18 | 2 (11%) |
| 3 | OMC | L3 | 3869 | 3 | 19,22,23 | 0.59 | 0 | 26,31,34 | 0.68 | 0 |
| 3 | OMC | L3 | 2861 | 3 | 19,22,23 | 0.56 | 0 | 26,31,34 | 0.69 | 0 |
| 3 | A2M | L3 | 4571 | 3 | 18,25,26 | 1.19 | 2 (11%) | 18,36,39 | 1.21 | 2 (11%) |
| 3 | PSU | L3 | 3844 | 3 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.83 | 5 (22%) |
| 39 | PTR | NR | 127 | 39 | 15,16,17 | 1.27 | 1 (6%) | 19,22,24 | 0.60 | 0 |
| 3 | OMG | L3 | 4623 | 3 | 18,26,27 | 1.16 | 2 (11%) | 19,38,41 | 0.97 | 1 (5%) |
| 3 | UR3 | L3 | 4530 | 3 | 19,22,23 | 1.11 | 3 (15%) | 26,32,35 | 1.24 | 1 (3%) |
| 3 | OMG | L3 | 1522 | 3 | 18,26,27 | 1.21 | 3 (16%) | 19,38,41 | 0.92 | 1 (5%) |
| 3 | OMU | L3 | 4306 | 3 | 19,22,23 | 1.98 | 6 (31%) | 26,31,34 | 1.81 | 4 (15%) |
| 3 | PSU | L3 | 3639 | 3 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.80 | 5 (22%) |
| 3 | OMC | L3 | 3701 | 3 | 19,22,23 | 0.53 | 0 | 26,31,34 | 0.57 | 0 |
| 3 | OMU | L3 | 4498 | 3 | 19,22,23 | 2.09 | 7 (36%) | 26,31,34 | 1.68 | 4 (15%) |
| 3 | OMG | L3 | 4228 | 3 | 18,26,27 | 1.24 | 3 (16%) | 19,38,41 | 0.96 | 1 (5%) |
| 3 | PSU | L3 | 3884 | 3 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.74 | 4 (18%) |
| 3 | OMU | L3 | 4227 | 3 | 19,22,23 | 1.97 | 6 (31%) | 26,31,34 | 1.75 | 4 (15%) |
| 3 | PSU | L3 | 4628 | 3 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.79 | 6 (27%) |
| 3 | A2M | L3 | 3830 | 3 | 18,25,26 | 1.21 | 2 (11%) | 18,36,39 | 1.29 | 2 (11%) |
| 3 | PSU | L3 | 1536 | 3 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.79 | 4 (18%) |
| 3 | A2M | L3 | 2401 | 3 | 18,25,26 | 1.20 | 2 (11%) | 18,36,39 | 1.32 | 2 (11%) |
| 3 | A2M | L3 | 1326 | 3 | 18,25,26 | 1.21 | 2 (11%) | 18,36,39 | 1.25 | 2 (11%) |
| 3 | OMG | L3 | 4370 | 3 | 18,26,27 | 1.23 | 3 (16%) | 19,38,41 | 0.94 | 1 (5%) |
| 3 | OMG | L3 | 1625 | 3 | 18,26,27 | 1.19 | 2 (11%) | 19,38,41 | 0.82 | 1 (5%) |
| 3 | PSU | L3 | 2632 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 3 | PSU | L3 | 3637 | 3 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.84 | 5 (22%) |
| 3 | PSU | L3 | 4431 | 3 | 18,21,22 | 1.10 | 1 (5%) | 22,30,33 | 1.80 | 5 (22%) |
| 3 | OMU | L3 | 3925 | 3 | 19,22,23 | 1.97 | 6 (31%) | 26,31,34 | 1.78 | 5 (19%) |
| 3 | OMG | L3 | 4494 | 3 | 18,26,27 | 1.21 | 2 (11%) | 19,38,41 | 0.86 | 1 (5%) |
| 3 | OMG | L3 | 3744 | 3 | 18,26,27 | 1.14 | 2 (11%) | 19,38,41 | 0.89 | 1 (5%) |
| 3 | PSU | L3 | 4576 | 3 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.78 | 5 (22%) |
| 3 | OMG | L3 | 4637 | 3 | 18,26,27 | 1.17 | 2 (11%) | 19,38,41 | 0.88 | 1 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | PSU | L3 | 4521 | 3 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 3 | PSU | L3 | 4636 | 3 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 1.91 | 6 (27%) |
| 3 | PSU | L3 | 1792 | 3 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.78 | 5 (22%) |
| 3 | PSU | L3 | 3851 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 3 | OMC | L3 | 2422 | 3,55 | 19,22,23 | 0.57 | 0 | 26,31,34 | 0.69 | 0 |
| 3 | OMG | L3 | 2424 | 3 | 18,26,27 | 1.21 | 2 (11%) | 19,38,41 | 0.80 | 1 (5%) |
| 3 | PSU | L3 | 4532 | 3 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.85 | 5 (22%) |
| 3 | OMG | L3 | 4392 | 3 | 18,26,27 | 1.21 | 2 (11%) | 19,38,41 | 0.87 | 1 (5%) |
| 3 | PSU | L3 | 4361 | 3 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.85 | 4 (18%) |
| 3 | PSU | L3 | 1683 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.89 | 5 (22%) |
| 3 | PSU | L3 | 4471 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.83 | 5 (22%) |
| 3 | PSU | L3 | 1677 | 3 | 18,21,22 | 0.98 | 1 (5%) | 22,30,33 | 1.76 | 4 (18%) |
| 3 | OMG | L3 | 2876 | 3 | 18,26,27 | 1.16 | 2 (11%) | 19,38,41 | 0.80 | 1 (5%) |
| 3 | PSU | L3 | 4353 | 3 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.90 | 5 (22%) |
| 3 | PSU | L3 | 4293 | 3 | 18,21,22 | 0.99 | 1 (5%) | 22,30,33 | 1.66 | 4 (18%) |
| 3 | OMG | L3 | 1316 | 3 | 18,26,27 | 1.21 | 3 (16%) | 19,38,41 | 0.89 | 1 (5%) |
| 3 | PSU | L3 | 4493 | 3 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 3 | PSU | L3 | 4403 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.81 | 6 (27%) |
| 3 | A2M | L3 | 1871 | 3 | 18,25,26 | 1.19 | 2 (11%) | 18,36,39 | 1.42 | 2 (11%) |
| 3 | PSU | L3 | 5001 | 3 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.72 | 4 (18%) |
| 3 | A2M | L3 | 398 | 3 | 18,25,26 | 1.21 | 2 (11%) | 18,36,39 | 1.33 | 2 (11%) |
| 3 | PSU | L3 | 4312 | 3 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.83 | 4 (18%) |
| 3 | OMC | L3 | 4536 | 3 | 19,22,23 | 0.59 | 0 | 26,31,34 | 0.67 | 0 |
| 3 | PSU | L3 | 1582 | 3 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.86 | 4 (18%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | PSU | L3 | 3730 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4500 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 2787 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | OMC | L3 | 2351 | 3,55 | - | 4/9/27/28 | 0/2/2/2 |
| 3 | PSU | L3 | 3853 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 1534 | 3,55 | - | 2/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | 6MZ | L3 | 4220 | 3 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 1862 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 3718 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMU | L3 | 4620 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | L1 | 75 | 2 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMC | L3 | 2804 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMU | L3 | 2837 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 23 | HIC | LN | 245 | 23 | - | 2/5/6/8 | 0/1/1/1 |
| 3 | A2M | L3 | 2815 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 2508 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 3920 | 3,55 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4299 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 2363 | 3,55 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMC | L3 | 2824 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | A2M | L3 | 3825 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4579 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 3899 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | A2M | L3 | 3867 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4552 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 3724 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 3695 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4457 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 1524 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMC | L3 | 3887 | 3 | - | 2/9/27/28 | 0/2/2/2 |
| 2 | PSU | L1 | 55 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 4590 | 3 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4296 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 3627 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | A2M | L3 | 400 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 5010 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 1860 | 3 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | PSU | L1 | 69 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 3734 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 4523 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 3715 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L3 | 4456 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMG | L3 | 4499 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 3822 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4972 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L3 | 1340 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | L3 | 4689 | 3 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | PSU | L3 | 4673 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMU | L3 | 2415 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMC | L3 | 3841 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | OMC | L3 | 2365 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L3 | 2839 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 2364 | 3 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | OMG | L3 | 4618 | 3 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | 1MA | L3 | 1322 | 3 | - | 0/3/25/26 | 0/3/3/3 |
| 3 | OMC | L3 | 3869 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | OMC | L3 | 2861 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | A2M | L3 | 4571 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 3844 | 3 | - | 1/7/25/26 | 0/2/2/2 |
| 39 | PTR | NR | 127 | 39 | - | 1/10/11/13 | 0/1/1/1 |
| 3 | OMG | L3 | 4623 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | UR3 | L3 | 4530 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 1522 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMU | L3 | 4306 | 3 | - | 4/9/27/28 | 0/2/2/2 |
| 3 | PSU | L3 | 3639 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L3 | 3701 | 3 | - | 7/9/27/28 | 0/2/2/2 |
| 3 | OMU | L3 | 4498 | 3 | - | 2/9/27/28 | 0/2/2/2 |
| 3 | OMG | L3 | 4228 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 3884 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMU | L3 | 4227 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | L3 | 4628 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 3830 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 1536 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 2401 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | A2M | L3 | 1326 | 3 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | OMG | L3 | 4370 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMG | L3 | 1625 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 2632 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 3637 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4431 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMU | L3 | 3925 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | OMG | L3 | 4494 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMG | L3 | 3744 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4576 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 4637 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4521 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4636 | 3 | - | 4/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | PSU | L3 | 1792 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 3851 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L3 | 2422 | 3,55 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | OMG | L3 | 2424 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4532 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 4392 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4361 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 1683 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4471 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 1677 | 3 | - | 4/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 2876 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4353 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4293 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L3 | 1316 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4493 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L3 | 4403 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 1871 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 5001 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L3 | 398 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L3 | 4312 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L3 | 4536 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L3 | 1582 | 3 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 185 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | L3 | 4498 | OMU | C6-N1 | 4.85 | 1.49 | 1.38 |
| 3 | L3 | 2415 | OMU | C6-N1 | 4.64 | 1.49 | 1.38 |
| 3 | L3 | 2837 | OMU | C6-N1 | 4.64 | 1.49 | 1.38 |
| 3 | L3 | 4306 | OMU | C6-N1 | 4.62 | 1.49 | 1.38 |
| 3 | L3 | 4620 | OMU | C6-N1 | 4.55 | 1.49 | 1.38 |

The worst 5 of 316 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | L3 | 3925 | OMU | C4-N3-C2 | -5.33 | 119.55 | 126.58 |
| 3 | L3 | 4227 | OMU | C4-N3-C2 | -5.27 | 119.63 | 126.58 |
| 3 | L3 | 4306 | OMU | C4-N3-C2 | -5.22 | 119.69 | 126.58 |
| 3 | L3 | 2837 | OMU | C4-N3-C2 | -5.21 | 119.70 | 126.58 |
| 3 | L3 | 4220 | 6MZ | C2-N1-C6 | 5.18 | 121.03 | 116.59 |

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | L1 | 75 | OMG | C1'-C2'-O2'-CM2 |
| 3 | L3 | 398 | A2M | C1'-C2'-O2'-CM' |
| 3 | L3 | 1316 | OMG | C1'-C2'-O2'-CM2 |
| 3 | L3 | 1326 | A2M | O4'-C4'-C5'-O5' |
| 3 | L3 | 1326 | A2M | C3'-C4'-C5'-O5' |

There are no ring outliers.

57 monomers are involved in 78 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | L3 | 4500 | PSU | 1 | 0 |
| 3 | L3 | 2351 | OMC | 2 | 0 |
| 3 | L3 | 1534 | A2M | 3 | 0 |
| 3 | L3 | 4220 | 6MZ | 3 | 0 |
| 3 | L3 | 3718 | A2M | 2 | 0 |
| 3 | L3 | 4620 | OMU | 1 | 0 |
| 2 | L1 | 75 | OMG | 2 | 0 |
| 3 | L3 | 2837 | OMU | 1 | 0 |
| 3 | L3 | 2815 | A2M | 1 | 0 |
| 3 | L3 | 3920 | PSU | 1 | 0 |
| 3 | L3 | 2363 | A2M | 3 | 0 |
| 3 | L3 | 2824 | OMC | 1 | 0 |
| 3 | L3 | 3899 | OMG | 1 | 0 |
| 3 | L3 | 3867 | A2M | 1 | 0 |
| 3 | L3 | 3724 | A2M | 2 | 0 |
| 3 | L3 | 4457 | PSU | 1 | 0 |
| 3 | L3 | 1524 | A2M | 1 | 0 |
| 3 | L3 | 3887 | OMC | 1 | 0 |
| 3 | L3 | 4296 | PSU | 1 | 0 |
| 3 | L3 | 400 | A2M | 2 | 0 |
| 2 | L1 | 69 | PSU | 2 | 0 |
| 3 | L3 | 3734 | PSU | 1 | 0 |
| 3 | L3 | 3715 | PSU | 1 | 0 |
| 3 | L3 | 1340 | OMC | 1 | 0 |
| 3 | L3 | 2415 | OMU | 1 | 0 |
| 3 | L3 | 3841 | OMC | 1 | 0 |
| 3 | L3 | 2364 | OMG | 1 | 0 |
| 3 | L3 | 4618 | OMG | 1 | 0 |
| 3 | L3 | 1322 | 1MA | 4 | 0 |
| 3 | L3 | 3869 | OMC | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | L3 | 2861 | OMC | 1 | 0 |
| 3 | L3 | 4571 | A2M | 1 | 0 |
| 3 | L3 | 4623 | OMG | 1 | 0 |
| 3 | L3 | 1522 | OMG | 1 | 0 |
| 3 | L3 | 4306 | OMU | 3 | 0 |
| 3 | L3 | 3701 | OMC | 1 | 0 |
| 3 | L3 | 4498 | OMU | 1 | 0 |
| 3 | L3 | 4227 | OMU | 1 | 0 |
| 3 | L3 | 3830 | A2M | 1 | 0 |
| 3 | L3 | 1326 | A2M | 2 | 0 |
| 3 | L3 | 2632 | PSU | 1 | 0 |
| 3 | L3 | 3925 | OMU | 1 | 0 |
| 3 | L3 | 4494 | OMG | 1 | 0 |
| 3 | L3 | 3744 | OMG | 1 | 0 |
| 3 | L3 | 4637 | OMG | 1 | 0 |
| 3 | L3 | 4636 | PSU | 1 | 0 |
| 3 | L3 | 2424 | OMG | 1 | 0 |
| 3 | L3 | 4392 | OMG | 1 | 0 |
| 3 | L3 | 4361 | PSU | 1 | 0 |
| 3 | L3 | 1683 | PSU | 1 | 0 |
| 3 | L3 | 4471 | PSU | 1 | 0 |
| 3 | L3 | 1677 | PSU | 3 | 0 |
| 3 | L3 | 2876 | OMG | 2 | 0 |
| 3 | L3 | 5001 | PSU | 1 | 0 |
| 3 | L3 | 398 | A2M | 2 | 0 |
| 3 | L3 | 4312 | PSU | 1 | 0 |
| 3 | L3 | 4536 | OMC | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 96 ligands modelled in this entry, 95 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 57 | GDP | SR | 1001 | 55,58 | 24,30,30 | 2.55 | 7 (29%) | 30,47,47 | 1.76 | 9 (30%) |

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 |
|---|---|---|---|---|---|---|---|
| 57 | GDP | SR | 1001 | 55,58 | - | 0/12/32/32 | 0/3/3/3 |

The worst 5 of 7 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 57 | SR | 1001 | GDP | O6-C6 | 8.33 | 1.40 | 1.23 |
| 57 | SR | 1001 | GDP | C2-N2 | 4.76 | 1.45 | 1.34 |
| 57 | SR | 1001 | GDP | O4'-C1' | 4.42 | 1.47 | 1.41 |
| 57 | SR | 1001 | GDP | C5-C4 | 2.40 | 1.49 | 1.43 |
| 57 | SR | 1001 | GDP | PB-O2B | -2.27 | 1.46 | 1.54 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | SR | 1001 | GDP | C3'-C2'-C1' | 4.21 | 107.31 | 100.98 |
| 57 | SR | 1001 | GDP | C5-C6-N1 | 3.36 | 119.88 | 113.95 |
| 57 | SR | 1001 | GDP | O2B-PB-O3A | 2.96 | 114.56 | 104.64 |
| 57 | SR | 1001 | GDP | C2-N1-C6 | -2.93 | 119.71 | 125.10 |
| 57 | SR | 1001 | GDP | O3B-PB-O3A | 2.81 | 114.05 | 104.64 |

There are no chirality outliers.

There are no torsion outliers.

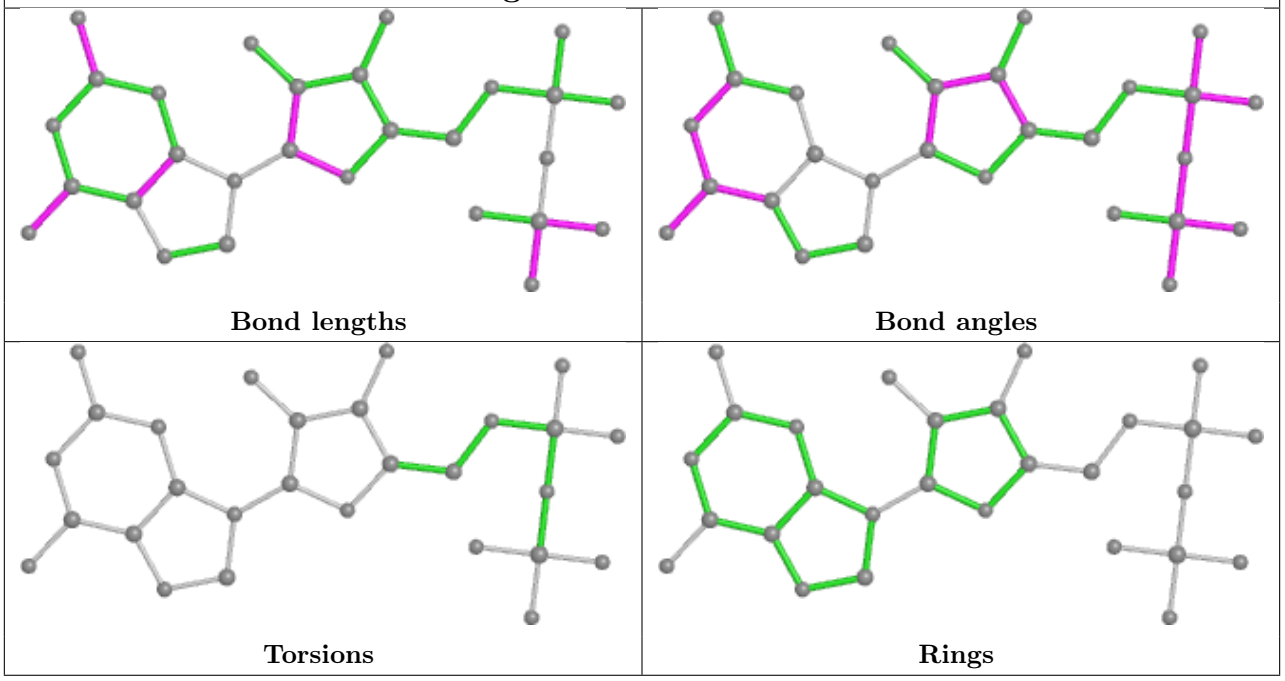
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

**Ligand GDP SR 1001**




## 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.

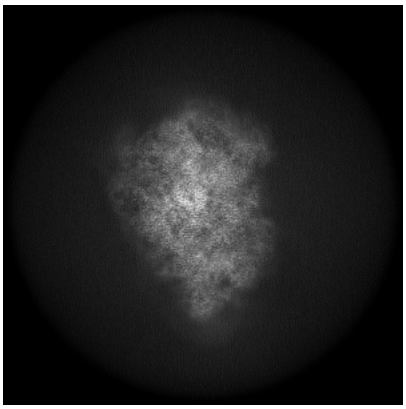
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29273. These allow visual inspection of the internal detail of the map and identification of artifacts.

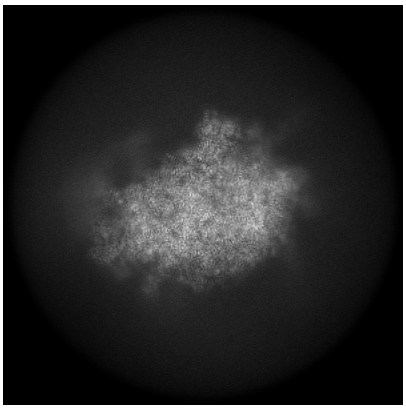
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

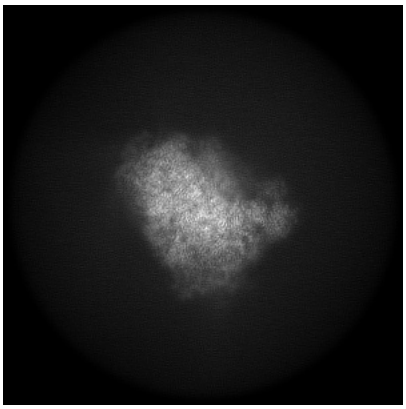
### 6.1.1 Primary map



X

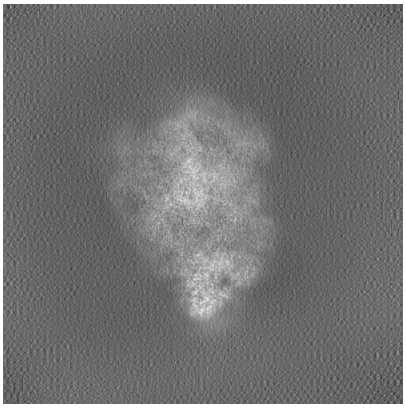


Y

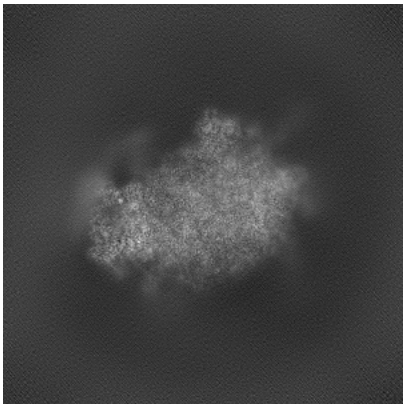


Z

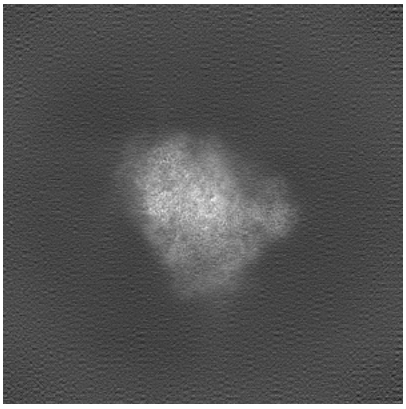
### 6.1.2 Raw map



X



Y

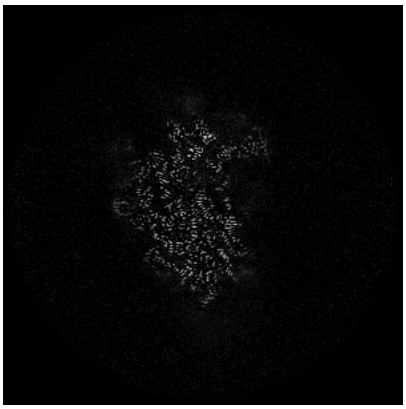


Z

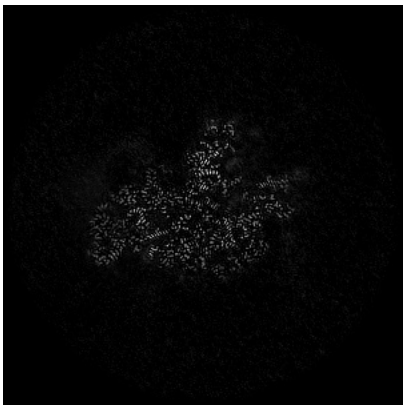
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

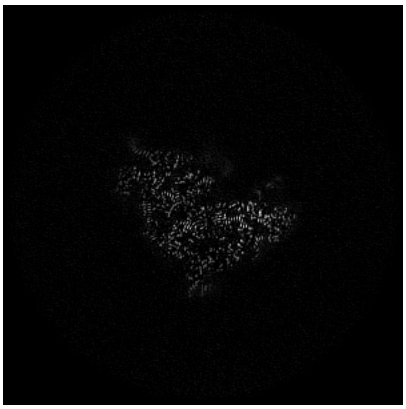
### 6.2.1 Primary map



X Index: 240

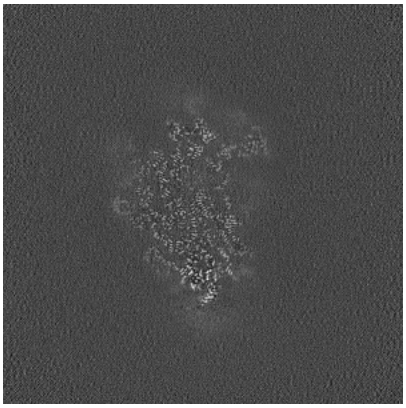


Y Index: 240

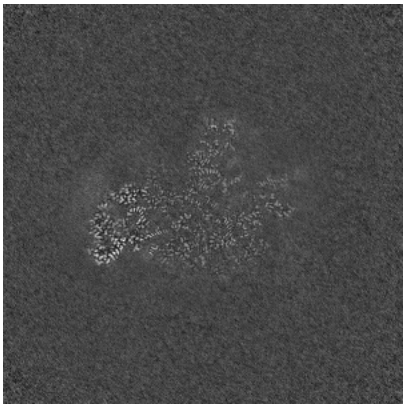


Z Index: 240

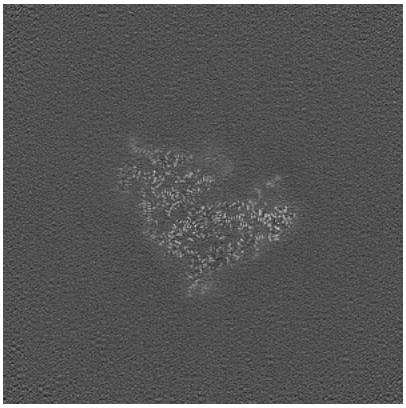
### 6.2.2 Raw map



X Index: 240



Y Index: 240

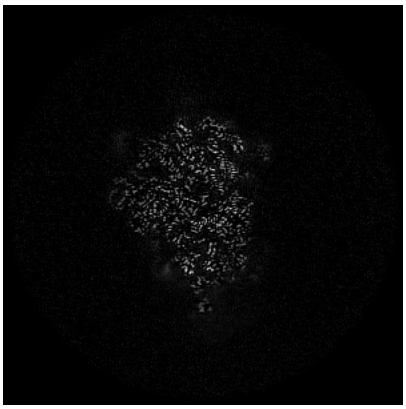


Z Index: 240

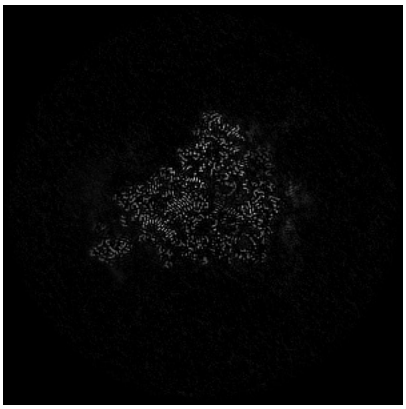
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

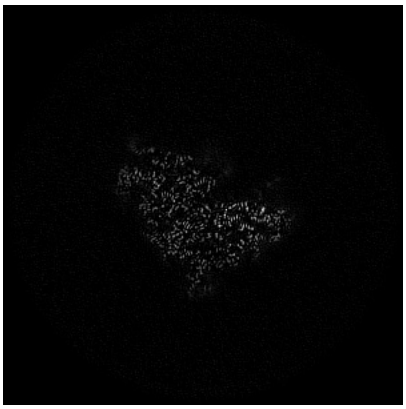
### 6.3.1 Primary map



X Index: 226

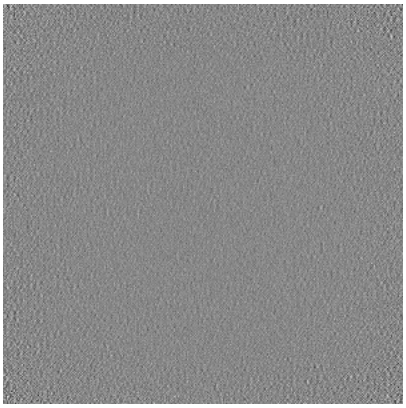


Y Index: 227

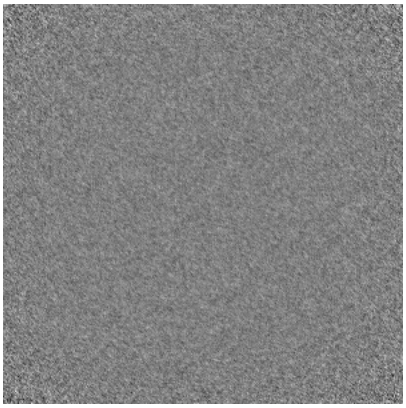


Z Index: 239

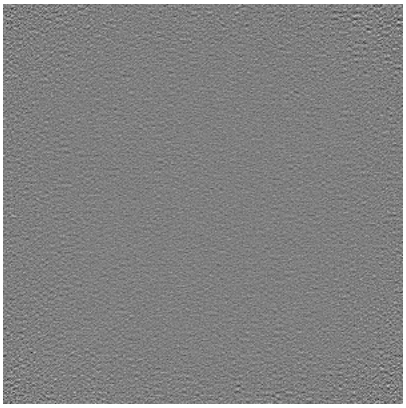
### 6.3.2 Raw map



X Index: 0



Y Index: 0

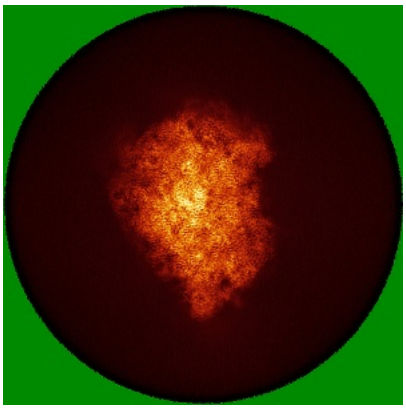


Z Index: 0

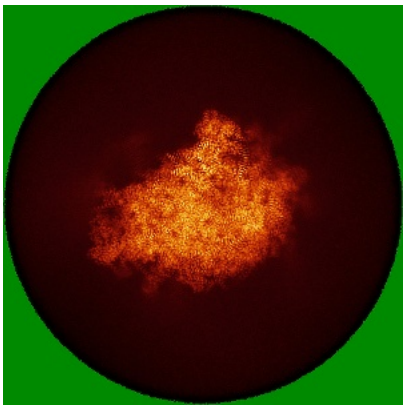
The images above show the largest variance slices of the map in three orthogonal directions.

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

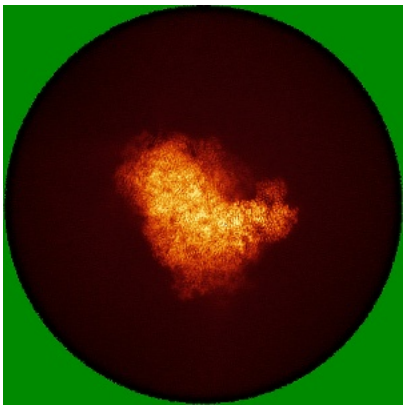
### 6.4.1 Primary map



X

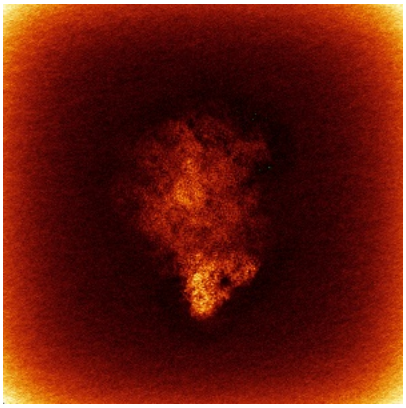


Y

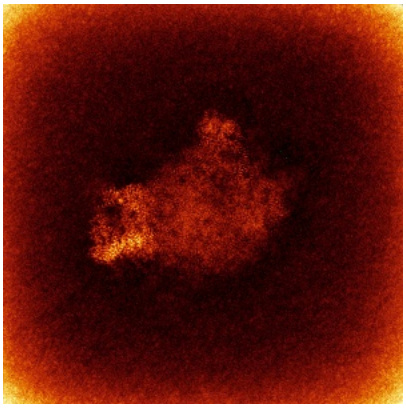


Z

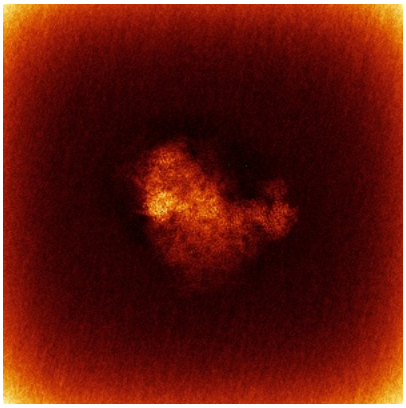
### 6.4.2 Raw map



X



Y



Z

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

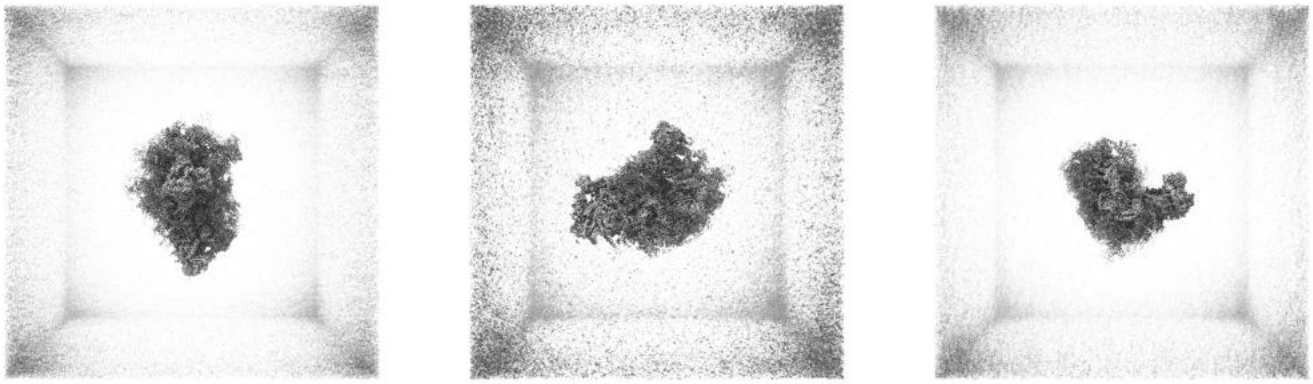
## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

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

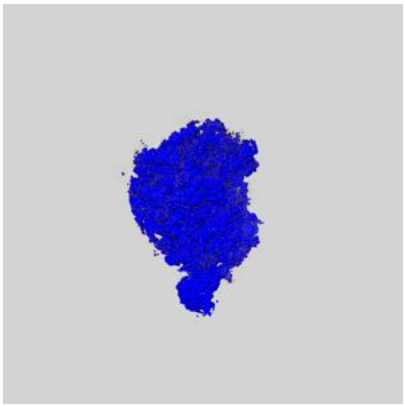
## 6.6 Mask visualisation

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

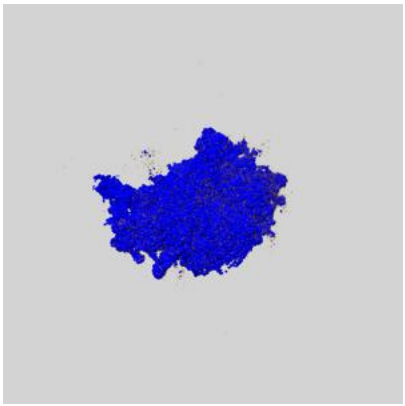
A mask typically either:

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

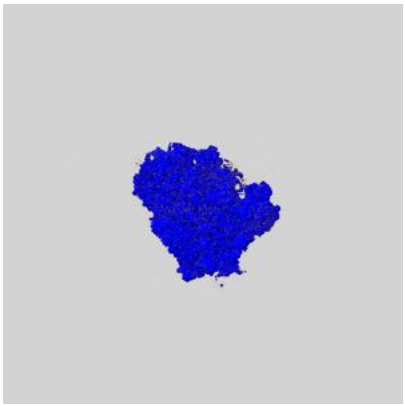
### 6.6.1 emd_29273_msk_1.map



X



Y

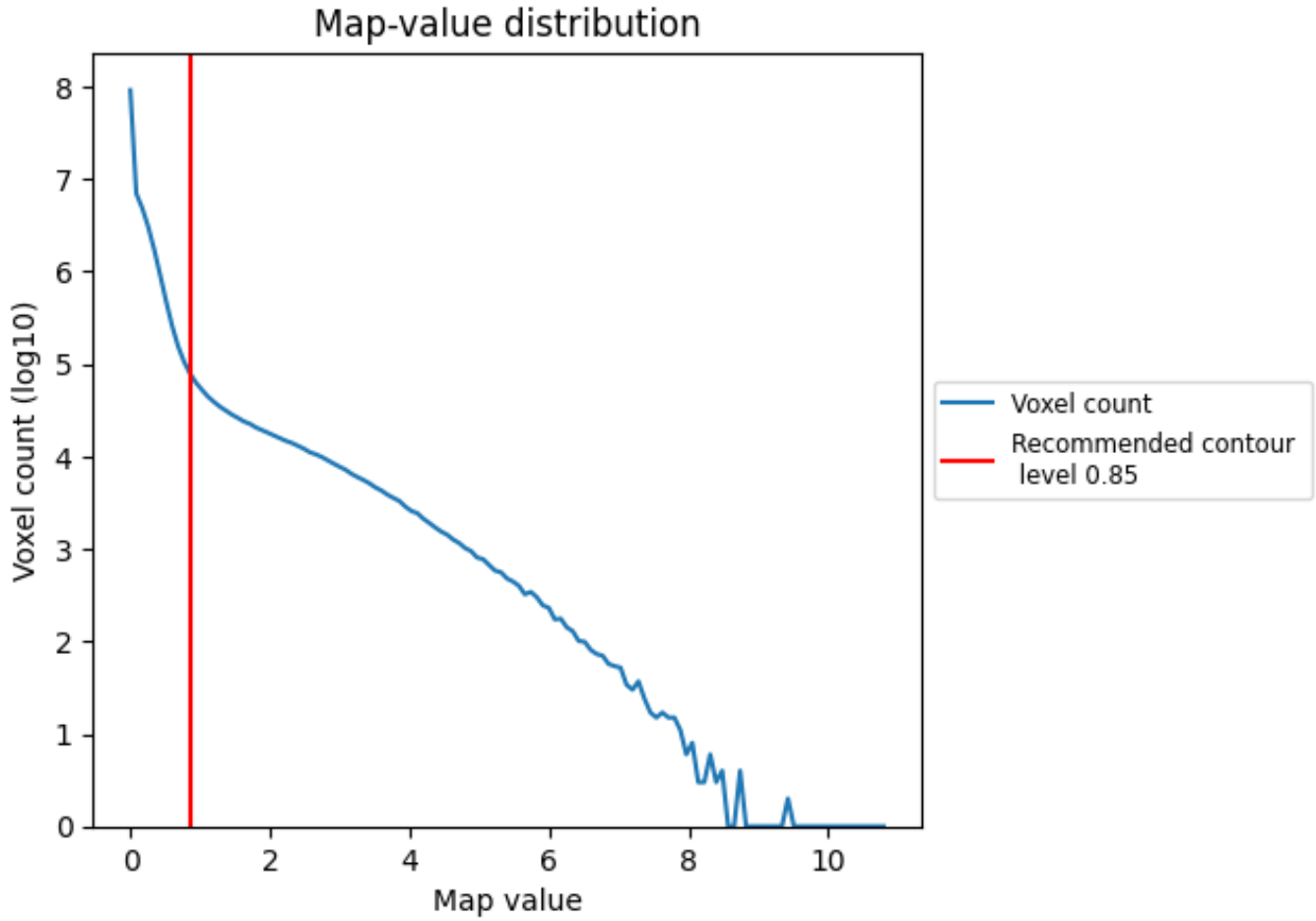


Z

# 7 Map analysis

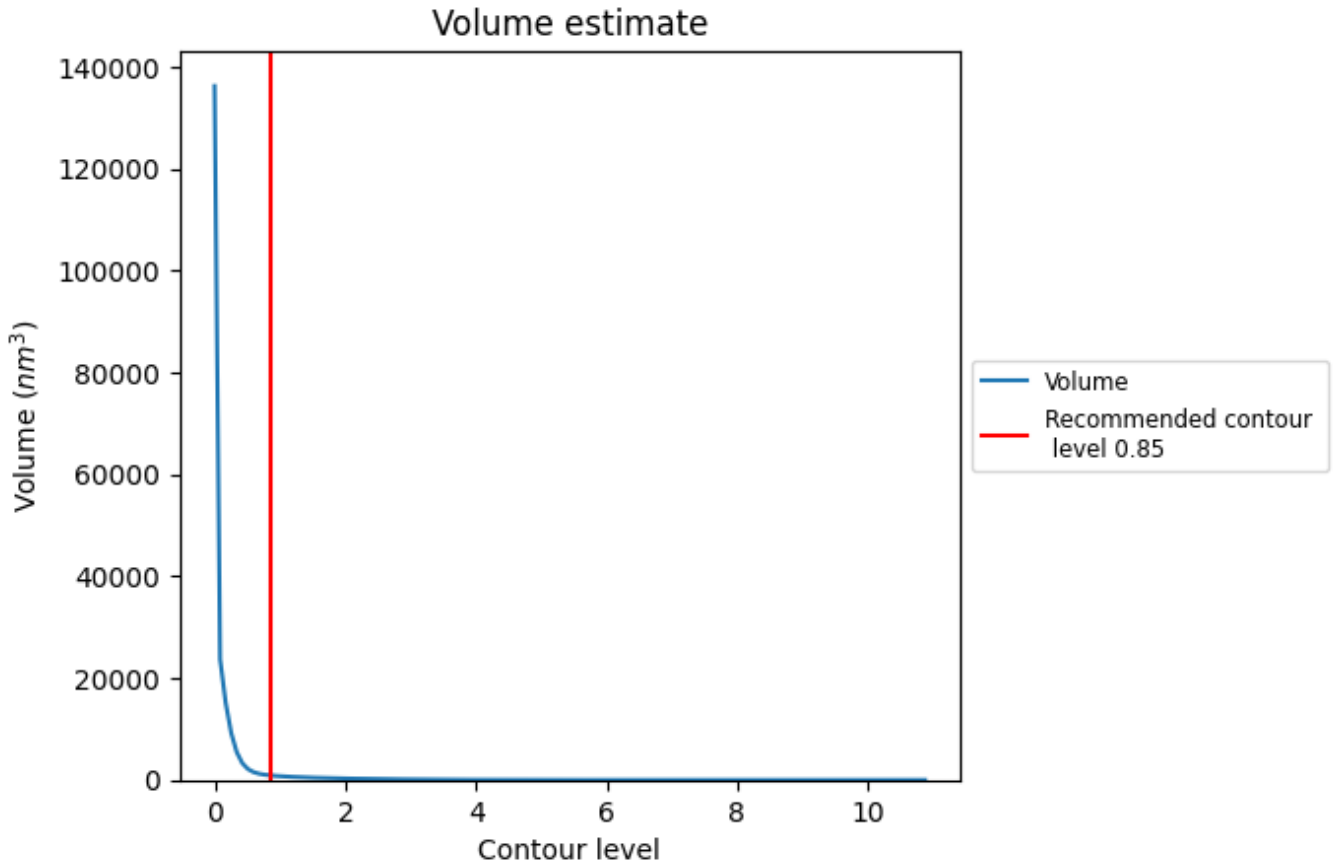
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

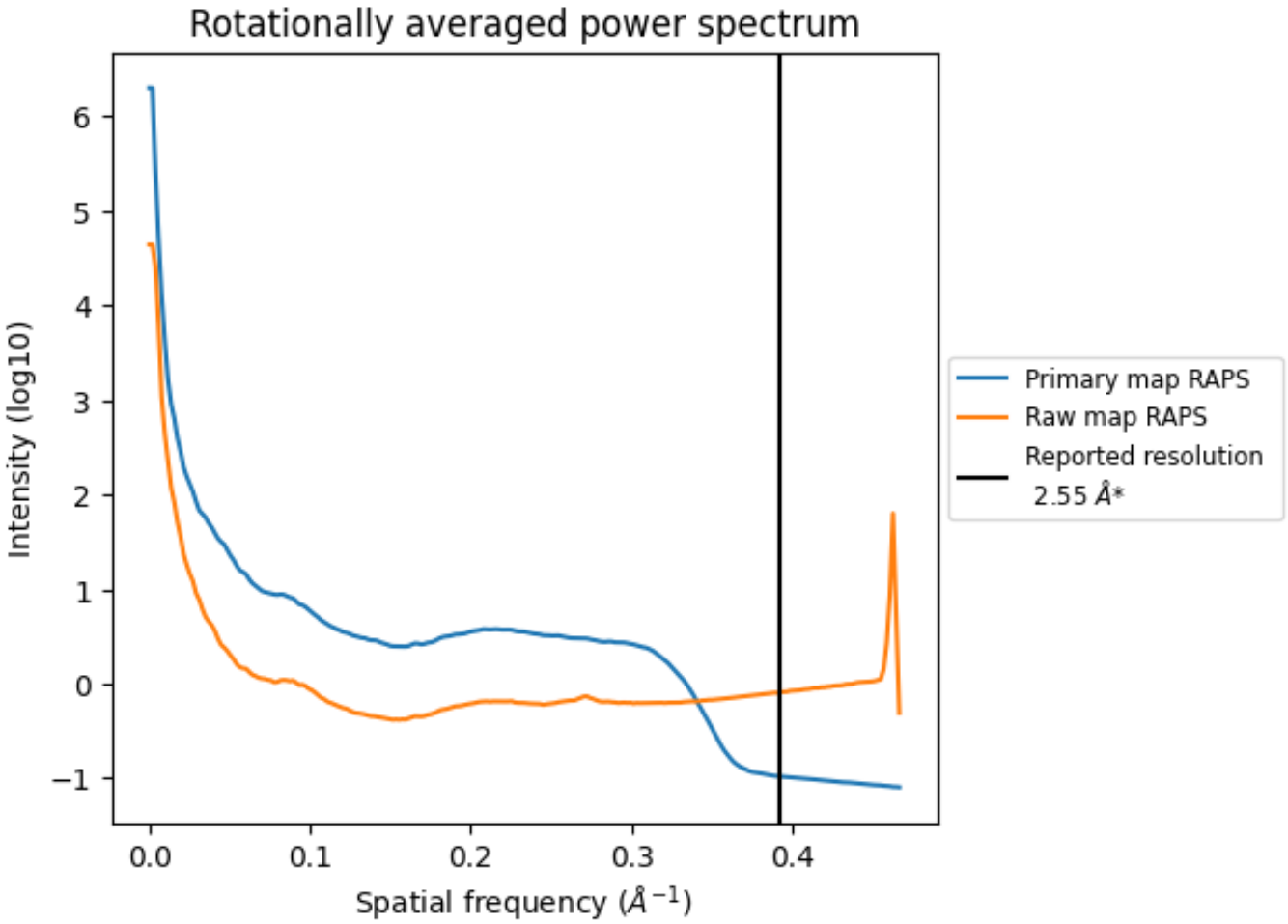
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 895 $nm^3$; this corresponds to an approximate mass of 809 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)

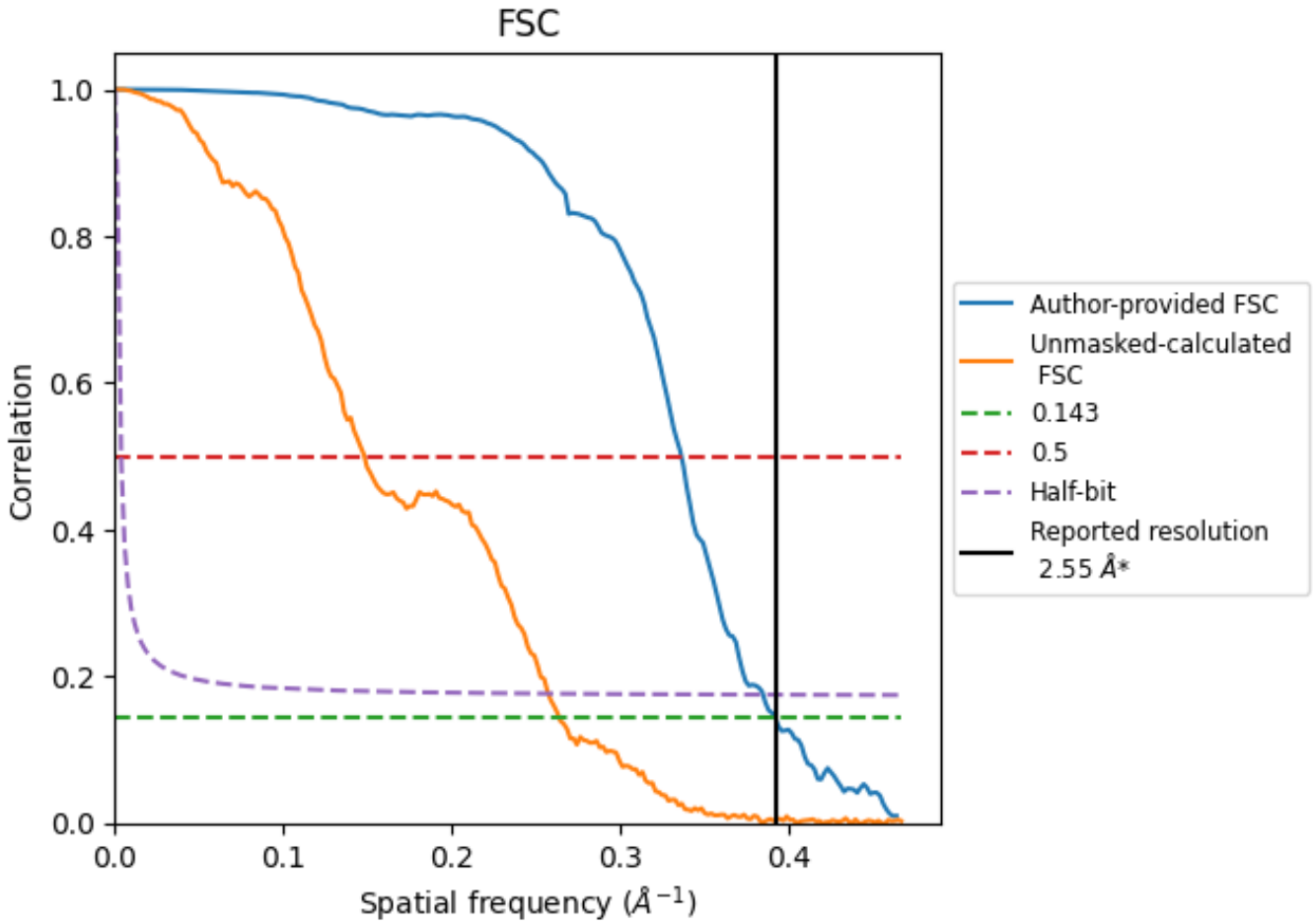



*Reported resolution corresponds to spatial frequency of 0.392 $Å^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.392 Å$^{-1}$

## 8.2 Resolution estimates (i)

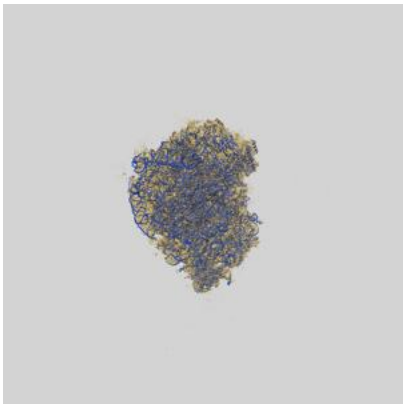
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.55 | - | - |
| Author-provided FSC curve | 2.55 | 2.98 | 2.60 |
| Unmasked-calculated* | 3.79 | 6.76 | 3.89 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.55 by more than 10 %

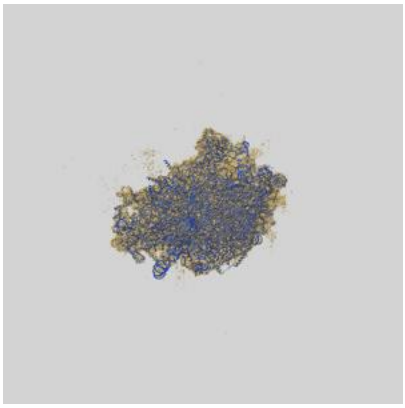
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29273 and PDB model 8FLB. Per-residue inclusion information can be found in section 3 on page 15.

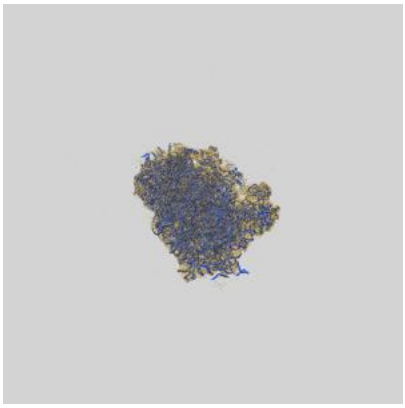
## 9.1 Map-model overlay



X



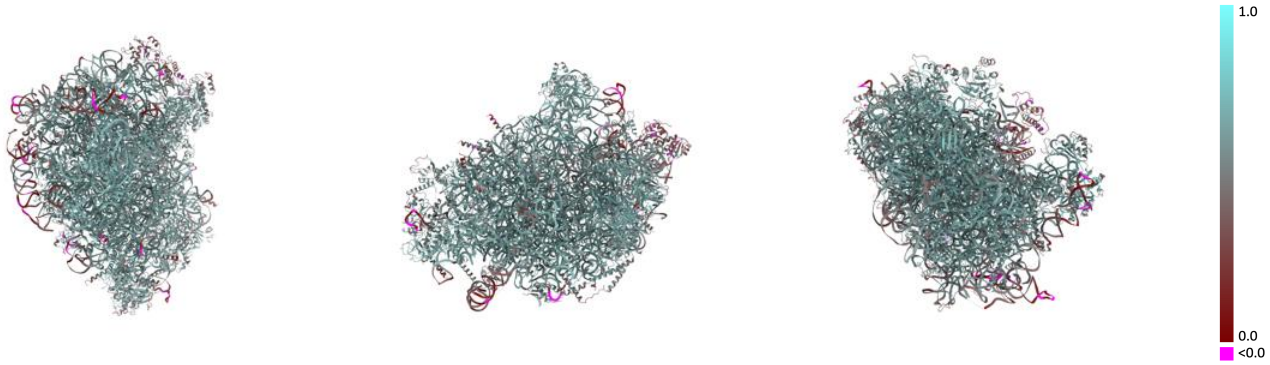
Y



Z

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

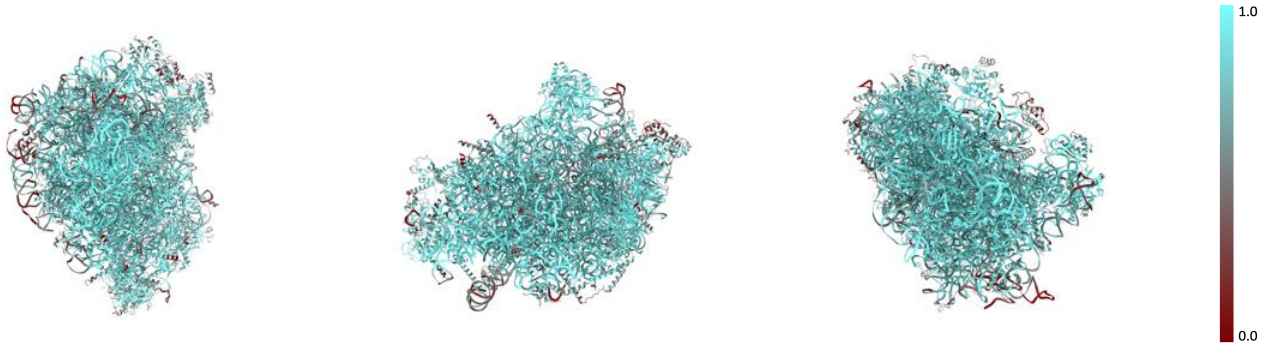
## 9.2 Q-score mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according 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.

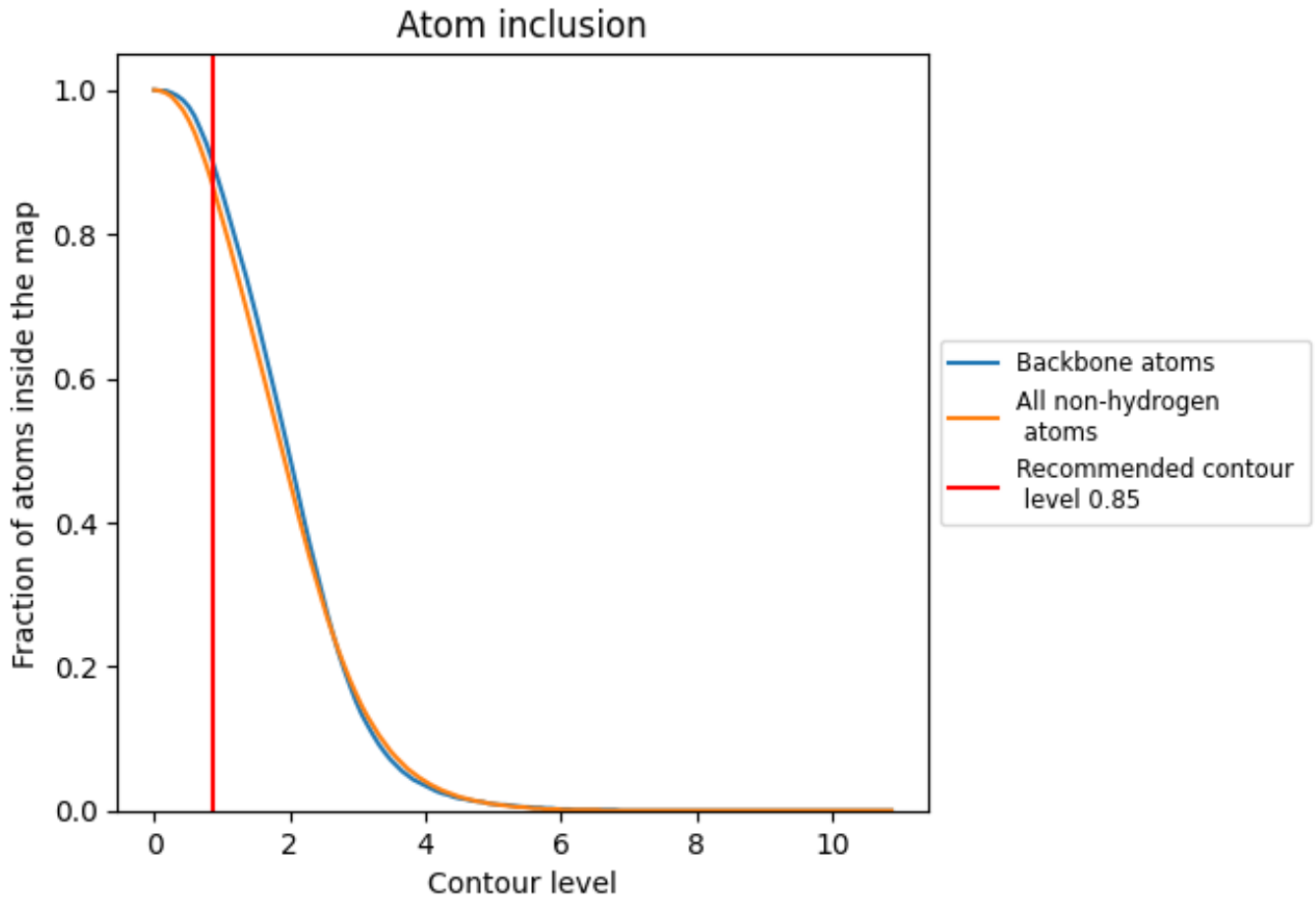
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).

## 9.4 Atom inclusion (i)




At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8710 | 0.5870 |
| BA | 0.3030 | 0.2780 |
| L1 | 0.9500 | 0.6260 |
| L3 | 0.8850 | 0.5750 |
| L4 | 0.9790 | 0.6330 |
| L5 | 0.8200 | 0.5590 |
| L6 | 0.8020 | 0.5790 |
| L7 | 0.9030 | 0.6290 |
| L8 | 0.8980 | 0.6220 |
| L9 | 0.9670 | 0.6580 |
| LA | 0.8850 | 0.6160 |
| LB | 0.9200 | 0.6320 |
| LC | 0.9630 | 0.6630 |
| LD | 0.8400 | 0.6000 |
| LE | 0.8890 | 0.6040 |
| LF | 0.7830 | 0.5740 |
| LG | 0.9050 | 0.6230 |
| LH | 0.8680 | 0.6240 |
| LI | 0.8510 | 0.5950 |
| LJ | 0.9210 | 0.6290 |
| LK | 0.9230 | 0.6380 |
| LL | 0.8790 | 0.6050 |
| LM | 0.7290 | 0.5260 |
| LN | 0.8920 | 0.6210 |
| LO | 0.8040 | 0.5850 |
| LP | 0.8400 | 0.6000 |
| LQ | 0.8940 | 0.6210 |
| LR | 0.9180 | 0.6230 |
| LS | 0.8590 | 0.6110 |
| LT | 0.9410 | 0.6420 |
| LU | 0.7890 | 0.5700 |
| LV | 0.8900 | 0.6120 |
| LW | 0.9420 | 0.6400 |
| LX | 0.8070 | 0.5880 |
| LY | 0.7380 | 0.5760 |


*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| LZ | 0.9410 | 0.6340 |
| NK | 0.6580 | 0.5250 |
| NL | 0.8070 | 0.5740 |
| NP | 0.8310 | 0.5860 |
| NR | 0.7370 | 0.5450 |
| SA | 0.8940 | 0.6190 |
| SB | 0.8880 | 0.6060 |
| SC | 0.7640 | 0.5620 |
| SD | 0.8830 | 0.6170 |
| SE | 0.8610 | 0.5990 |
| SF | 0.9230 | 0.6360 |
| SG | 0.9000 | 0.6130 |
| SH | 0.6820 | 0.5050 |
| SI | 0.7270 | 0.5360 |
| SK | 0.8420 | 0.5870 |
| SM | 0.9010 | 0.6190 |
| SQ | 0.6030 | 0.3730 |
| SR | 0.7780 | 0.5580 |
| SV | 0.8330 | 0.5850 |
| VB | 0.6450 | 0.5280 |