



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2023 – 03:12 PM EST

PDB ID : 8G5Y
EMDB ID : EMD-29757
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (IC state)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-02-14
Resolution : 2.29 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:

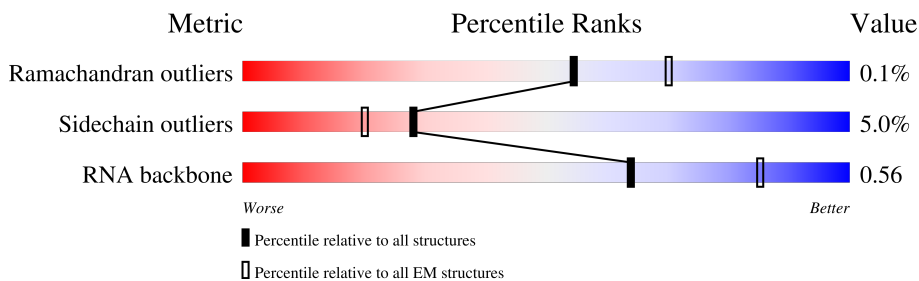
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.29 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.



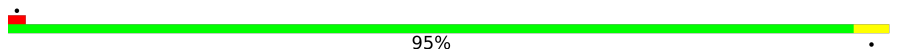



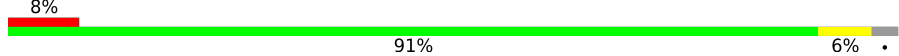
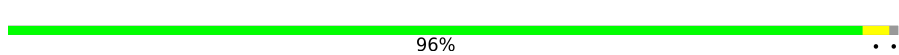
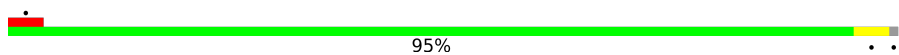
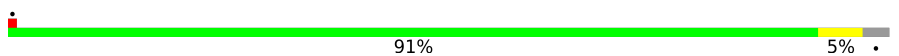



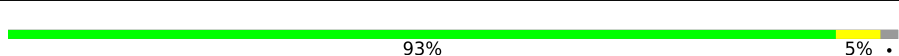
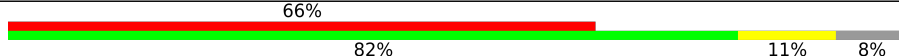
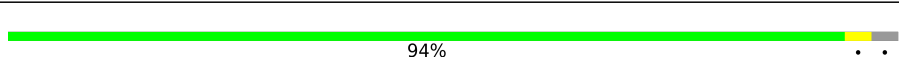
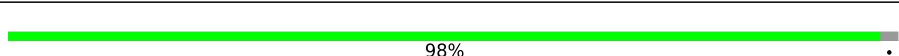
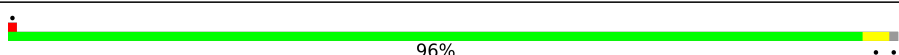
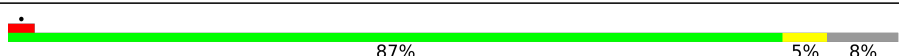
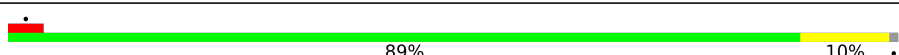
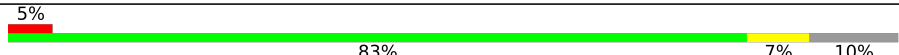
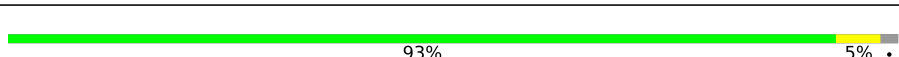
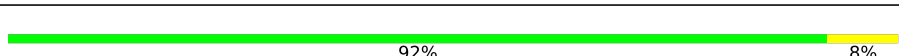
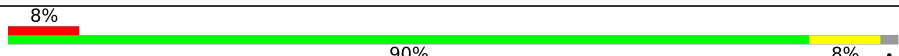


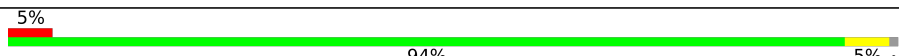
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | S2 | 1869 | |
| 2 | L8 | 156 | |
| 3 | L5 | 5069 | |
| 4 | L7 | 120 | |
| 5 | SB | 264 | |
| 6 | SA | 295 | |
| 7 | SD | 243 | |
| 8 | SJ | 194 | |

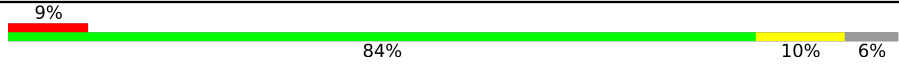




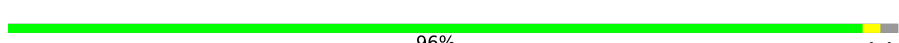
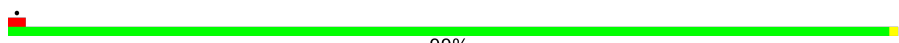

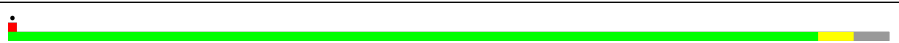

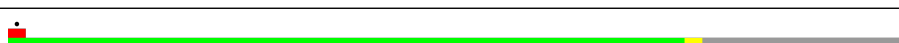


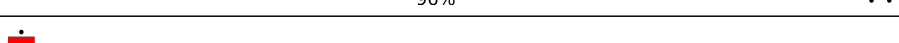
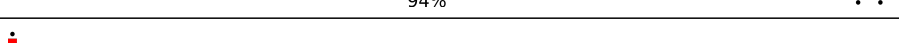
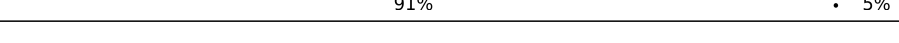
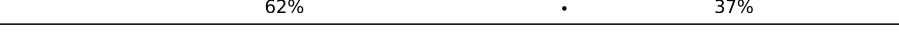
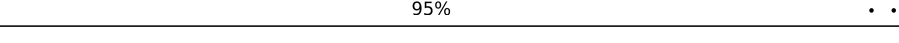
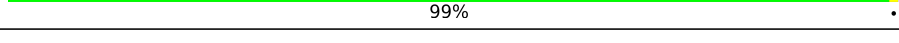
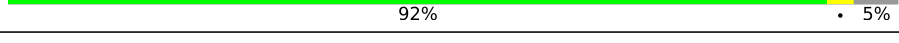
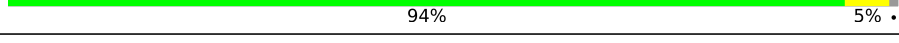
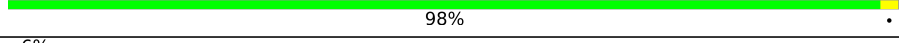
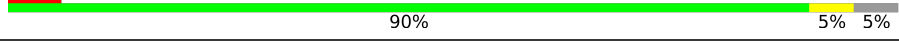
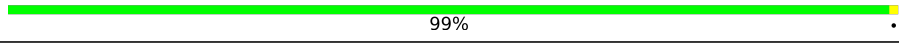
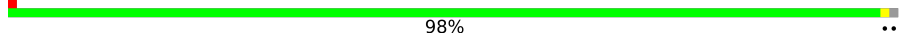
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 9 | SE | 263 |  95% |
| 10 | SC | 293 |  71% 5% 24% |
| 11 | SG | 249 |  89% 6% 5% 8% |
| 12 | SF | 204 |  89% 7% |
| 13 | SH | 194 |  91% 6% |
| 14 | SW | 130 |  96% |
| 15 | SI | 208 |  95% |
| 16 | SQ | 146 |  91% 5% |
| 17 | SU | 119 |  78% 7% 15% 10% |
| 18 | SK | 165 |  55% 42% |
| 19 | SO | 151 |  87% 11% |
| 20 | SX | 143 |  93% 5% |
| 21 | SM | 132 |  82% 11% 8% 66% |
| 22 | SS | 152 |  94% |
| 23 | Sd | 56 |  98% |
| 24 | SN | 151 |  96% |
| 25 | SL | 158 |  87% 5% 8% |
| 26 | SR | 135 |  89% 10% |
| 27 | SP | 145 |  83% 7% 10% 5% |
| 28 | ST | 145 |  93% 5% |
| 29 | SV | 83 |  92% 8% |
| 30 | SY | 133 |  90% 8% |
| 31 | SZ | 125 |  64% 33% |
| 32 | Sa | 115 |  85% 14% |
| 33 | Sb | 84 |  94% 5% |





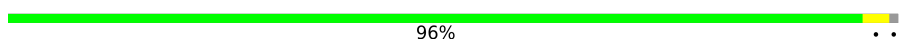

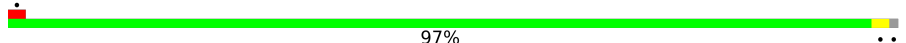



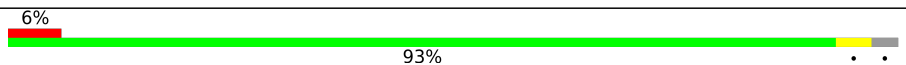
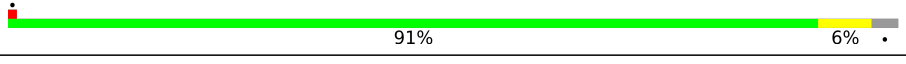




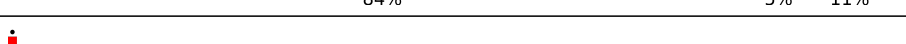
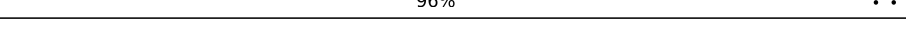
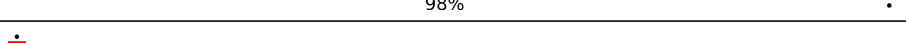

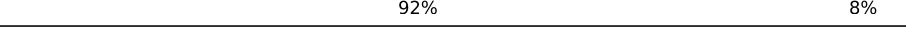
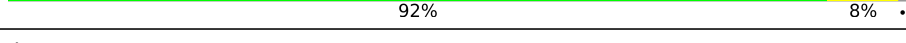
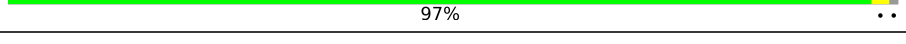
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 34 | Sc | 69 |  |
| 35 | Se | 133 |  |
| 36 | Sf | 156 |  |
| 37 | Sg | 317 |  |
| 38 | Lz | 217 |  |
| 39 | LA | 257 |  |
| 40 | LB | 403 |  |
| 41 | LC | 427 |  |
| 42 | LJ | 178 |  |
| 43 | LH | 192 |  |
| 44 | LE | 288 |  |
| 45 | LG | 266 |  |
| 46 | LO | 203 |  |
| 47 | LL | 211 |  |
| 48 | LV | 140 |  |
| 49 | LM | 215 |  |
| 50 | La | 148 |  |
| 51 | LN | 204 |  |
| 52 | LI | 214 |  |
| 53 | LD | 297 |  |
| 54 | LQ | 188 |  |
| 55 | LR | 196 |  |
| 56 | LS | 176 |  |
| 57 | LT | 160 |  |
| 58 | LP | 184 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 59 | LU | 128 |  |
| 60 | LX | 156 |  |
| 61 | LY | 145 |  |
| 62 | LW | 157 |  |
| 63 | LZ | 136 |  |
| 64 | Lr | 137 |  |
| 65 | Lh | 123 |  |
| 66 | Lb | 159 |  |
| 67 | LF | 248 |  |
| 68 | Lc | 115 |  |
| 69 | Ld | 125 |  |
| 70 | Le | 135 |  |
| 71 | Lf | 110 |  |
| 72 | Lg | 117 |  |
| 73 | Li | 105 |  |
| 74 | Lj | 97 |  |
| 75 | Lk | 70 |  |
| 76 | Ll | 51 |  |
| 77 | Lm | 128 |  |
| 78 | Ln | 25 |  |
| 79 | Lo | 106 |  |
| 80 | Lp | 92 |  |
| 81 | mR | 60 |  |
| 82 | Pt | 77 | |
| 83 | 5A | 154 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 6 | SAC | SA | 2 | - | X | - | - |
| 64 | SAC | Lr | 2 | - | X | - | - |

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 219823 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 1 | S2 | 1680 | 35800 | 16005 | 6403 | 11713 | 1679 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| | | | Total | C | N | O | P | | |
| 2 | L8 | 156 | 3316 | 1482 | 585 | 1094 | 155 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 3 | L5 | 3721 | 79154 | 35258 | 14402 | 25772 | 3722 | 2 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | P | | |
| 4 | L7 | 120 | 2558 | 1141 | 456 | 842 | 119 | 0 | 0 |

- Molecule 5 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | SB | 223 | 1806 | 1145 | 325 | 322 | 14 | 0 | 0 |

- Molecule 6 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | SA | 222 | 1750 | 1111 | 306 | 325 | 8 | 0 | 0 |

- Molecule 7 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | SD | 226 | 1756 | 1119 | 315 | 314 | 8 | 0 | 0 |

- Molecule 8 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | SJ | 185 | 1525 | 969 | 306 | 248 | 2 | 0 | 0 |

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | SE | 262 | 2076 | 1324 | 386 | 358 | 8 | 0 | 0 |

- Molecule 10 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | SC | 222 | 1725 | 1115 | 298 | 302 | 10 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | SG | 237 | 1923 | 1200 | 387 | 329 | 7 | 0 | 0 |

- Molecule 12 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | SF | 189 | 1494 | 934 | 284 | 269 | 7 | 0 | 0 |

- Molecule 13 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 13 | SH | 189 | 1517 | 966 | 279 | 271 | 1 | 0 | 0 |

- Molecule 14 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | SW | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1034 | 659 | 193 | 176 | 6 | | |

- Molecule 15 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15 | SI | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1686 | 1058 | 332 | 291 | 5 | | |

- Molecule 16 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | SQ | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 715 | 212 | 193 | 3 | | |

- Molecule 17 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | SU | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 803 | 504 | 153 | 142 | 4 | | |

- Molecule 18 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | SK | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 810 | 530 | 143 | 131 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | SO | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1009 | 618 | 198 | 187 | 6 | | |

- Molecule 20 is a protein called uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | SX | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1088 | 687 | 215 | 183 | 3 | | |

- Molecule 21 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 21 | SM | 122 | 950 | 596 | 168 | 177 | 9 | 0 | 0 |

- Molecule 22 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 22 | SS | 148 | 1214 | 761 | 245 | 207 | 1 | 0 | 0 |

- Molecule 23 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 23 | Sd | 55 | 458 | 286 | 94 | 73 | 5 | 0 | 0 |

- Molecule 24 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 24 | SN | 150 | 1214 | 778 | 231 | 204 | 1 | 1 | 0 |

- Molecule 25 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 25 | SL | 146 | 1200 | 766 | 226 | 202 | 6 | 0 | 0 |

- Molecule 26 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 26 | SR | 134 | 1082 | 680 | 201 | 197 | 4 | 0 | 0 |

- Molecule 27 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 27 | SP | 131 | 1078 | 684 | 204 | 183 | 7 | 0 | 0 |

- Molecule 28 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 28 | ST | 142 | 1121 | 707 | 212 | 199 | 3 | 1 | 0 |

- Molecule 29 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 29 | SV | 83 | 639 | 395 | 117 | 122 | 5 | 0 | 0 |

- Molecule 30 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 30 | SY | 131 | 1065 | 673 | 209 | 178 | 5 | 0 | 0 |

- Molecule 31 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 31 | SZ | 84 | 674 | 433 | 126 | 114 | 1 | 0 | 0 |

- Molecule 32 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 32 | Sa | 99 | 800 | 497 | 168 | 130 | 5 | 1 | 0 |

- Molecule 33 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 33 | Sb | 83 | 651 | 408 | 121 | 115 | 7 | 0 | 0 |

- Molecule 34 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 34 | Sc | 65 | 512 | 311 | 103 | 96 | 2 | 0 | 0 |

- Molecule 35 is a protein called FAU ubiquitin-like and ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35 | Se | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 394 | 241 | 88 | 64 | 1 | | |

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 36 | Sf | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 515 | 324 | 98 | 86 | 7 | | |

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37 | Sg | 313 | Total | C | N | O | S | 0 | 0 |
| | | | 2436 | 1535 | 424 | 465 | 12 | | |

- Molecule 38 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38 | Lz | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1695 | 1086 | 304 | 297 | 8 | | |

- Molecule 39 is a protein called uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39 | LA | 251 | Total | C | N | O | S | 1 | 0 |
| | | | 1930 | 1209 | 396 | 319 | 6 | | |

- Molecule 40 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40 | LB | 402 | Total | C | N | O | S | 0 | 0 |
| | | | 3239 | 2061 | 608 | 556 | 14 | | |

- Molecule 41 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41 | LC | 366 | Total | C | N | O | S | 0 | 0 |
| | | | 2914 | 1832 | 581 | 487 | 14 | | |

- Molecule 42 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 42 | LJ | 170 | 1362 | 861 | 254 | 241 | 6 | 0 | 0 |

- Molecule 43 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 43 | LH | 190 | 1518 | 956 | 284 | 272 | 6 | 0 | 0 |

- Molecule 44 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 44 | LE | 223 | 1786 | 1150 | 339 | 293 | 4 | 0 | 0 |

- Molecule 45 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 45 | LG | 241 | 1926 | 1228 | 371 | 323 | 4 | 0 | 0 |

- Molecule 46 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 46 | LO | 199 | 1633 | 1053 | 319 | 256 | 5 | 0 | 0 |

- Molecule 47 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 47 | LL | 206 | 1664 | 1041 | 345 | 274 | 4 | 0 | 0 |

- Molecule 48 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 48 | LV | 133 | 988 | 623 | 186 | 174 | 5 | 0 | 0 |

- Molecule 49 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 49 | LM | 136 | 1120 | 719 | 215 | 179 | 7 | 0 | 0 |

- Molecule 50 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 50 | La | 147 | 1162 | 736 | 237 | 186 | 3 | 0 | 0 |

- Molecule 51 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 51 | LN | 203 | 1700 | 1072 | 359 | 265 | 4 | 0 | 0 |

- Molecule 52 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 52 | LI | 203 | 1645 | 1045 | 317 | 270 | 13 | 0 | 0 |

- Molecule 53 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 53 | LD | 294 | 2391 | 1513 | 436 | 428 | 14 | 0 | 0 |

- Molecule 54 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 54 | LQ | 187 | 1512 | 944 | 314 | 249 | 5 | 0 | 0 |

- Molecule 55 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 55 | LR | 187 | 1566 | 971 | 336 | 250 | 9 | 0 | 0 |

- Molecule 56 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 56 | LS | 176 | 1460 | 930 | 284 | 235 | 11 | 0 | 0 |

- Molecule 57 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 57 | LT | 159 | 1311 | 833 | 256 | 216 | 6 | 2 | 0 |

- Molecule 58 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 58 | LP | 153 | 1248 | 780 | 242 | 217 | 9 | 1 | 0 |

- Molecule 59 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 59 | LU | 99 | 808 | 518 | 141 | 147 | 2 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 60 | LX | 118 | 966 | 618 | 181 | 166 | 1 | 0 | 0 |

- Molecule 61 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 61 | LY | 134 | 1115 | 700 | 226 | 186 | 3 | 0 | 0 |

- Molecule 62 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 62 | LW | 118 | 955 | 599 | 192 | 159 | 5 | 1 | 0 |

- Molecule 63 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 63 | LZ | 135 | 1115 | 719 | 211 | 182 | 3 | 1 | 0 |

- Molecule 64 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 64 | Lr | 125 | 1011 | 629 | 208 | 169 | 5 | 1 | 0 |

- Molecule 65 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 65 | Lh | 122 | 1014 | 641 | 205 | 167 | 1 | 0 | 0 |

- Molecule 66 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 66 | Lb | 111 | 898 | 560 | 195 | 139 | 4 | 0 | 0 |

- Molecule 67 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 67 | LF | 225 | 1869 | 1202 | 358 | 300 | 9 | 0 | 0 |

- Molecule 68 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 68 | Lc | 99 | 770 | 488 | 136 | 140 | 6 | 0 | 0 |

- Molecule 69 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 69 | Ld | 107 | 888 | 560 | 171 | 155 | 2 | 0 | 0 |

- Molecule 70 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 70 | Le | 128 | 1053 | 667 | 216 | 165 | 5 | 0 | 0 |

- Molecule 71 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 71 | Lf | 110 | 883 | 560 | 175 | 144 | 4 | 0 | 0 |

- Molecule 72 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 72 | Lg | 114 | 906 | 566 | 187 | 147 | 6 | 0 | 0 |

- Molecule 73 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 73 | Li | 102 | 832 | 521 | 177 | 129 | 5 | 0 | 0 |

- Molecule 74 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 74 | Lj | 86 | 712 | 439 | 157 | 111 | 5 | 1 | 0 |

- Molecule 75 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 75 | Lk | 69 | 568 | 366 | 103 | 98 | 1 | 0 | 0 |

- Molecule 76 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 76 | Ll | 50 | 443 | 281 | 98 | 63 | 1 | 0 | 0 |

- Molecule 77 is a protein called eL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 77 | Lm | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 431 | 269 | 90 | 66 | 6 | | |

- Molecule 78 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78 | Ln | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 145 | 64 | 27 | 3 | | |

- Molecule 79 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79 | Lo | 105 | Total | C | N | O | S | 2 | 0 |
| | | | 878 | 553 | 180 | 139 | 6 | | |

- Molecule 80 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80 | Lp | 91 | Total | C | N | O | S | 1 | 0 |
| | | | 715 | 450 | 139 | 119 | 7 | | |

- Molecule 81 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 81 | mR | 8 | Total | C | N | O | P | 0 | 0 |
| | | | 172 | 77 | 32 | 55 | 8 | | |

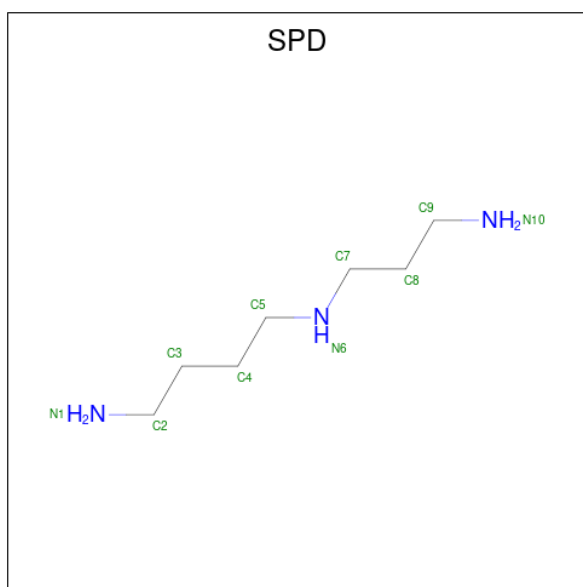
- Molecule 82 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 82 | Pt | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1645 | 734 | 298 | 535 | 77 | 1 | | |

- Molecule 83 is a protein called eIF5A1.

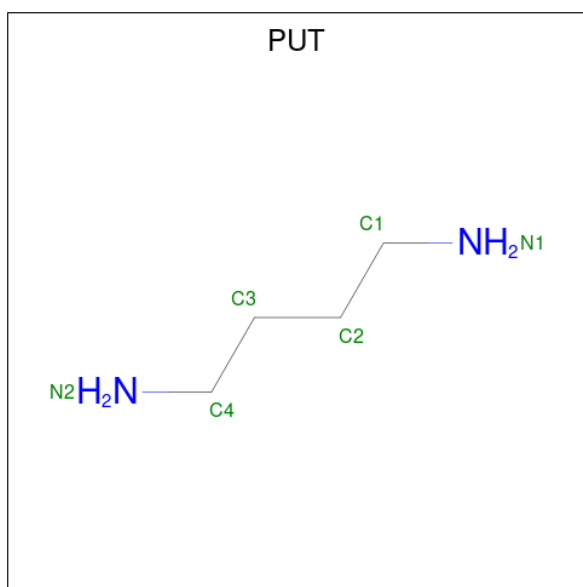
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83 | 5A | 138 | Total | C | N | O | S | 1 | 0 |
| | | | 1073 | 676 | 184 | 204 | 9 | | |

- Molecule 84 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|---|---------|
| | | | Total | C | N | |
| 84 | S2 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |
| 84 | L5 | 1 | 10 | 7 | 3 | 0 |

- Molecule 85 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|--------------------|---------|
| 85 | S2 | 1 | Total C N 6 4 2 | 0 |
| 85 | S2 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |
| 85 | L5 | 1 | Total C N 6 4 2 | 0 |

- Molecule 86 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 86 | S2 | 17 | Total K 17 17 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 86 | L8 | 1 | Total K 1 1 | 0 |
| 86 | L5 | 52 | Total K 52 52 | 0 |
| 86 | L7 | 1 | Total K 1 1 | 0 |
| 86 | SL | 1 | Total K 1 1 | 0 |
| 86 | Sa | 1 | Total K 1 1 | 0 |
| 86 | LA | 1 | Total K 1 1 | 0 |
| 86 | LH | 1 | Total K 1 1 | 0 |
| 86 | Lf | 1 | Total K 1 1 | 0 |
| 86 | Lg | 1 | Total K 1 1 | 0 |

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|---------------------|---------|
| 87 | S2 | 124 | Total Mg 124 124 | 0 |
| 87 | L8 | 10 | Total Mg 10 10 | 0 |
| 87 | L5 | 344 | Total Mg 344 344 | 0 |
| 87 | L7 | 5 | Total Mg 5 5 | 0 |
| 87 | SJ | 1 | Total Mg 1 1 | 0 |
| 87 | SE | 1 | Total Mg 1 1 | 0 |
| 87 | SC | 1 | Total Mg 1 1 | 0 |
| 87 | SX | 1 | Total Mg 1 1 | 0 |
| 87 | Sd | 1 | Total Mg 1 1 | 0 |
| 87 | SN | 1 | Total Mg 1 1 | 0 |

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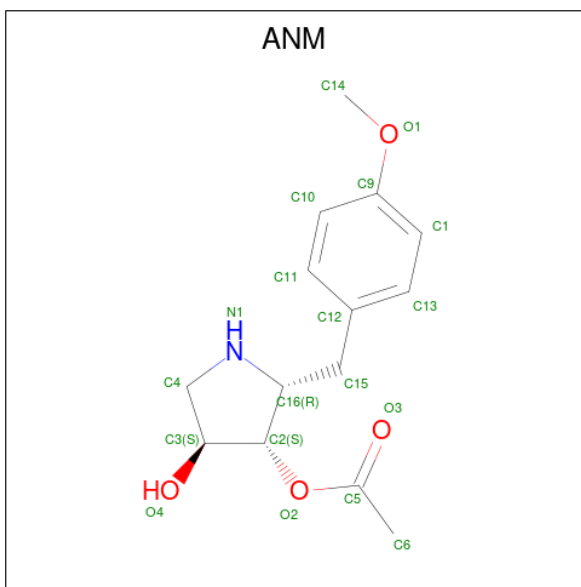
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Mg | |
| 87 | ST | 1 | 1 | 1 | 0 |
| 87 | Sb | 1 | 1 | 1 | 0 |
| 87 | LA | 2 | 2 | 2 | 0 |
| 87 | LB | 2 | 2 | 2 | 0 |
| 87 | LC | 2 | 2 | 2 | 0 |
| 87 | LO | 1 | 1 | 1 | 0 |
| 87 | LL | 2 | 2 | 2 | 0 |
| 87 | LV | 1 | 1 | 1 | 0 |
| 87 | LN | 1 | 1 | 1 | 0 |
| 87 | LI | 1 | 1 | 1 | 0 |
| 87 | LD | 1 | 1 | 1 | 0 |
| 87 | LQ | 1 | 1 | 1 | 0 |
| 87 | LR | 2 | 2 | 2 | 0 |
| 87 | LS | 2 | 2 | 2 | 0 |
| 87 | LP | 3 | 3 | 3 | 0 |
| 87 | Lr | 1 | 1 | 1 | 0 |
| 87 | Lc | 1 | 1 | 1 | 0 |
| 87 | Le | 1 | 1 | 1 | 0 |
| 87 | Lg | 1 | 1 | 1 | 0 |
| 87 | Lj | 1 | 1 | 1 | 0 |
| 87 | Lo | 1 | 1 | 1 | 0 |

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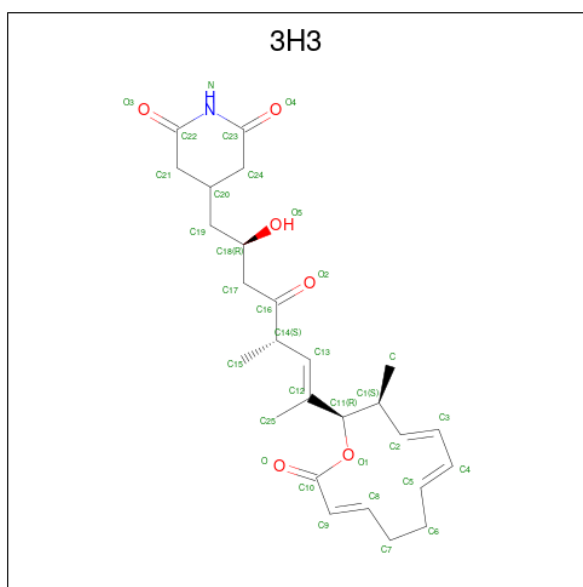
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 87 | Lp | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 87 | Pt | 4 | Total | Mg | 0 |
| | | | 4 | 4 | |
| 87 | 5A | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 88 is ANISOMYCIN (three-letter code: ANM) (formula: $C_{14}H_{19}NO_4$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 88 | L5 | 1 | Total | C | N | O | 0 |
| | | | 19 | 14 | 1 | 4 | |

- Molecule 89 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxooxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (three-letter code: 3H3) (formula: $C_{26}H_{35}NO_6$) (labeled as "Ligand of Interest" by depositor).

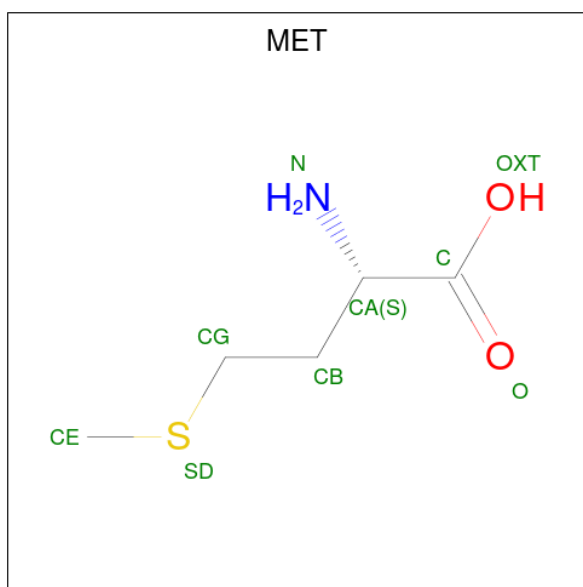


| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| | | | Total | C | N | O | |
| 89 | L5 | 1 | 33 | 26 | 1 | 6 | 0 |

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Zn | |
| 90 | Sd | 1 | 1 | 1 | 0 |
| 90 | Sa | 1 | 1 | 1 | 0 |
| 90 | Sf | 1 | 1 | 1 | 0 |
| 90 | Lg | 1 | 1 | 1 | 0 |
| 90 | Lj | 1 | 1 | 1 | 0 |
| 90 | Lm | 1 | 1 | 1 | 0 |
| 90 | Lo | 1 | 1 | 1 | 0 |
| 90 | Lp | 1 | 1 | 1 | 0 |

- Molecule 91 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| | | | Total | C | N | O | S | |
| 91 | Pt | 1 | 8 | 5 | 1 | 1 | 1 | 0 |

- Molecule 92 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 92 | S2 | 123 | Total | O | 0 |
| | | | 123 | 123 | |
| 92 | L8 | 11 | Total | O | 0 |
| | | | 11 | 11 | |
| 92 | L5 | 996 | Total | O | 0 |
| | | | 996 | 996 | |
| 92 | L7 | 8 | Total | O | 0 |
| | | | 8 | 8 | |
| 92 | SA | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 92 | SF | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 92 | SQ | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 92 | SS | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 92 | SN | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 92 | Sa | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 92 | LA | 18 | Total | O | 0 |
| | | | 18 | 18 | |

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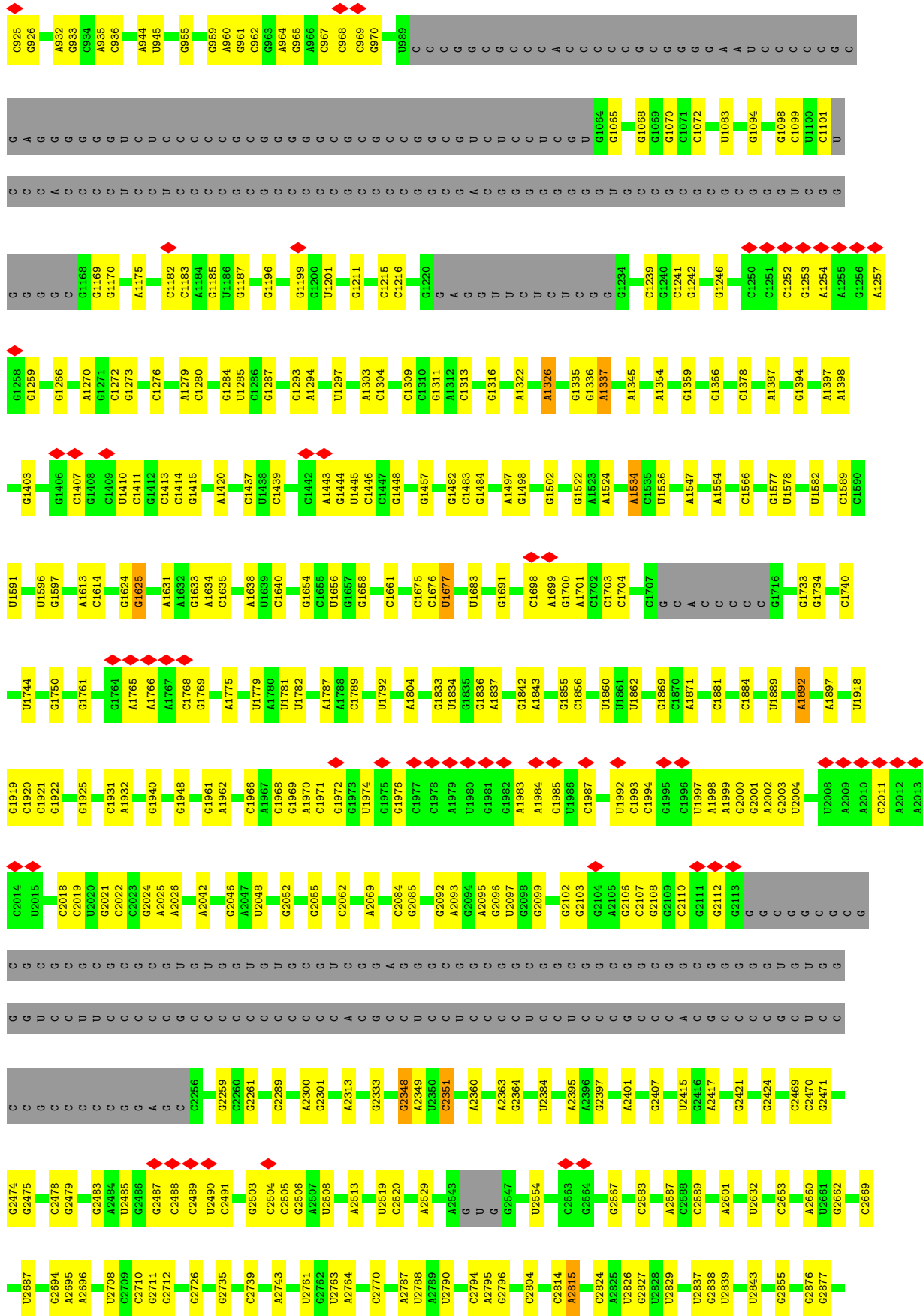
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 92 | LB | 8 | Total 8 | O 8 | 0 |
| 92 | LC | 21 | Total 21 | O 21 | 0 |
| 92 | LO | 3 | Total 3 | O 3 | 0 |
| 92 | LL | 3 | Total 3 | O 3 | 0 |
| 92 | LV | 2 | Total 2 | O 2 | 0 |
| 92 | La | 10 | Total 10 | O 10 | 0 |
| 92 | LN | 4 | Total 4 | O 4 | 0 |
| 92 | LI | 2 | Total 2 | O 2 | 0 |
| 92 | LD | 1 | Total 1 | O 1 | 0 |
| 92 | LQ | 6 | Total 6 | O 6 | 0 |
| 92 | LR | 1 | Total 1 | O 1 | 0 |
| 92 | LT | 1 | Total 1 | O 1 | 0 |
| 92 | LP | 2 | Total 2 | O 2 | 0 |
| 92 | LX | 2 | Total 2 | O 2 | 0 |
| 92 | LZ | 1 | Total 1 | O 1 | 0 |
| 92 | Lr | 1 | Total 1 | O 1 | 0 |
| 92 | Lb | 2 | Total 2 | O 2 | 0 |
| 92 | LF | 4 | Total 4 | O 4 | 0 |
| 92 | Lc | 1 | Total 1 | O 1 | 0 |
| 92 | Ld | 1 | Total 1 | O 1 | 0 |
| 92 | Le | 14 | Total 14 | O 14 | 0 |

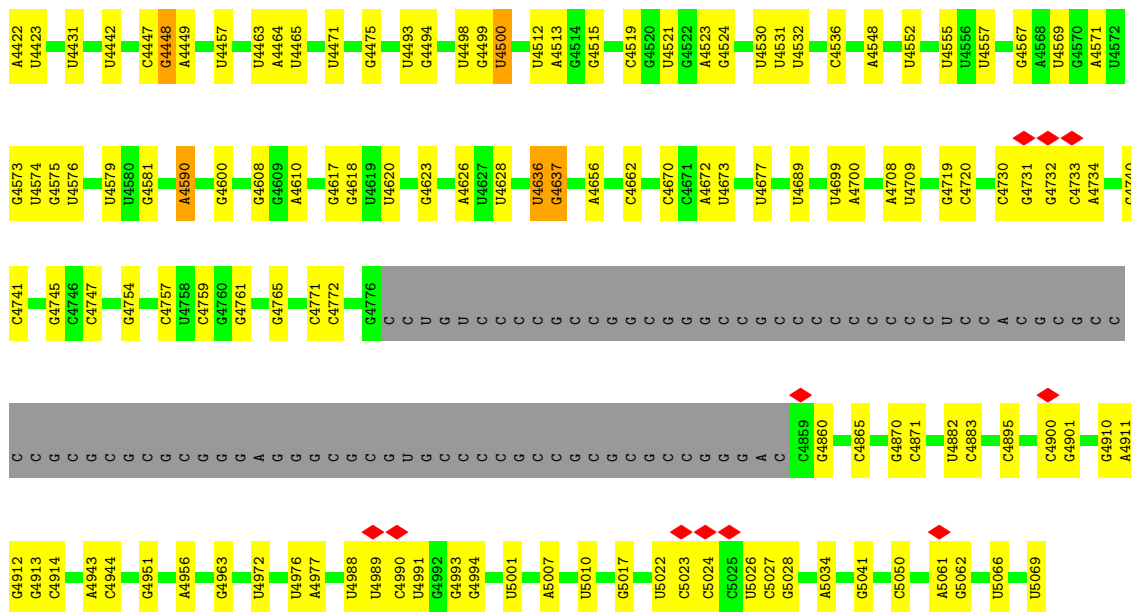
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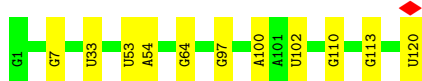
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 92 | Lf | 3 | Total 3 | O 3 | 0 |
| 92 | Lg | 4 | Total 4 | O 4 | 0 |
| 92 | Lj | 6 | Total 6 | O 6 | 0 |
| 92 | Ln | 1 | Total 1 | O 1 | 0 |
| 92 | Lo | 1 | Total 1 | O 1 | 0 |
| 92 | Lp | 2 | Total 2 | O 2 | 0 |
| 92 | Pt | 1 | Total 1 | O 1 | 0 |
| 92 | 5A | 1 | Total 1 | O 1 | 0 |



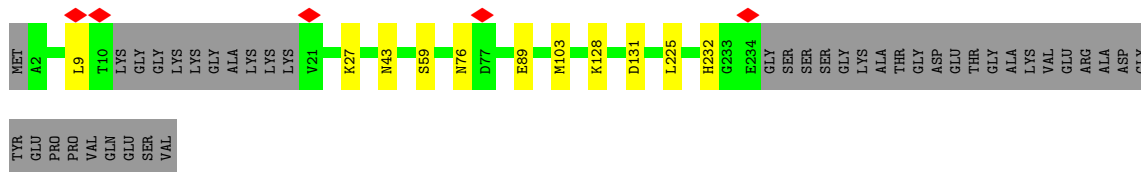
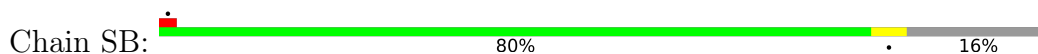
| | | | | | | | |
|-------|-------|-------|-------|-------|---------|---------|---|
| A4251 | G4305 | U4113 | G4026 | A3966 | U8222 | A3662 | G |
| C4252 | U4306 | C4114 | C4027 | G3967 | U8851 | A3673 | C |
| A4253 | U4299 | C4115 | G4038 | U3968 | A3852 | C3673 | G |
| G4254 | U4296 | C4116 | C4039 | G3969 | U3853 | U3695 | G |
| G4266 | U4299 | C4119 | C4040 | G3970 | A3867 | U3713 | U |
| G4267 | U4299 | C4122 | G4041 | A3971 | G3868 | U3714 | C |
| A4268 | U4299 | G4127 | G4042 | G3972 | C3869 | U3715 | U |
| A4273 | U4281 | A4127 | G4043 | G3973 | C3876 | G3718 | G |
| A4281 | U4291 | C4133 | C4034 | C3974 | U3844 | A3718 | C |
| G4291 | A4292 | G4136 | G4037 | C3976 | U3944 | A3723 | G |
| A4292 | U4293 | C4137 | C4038 | C3977 | U3851 | A3724 | C |
| U4293 | U4293 | G4137 | G4039 | C3978 | A3852 | A3724 | G |
| U4296 | U4296 | C4140 | C4040 | C3979 | U3853 | U3729 | C |
| U4299 | U4299 | G4141 | G4041 | G3980 | A3867 | U3734 | G |
| G4305 | U4306 | C4142 | G4042 | C3981 | G3868 | G3741 | C |
| U4306 | U4306 | G4143 | G4043 | C3982 | C3869 | C3741 | G |
| U4312 | U4312 | C4144 | G4044 | G3983 | A3876 | G3744 | C |
| A4313 | U4314 | A4144 | A4045 | C3984 | A3877 | A3744 | G |
| C4314 | U4314 | C4145 | A4046 | C3985 | C3878 | A3748 | C |
| G4329 | G4330 | C4146 | A4047 | C3986 | G3879 | A3748 | G |
| C4330 | U4339 | G4147 | A4048 | C3987 | C3879 | A3748 | C |
| A4339 | U4353 | C4148 | U4049 | C3988 | U3884 | G3753 | G |
| U4353 | U4361 | G4149 | A4050 | C3989 | U3884 | G3753 | C |
| G4370 | G4370 | C4150 | C4051 | C3990 | G3897 | U3758 | C |
| G4373 | U4361 | C4151 | G4052 | C3991 | A3759 | A3758 | G |
| A4376 | U4361 | C4152 | A4053 | C3992 | A3760 | A3759 | C |
| A4377 | U4361 | C4153 | C4054 | G3993 | C3898 | A3760 | G |
| A4378 | U4361 | C4154 | G4055 | C3994 | C3899 | C3761 | C |
| A4385 | G4370 | C4155 | U4055 | G3995 | G3900 | C3761 | G |
| C4386 | U4361 | C4156 | A4056 | C3996 | A3901 | U3762 | C |
| C4387 | U4361 | C4157 | A4056 | C3997 | A3901 | A3763 | G |
| G4391 | U4361 | C4158 | C4059 | C3998 | A3906 | A3764 | C |
| G4392 | U4361 | C4159 | U4060 | C4000 | C3907 | G3764 | G |
| A4394 | U4361 | C4160 | G4061 | C4001 | A3766 | U3765 | C |
| U4395 | U4361 | C4161 | A4062 | A4002 | C3767 | A3766 | G |
| A4396 | U4361 | C4162 | U4063 | A4003 | U3768 | C3767 | C |
| U4403 | U4403 | C4163 | U4064 | G4004 | C3769 | U3768 | G |
| U4420 | U4420 | C4164 | G4065 | G4005 | U3914 | C3769 | C |
| C4421 | U4420 | C4165 | G4065 | C3999 | U3915 | U3770 | G |
| | | C4166 | C4076 | C4000 | U3920 | G3776 | C |
| | | C4167 | G4076 | C4001 | G3777 | G3776 | G |
| | | C4168 | G4094 | G4002 | G3615 | G3615 | C |
| | | C4169 | G4095 | G4003 | U3616 | U3616 | G |
| | | C4170 | C4096 | A4003 | G3617 | G3617 | C |
| | | C4171 | G4097 | G4004 | C3618 | C3618 | G |
| | | C4172 | A4098 | G4005 | A3621 | A3621 | C |
| | | C4173 | G4099 | G4006 | G3626 | G3626 | G |
| | | C4174 | C4100 | G4007 | G3627 | G3627 | C |
| | | C4175 | C4101 | C4008 | A3635 | A3635 | G |
| | | C4176 | C4102 | C4009 | C3636 | C3636 | C |
| | | C4177 | C4103 | C4010 | U3637 | U3637 | G |
| | | C4178 | G4104 | G4011 | A3638 | A3638 | C |
| | | C4179 | A4105 | G4012 | U3639 | U3639 | G |
| | | C4180 | G4106 | G4013 | U3644 | U3644 | C |
| | | C4181 | G4107 | G4014 | A3817 | A3817 | G |
| | | C4182 | G4108 | C4015 | UY13818 | UY13818 | C |
| | | C4183 | G4109 | C4016 | G3819 | G3819 | G |
| | | C4184 | U4110 | G4017 | | | C |
| | | C4185 | C4111 | G4018 | | | G |
| | | C4186 | C4112 | G4019 | | | C |
| | | C4187 | | U4020 | | | G |
| | | C4188 | | C4021 | | | C |
| | | C4189 | | G4022 | | | G |
| | | C4190 | | G4023 | | | C |
| | | C4191 | | G4024 | | | G |
| | | C4192 | | C4025 | | | C |



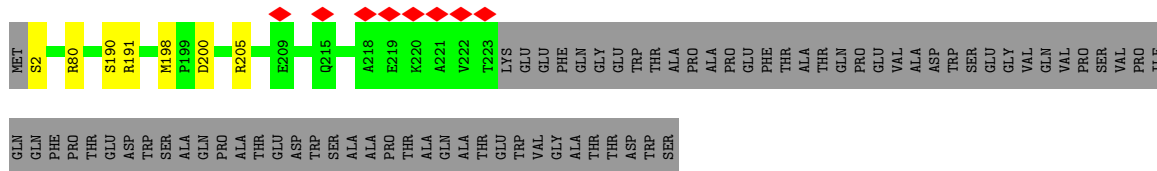
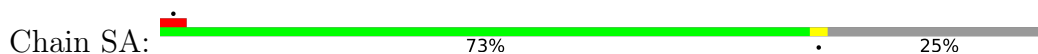
• Molecule 4: 5S rRNA



• Molecule 5: 40S ribosomal protein S3a

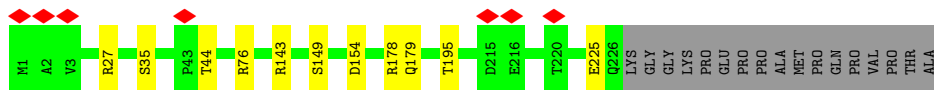


• Molecule 6: 40S ribosomal protein SA

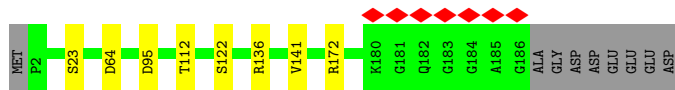
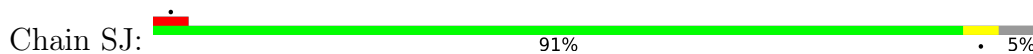


• Molecule 7: 40S ribosomal protein S3





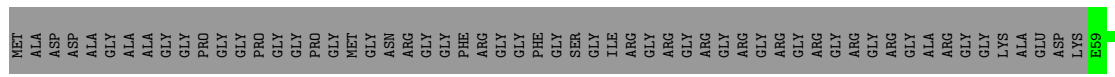
• Molecule 8: 40S ribosomal protein S9



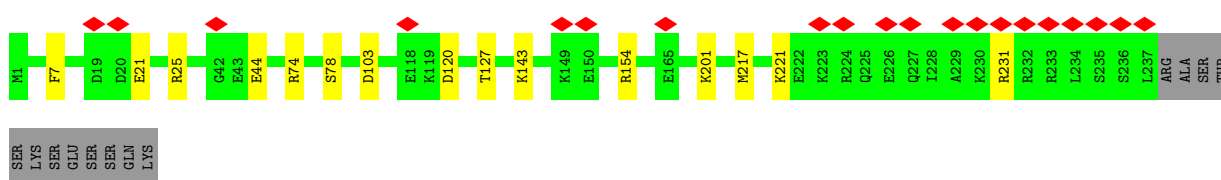
• Molecule 9: 40S ribosomal protein S4, X isoform



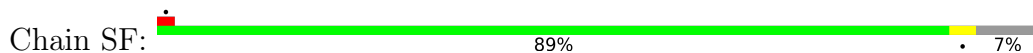
• Molecule 10: 40S ribosomal protein S2



• Molecule 11: 40S ribosomal protein S6



• Molecule 12: 40S ribosomal protein S5



• Molecule 13: 40S ribosomal protein S7

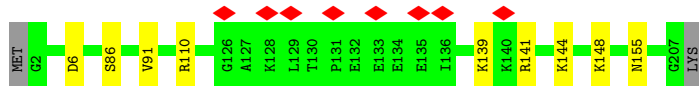




• Molecule 14: 40S ribosomal protein S15a



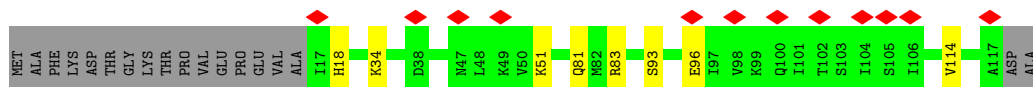
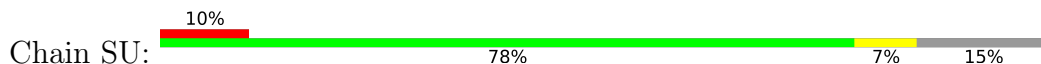
• Molecule 15: 40S ribosomal protein S8



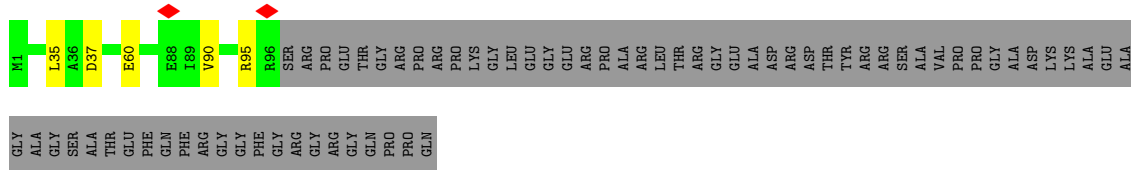
• Molecule 16: 40S ribosomal protein S16



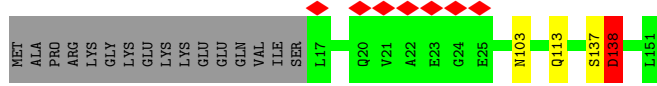
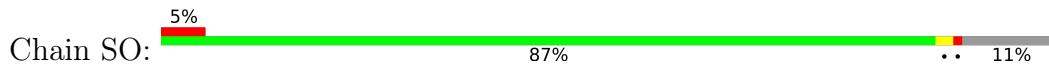
• Molecule 17: 40S ribosomal protein S20



• Molecule 18: 40S ribosomal protein S10



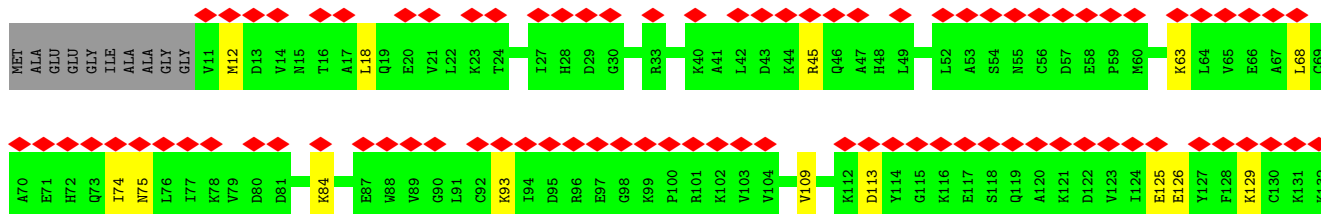
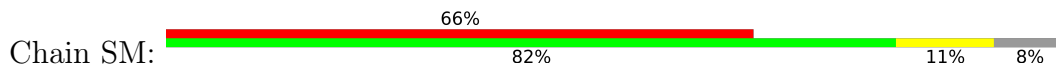
• Molecule 19: 40S ribosomal protein S14



• Molecule 20: uS12



• Molecule 21: 40S ribosomal protein S12



• Molecule 22: 40S ribosomal protein S18



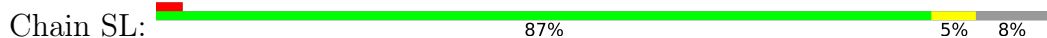
• Molecule 23: 40S ribosomal protein S29



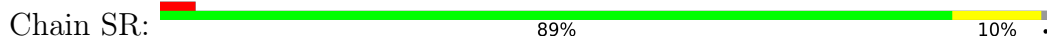
• Molecule 24: 40S ribosomal protein S13

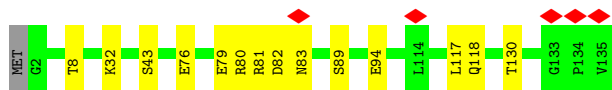


• Molecule 25: 40S ribosomal protein S11

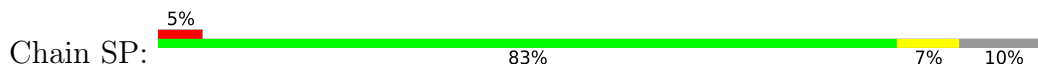


• Molecule 26: 40S ribosomal protein S17





• Molecule 27: 40S ribosomal protein S15



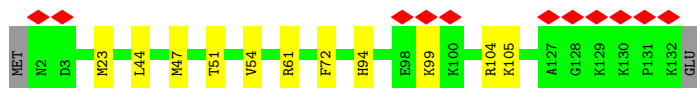
• Molecule 28: 40S ribosomal protein S19



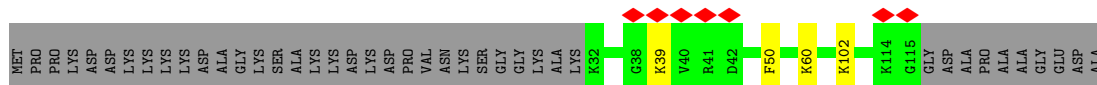
• Molecule 29: 40S ribosomal protein S21



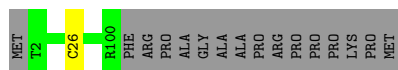
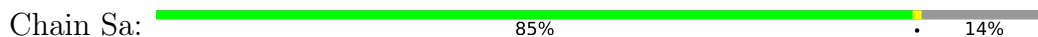
• Molecule 30: 40S ribosomal protein S24



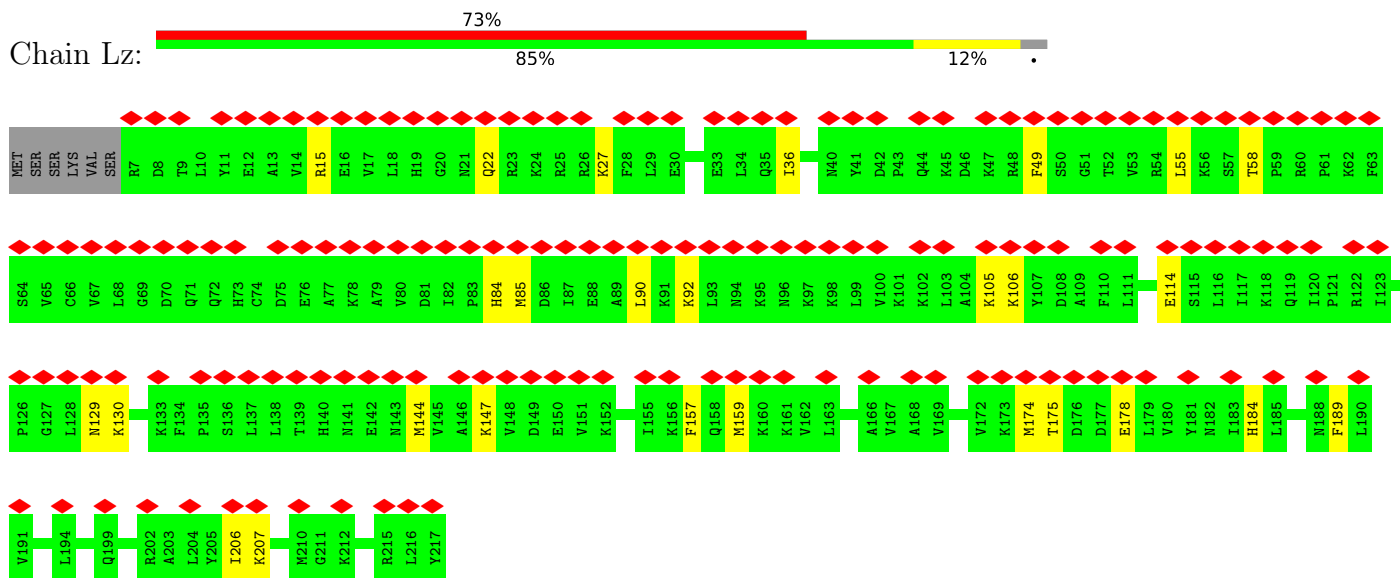
• Molecule 31: 40S ribosomal protein S25



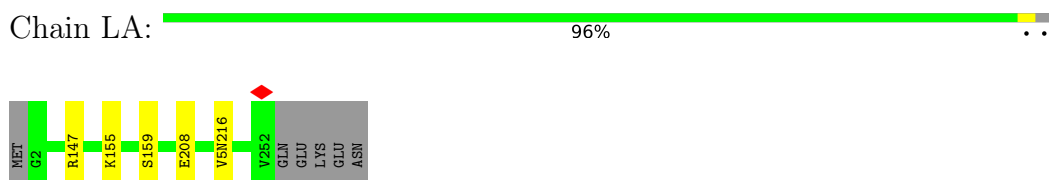
• Molecule 32: 40S ribosomal protein S26



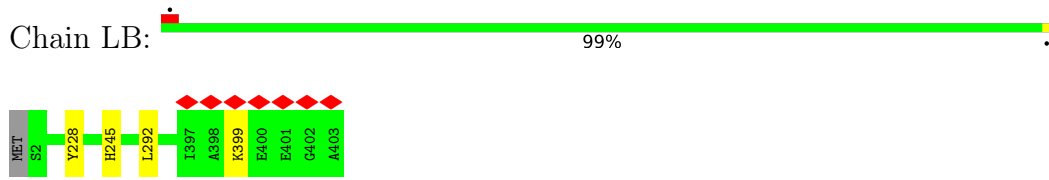
• Molecule 33: 40S ribosomal protein S27



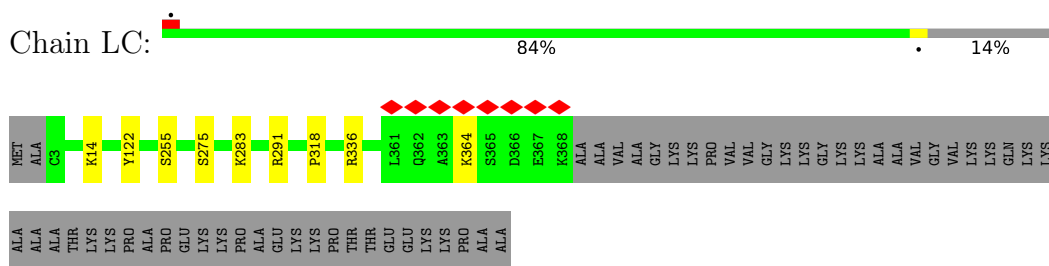
• Molecule 39: uL2



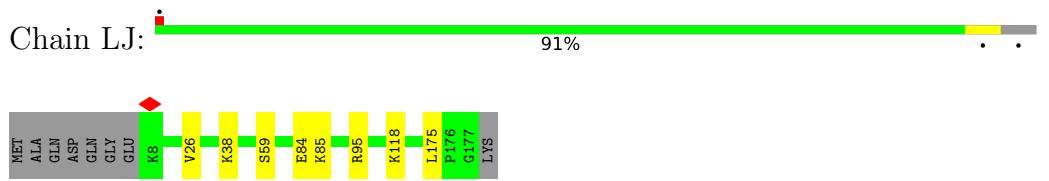
• Molecule 40: 60S ribosomal protein L3



• Molecule 41: 60S ribosomal protein L4

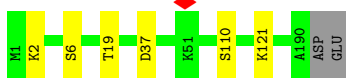


• Molecule 42: 60S ribosomal protein L11




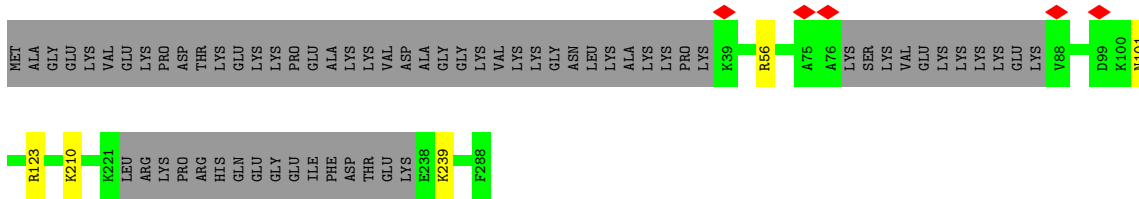
• Molecule 43: 60S ribosomal protein L9

Chain LH:  96%




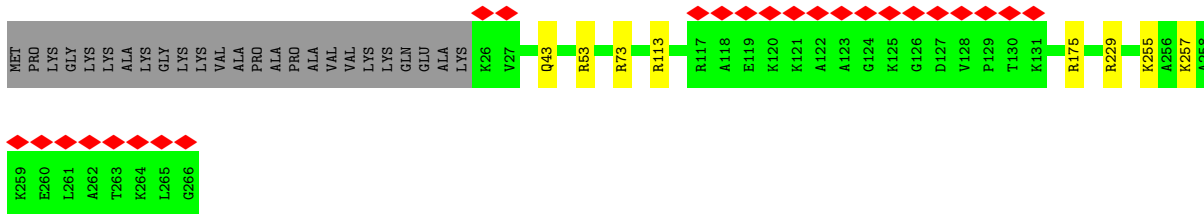
- Molecule 44: 60S ribosomal protein L6

Chain LE:  76%



- Molecule 45: 60S ribosomal protein L7a

Chain LG:  9%



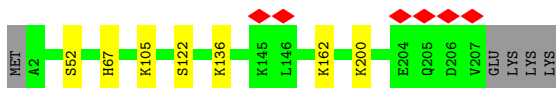
- Molecule 46: 60S ribosomal protein L13a

Chain LO:  96%



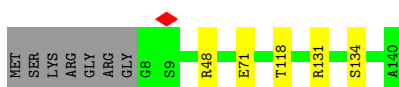
- Molecule 47: 60S ribosomal protein L13

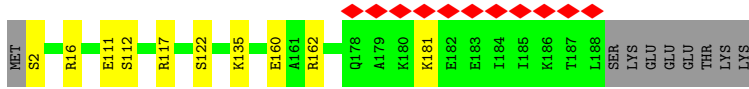
Chain LL:  94%



- Molecule 48: 60S ribosomal protein L23

Chain LV:  91%

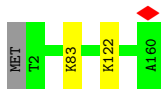




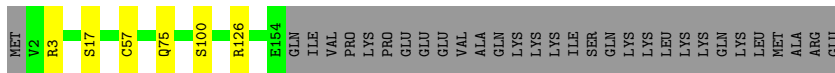
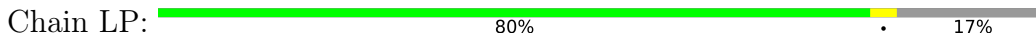
• Molecule 56: 60S ribosomal protein L18a



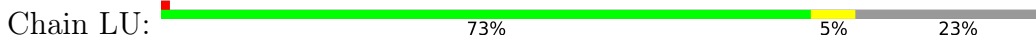
• Molecule 57: 60S ribosomal protein L21



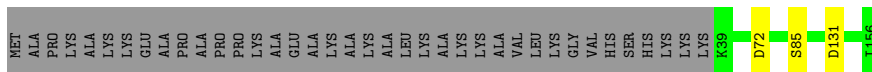
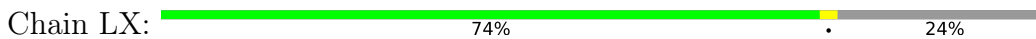
• Molecule 58: 60S ribosomal protein L17



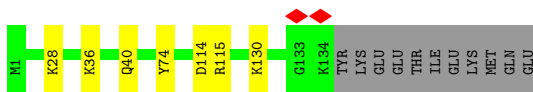
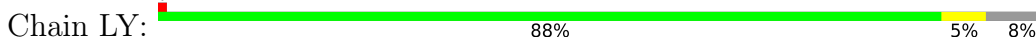
• Molecule 59: 60S ribosomal protein L22



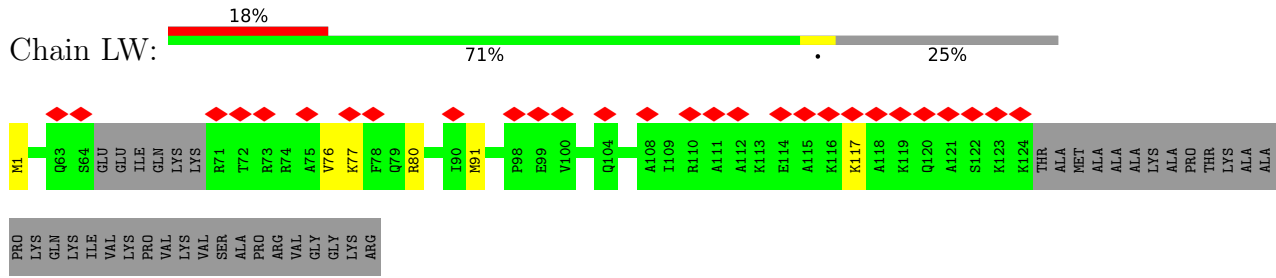
• Molecule 60: 60S ribosomal protein L23a



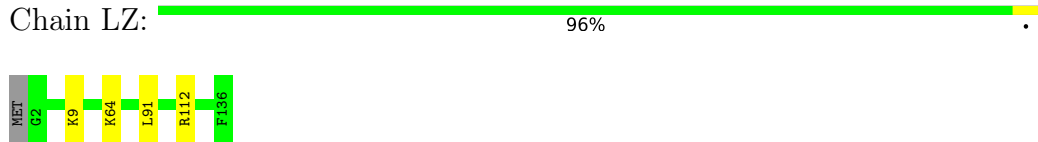
• Molecule 61: 60S ribosomal protein L26



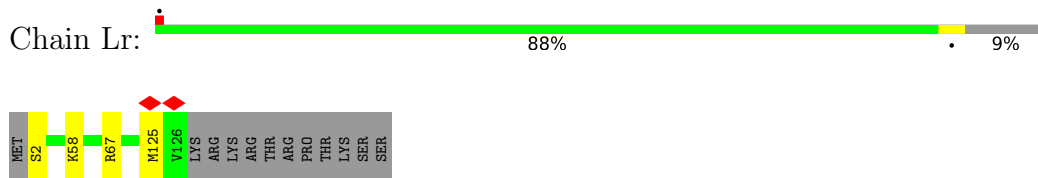
• Molecule 62: 60S ribosomal protein L24



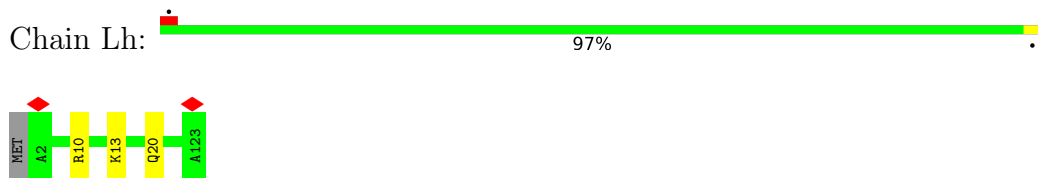
• Molecule 63: 60S ribosomal protein L27



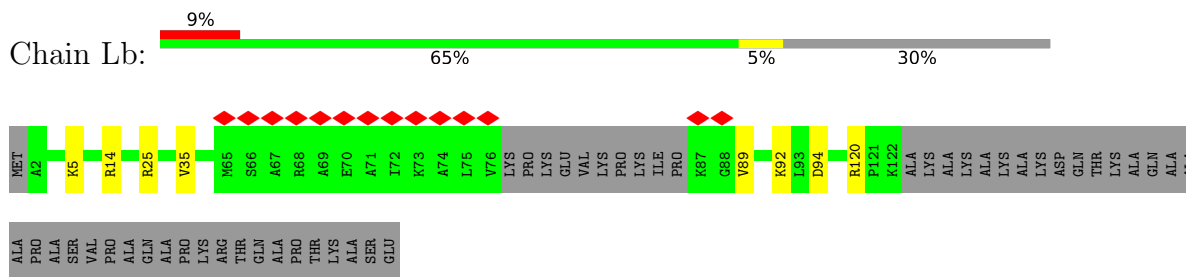
• Molecule 64: 60S ribosomal protein L28



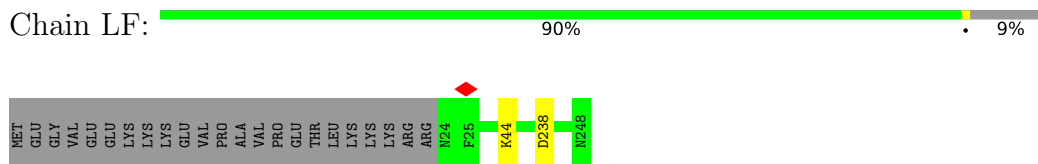
• Molecule 65: 60S ribosomal protein L35



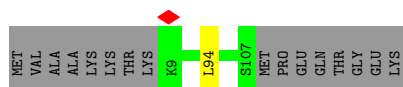
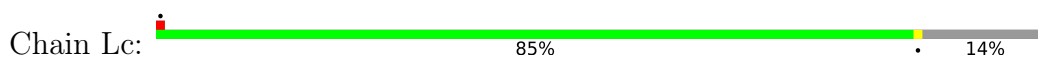
• Molecule 66: 60S ribosomal protein L29



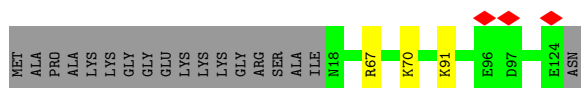
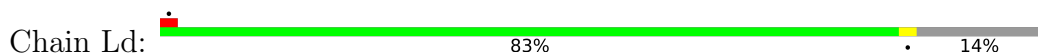
• Molecule 67: 60S ribosomal protein L7



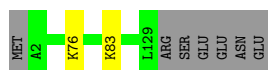
• Molecule 68: 60S ribosomal protein L30



• Molecule 69: 60S ribosomal protein L31



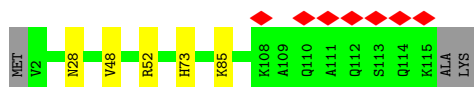
• Molecule 70: 60S ribosomal protein L32



• Molecule 71: 60S ribosomal protein L35a



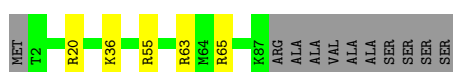
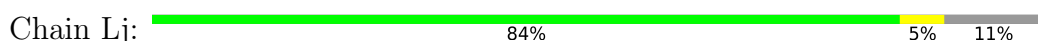
• Molecule 72: 60S ribosomal protein L34



• Molecule 73: 60S ribosomal protein L36

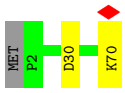


• Molecule 74: 60S ribosomal protein L37



- Molecule 75: 60S ribosomal protein L38

Chain Lk:  96%



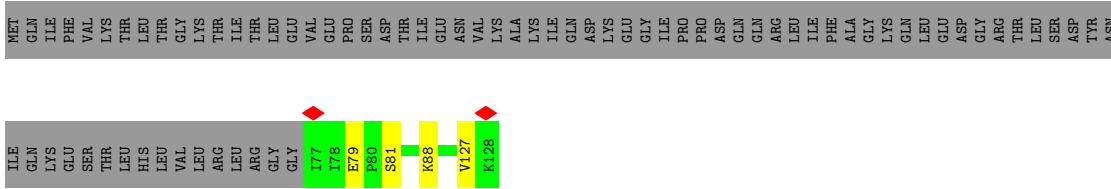
- Molecule 76: 60S ribosomal protein L39

Chain Ll:  98%



- Molecule 77: eL40

Chain Lm:  38%



- Molecule 78: 60S ribosomal protein L41

Chain Ln:  92%



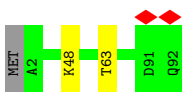
- Molecule 79: 60S ribosomal protein L36a

Chain Lo:  92%



- Molecule 80: 60S ribosomal protein L37a

Chain Lp:  97%

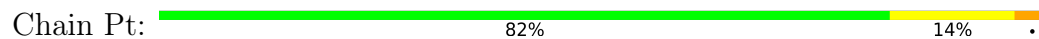


- Molecule 81: mRNA

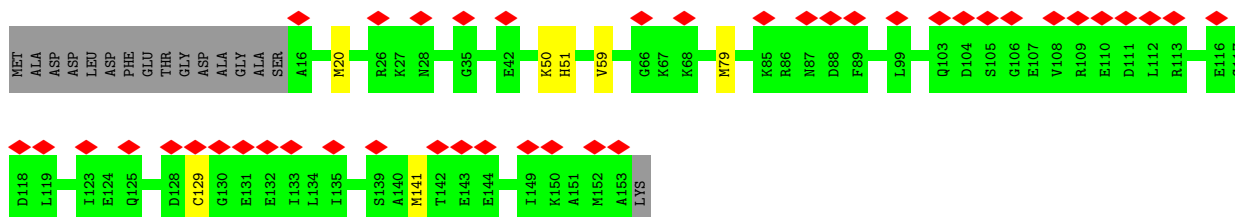
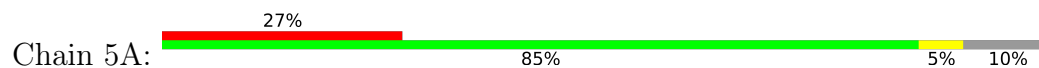
Chain mR:  10%



- Molecule 82: P-site tRNA



- Molecule 83: eIF5A1



4 Experimental information

| Property | Value | Source |
|--------------------------------------|------------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 55836 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 79 | Depositor |
| Minimum defocus (nm) | -500 | Depositor |
| Maximum defocus (nm) | -1500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.053 | Depositor |
| Minimum map value | -0.014 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.005 | Depositor |
| Map size (\AA) | 528.64, 528.64, 528.64 | wwPDB |
| Map dimensions | 640, 640, 640 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 0.82600003, 0.82600003, 0.82600003 | 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: 1MA, ANM, PUT, PSU, G7M, HIC, 5MC, 6MZ, MLZ, K, OMU, A2M, HY3, UR3, OMG, V5N, AME, MG, OMC, 4AC, UY1, SPD, ZN, B8N, 3H3, 4SU, 5CT, SAC, MA6, M3L, H2U

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 | S2 | 0.75 | 0/38000 | 0.83 | 9/59217 (0.0%) |
| 2 | L8 | 0.90 | 0/3609 | 0.90 | 1/5623 (0.0%) |
| 3 | L5 | 0.87 | 3/85432 (0.0%) | 0.97 | 50/133204 (0.0%) |
| 4 | L7 | 0.91 | 0/2858 | 0.86 | 0/4455 |
| 5 | SB | 0.34 | 0/1832 | 0.52 | 0/2449 |
| 6 | SA | 0.36 | 0/1778 | 0.50 | 0/2416 |
| 7 | SD | 0.34 | 0/1784 | 0.54 | 0/2403 |
| 8 | SJ | 0.33 | 0/1550 | 0.55 | 0/2069 |
| 9 | SE | 0.34 | 0/2118 | 0.55 | 0/2849 |
| 10 | SC | 0.37 | 0/1762 | 0.49 | 0/2381 |
| 11 | SG | 0.30 | 0/1946 | 0.55 | 0/2590 |
| 12 | SF | 0.34 | 0/1515 | 0.53 | 0/2037 |
| 13 | SH | 0.30 | 0/1540 | 0.53 | 0/2064 |
| 14 | SW | 0.35 | 0/1051 | 0.56 | 0/1406 |
| 15 | SI | 0.38 | 0/1715 | 0.57 | 0/2287 |
| 16 | SQ | 0.36 | 0/1141 | 0.53 | 0/1528 |
| 17 | SU | 0.33 | 0/813 | 0.56 | 0/1092 |
| 18 | SK | 0.33 | 0/834 | 0.54 | 1/1125 (0.1%) |
| 19 | SO | 0.34 | 0/1022 | 0.58 | 0/1372 |
| 20 | SX | 0.36 | 0/1096 | 0.54 | 0/1461 |
| 21 | SM | 0.25 | 0/960 | 0.58 | 0/1286 |
| 22 | SS | 0.32 | 0/1232 | 0.57 | 0/1651 |
| 23 | Sd | 0.38 | 0/469 | 0.59 | 0/623 |
| 24 | SN | 0.36 | 0/1242 | 0.54 | 0/1671 |
| 25 | SL | 0.40 | 0/1221 | 0.57 | 0/1632 |
| 26 | SR | 0.37 | 0/1097 | 0.57 | 0/1474 |
| 27 | SP | 0.33 | 0/1100 | 0.54 | 0/1470 |
| 28 | ST | 0.34 | 0/1148 | 0.53 | 0/1540 |
| 29 | SV | 0.38 | 0/635 | 0.54 | 0/850 |
| 30 | SY | 0.31 | 0/1083 | 0.55 | 0/1438 |
| 31 | SZ | 0.29 | 0/682 | 0.52 | 0/911 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | Sa | 0.38 | 0/816 | 0.60 | 0/1093 |
| 33 | Sb | 0.34 | 0/665 | 0.51 | 0/891 |
| 34 | Sc | 0.33 | 0/514 | 0.62 | 0/688 |
| 35 | Se | 0.31 | 0/396 | 0.55 | 0/519 |
| 36 | Sf | 0.37 | 0/525 | 0.62 | 0/695 |
| 37 | Sg | 0.30 | 0/2493 | 0.55 | 0/3394 |
| 38 | Lz | 0.26 | 0/1723 | 0.54 | 0/2313 |
| 39 | LA | 0.43 | 0/1958 | 0.64 | 0/2623 |
| 40 | LB | 0.41 | 0/3294 | 0.56 | 0/4406 |
| 41 | LC | 0.40 | 0/2968 | 0.59 | 0/3985 |
| 42 | LJ | 0.35 | 0/1385 | 0.55 | 0/1852 |
| 43 | LH | 0.36 | 0/1537 | 0.52 | 0/2066 |
| 44 | LE | 0.35 | 0/1820 | 0.54 | 0/2442 |
| 45 | LG | 0.36 | 0/1959 | 0.52 | 0/2637 |
| 46 | LO | 0.38 | 0/1665 | 0.56 | 0/2228 |
| 47 | LL | 0.37 | 0/1695 | 0.62 | 0/2270 |
| 48 | LV | 0.38 | 0/1002 | 0.57 | 0/1345 |
| 49 | LM | 0.37 | 0/1142 | 0.54 | 0/1527 |
| 50 | La | 0.43 | 0/1178 | 0.62 | 0/1573 |
| 51 | LN | 0.47 | 0/1745 | 0.65 | 0/2338 |
| 52 | LI | 0.38 | 0/1683 | 0.55 | 0/2247 |
| 53 | LD | 0.39 | 0/2437 | 0.52 | 0/3263 |
| 54 | LQ | 0.40 | 0/1536 | 0.65 | 0/2052 |
| 55 | LR | 0.33 | 0/1582 | 0.57 | 0/2091 |
| 56 | LS | 0.45 | 0/1500 | 0.58 | 0/2013 |
| 57 | LT | 0.42 | 0/1345 | 0.55 | 0/1795 |
| 58 | LP | 0.39 | 0/1277 | 0.57 | 0/1713 |
| 59 | LU | 0.34 | 0/822 | 0.51 | 0/1103 |
| 60 | LX | 0.41 | 0/983 | 0.54 | 0/1323 |
| 61 | LY | 0.39 | 0/1132 | 0.57 | 0/1504 |
| 62 | LW | 0.35 | 0/972 | 0.55 | 0/1288 |
| 63 | LZ | 0.41 | 0/1141 | 0.54 | 0/1521 |
| 64 | Lr | 0.39 | 0/1020 | 0.59 | 0/1367 |
| 65 | Lh | 0.34 | 0/1022 | 0.55 | 0/1351 |
| 66 | Lb | 0.38 | 0/900 | 0.55 | 0/1187 |
| 67 | LF | 0.43 | 0/1904 | 0.57 | 0/2539 |
| 68 | Lc | 0.40 | 0/780 | 0.52 | 0/1046 |
| 69 | Ld | 0.38 | 0/903 | 0.59 | 0/1216 |
| 70 | Le | 0.44 | 0/1071 | 0.64 | 0/1429 |
| 71 | Lf | 0.43 | 0/902 | 0.62 | 0/1208 |
| 72 | Lg | 0.41 | 0/916 | 0.59 | 0/1220 |
| 73 | Li | 0.35 | 0/843 | 0.57 | 0/1115 |
| 74 | Lj | 0.47 | 0/731 | 0.64 | 0/967 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 75 | Lk | 0.36 | 0/574 | 0.51 | 0/761 |
| 76 | Ll | 0.38 | 0/453 | 0.59 | 0/599 |
| 77 | Lm | 0.41 | 0/425 | 0.59 | 0/564 |
| 78 | Ln | 0.41 | 0/240 | 0.79 | 0/305 |
| 79 | Lo | 0.42 | 0/888 | 0.59 | 0/1170 |
| 80 | Lp | 0.37 | 0/728 | 0.59 | 0/967 |
| 81 | mR | 0.43 | 0/192 | 0.76 | 0/297 |
| 82 | Pt | 0.86 | 6/1721 (0.3%) | 1.03 | 11/2679 (0.4%) |
| 83 | 5A | 0.31 | 0/1060 | 0.61 | 0/1425 |
| All | All | 0.68 | 9/228428 (0.0%) | 0.80 | 72/334784 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 19 | SO | 0 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 82 | Pt | 77 | A | C5-C4 | 11.16 | 1.46 | 1.38 |
| 82 | Pt | 1 | C | OP3-P | -10.42 | 1.48 | 1.61 |
| 82 | Pt | 77 | A | N7-C5 | -7.90 | 1.34 | 1.39 |
| 82 | Pt | 77 | A | N9-C4 | -7.68 | 1.33 | 1.37 |
| 82 | Pt | 77 | A | C5-C6 | 6.85 | 1.47 | 1.41 |

The worst 5 of 72 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 82 | Pt | 77 | A | C2-N3-C4 | 20.00 | 120.60 | 110.60 |
| 82 | Pt | 77 | A | N1-C2-N3 | -11.94 | 123.33 | 129.30 |
| 82 | Pt | 77 | A | N3-C4-C5 | -10.89 | 119.18 | 126.80 |
| 82 | Pt | 77 | A | N3-C4-N9 | 9.14 | 134.72 | 127.40 |
| 82 | Pt | 77 | A | C4-C5-N7 | -7.65 | 106.87 | 110.70 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 19 | SO | 138 | ASP | Peptide |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 5 | SB | 219/264 (83%) | 213 (97%) | 6 (3%) | 0 | 100 | 100 |
| 6 | SA | 220/295 (75%) | 215 (98%) | 5 (2%) | 0 | 100 | 100 |
| 7 | SD | 224/243 (92%) | 212 (95%) | 12 (5%) | 0 | 100 | 100 |
| 8 | SJ | 183/194 (94%) | 179 (98%) | 4 (2%) | 0 | 100 | 100 |
| 9 | SE | 260/263 (99%) | 252 (97%) | 8 (3%) | 0 | 100 | 100 |
| 10 | SC | 220/293 (75%) | 215 (98%) | 5 (2%) | 0 | 100 | 100 |
| 11 | SG | 235/249 (94%) | 229 (97%) | 6 (3%) | 0 | 100 | 100 |
| 12 | SF | 187/204 (92%) | 180 (96%) | 6 (3%) | 1 (0%) | 29 | 35 |
| 13 | SH | 187/194 (96%) | 179 (96%) | 8 (4%) | 0 | 100 | 100 |
| 14 | SW | 127/130 (98%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |
| 15 | SI | 204/208 (98%) | 197 (97%) | 7 (3%) | 0 | 100 | 100 |
| 16 | SQ | 139/146 (95%) | 135 (97%) | 4 (3%) | 0 | 100 | 100 |
| 17 | SU | 99/119 (83%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | SK | 94/165 (57%) | 89 (95%) | 5 (5%) | 0 | 100 | 100 |
| 19 | SO | 133/151 (88%) | 129 (97%) | 3 (2%) | 1 (1%) | 19 | 23 |
| 20 | SX | 137/143 (96%) | 134 (98%) | 3 (2%) | 0 | 100 | 100 |
| 21 | SM | 120/132 (91%) | 117 (98%) | 3 (2%) | 0 | 100 | 100 |
| 22 | SS | 146/152 (96%) | 143 (98%) | 3 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 23 | Sd | 53/56 (95%) | 53 (100%) | 0 | 0 | 100 | 100 |
| 24 | SN | 149/151 (99%) | 147 (99%) | 2 (1%) | 0 | 100 | 100 |
| 25 | SL | 142/158 (90%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 26 | SR | 132/135 (98%) | 123 (93%) | 9 (7%) | 0 | 100 | 100 |
| 27 | SP | 129/145 (89%) | 125 (97%) | 4 (3%) | 0 | 100 | 100 |
| 28 | ST | 142/145 (98%) | 135 (95%) | 7 (5%) | 0 | 100 | 100 |
| 29 | SV | 81/83 (98%) | 81 (100%) | 0 | 0 | 100 | 100 |
| 30 | SY | 129/133 (97%) | 126 (98%) | 3 (2%) | 0 | 100 | 100 |
| 31 | SZ | 82/125 (66%) | 79 (96%) | 3 (4%) | 0 | 100 | 100 |
| 32 | Sa | 98/115 (85%) | 98 (100%) | 0 | 0 | 100 | 100 |
| 33 | Sb | 81/84 (96%) | 77 (95%) | 4 (5%) | 0 | 100 | 100 |
| 34 | Sc | 63/69 (91%) | 59 (94%) | 4 (6%) | 0 | 100 | 100 |
| 35 | Se | 46/133 (35%) | 45 (98%) | 0 | 1 (2%) | 6 | 5 |
| 36 | Sf | 61/156 (39%) | 49 (80%) | 10 (16%) | 2 (3%) | 4 | 2 |
| 37 | Sg | 311/317 (98%) | 287 (92%) | 23 (7%) | 1 (0%) | 41 | 50 |
| 38 | Lz | 209/217 (96%) | 201 (96%) | 8 (4%) | 0 | 100 | 100 |
| 39 | LA | 249/257 (97%) | 240 (96%) | 9 (4%) | 0 | 100 | 100 |
| 40 | LB | 399/403 (99%) | 390 (98%) | 9 (2%) | 0 | 100 | 100 |
| 41 | LC | 364/427 (85%) | 359 (99%) | 5 (1%) | 0 | 100 | 100 |
| 42 | LJ | 168/178 (94%) | 166 (99%) | 2 (1%) | 0 | 100 | 100 |
| 43 | LH | 188/192 (98%) | 186 (99%) | 2 (1%) | 0 | 100 | 100 |
| 44 | LE | 217/288 (75%) | 212 (98%) | 5 (2%) | 0 | 100 | 100 |
| 45 | LG | 239/266 (90%) | 230 (96%) | 9 (4%) | 0 | 100 | 100 |
| 46 | LO | 197/203 (97%) | 194 (98%) | 3 (2%) | 0 | 100 | 100 |
| 47 | LL | 204/211 (97%) | 195 (96%) | 9 (4%) | 0 | 100 | 100 |
| 48 | LV | 131/140 (94%) | 130 (99%) | 1 (1%) | 0 | 100 | 100 |
| 49 | LM | 134/215 (62%) | 130 (97%) | 4 (3%) | 0 | 100 | 100 |
| 50 | La | 144/148 (97%) | 143 (99%) | 1 (1%) | 0 | 100 | 100 |
| 51 | LN | 201/204 (98%) | 198 (98%) | 3 (2%) | 0 | 100 | 100 |
| 52 | LI | 199/214 (93%) | 197 (99%) | 2 (1%) | 0 | 100 | 100 |
| 53 | LD | 292/297 (98%) | 286 (98%) | 6 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 54 | LQ | 185/188 (98%) | 180 (97%) | 5 (3%) | 0 | 100 | 100 |
| 55 | LR | 185/196 (94%) | 184 (100%) | 1 (0%) | 0 | 100 | 100 |
| 56 | LS | 174/176 (99%) | 171 (98%) | 3 (2%) | 0 | 100 | 100 |
| 57 | LT | 159/160 (99%) | 157 (99%) | 2 (1%) | 0 | 100 | 100 |
| 58 | LP | 152/184 (83%) | 149 (98%) | 3 (2%) | 0 | 100 | 100 |
| 59 | LU | 97/128 (76%) | 96 (99%) | 1 (1%) | 0 | 100 | 100 |
| 60 | LX | 116/156 (74%) | 115 (99%) | 1 (1%) | 0 | 100 | 100 |
| 61 | LY | 132/145 (91%) | 132 (100%) | 0 | 0 | 100 | 100 |
| 62 | LW | 114/157 (73%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 63 | LZ | 134/136 (98%) | 131 (98%) | 3 (2%) | 0 | 100 | 100 |
| 64 | Lr | 124/137 (90%) | 124 (100%) | 0 | 0 | 100 | 100 |
| 65 | Lh | 120/123 (98%) | 120 (100%) | 0 | 0 | 100 | 100 |
| 66 | Lb | 106/159 (67%) | 104 (98%) | 2 (2%) | 0 | 100 | 100 |
| 67 | LF | 223/248 (90%) | 217 (97%) | 6 (3%) | 0 | 100 | 100 |
| 68 | Lc | 97/115 (84%) | 97 (100%) | 0 | 0 | 100 | 100 |
| 69 | Ld | 105/125 (84%) | 104 (99%) | 1 (1%) | 0 | 100 | 100 |
| 70 | Le | 126/135 (93%) | 125 (99%) | 1 (1%) | 0 | 100 | 100 |
| 71 | Lf | 108/110 (98%) | 107 (99%) | 1 (1%) | 0 | 100 | 100 |
| 72 | Lg | 112/117 (96%) | 110 (98%) | 2 (2%) | 0 | 100 | 100 |
| 73 | Li | 100/105 (95%) | 98 (98%) | 2 (2%) | 0 | 100 | 100 |
| 74 | Lj | 85/97 (88%) | 83 (98%) | 2 (2%) | 0 | 100 | 100 |
| 75 | Lk | 67/70 (96%) | 67 (100%) | 0 | 0 | 100 | 100 |
| 76 | Ll | 48/51 (94%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 77 | Lm | 49/128 (38%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 78 | Ln | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 79 | Lo | 104/106 (98%) | 103 (99%) | 1 (1%) | 0 | 100 | 100 |
| 80 | Lp | 90/92 (98%) | 85 (94%) | 5 (6%) | 0 | 100 | 100 |
| 83 | 5A | 135/154 (88%) | 127 (94%) | 7 (5%) | 1 (1%) | 22 | 26 |
| All | All | 11638/13133 (89%) | 11331 (97%) | 300 (3%) | 7 (0%) | 54 | 64 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | SF | 79 | HIS |
| 35 | Se | 119 | VAL |
| 37 | Sg | 234 | ASP |
| 83 | 5A | 141 | MET |
| 19 | SO | 138 | 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 | SB | 202/231 (87%) | 191 (95%) | 11 (5%) | 22 | 30 |
| 6 | SA | 183/242 (76%) | 177 (97%) | 6 (3%) | 38 | 53 |
| 7 | SD | 189/202 (94%) | 178 (94%) | 11 (6%) | 20 | 27 |
| 8 | SJ | 161/168 (96%) | 153 (95%) | 8 (5%) | 24 | 34 |
| 9 | SE | 224/225 (100%) | 213 (95%) | 11 (5%) | 25 | 35 |
| 10 | SC | 188/225 (84%) | 174 (93%) | 14 (7%) | 13 | 17 |
| 11 | SG | 207/218 (95%) | 192 (93%) | 15 (7%) | 14 | 18 |
| 12 | SF | 159/170 (94%) | 152 (96%) | 7 (4%) | 28 | 39 |
| 13 | SH | 168/174 (97%) | 156 (93%) | 12 (7%) | 14 | 19 |
| 14 | SW | 112/113 (99%) | 108 (96%) | 4 (4%) | 35 | 49 |
| 15 | SI | 178/180 (99%) | 169 (95%) | 9 (5%) | 24 | 33 |
| 16 | SQ | 117/121 (97%) | 109 (93%) | 8 (7%) | 16 | 21 |
| 17 | SU | 93/107 (87%) | 85 (91%) | 8 (9%) | 10 | 12 |
| 18 | SK | 87/136 (64%) | 83 (95%) | 4 (5%) | 27 | 38 |
| 19 | SO | 105/119 (88%) | 101 (96%) | 4 (4%) | 33 | 47 |
| 20 | SX | 111/114 (97%) | 105 (95%) | 6 (5%) | 22 | 30 |
| 21 | SM | 104/108 (96%) | 90 (86%) | 14 (14%) | 4 | 4 |
| 22 | SS | 128/132 (97%) | 123 (96%) | 5 (4%) | 32 | 46 |
| 23 | Sd | 48/49 (98%) | 48 (100%) | 0 | 100 | 100 |
| 24 | SN | 131/131 (100%) | 125 (95%) | 6 (5%) | 27 | 38 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 25 | SL | 132/142 (93%) | 124 (94%) | 8 (6%) | 18 | 25 |
| 26 | SR | 121/122 (99%) | 107 (88%) | 14 (12%) | 5 | 6 |
| 27 | SP | 117/130 (90%) | 107 (92%) | 10 (8%) | 10 | 13 |
| 28 | ST | 114/115 (99%) | 107 (94%) | 7 (6%) | 18 | 25 |
| 29 | SV | 66/66 (100%) | 60 (91%) | 6 (9%) | 9 | 11 |
| 30 | SY | 113/115 (98%) | 102 (90%) | 11 (10%) | 8 | 9 |
| 31 | SZ | 74/103 (72%) | 70 (95%) | 4 (5%) | 22 | 30 |
| 32 | Sa | 87/98 (89%) | 86 (99%) | 1 (1%) | 73 | 86 |
| 33 | Sb | 75/76 (99%) | 71 (95%) | 4 (5%) | 22 | 31 |
| 34 | Sc | 58/62 (94%) | 51 (88%) | 7 (12%) | 5 | 5 |
| 35 | Se | 40/104 (38%) | 38 (95%) | 2 (5%) | 24 | 34 |
| 36 | Sf | 56/140 (40%) | 44 (79%) | 12 (21%) | 1 | 1 |
| 37 | Sg | 272/275 (99%) | 240 (88%) | 32 (12%) | 5 | 5 |
| 38 | Lz | 189/196 (96%) | 162 (86%) | 27 (14%) | 3 | 3 |
| 39 | LA | 193/198 (98%) | 189 (98%) | 4 (2%) | 53 | 70 |
| 40 | LB | 347/348 (100%) | 344 (99%) | 3 (1%) | 78 | 89 |
| 41 | LC | 305/348 (88%) | 296 (97%) | 9 (3%) | 41 | 57 |
| 42 | LJ | 143/149 (96%) | 135 (94%) | 8 (6%) | 21 | 29 |
| 43 | LH | 169/171 (99%) | 163 (96%) | 6 (4%) | 35 | 49 |
| 44 | LE | 196/252 (78%) | 191 (97%) | 5 (3%) | 46 | 63 |
| 45 | LG | 203/223 (91%) | 195 (96%) | 8 (4%) | 32 | 46 |
| 46 | LO | 171/174 (98%) | 167 (98%) | 4 (2%) | 50 | 67 |
| 47 | LL | 172/177 (97%) | 165 (96%) | 7 (4%) | 30 | 43 |
| 48 | LV | 102/107 (95%) | 97 (95%) | 5 (5%) | 25 | 35 |
| 49 | LM | 116/161 (72%) | 113 (97%) | 3 (3%) | 46 | 63 |
| 50 | La | 119/120 (99%) | 114 (96%) | 5 (4%) | 30 | 42 |
| 51 | LN | 171/172 (99%) | 169 (99%) | 2 (1%) | 71 | 84 |
| 52 | LI | 173/181 (96%) | 167 (96%) | 6 (4%) | 36 | 50 |
| 53 | LD | 247/250 (99%) | 232 (94%) | 15 (6%) | 18 | 25 |
| 54 | LQ | 164/165 (99%) | 161 (98%) | 3 (2%) | 59 | 75 |
| 55 | LR | 166/175 (95%) | 156 (94%) | 10 (6%) | 19 | 26 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|------------|----------|-------------|-----|
| 56 | LS | 157/157 (100%) | 155 (99%) | 2 (1%) | 69 | 82 |
| 57 | LT | 141/140 (101%) | 139 (99%) | 2 (1%) | 67 | 81 |
| 58 | LP | 135/163 (83%) | 128 (95%) | 7 (5%) | 23 | 32 |
| 59 | LU | 89/115 (77%) | 83 (93%) | 6 (7%) | 16 | 21 |
| 60 | LX | 106/133 (80%) | 103 (97%) | 3 (3%) | 43 | 60 |
| 61 | LY | 124/135 (92%) | 117 (94%) | 7 (6%) | 21 | 29 |
| 62 | LW | 96/126 (76%) | 89 (93%) | 7 (7%) | 14 | 18 |
| 63 | LZ | 118/118 (100%) | 114 (97%) | 4 (3%) | 37 | 51 |
| 64 | Lr | 109/120 (91%) | 106 (97%) | 3 (3%) | 43 | 60 |
| 65 | Lh | 109/110 (99%) | 106 (97%) | 3 (3%) | 43 | 60 |
| 66 | Lb | 90/125 (72%) | 83 (92%) | 7 (8%) | 12 | 16 |
| 67 | LF | 194/215 (90%) | 192 (99%) | 2 (1%) | 76 | 87 |
| 68 | Lc | 84/97 (87%) | 83 (99%) | 1 (1%) | 71 | 84 |
| 69 | Ld | 98/110 (89%) | 95 (97%) | 3 (3%) | 40 | 55 |
| 70 | Le | 114/121 (94%) | 112 (98%) | 2 (2%) | 59 | 75 |
| 71 | Lf | 89/89 (100%) | 86 (97%) | 3 (3%) | 37 | 51 |
| 72 | Lg | 98/100 (98%) | 93 (95%) | 5 (5%) | 24 | 33 |
| 73 | Li | 86/89 (97%) | 80 (93%) | 6 (7%) | 15 | 19 |
| 74 | Lj | 74/80 (92%) | 69 (93%) | 5 (7%) | 16 | 21 |
| 75 | Lk | 64/65 (98%) | 62 (97%) | 2 (3%) | 40 | 55 |
| 76 | Ll | 47/48 (98%) | 47 (100%) | 0 | 100 | 100 |
| 77 | Lm | 47/115 (41%) | 43 (92%) | 4 (8%) | 10 | 13 |
| 78 | Ln | 24/24 (100%) | 22 (92%) | 2 (8%) | 11 | 14 |
| 79 | Lo | 94/93 (101%) | 86 (92%) | 8 (8%) | 10 | 13 |
| 80 | Lp | 75/75 (100%) | 73 (97%) | 2 (3%) | 44 | 61 |
| 83 | 5A | 114/127 (90%) | 109 (96%) | 5 (4%) | 28 | 39 |
| All | All | 10142/11170 (91%) | 9630 (95%) | 512 (5%) | 28 | 34 |

5 of 512 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67 | LF | 238 | ASP |
| 72 | Lg | 73 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67 | LF | 44 | LYS |
| 27 | SP | 140 | ARG |
| 27 | SP | 55 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | SV | 2 | GLN |
| 50 | La | 89 | ASN |
| 36 | Sf | 139 | HIS |
| 70 | Le | 23 | HIS |
| 40 | LB | 354 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | S2 | 1661/1869 (88%) | 298 (17%) | 2 (0%) |
| 2 | L8 | 155/156 (99%) | 26 (16%) | 0 |
| 3 | L5 | 3650/5069 (72%) | 634 (17%) | 20 (0%) |
| 4 | L7 | 119/120 (99%) | 11 (9%) | 0 |
| 81 | mR | 7/60 (11%) | 2 (28%) | 0 |
| 82 | Pt | 76/77 (98%) | 11 (14%) | 0 |
| All | All | 5668/7351 (77%) | 982 (17%) | 22 (0%) |

5 of 982 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S2 | 3 | C |
| 1 | S2 | 25 | A |
| 1 | S2 | 33 | G |
| 1 | S2 | 41 | G |
| 1 | S2 | 45 | A |

5 of 22 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | L5 | 3958 | G |
| 3 | L5 | 4449 | A |
| 3 | L5 | 4115 | G |
| 3 | L5 | 4699 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | L5 | 1482 | G |

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

235 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 | OMC | L5 | 4456 | 3 | 19,22,23 | 0.84 | 0 | 26,31,34 | 0.69 | 0 |
| 3 | PSU | L5 | 2508 | 3 | 18,21,22 | 1.31 | 2 (11%) | 22,30,33 | 1.84 | 4 (18%) |
| 3 | PSU | L5 | 2632 | 3 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.90 | 4 (18%) |
| 1 | OMG | S2 | 1447 | 1 | 18,26,27 | 0.98 | 1 (5%) | 19,38,41 | 1.12 | 2 (10%) |
| 1 | PSU | S2 | 814 | 1 | 18,21,22 | 1.43 | 3 (16%) | 22,30,33 | 1.89 | 3 (13%) |
| 3 | PSU | L5 | 1779 | 3 | 18,21,22 | 1.41 | 4 (22%) | 22,30,33 | 1.93 | 3 (13%) |
| 1 | G7M | S2 | 1639 | 82,1 | 20,26,27 | 2.55 | 5 (25%) | 17,39,42 | 1.07 | 2 (11%) |
| 1 | PSU | S2 | 1244 | 1 | 18,21,22 | 1.41 | 4 (22%) | 22,30,33 | 1.97 | 3 (13%) |
| 3 | PSU | L5 | 3695 | 3 | 18,21,22 | 1.41 | 4 (22%) | 22,30,33 | 2.00 | 3 (13%) |
| 3 | PSU | L5 | 3920 | 87,3 | 18,21,22 | 1.43 | 3 (16%) | 22,30,33 | 2.15 | 4 (18%) |
| 3 | PSU | L5 | 4361 | 3 | 18,21,22 | 1.41 | 3 (16%) | 22,30,33 | 1.93 | 4 (18%) |
| 3 | OMG | L5 | 1625 | 86,87,3 | 18,26,27 | 1.07 | 1 (5%) | 19,38,41 | 1.27 | 4 (21%) |
| 1 | MA6 | S2 | 1850 | 1 | 19,26,27 | 0.83 | 0 | 18,38,41 | 1.49 | 3 (16%) |
| 3 | PSU | L5 | 4431 | 3 | 18,21,22 | 1.42 | 3 (16%) | 22,30,33 | 1.86 | 4 (18%) |
| 3 | PSU | L5 | 2843 | 3 | 18,21,22 | 1.46 | 3 (16%) | 22,30,33 | 2.08 | 5 (22%) |
| 1 | OMG | S2 | 601 | 1 | 18,26,27 | 1.03 | 1 (5%) | 19,38,41 | 1.04 | 2 (10%) |
| 1 | OMG | S2 | 436 | 1 | 18,26,27 | 1.01 | 1 (5%) | 19,38,41 | 1.18 | 2 (10%) |
| 3 | OMG | L5 | 4618 | 3 | 18,26,27 | 0.91 | 1 (5%) | 19,38,41 | 1.22 | 2 (10%) |
| 1 | A2M | S2 | 468 | 1 | 18,25,26 | 0.96 | 1 (5%) | 18,36,39 | 1.29 | 3 (16%) |
| 1 | PSU | S2 | 1239 | 1 | 18,21,22 | 1.43 | 4 (22%) | 22,30,33 | 1.98 | 3 (13%) |
| 1 | PSU | S2 | 815 | 1 | 18,21,22 | 1.39 | 3 (16%) | 22,30,33 | 1.90 | 4 (18%) |
| 3 | PSU | L5 | 4552 | 3 | 18,21,22 | 1.50 | 5 (27%) | 22,30,33 | 1.88 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | PSU | S2 | 649 | 1 | 18,21,22 | 1.39 | 4 (22%) | 22,30,33 | 2.03 | 3 (13%) |
| 1 | A2M | S2 | 1031 | 1 | 18,25,26 | 0.91 | 1 (5%) | 18,36,39 | 1.30 | 3 (16%) |
| 1 | PSU | S2 | 651 | 1 | 18,21,22 | 1.45 | 4 (22%) | 22,30,33 | 1.98 | 3 (13%) |
| 3 | PSU | L5 | 4293 | 3 | 18,21,22 | 1.46 | 3 (16%) | 22,30,33 | 1.98 | 5 (22%) |
| 1 | OMU | S2 | 1442 | 1,87 | 19,22,23 | 1.26 | 3 (15%) | 26,31,34 | 1.70 | 4 (15%) |
| 3 | OMC | L5 | 2804 | 3 | 19,22,23 | 0.81 | 0 | 26,31,34 | 0.95 | 2 (7%) |
| 40 | HIC | LB | 245 | 40 | 8,11,12 | 1.62 | 2 (25%) | 6,14,16 | 1.10 | 0 |
| 3 | A2M | L5 | 4590 | 3 | 18,25,26 | 1.02 | 2 (11%) | 18,36,39 | 1.50 | 4 (22%) |
| 3 | PSU | L5 | 4296 | 3 | 18,21,22 | 1.44 | 4 (22%) | 22,30,33 | 2.01 | 4 (18%) |
| 3 | OMU | L5 | 2837 | 3 | 19,22,23 | 1.33 | 3 (15%) | 26,31,34 | 1.93 | 6 (23%) |
| 3 | OMC | L5 | 3808 | 87,3 | 19,22,23 | 0.83 | 0 | 26,31,34 | 0.80 | 1 (3%) |
| 1 | OMU | S2 | 354 | 1 | 19,22,23 | 1.26 | 3 (15%) | 26,31,34 | 1.68 | 4 (15%) |
| 3 | PSU | L5 | 3729 | 3 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 1.95 | 3 (13%) |
| 3 | OMG | L5 | 4370 | 3 | 18,26,27 | 0.91 | 1 (5%) | 19,38,41 | 1.15 | 3 (15%) |
| 3 | A2M | L5 | 1871 | 87,3 | 18,25,26 | 0.82 | 0 | 18,36,39 | 1.52 | 2 (11%) |
| 3 | A2M | L5 | 3718 | 3 | 18,25,26 | 0.94 | 1 (5%) | 18,36,39 | 1.17 | 2 (11%) |
| 1 | OMC | S2 | 1703 | 1,87 | 19,22,23 | 0.77 | 0 | 26,31,34 | 0.73 | 0 |
| 3 | PSU | L5 | 4531 | 3 | 18,21,22 | 1.39 | 4 (22%) | 22,30,33 | 1.94 | 3 (13%) |
| 3 | OMC | L5 | 4536 | 3 | 19,22,23 | 0.90 | 2 (10%) | 26,31,34 | 0.95 | 1 (3%) |
| 3 | A2M | L5 | 1326 | 3 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.68 | 5 (27%) |
| 3 | OMG | L5 | 2876 | 3 | 18,26,27 | 1.05 | 1 (5%) | 19,38,41 | 1.16 | 2 (10%) |
| 1 | PSU | S2 | 1232 | 1 | 18,21,22 | 1.49 | 4 (22%) | 22,30,33 | 2.00 | 4 (18%) |
| 3 | PSU | L5 | 1744 | 87,3 | 18,21,22 | 1.43 | 3 (16%) | 22,30,33 | 1.93 | 3 (13%) |
| 1 | OMG | S2 | 1490 | 1,87 | 18,26,27 | 1.04 | 1 (5%) | 19,38,41 | 1.25 | 3 (15%) |
| 3 | PSU | L5 | 4423 | 3 | 18,21,22 | 1.46 | 3 (16%) | 22,30,33 | 2.02 | 4 (18%) |
| 1 | PSU | S2 | 609 | 1 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.94 | 3 (13%) |
| 3 | PSU | L5 | 3851 | 87,3 | 18,21,22 | 1.46 | 4 (22%) | 22,30,33 | 1.98 | 6 (27%) |
| 1 | PSU | S2 | 866 | 1 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 1.94 | 3 (13%) |
| 3 | OMG | L5 | 1316 | 3 | 18,26,27 | 1.05 | 1 (5%) | 19,38,41 | 1.34 | 3 (15%) |
| 6 | SAC | SA | 2 | 6 | 7,8,9 | 3.75 | 2 (28%) | 8,9,11 | 4.33 | 4 (50%) |
| 3 | PSU | L5 | 4569 | 3 | 18,21,22 | 1.46 | 4 (22%) | 22,30,33 | 2.12 | 6 (27%) |
| 3 | OMC | L5 | 2365 | 87,3 | 19,22,23 | 0.79 | 0 | 26,31,34 | 0.78 | 0 |
| 3 | PSU | L5 | 4353 | 3 | 18,21,22 | 1.51 | 4 (22%) | 22,30,33 | 2.12 | 3 (13%) |
| 1 | OMU | S2 | 116 | 1 | 19,22,23 | 1.27 | 3 (15%) | 26,31,34 | 1.67 | 4 (15%) |
| 1 | PSU | S2 | 1081 | 1 | 18,21,22 | 1.46 | 4 (22%) | 22,30,33 | 1.94 | 5 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | A2M | L5 | 398 | 3 | 18,25,26 | 0.99 | 1 (5%) | 18,36,39 | 1.23 | 2 (11%) |
| 3 | OMG | L5 | 4499 | 3 | 18,26,27 | 0.97 | 1 (5%) | 19,38,41 | 1.13 | 2 (10%) |
| 3 | PSU | L5 | 3762 | 3 | 18,21,22 | 1.38 | 3 (16%) | 22,30,33 | 1.91 | 3 (13%) |
| 1 | A2M | S2 | 512 | 1 | 18,25,26 | 0.91 | 1 (5%) | 18,36,39 | 1.17 | 2 (11%) |
| 1 | OMC | S2 | 174 | 1 | 19,22,23 | 0.80 | 0 | 26,31,34 | 0.87 | 0 |
| 1 | PSU | S2 | 406 | 1 | 18,21,22 | 1.43 | 4 (22%) | 22,30,33 | 1.96 | 4 (18%) |
| 3 | PSU | L5 | 4493 | 87,3 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.88 | 3 (13%) |
| 3 | PSU | L5 | 3639 | 3 | 18,21,22 | 1.69 | 4 (22%) | 22,30,33 | 1.88 | 5 (22%) |
| 3 | A2M | L5 | 3724 | 3 | 18,25,26 | 0.96 | 1 (5%) | 18,36,39 | 1.27 | 2 (11%) |
| 1 | PSU | S2 | 1174 | 1,87 | 18,21,22 | 1.44 | 4 (22%) | 22,30,33 | 1.94 | 4 (18%) |
| 64 | SAC | Lr | 2 | 64 | 7,8,9 | 3.76 | 2 (28%) | 8,9,11 | 4.27 | 4 (50%) |
| 1 | PSU | S2 | 918 | 1 | 18,21,22 | 1.55 | 5 (27%) | 22,30,33 | 2.13 | 5 (22%) |
| 1 | PSU | S2 | 1004 | 1 | 18,21,22 | 1.60 | 5 (27%) | 22,30,33 | 2.02 | 4 (18%) |
| 3 | A2M | L5 | 4523 | 87,3 | 18,25,26 | 0.88 | 1 (5%) | 18,36,39 | 1.44 | 3 (16%) |
| 3 | PSU | L5 | 4532 | 3 | 18,21,22 | 1.55 | 3 (16%) | 22,30,33 | 1.81 | 4 (18%) |
| 3 | 1MA | L5 | 1322 | 87,3 | 16,25,26 | 1.45 | 3 (18%) | 18,37,40 | 1.23 | 3 (16%) |
| 1 | PSU | S2 | 822 | 1 | 18,21,22 | 1.45 | 3 (16%) | 22,30,33 | 2.13 | 5 (22%) |
| 1 | PSU | S2 | 1243 | 1 | 18,21,22 | 1.45 | 4 (22%) | 22,30,33 | 1.98 | 3 (13%) |
| 3 | PSU | L5 | 3715 | 3 | 18,21,22 | 1.41 | 4 (22%) | 22,30,33 | 2.05 | 4 (18%) |
| 3 | PSU | L5 | 1782 | 3 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 1.96 | 3 (13%) |
| 1 | A2M | S2 | 27 | 1,87 | 18,25,26 | 0.94 | 1 (5%) | 18,36,39 | 1.28 | 3 (16%) |
| 3 | PSU | L5 | 3637 | 86,87,3 | 18,21,22 | 1.39 | 2 (11%) | 22,30,33 | 2.25 | 3 (13%) |
| 82 | H2U | Pt | 21 | 82 | 18,21,22 | 0.97 | 2 (11%) | 21,30,33 | 1.42 | 2 (9%) |
| 1 | PSU | S2 | 801 | 1 | 18,21,22 | 1.38 | 3 (16%) | 22,30,33 | 1.94 | 4 (18%) |
| 3 | A2M | L5 | 3825 | 3 | 18,25,26 | 1.00 | 1 (5%) | 18,36,39 | 1.43 | 4 (22%) |
| 1 | PSU | S2 | 1692 | 1 | 18,21,22 | 1.45 | 4 (22%) | 22,30,33 | 1.94 | 3 (13%) |
| 3 | PSU | L5 | 4471 | 3 | 18,21,22 | 1.41 | 3 (16%) | 22,30,33 | 1.82 | 3 (13%) |
| 3 | PSU | L5 | 4500 | 3 | 18,21,22 | 1.38 | 4 (22%) | 22,30,33 | 2.03 | 4 (18%) |
| 3 | PSU | L5 | 1536 | 3 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 2.09 | 4 (18%) |
| 3 | OMG | L5 | 2364 | 3 | 18,26,27 | 1.23 | 1 (5%) | 19,38,41 | 1.16 | 2 (10%) |
| 39 | V5N | LA | 216 | 39 | 4,11,12 | 0.38 | 0 | 5,14,16 | 1.61 | 2 (40%) |
| 3 | OMC | L5 | 3841 | 3 | 19,22,23 | 0.82 | 1 (5%) | 26,31,34 | 0.94 | 0 |
| 1 | A2M | S2 | 668 | 1,87 | 18,25,26 | 0.93 | 1 (5%) | 18,36,39 | 1.60 | 4 (22%) |
| 1 | PSU | S2 | 573 | 1 | 18,21,22 | 1.41 | 3 (16%) | 22,30,33 | 1.93 | 3 (13%) |
| 79 | MLZ | Lo | 53 | 79 | 8,9,10 | 0.72 | 0 | 4,9,11 | 0.80 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | OMG | S2 | 1328 | 1,86 | 18,26,27 | 0.96 | 1 (5%) | 19,38,41 | 1.05 | 2 (10%) |
| 3 | OMG | L5 | 4637 | 86,3 | 18,26,27 | 1.00 | 1 (5%) | 19,38,41 | 1.11 | 2 (10%) |
| 2 | OMG | L8 | 75 | 2 | 18,26,27 | 0.95 | 1 (5%) | 19,38,41 | 1.10 | 2 (10%) |
| 1 | PSU | S2 | 36 | 1 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.90 | 3 (13%) |
| 1 | OMU | S2 | 428 | 1 | 19,22,23 | 1.22 | 3 (15%) | 26,31,34 | 1.75 | 5 (19%) |
| 3 | OMC | L5 | 2351 | 87,3 | 19,22,23 | 0.83 | 0 | 26,31,34 | 1.20 | 3 (11%) |
| 3 | OMU | L5 | 2415 | 3 | 19,22,23 | 1.29 | 2 (10%) | 26,31,34 | 1.71 | 5 (19%) |
| 3 | PSU | L5 | 1683 | 86,3 | 18,21,22 | 1.44 | 4 (22%) | 22,30,33 | 2.05 | 3 (13%) |
| 1 | OMC | S2 | 462 | 1 | 19,22,23 | 0.81 | 0 | 26,31,34 | 0.80 | 0 |
| 1 | PSU | S2 | 1367 | 1 | 18,21,22 | 1.47 | 4 (22%) | 22,30,33 | 1.96 | 3 (13%) |
| 1 | MA6 | S2 | 1851 | 1 | 19,26,27 | 0.79 | 1 (5%) | 18,38,41 | 1.51 | 3 (16%) |
| 1 | A2M | S2 | 1383 | 1 | 18,25,26 | 1.01 | 1 (5%) | 18,36,39 | 1.32 | 2 (11%) |
| 3 | A2M | L5 | 3785 | 3 | 18,25,26 | 0.89 | 0 | 18,36,39 | 1.47 | 2 (11%) |
| 3 | PSU | L5 | 2839 | 3 | 18,21,22 | 1.60 | 3 (16%) | 22,30,33 | 1.79 | 4 (18%) |
| 1 | PSU | S2 | 119 | 1 | 18,21,22 | 1.37 | 4 (22%) | 22,30,33 | 1.96 | 4 (18%) |
| 3 | A2M | L5 | 1534 | 87,3 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.37 | 3 (16%) |
| 3 | A2M | L5 | 3830 | 3 | 18,25,26 | 0.90 | 1 (5%) | 18,36,39 | 1.51 | 3 (16%) |
| 3 | PSU | L5 | 3758 | 3 | 18,21,22 | 1.44 | 4 (22%) | 22,30,33 | 1.94 | 4 (18%) |
| 1 | PSU | S2 | 1136 | 1 | 18,21,22 | 1.44 | 3 (16%) | 22,30,33 | 2.06 | 4 (18%) |
| 1 | PSU | S2 | 93 | 1 | 18,21,22 | 1.52 | 3 (16%) | 22,30,33 | 1.81 | 4 (18%) |
| 1 | PSU | S2 | 109 | 1,86 | 18,21,22 | 1.66 | 6 (33%) | 22,30,33 | 2.18 | 4 (18%) |
| 1 | OMG | S2 | 683 | 1 | 18,26,27 | 0.91 | 1 (5%) | 19,38,41 | 1.20 | 2 (10%) |
| 3 | OMG | L5 | 3744 | 3 | 18,26,27 | 0.88 | 1 (5%) | 19,38,41 | 1.24 | 3 (15%) |
| 3 | OMC | L5 | 2861 | 3 | 19,22,23 | 0.75 | 0 | 26,31,34 | 0.71 | 0 |
| 3 | PSU | L5 | 1792 | 3 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 1.90 | 3 (13%) |
| 3 | OMC | L5 | 3887 | 3 | 19,22,23 | 0.84 | 0 | 26,31,34 | 0.80 | 0 |
| 3 | OMU | L5 | 4227 | 3 | 19,22,23 | 1.25 | 2 (10%) | 26,31,34 | 1.73 | 5 (19%) |
| 3 | OMU | L5 | 4306 | 3 | 19,22,23 | 1.21 | 2 (10%) | 26,31,34 | 1.50 | 5 (19%) |
| 3 | PSU | L5 | 4521 | 86,87,3 | 18,21,22 | 1.48 | 3 (16%) | 22,30,33 | 2.03 | 5 (22%) |
| 3 | OMG | L5 | 4623 | 3 | 18,26,27 | 1.01 | 1 (5%) | 19,38,41 | 1.04 | 2 (10%) |
| 3 | A2M | L5 | 2815 | 87,3 | 18,25,26 | 0.86 | 0 | 18,36,39 | 1.41 | 2 (11%) |
| 3 | OMG | L5 | 1522 | 3 | 18,26,27 | 0.89 | 0 | 19,38,41 | 1.26 | 4 (21%) |
| 3 | OMG | L5 | 4196 | 87,82,3 | 18,26,27 | 1.00 | 1 (5%) | 19,38,41 | 0.98 | 2 (10%) |
| 3 | PSU | L5 | 5001 | 87,3 | 18,21,22 | 1.53 | 4 (22%) | 22,30,33 | 2.06 | 5 (22%) |
| 1 | PSU | S2 | 572 | 1 | 18,21,22 | 1.42 | 3 (16%) | 22,30,33 | 1.97 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | PSU | S2 | 296 | 1 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.95 | 3 (13%) |
| 1 | 6MZ | S2 | 1832 | 87,1,86 | 18,25,26 | 0.82 | 1 (5%) | 16,36,39 | 2.38 | 3 (18%) |
| 83 | 5CT | 5A | 50[B] | - | 13,14,15 | 1.06 | 1 (7%) | 9,15,17 | 1.09 | 0 |
| 29 | AME | SV | 1 | 29 | 9,10,11 | 3.20 | 2 (22%) | 9,11,13 | 4.44 | 4 (44%) |
| 3 | PSU | L5 | 3734 | 3 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.88 | 4 (18%) |
| 3 | OMG | L5 | 4392 | 3 | 18,26,27 | 0.95 | 1 (5%) | 19,38,41 | 1.09 | 2 (10%) |
| 1 | 4AC | S2 | 1842 | 1 | 21,24,25 | 1.10 | 2 (9%) | 29,34,37 | 1.26 | 5 (17%) |
| 50 | V5N | La | 39 | 50 | 4,11,12 | 0.52 | 0 | 5,14,16 | 1.99 | 3 (60%) |
| 3 | PSU | L5 | 3884 | 87,3 | 18,21,22 | 1.43 | 3 (16%) | 22,30,33 | 2.12 | 4 (18%) |
| 20 | HY3 | SX | 62 | 20 | 6,8,9 | 1.43 | 1 (16%) | 5,10,12 | 1.13 | 0 |
| 1 | OMU | S2 | 121 | 1 | 19,22,23 | 1.29 | 3 (15%) | 26,31,34 | 1.70 | 4 (15%) |
| 3 | PSU | L5 | 3844 | 3 | 18,21,22 | 1.50 | 5 (27%) | 22,30,33 | 1.95 | 4 (18%) |
| 1 | PSU | S2 | 1625 | 1 | 18,21,22 | 1.44 | 3 (16%) | 22,30,33 | 1.95 | 3 (13%) |
| 1 | PSU | S2 | 34 | 1 | 18,21,22 | 1.44 | 4 (22%) | 22,30,33 | 2.03 | 4 (18%) |
| 2 | OMU | L8 | 14 | 2,3 | 19,22,23 | 1.27 | 3 (15%) | 26,31,34 | 1.55 | 5 (19%) |
| 3 | PSU | L5 | 4457 | 3 | 18,21,22 | 1.52 | 4 (22%) | 22,30,33 | 1.79 | 3 (13%) |
| 1 | A2M | S2 | 159 | 1 | 18,25,26 | 0.96 | 1 (5%) | 18,36,39 | 1.26 | 2 (11%) |
| 1 | OMG | S2 | 509 | 1,87 | 18,26,27 | 0.92 | 1 (5%) | 19,38,41 | 1.15 | 2 (10%) |
| 1 | A2M | S2 | 166 | 1 | 18,25,26 | 0.99 | 1 (5%) | 18,36,39 | 1.22 | 2 (11%) |
| 3 | 5MC | L5 | 3782 | 87,3 | 18,22,23 | 1.04 | 2 (11%) | 26,32,35 | 1.18 | 3 (11%) |
| 3 | OMC | L5 | 2824 | 3 | 19,22,23 | 0.83 | 1 (5%) | 26,31,34 | 0.84 | 0 |
| 3 | OMG | L5 | 3944 | 3 | 18,26,27 | 0.96 | 1 (5%) | 19,38,41 | 1.12 | 2 (10%) |
| 3 | A2M | L5 | 2401 | 3 | 18,25,26 | 0.95 | 1 (5%) | 18,36,39 | 1.37 | 2 (11%) |
| 3 | PSU | L5 | 4442 | 3 | 18,21,22 | 1.47 | 5 (27%) | 22,30,33 | 1.99 | 5 (22%) |
| 1 | PSU | S2 | 686 | 1 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.96 | 3 (13%) |
| 3 | PSU | L5 | 4972 | 3 | 18,21,22 | 1.62 | 5 (27%) | 22,30,33 | 2.15 | 5 (22%) |
| 3 | OMC | L5 | 2422 | 87,3 | 19,22,23 | 0.83 | 0 | 26,31,34 | 0.79 | 0 |
| 3 | PSU | L5 | 4576 | 3 | 18,21,22 | 1.41 | 4 (22%) | 22,30,33 | 1.95 | 3 (13%) |
| 1 | PSU | S2 | 105 | 1 | 18,21,22 | 1.50 | 4 (22%) | 22,30,33 | 2.02 | 4 (18%) |
| 3 | PSU | L5 | 4636 | 3 | 18,21,22 | 1.50 | 4 (22%) | 22,30,33 | 1.95 | 4 (18%) |
| 3 | PSU | L5 | 4673 | 87,3 | 18,21,22 | 1.44 | 3 (16%) | 22,30,33 | 1.92 | 5 (22%) |
| 1 | A2M | S2 | 99 | 1,87 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.22 | 2 (11%) |
| 3 | UY1 | L5 | 3818 | 86,87,3 | 19,22,23 | 1.49 | 4 (21%) | 22,31,34 | 1.85 | 4 (18%) |
| 1 | OMU | S2 | 172 | 1 | 19,22,23 | 1.25 | 4 (21%) | 26,31,34 | 1.77 | 5 (19%) |
| 3 | PSU | L5 | 1677 | 3 | 18,21,22 | 1.52 | 5 (27%) | 22,30,33 | 2.21 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 66 | MLZ | Lb | 5 | 66 | 8,9,10 | 0.95 | 0 | 4,9,11 | 1.17 | 1 (25%) |
| 1 | OMC | S2 | 517 | 1 | 19,22,23 | 0.80 | 0 | 26,31,34 | 0.68 | 0 |
| 77 | M3L | Lm | 98 | 77 | 10,11,12 | 0.55 | 0 | 9,14,16 | 0.49 | 0 |
| 1 | A2M | S2 | 484 | 1 | 18,25,26 | 0.95 | 1 (5%) | 18,36,39 | 1.26 | 2 (11%) |
| 3 | A2M | L5 | 3723 | 3 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.18 | 2 (11%) |
| 3 | OMC | L5 | 3701 | 86,3 | 19,22,23 | 0.84 | 0 | 26,31,34 | 0.98 | 0 |
| 3 | OMC | L5 | 3869 | 3 | 19,22,23 | 0.85 | 1 (5%) | 26,31,34 | 1.04 | 1 (3%) |
| 3 | OMG | L5 | 3627 | 3 | 18,26,27 | 0.99 | 1 (5%) | 19,38,41 | 1.21 | 2 (10%) |
| 3 | PSU | L5 | 3853 | 87,3 | 18,21,22 | 1.42 | 3 (16%) | 22,30,33 | 2.12 | 4 (18%) |
| 1 | UY1 | S2 | 1326 | 1,87 | 19,22,23 | 1.47 | 4 (21%) | 22,31,34 | 2.14 | 4 (18%) |
| 1 | A2M | S2 | 590 | 1 | 18,25,26 | 0.95 | 1 (5%) | 18,36,39 | 1.21 | 2 (11%) |
| 3 | A2M | L5 | 3760 | 87,1,3 | 18,25,26 | 0.99 | 1 (5%) | 18,36,39 | 1.14 | 2 (11%) |
| 2 | PSU | L8 | 55 | 2 | 18,21,22 | 1.43 | 3 (16%) | 22,30,33 | 1.93 | 4 (18%) |
| 3 | PSU | L5 | 5010 | 3 | 18,21,22 | 1.47 | 4 (22%) | 22,30,33 | 1.99 | 3 (13%) |
| 3 | PSU | L5 | 1582 | 3 | 18,21,22 | 1.50 | 4 (22%) | 22,30,33 | 1.95 | 4 (18%) |
| 1 | PSU | S2 | 966 | 1 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.92 | 3 (13%) |
| 82 | OMC | Pt | 33 | 82 | 19,22,23 | 0.82 | 0 | 26,31,34 | 0.72 | 0 |
| 2 | PSU | L8 | 69 | 2 | 18,21,22 | 1.44 | 3 (16%) | 22,30,33 | 1.94 | 4 (18%) |
| 3 | A2M | L5 | 2363 | 87,3 | 18,25,26 | 1.00 | 0 | 18,36,39 | 1.32 | 2 (11%) |
| 3 | 6MZ | L5 | 4220 | 3 | 18,25,26 | 0.86 | 1 (5%) | 16,36,39 | 2.52 | 4 (25%) |
| 3 | UR3 | L5 | 4530 | 3 | 19,22,23 | 0.83 | 1 (5%) | 26,32,35 | 1.50 | 2 (7%) |
| 1 | A2M | S2 | 1678 | 1 | 18,25,26 | 0.96 | 1 (5%) | 18,36,39 | 1.25 | 2 (11%) |
| 1 | PSU | S2 | 218 | 1 | 18,21,22 | 1.41 | 4 (22%) | 22,30,33 | 1.95 | 4 (18%) |
| 3 | OMU | L5 | 4498 | 87,3 | 19,22,23 | 1.30 | 3 (15%) | 26,31,34 | 1.77 | 5 (19%) |
| 1 | B8N | S2 | 1248 | 1 | 24,29,30 | 0.91 | 1 (4%) | 29,42,45 | 1.64 | 7 (24%) |
| 1 | OMU | S2 | 1804 | 1 | 19,22,23 | 1.30 | 3 (15%) | 26,31,34 | 1.82 | 5 (19%) |
| 82 | 4SU | Pt | 8 | 82 | 18,21,22 | 2.03 | 4 (22%) | 26,30,33 | 2.40 | 5 (19%) |
| 1 | PSU | S2 | 1445 | 1 | 18,21,22 | 1.37 | 3 (16%) | 22,30,33 | 1.90 | 3 (13%) |
| 3 | OMC | L5 | 1881 | 87,3 | 19,22,23 | 0.83 | 0 | 26,31,34 | 1.05 | 1 (3%) |
| 1 | OMG | S2 | 867 | 1 | 18,26,27 | 0.90 | 1 (5%) | 19,38,41 | 1.09 | 2 (10%) |
| 1 | A2M | S2 | 576 | 1 | 18,25,26 | 0.93 | 1 (5%) | 18,36,39 | 1.21 | 2 (11%) |
| 1 | PSU | S2 | 1238 | 1 | 18,21,22 | 1.40 | 4 (22%) | 22,30,33 | 1.91 | 3 (13%) |
| 1 | OMU | S2 | 1288 | 1 | 19,22,23 | 1.27 | 3 (15%) | 26,31,34 | 1.87 | 6 (23%) |
| 3 | OMU | L5 | 3925 | 3 | 19,22,23 | 1.30 | 2 (10%) | 26,31,34 | 1.91 | 5 (19%) |
| 3 | PSU | L5 | 4403 | 3 | 18,21,22 | 1.46 | 4 (22%) | 22,30,33 | 1.99 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | PSU | L5 | 4312 | 3 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 1.86 | 3 (13%) |
| 1 | OMC | S2 | 1391 | 1 | 19,22,23 | 0.81 | 0 | 26,31,34 | 0.82 | 0 |
| 3 | PSU | L5 | 3764 | 3 | 18,21,22 | 1.45 | 4 (22%) | 22,30,33 | 1.90 | 3 (13%) |
| 1 | PSU | S2 | 1056 | 1 | 18,21,22 | 1.43 | 3 (16%) | 22,30,33 | 1.98 | 5 (22%) |
| 3 | A2M | L5 | 4571 | 3 | 18,25,26 | 1.02 | 1 (5%) | 18,36,39 | 1.26 | 2 (11%) |
| 3 | PSU | L5 | 1860 | 3 | 18,21,22 | 1.39 | 3 (16%) | 22,30,33 | 1.85 | 4 (18%) |
| 3 | OMG | L5 | 3792 | 3 | 18,26,27 | 0.91 | 1 (5%) | 19,38,41 | 1.09 | 3 (15%) |
| 82 | G7M | Pt | 47 | 82 | 20,26,27 | 2.38 | 3 (15%) | 17,39,42 | 0.71 | 0 |
| 3 | OMG | L5 | 4228 | 3 | 18,26,27 | 0.88 | 1 (5%) | 19,38,41 | 1.27 | 3 (15%) |
| 1 | PSU | S2 | 1177 | 1 | 18,21,22 | 1.54 | 4 (22%) | 22,30,33 | 1.90 | 3 (13%) |
| 1 | OMU | S2 | 627 | 1 | 19,22,23 | 1.21 | 2 (10%) | 26,31,34 | 1.74 | 5 (19%) |
| 1 | PSU | S2 | 681 | 1 | 18,21,22 | 1.46 | 4 (22%) | 22,30,33 | 2.01 | 4 (18%) |
| 3 | OMG | L5 | 4494 | 87,3 | 18,26,27 | 1.08 | 1 (5%) | 19,38,41 | 1.17 | 2 (10%) |
| 3 | 5MC | L5 | 4447 | 86,3 | 18,22,23 | 1.03 | 2 (11%) | 26,32,35 | 1.31 | 3 (11%) |
| 82 | PSU | Pt | 56 | 82 | 18,21,22 | 1.34 | 3 (16%) | 22,30,33 | 1.94 | 4 (18%) |
| 1 | PSU | S2 | 863 | 1 | 18,21,22 | 1.40 | 4 (22%) | 22,30,33 | 1.91 | 3 (13%) |
| 3 | A2M | L5 | 3867 | 3 | 18,25,26 | 0.99 | 1 (5%) | 18,36,39 | 1.47 | 3 (16%) |
| 3 | A2M | L5 | 1524 | 3 | 18,25,26 | 0.94 | 1 (5%) | 18,36,39 | 1.52 | 2 (11%) |
| 3 | PSU | L5 | 4420 | 3 | 18,21,22 | 1.47 | 5 (27%) | 22,30,33 | 1.87 | 3 (13%) |
| 1 | PSU | S2 | 1347 | 1 | 18,21,22 | 1.49 | 4 (22%) | 22,30,33 | 1.95 | 4 (18%) |
| 83 | 5CT | 5A | 50[A] | 87 | 13,14,15 | 1.04 | 1 (7%) | 9,15,17 | 1.36 | 1 (11%) |
| 3 | A2M | L5 | 400 | 3 | 18,25,26 | 0.95 | 1 (5%) | 18,36,39 | 1.24 | 2 (11%) |
| 3 | OMU | L5 | 4620 | 3 | 19,22,23 | 1.23 | 3 (15%) | 26,31,34 | 1.81 | 5 (19%) |
| 3 | PSU | L5 | 1781 | 3 | 18,21,22 | 1.49 | 4 (22%) | 22,30,33 | 1.98 | 3 (13%) |
| 1 | 4AC | S2 | 1337 | 1 | 21,24,25 | 1.08 | 2 (9%) | 29,34,37 | 1.13 | 4 (13%) |
| 3 | PSU | L5 | 3770 | 3 | 18,21,22 | 1.47 | 5 (27%) | 22,30,33 | 1.97 | 3 (13%) |
| 3 | PSU | L5 | 4299 | 3 | 18,21,22 | 1.52 | 5 (27%) | 22,30,33 | 1.96 | 3 (13%) |
| 3 | OMG | L5 | 2424 | 3 | 18,26,27 | 0.97 | 1 (5%) | 19,38,41 | 1.04 | 2 (10%) |
| 1 | PSU | S2 | 1643 | 1,87 | 18,21,22 | 1.48 | 3 (16%) | 22,30,33 | 1.99 | 4 (18%) |
| 3 | PSU | L5 | 4628 | 3 | 18,21,22 | 1.44 | 5 (27%) | 22,30,33 | 2.02 | 5 (22%) |
| 3 | A2M | L5 | 2787 | 3 | 18,25,26 | 1.04 | 1 (5%) | 18,36,39 | 1.58 | 3 (16%) |
| 3 | PSU | L5 | 4579 | 3 | 18,21,22 | 1.45 | 4 (22%) | 22,30,33 | 1.89 | 3 (13%) |
| 3 | OMG | L5 | 3899 | 3 | 18,26,27 | 0.92 | 1 (5%) | 19,38,41 | 1.25 | 3 (15%) |
| 3 | OMC | L5 | 1340 | 3 | 19,22,23 | 0.76 | 0 | 26,31,34 | 0.92 | 0 |
| 1 | OMG | S2 | 644 | 1 | 18,26,27 | 0.98 | 1 (5%) | 19,38,41 | 1.11 | 2 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | PSU | L5 | 4689 | 3 | 18,21,22 | 1.47 | 4 (22%) | 22,30,33 | 2.04 | 4 (18%) |
| 3 | PSU | L5 | 3768 | 3 | 18,21,22 | 1.40 | 4 (22%) | 22,30,33 | 1.99 | 3 (13%) |
| 3 | PSU | L5 | 1862 | 3 | 18,21,22 | 1.55 | 3 (16%) | 22,30,33 | 1.84 | 5 (22%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|-----------|---------|
| 3 | OMC | L5 | 4456 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 2508 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 2632 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | S2 | 1447 | 1 | - | 3/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 814 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 1779 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | G7M | S2 | 1639 | 82,1 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | PSU | S2 | 1244 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 3695 | 3 | - | 1/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 3920 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4361 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 1625 | 86,87,3 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | MA6 | S2 | 1850 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 3 | PSU | L5 | 4431 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 2843 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | S2 | 601 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | S2 | 436 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMG | L5 | 4618 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | S2 | 468 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 1239 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 815 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4552 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 649 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | S2 | 1031 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 651 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4293 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | S2 | 1442 | 1,87 | - | 3/9/27/28 | 0/2/2/2 |
| 3 | OMC | L5 | 2804 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 40 | HIC | LB | 245 | 40 | - | 0/5/6/8 | 0/1/1/1 |
| 3 | A2M | L5 | 4590 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 4296 | 3 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 3 | OMU | L5 | 2837 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMC | L5 | 3808 | 87,3 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMU | S2 | 354 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 3729 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 4370 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 1871 | 87,3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 3718 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | OMC | S2 | 1703 | 1,87 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 4531 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L5 | 4536 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | A2M | L5 | 1326 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMG | L5 | 2876 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 1232 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 1744 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | S2 | 1490 | 1,87 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 4423 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 609 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 3851 | 87,3 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 866 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 1316 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 6 | SAC | SA | 2 | 6 | - | 4/7/8/10 | - |
| 3 | PSU | L5 | 4569 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L5 | 2365 | 87,3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 4353 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | S2 | 116 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | S2 | 1081 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 398 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMG | L5 | 4499 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 3762 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | S2 | 512 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMC | S2 | 174 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | S2 | 406 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4493 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 3639 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 3724 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 1174 | 1,87 | - | 0/7/25/26 | 0/2/2/2 |
| 64 | SAC | Lr | 2 | 64 | - | 4/7/8/10 | - |
| 1 | PSU | S2 | 918 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 1004 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 4523 | 87,3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 4532 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | 1MA | L5 | 1322 | 87,3 | - | 0/3/25/26 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|-----------|---------|
| 1 | PSU | S2 | 822 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 1243 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 3715 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 1782 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | S2 | 27 | 1,87 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 3637 | 86,87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 82 | H2U | Pt | 21 | 82 | - | 3/7/38/39 | 0/2/2/2 |
| 1 | PSU | S2 | 801 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 3825 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 1692 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4471 | 3 | - | 1/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4500 | 3 | - | 3/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 1536 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 2364 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 39 | V5N | LA | 216 | 39 | - | 1/5/10/12 | 0/1/1/1 |
| 3 | OMC | L5 | 3841 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | A2M | S2 | 668 | 1,87 | - | 3/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 573 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 79 | MLZ | Lo | 53 | 79 | - | 3/7/8/10 | - |
| 1 | OMG | S2 | 1328 | 1,86 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMG | L5 | 4637 | 86,3 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | OMG | L8 | 75 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 36 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | S2 | 428 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 3 | OMC | L5 | 2351 | 87,3 | - | 3/9/27/28 | 0/2/2/2 |
| 3 | OMU | L5 | 2415 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 1683 | 86,3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | S2 | 462 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 1 | PSU | S2 | 1367 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | S2 | 1851 | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 1 | A2M | S2 | 1383 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 3785 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 2839 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 119 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 1534 | 87,3 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 3830 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 3758 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 1136 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 93 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 109 | 1,86 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-------|---------|---------|------------|---------|
| 1 | OMG | S2 | 683 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | OMG | L5 | 3744 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMC | L5 | 2861 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 1792 | 3 | - | 1/7/25/26 | 0/2/2/2 |
| 3 | OMC | L5 | 3887 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMU | L5 | 4227 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMU | L5 | 4306 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 4521 | 86,87,3 | - | 2/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 4623 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 2815 | 87,3 | - | 4/5/27/28 | 0/3/3/3 |
| 3 | OMG | L5 | 1522 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMG | L5 | 4196 | 87,82,3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 5001 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 572 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 296 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 6MZ | S2 | 1832 | 87,1,86 | - | 0/5/27/28 | 0/3/3/3 |
| 83 | 5CT | 5A | 50[B] | - | - | 9/13/14/16 | - |
| 29 | AME | SV | 1 | 29 | - | 3/9/10/12 | - |
| 3 | PSU | L5 | 3734 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 4392 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 4AC | S2 | 1842 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 50 | V5N | La | 39 | 50 | - | 0/5/10/12 | 0/1/1/1 |
| 3 | PSU | L5 | 3884 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | HY3 | SX | 62 | 20 | - | 1/1/12/14 | 0/1/1/1 |
| 1 | OMU | S2 | 121 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 3844 | 3 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 1625 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 34 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | L8 | 14 | 2,3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 4457 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | S2 | 159 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | OMG | S2 | 509 | 1,87 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | S2 | 166 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | 5MC | L5 | 3782 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L5 | 2824 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMG | L5 | 3944 | 3 | - | 2/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 2401 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 4442 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 686 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4972 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L5 | 2422 | 87,3 | - | 2/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|------------|---------|
| 3 | PSU | L5 | 4576 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 105 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4636 | 3 | - | 2/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4673 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | S2 | 99 | 1,87 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | UY1 | L5 | 3818 | 86,87,3 | - | 1/9/27/28 | 0/2/2/2 |
| 1 | OMU | S2 | 172 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 1677 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 66 | MLZ | Lb | 5 | 66 | - | 0/7/8/10 | - |
| 1 | OMC | S2 | 517 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 77 | M3L | Lm | 98 | 77 | - | 0/9/10/12 | - |
| 1 | A2M | S2 | 484 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 3723 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMC | L5 | 3701 | 86,3 | - | 4/9/27/28 | 0/2/2/2 |
| 3 | OMC | L5 | 3869 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMG | L5 | 3627 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 3853 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | UY1 | S2 | 1326 | 1,87 | - | 3/9/27/28 | 0/2/2/2 |
| 1 | A2M | S2 | 590 | 1 | - | 3/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 3760 | 87,1,3 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | PSU | L8 | 55 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 5010 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 1582 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 966 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 82 | OMC | Pt | 33 | 82 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | PSU | L8 | 69 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 2363 | 87,3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | 6MZ | L5 | 4220 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | UR3 | L5 | 4530 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | S2 | 1678 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 218 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMU | L5 | 4498 | 87,3 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | B8N | S2 | 1248 | 1 | - | 2/16/34/35 | 0/2/2/2 |
| 1 | OMU | S2 | 1804 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 82 | 4SU | Pt | 8 | 82 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 1445 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | L5 | 1881 | 87,3 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMG | S2 | 867 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | A2M | S2 | 576 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 1238 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | S2 | 1288 | 1 | - | 1/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-------|------|---------|------------|---------|
| 3 | OMU | L5 | 3925 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 4403 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4312 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | S2 | 1391 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 3764 | 3 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 1056 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 4571 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 1860 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 3792 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 82 | G7M | Pt | 47 | 82 | - | 1/3/25/26 | 0/3/3/3 |
| 3 | OMG | L5 | 4228 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 1177 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | S2 | 627 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | S2 | 681 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 4494 | 87,3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | 5MC | L5 | 4447 | 86,3 | - | 4/7/25/26 | 0/2/2/2 |
| 82 | PSU | Pt | 56 | 82 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 863 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 3867 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | A2M | L5 | 1524 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 4420 | 3 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | S2 | 1347 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 83 | 5CT | 5A | 50[A] | 87 | - | 9/13/14/16 | - |
| 3 | A2M | L5 | 400 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 3 | OMU | L5 | 4620 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | L5 | 1781 | 3 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 4AC | S2 | 1337 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 3 | PSU | L5 | 3770 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4299 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 2424 | 3 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | PSU | S2 | 1643 | 1,87 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 4628 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | L5 | 2787 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 4579 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | L5 | 3899 | 3 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | OMC | L5 | 1340 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMG | S2 | 644 | 1 | - | 4/5/27/28 | 0/3/3/3 |
| 3 | PSU | L5 | 4689 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 3768 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | L5 | 1862 | 3 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 546 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 64 | Lr | 2 | SAC | OAC-C1A | 8.94 | 1.43 | 1.23 |
| 6 | SA | 2 | SAC | OAC-C1A | 8.86 | 1.43 | 1.23 |
| 29 | SV | 1 | AME | OT-CT1 | 8.71 | 1.42 | 1.23 |
| 82 | Pt | 47 | G7M | C8-N9 | 7.04 | 1.46 | 1.33 |
| 1 | S2 | 1639 | G7M | C8-N9 | 6.88 | 1.45 | 1.33 |

The worst 5 of 714 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | S2 | 1832 | 6MZ | C2-N1-C6 | 8.00 | 123.45 | 116.59 |
| 6 | SA | 2 | SAC | OAC-C1A-C2A | -7.97 | 107.26 | 122.06 |
| 29 | SV | 1 | AME | OT-CT1-N | -7.55 | 108.06 | 121.95 |
| 3 | L5 | 4220 | 6MZ | C2-N1-C6 | 7.54 | 123.06 | 116.59 |
| 82 | Pt | 8 | 4SU | C4-N3-C2 | -7.33 | 120.22 | 127.34 |

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | L8 | 14 | OMU | C1'-C2'-O2'-CM2 |
| 6 | SA | 2 | SAC | OAC-C1A-N-CA |
| 6 | SA | 2 | SAC | CB-CA-N-C1A |
| 6 | SA | 2 | SAC | O-C-CA-CB |
| 29 | SV | 1 | AME | OT-CT1-N-CA |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 636 ligands modelled in this entry, 609 are monoatomic - leaving 27 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$ |
| 84 | SPD | L5 | 5505 | - | 9,9,9 | 0.42 | 0 | 8,8,8 | 1.11 | 1 (12%) |
| 91 | MET | Pt | 78 | 82 | 6,7,8 | 0.69 | 0 | 2,7,9 | 1.99 | 1 (50%) |
| 85 | PUT | L5 | 5521 | - | 5,5,5 | 0.09 | 0 | 4,4,4 | 0.22 | 0 |
| 85 | PUT | L5 | 5515 | - | 5,5,5 | 0.15 | 0 | 4,4,4 | 0.18 | 0 |
| 84 | SPD | L5 | 5507 | - | 9,9,9 | 0.33 | 0 | 8,8,8 | 0.81 | 0 |
| 84 | SPD | L5 | 5513 | - | 9,9,9 | 0.29 | 0 | 8,8,8 | 0.80 | 0 |
| 85 | PUT | S2 | 1902 | - | 5,5,5 | 0.12 | 0 | 4,4,4 | 0.17 | 0 |
| 85 | PUT | L5 | 5522 | - | 5,5,5 | 0.07 | 0 | 4,4,4 | 0.17 | 0 |
| 84 | SPD | L5 | 5506 | - | 9,9,9 | 0.16 | 0 | 8,8,8 | 0.22 | 0 |
| 85 | PUT | L5 | 5516 | - | 5,5,5 | 0.13 | 0 | 4,4,4 | 0.18 | 0 |
| 85 | PUT | L5 | 5519 | - | 5,5,5 | 0.16 | 0 | 4,4,4 | 0.23 | 0 |
| 84 | SPD | L5 | 5511 | - | 9,9,9 | 0.28 | 0 | 8,8,8 | 0.97 | 1 (12%) |
| 85 | PUT | L5 | 5520 | - | 5,5,5 | 0.18 | 0 | 4,4,4 | 0.23 | 0 |
| 89 | 3H3 | L5 | 5523 | - | 33,34,34 | 3.33 | 13 (39%) | 34,45,45 | 3.99 | 19 (55%) |
| 84 | SPD | L5 | 5509 | - | 9,9,9 | 0.23 | 0 | 8,8,8 | 0.49 | 0 |
| 84 | SPD | L5 | 5502 | - | 9,9,9 | 0.35 | 0 | 8,8,8 | 0.71 | 0 |
| 84 | SPD | L5 | 5512 | - | 9,9,9 | 0.38 | 0 | 8,8,8 | 0.61 | 0 |
| 84 | SPD | L5 | 5504 | - | 9,9,9 | 0.39 | 0 | 8,8,8 | 1.02 | 0 |
| 85 | PUT | L5 | 5518 | - | 5,5,5 | 0.17 | 0 | 4,4,4 | 0.22 | 0 |
| 84 | SPD | S2 | 1901 | - | 9,9,9 | 0.31 | 0 | 8,8,8 | 0.68 | 0 |
| 85 | PUT | L5 | 5517 | - | 5,5,5 | 0.13 | 0 | 4,4,4 | 0.15 | 0 |
| 88 | ANM | L5 | 5501 | 86 | 20,20,20 | 1.20 | 2 (10%) | 22,27,27 | 1.58 | 5 (22%) |
| 84 | SPD | L5 | 5503 | - | 9,9,9 | 0.29 | 0 | 8,8,8 | 1.03 | 1 (12%) |
| 84 | SPD | L5 | 5508 | - | 9,9,9 | 0.36 | 0 | 8,8,8 | 0.56 | 0 |
| 85 | PUT | L5 | 5514 | - | 5,5,5 | 0.15 | 0 | 4,4,4 | 0.19 | 0 |
| 85 | PUT | S2 | 1903 | - | 5,5,5 | 0.08 | 0 | 4,4,4 | 0.17 | 0 |
| 84 | SPD | L5 | 5510 | - | 9,9,9 | 0.29 | 0 | 8,8,8 | 0.75 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 84 | SPD | L5 | 5505 | - | - | 4/7/7/7 | - |
| 91 | MET | Pt | 78 | 82 | - | 2/5/6/8 | - |
| 85 | PUT | L5 | 5521 | - | - | 0/3/3/3 | - |
| 85 | PUT | L5 | 5515 | - | - | 1/3/3/3 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 84 | SPD | L5 | 5507 | - | - | 4/7/7/7 | - |
| 84 | SPD | L5 | 5513 | - | - | 2/7/7/7 | - |
| 85 | PUT | S2 | 1902 | - | - | 1/3/3/3 | - |
| 85 | PUT | L5 | 5522 | - | - | 2/3/3/3 | - |
| 84 | SPD | L5 | 5506 | - | - | 4/7/7/7 | - |
| 85 | PUT | L5 | 5516 | - | - | 2/3/3/3 | - |
| 85 | PUT | L5 | 5519 | - | - | 1/3/3/3 | - |
| 84 | SPD | L5 | 5511 | - | - | 3/7/7/7 | - |
| 85 | PUT | L5 | 5520 | - | - | 1/3/3/3 | - |
| 89 | 3H3 | L5 | 5523 | - | - | 16/39/51/51 | 0/1/2/2 |
| 84 | SPD | L5 | 5509 | - | - | 3/7/7/7 | - |
| 84 | SPD | L5 | 5502 | - | - | 0/7/7/7 | - |
| 84 | SPD | L5 | 5512 | - | - | 2/7/7/7 | - |
| 84 | SPD | L5 | 5504 | - | - | 4/7/7/7 | - |
| 85 | PUT | L5 | 5518 | - | - | 1/3/3/3 | - |
| 84 | SPD | S2 | 1901 | - | - | 4/7/7/7 | - |
| 85 | PUT | L5 | 5517 | - | - | 0/3/3/3 | - |
| 88 | ANM | L5 | 5501 | 86 | - | 2/10/23/23 | 0/2/2/2 |
| 84 | SPD | L5 | 5503 | - | - | 3/7/7/7 | - |
| 84 | SPD | L5 | 5508 | - | - | 2/7/7/7 | - |
| 85 | PUT | L5 | 5514 | - | - | 0/3/3/3 | - |
| 85 | PUT | S2 | 1903 | - | - | 0/3/3/3 | - |
| 84 | SPD | L5 | 5510 | - | - | 4/7/7/7 | - |

The worst 5 of 15 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 89 | L5 | 5523 | 3H3 | C13-C12 | 9.39 | 1.53 | 1.33 |
| 89 | L5 | 5523 | 3H3 | O3-C22 | 7.47 | 1.38 | 1.23 |
| 89 | L5 | 5523 | 3H3 | O4-C23 | 7.09 | 1.37 | 1.23 |
| 89 | L5 | 5523 | 3H3 | C23-N | 6.52 | 1.48 | 1.37 |
| 89 | L5 | 5523 | 3H3 | C22-N | 5.47 | 1.46 | 1.37 |

The worst 5 of 28 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 89 | L5 | 5523 | 3H3 | O3-C22-N | -9.93 | 104.55 | 120.28 |
| 89 | L5 | 5523 | 3H3 | C22-N-C23 | -9.43 | 114.34 | 125.78 |
| 89 | L5 | 5523 | 3H3 | O4-C23-N | -8.53 | 106.76 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 89 | L5 | 5523 | 3H3 | O1-C11-C1 | 8.01 | 116.77 | 106.31 |
| 89 | L5 | 5523 | 3H3 | O3-C22-C21 | -6.43 | 110.10 | 122.62 |

There are no chirality outliers.

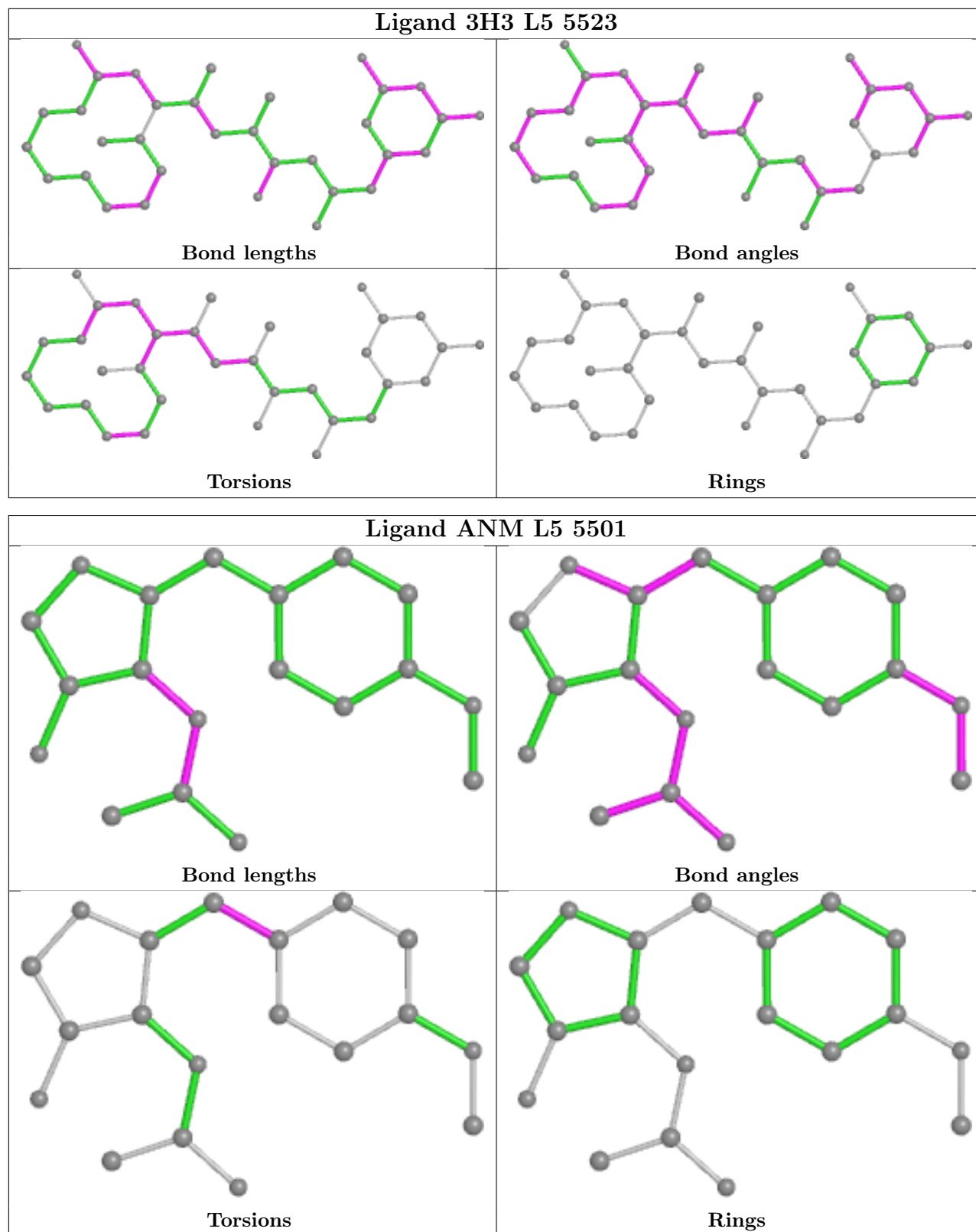
5 of 68 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 84 | S2 | 1901 | SPD | C4-C5-N6-C7 |
| 84 | L5 | 5509 | SPD | C8-C7-N6-C5 |
| 89 | L5 | 5523 | 3H3 | C2-C1-C11-O1 |
| 89 | L5 | 5523 | 3H3 | C2-C1-C11-C12 |
| 89 | L5 | 5523 | 3H3 | C-C1-C11-O1 |

There are no ring outliers.

No monomer is involved in short contacts.

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



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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

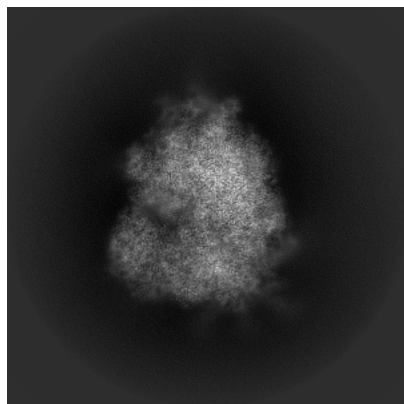
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29757. These allow visual inspection of the internal detail of the map and identification of artifacts.

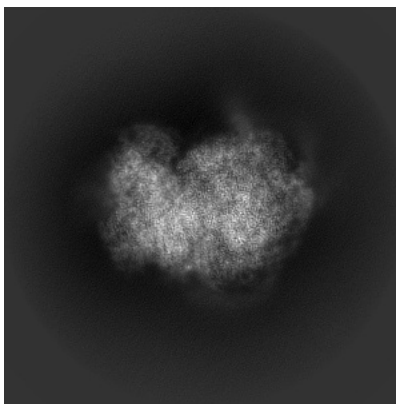
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

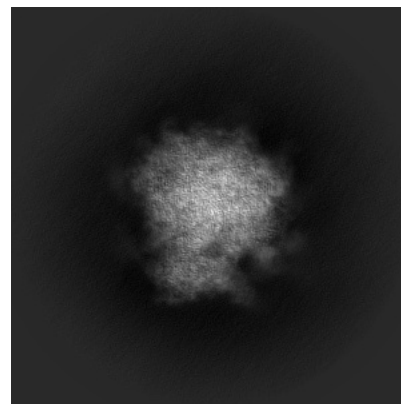
6.1.1 Primary map



X

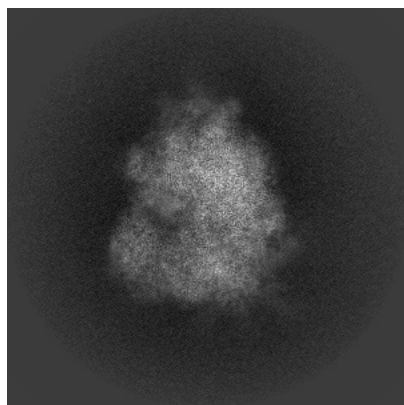


Y

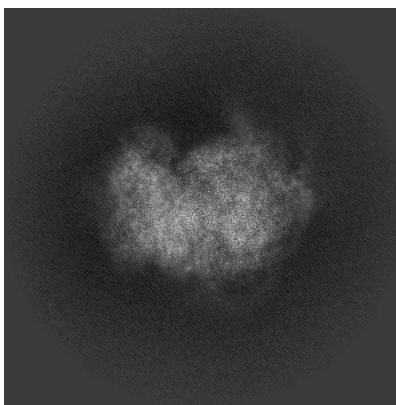


Z

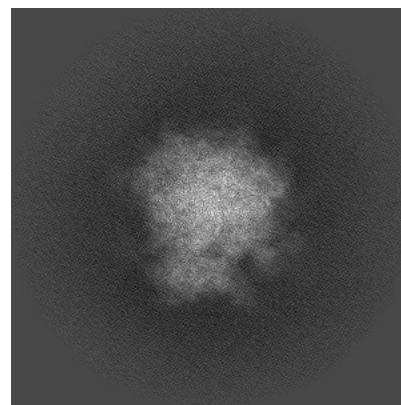
6.1.2 Raw map



X



Y

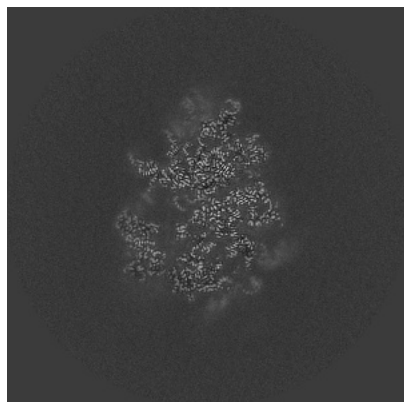


Z

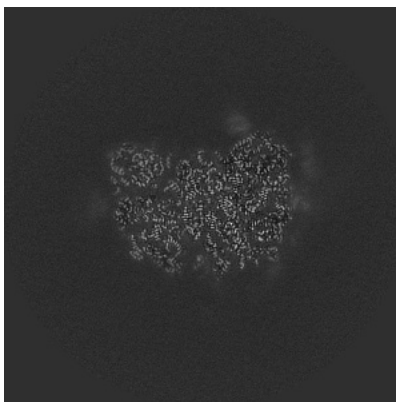
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

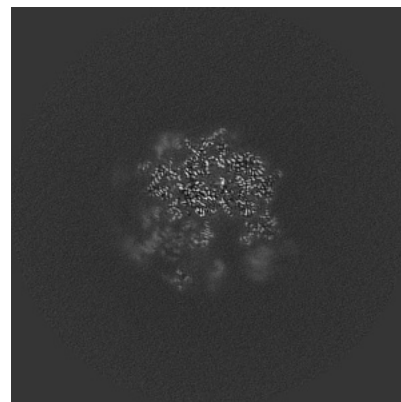
6.2.1 Primary map



X Index: 320

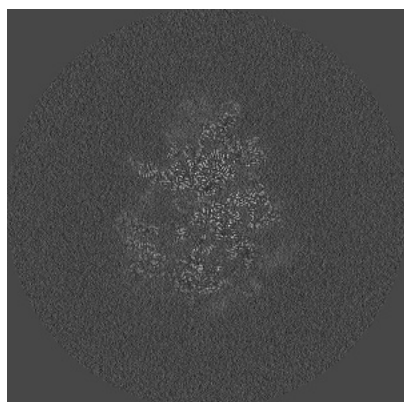


Y Index: 320

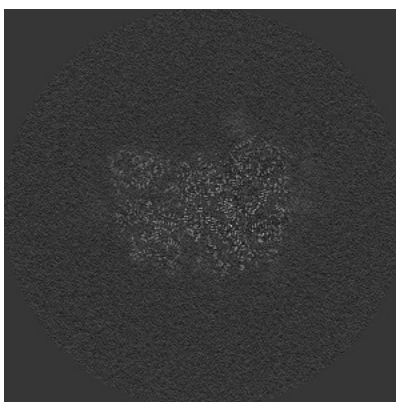


Z Index: 320

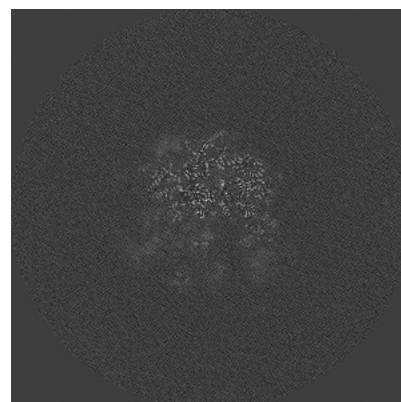
6.2.2 Raw map



X Index: 320



Y Index: 320

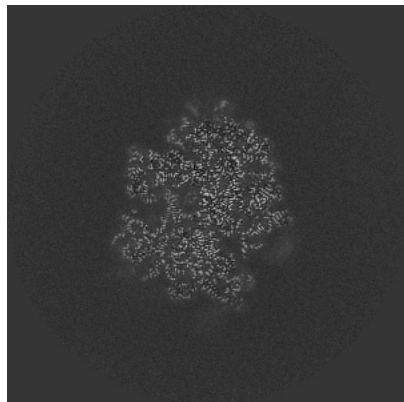


Z Index: 320

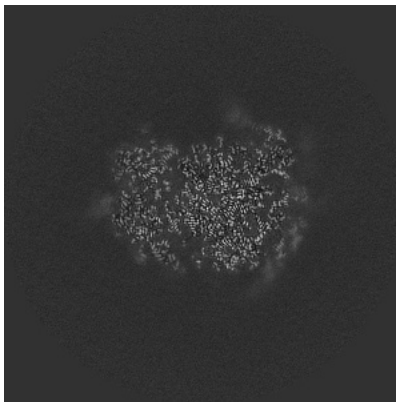
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

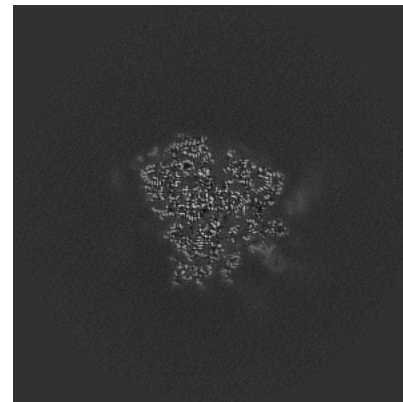
6.3.1 Primary map



X Index: 298

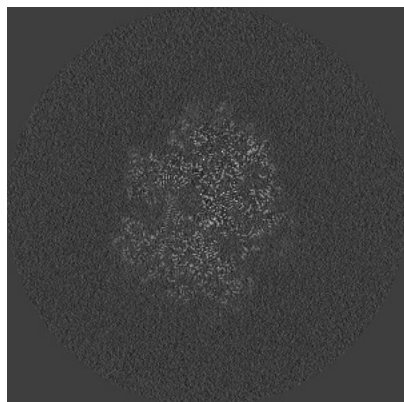


Y Index: 332

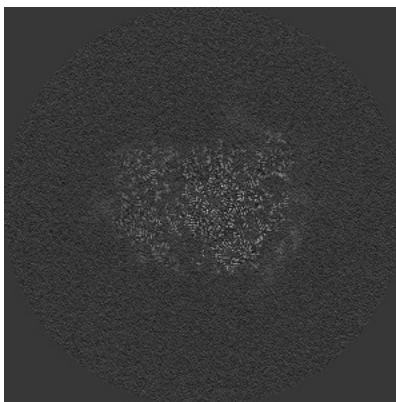


Z Index: 367

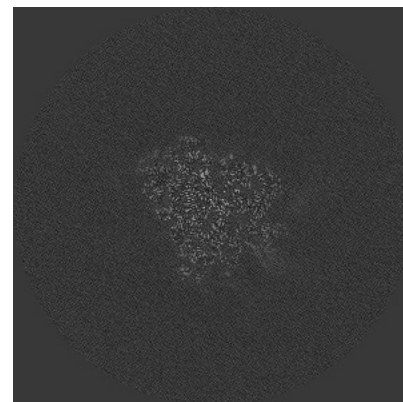
6.3.2 Raw map



X Index: 299



Y Index: 332

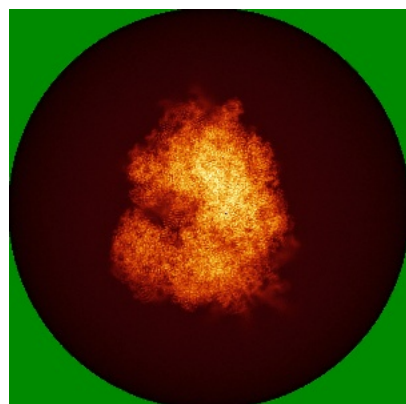


Z Index: 362

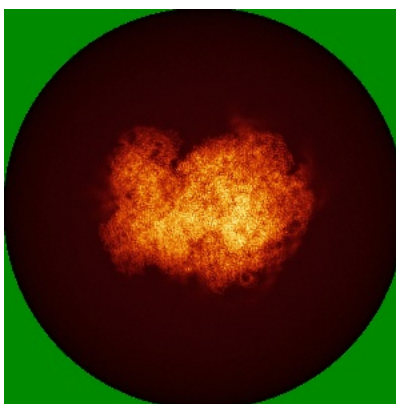
The images above show the largest variance slices of the map in three orthogonal directions.

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

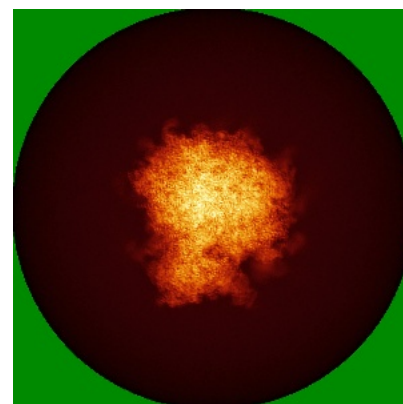
6.4.1 Primary map



X

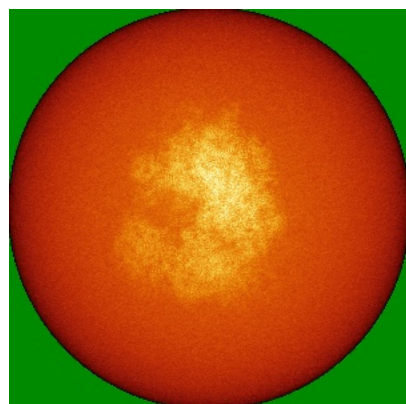


Y

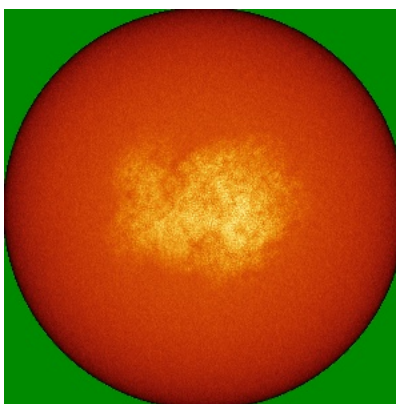


Z

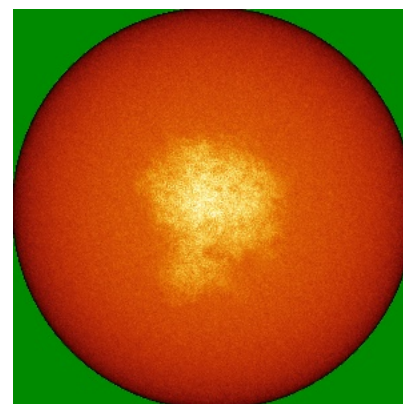
6.4.2 Raw map



X



Y

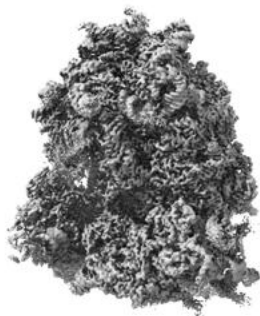


Z

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



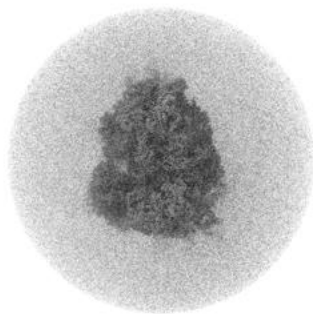
Y



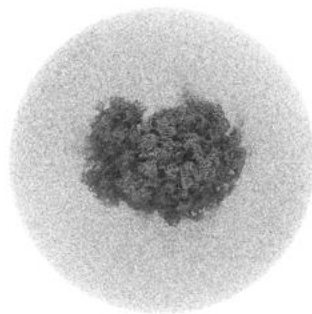
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

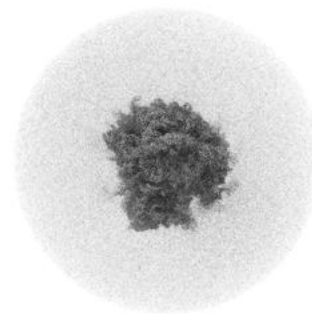
6.5.2 Raw map



X



Y



Z

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

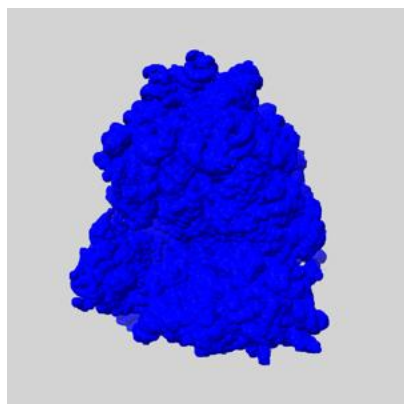
6.6 Mask visualisation [i](#)

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

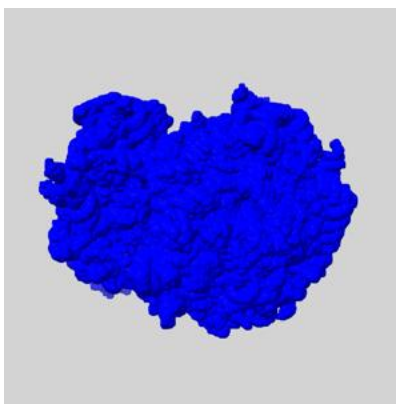
A mask typically either:

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

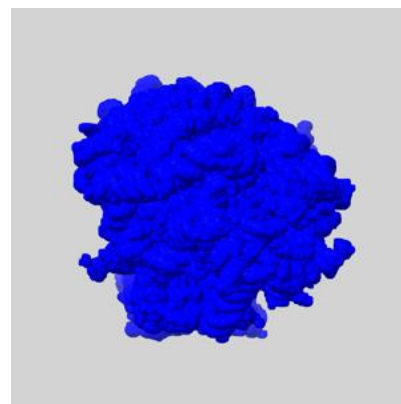
6.6.1 emd_29757_msk_1.map [i](#)



X



Y

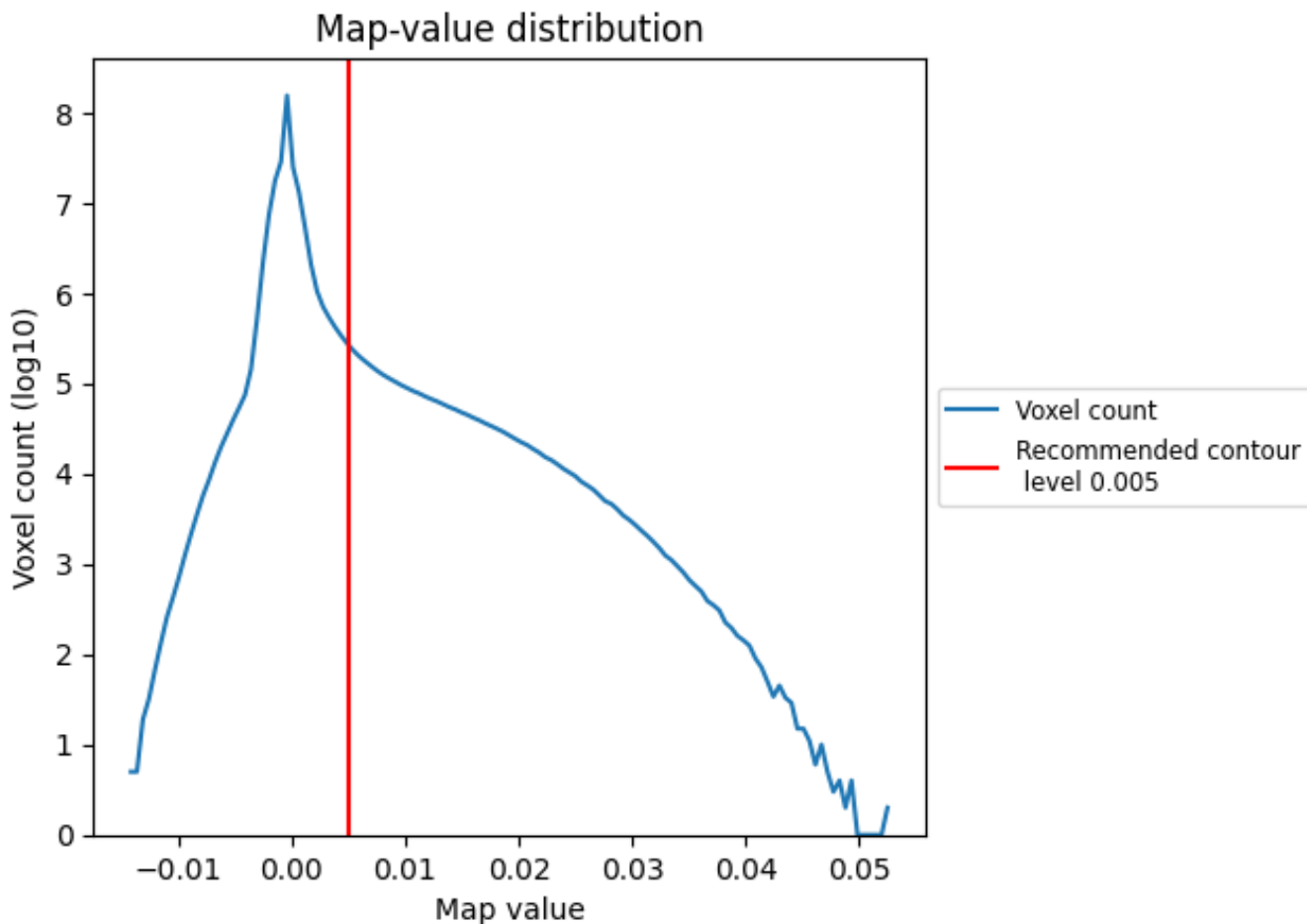


Z

7 Map analysis [i](#)

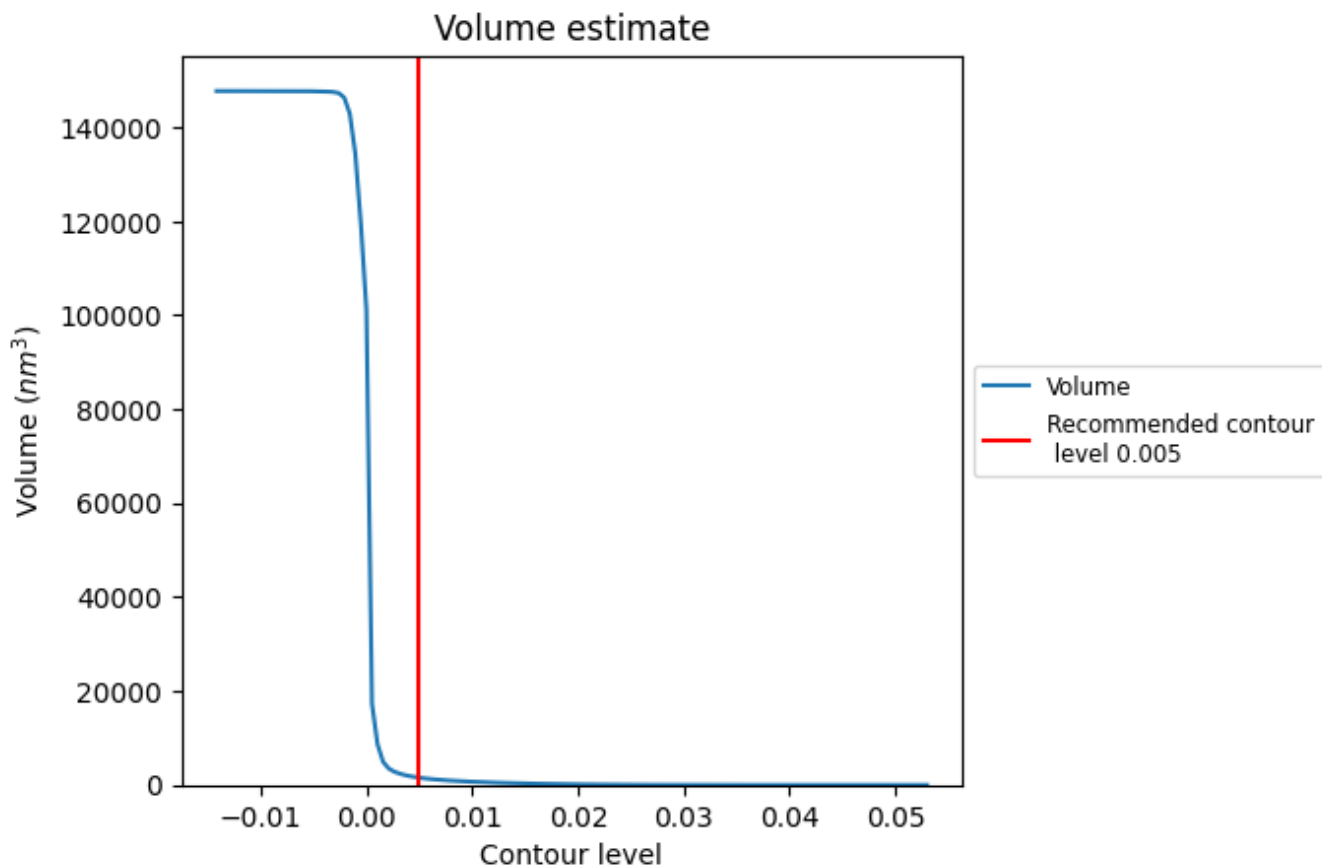
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

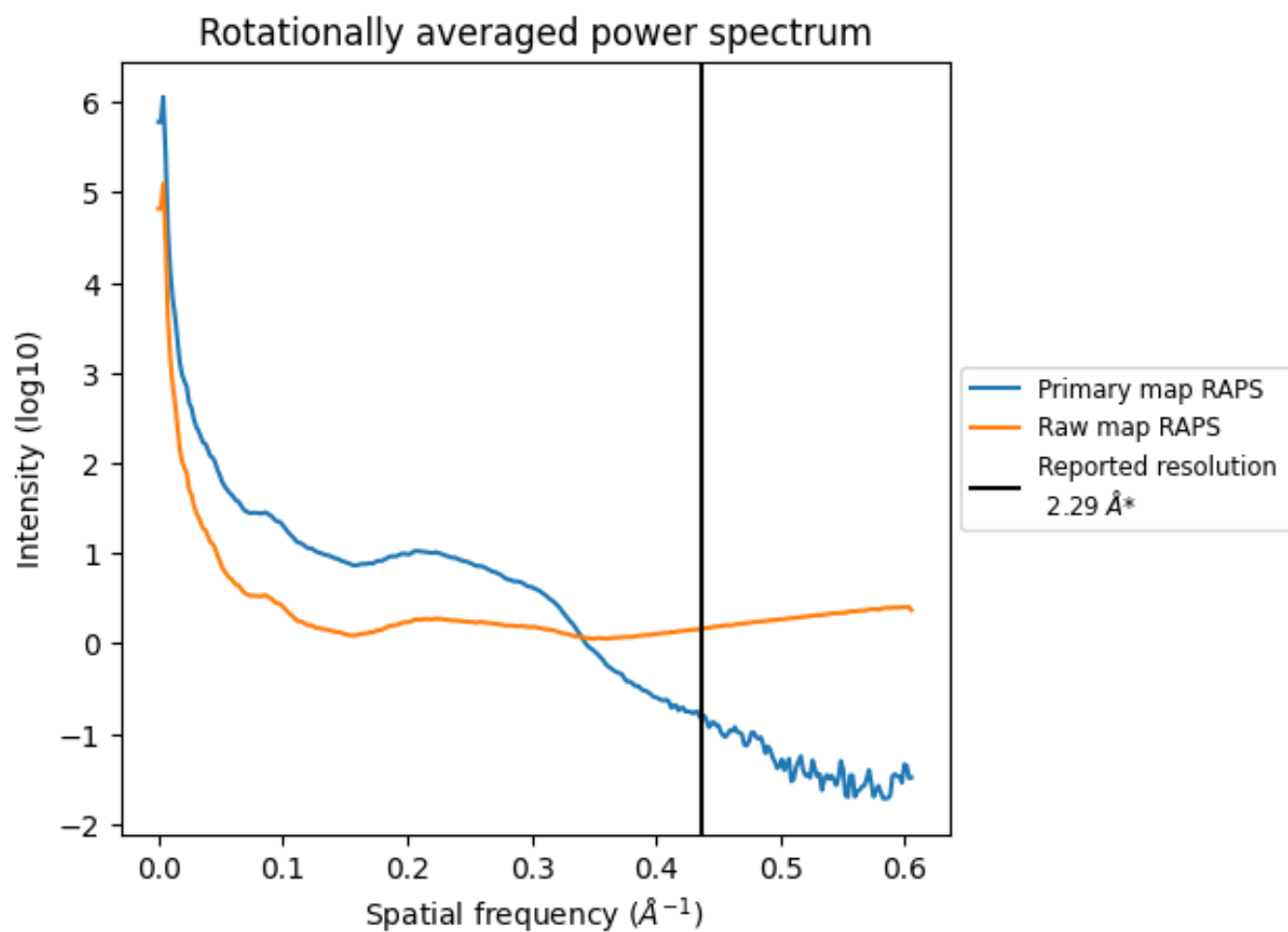
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1549 nm^3 ; this corresponds to an approximate mass of 1399 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](#)

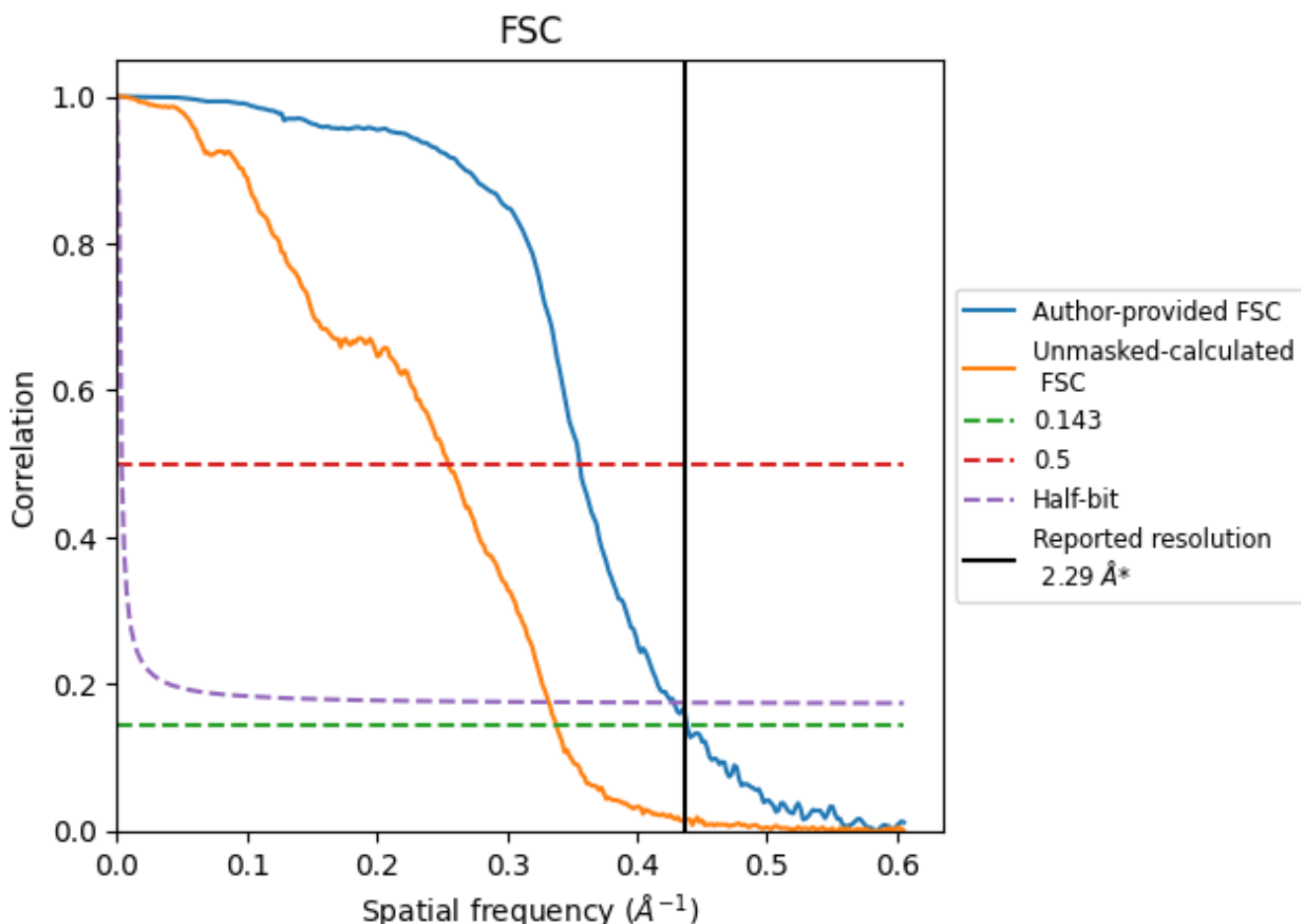


*Reported resolution corresponds to spatial frequency of 0.437 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.437 Å⁻¹

8.2 Resolution estimates [i](#)

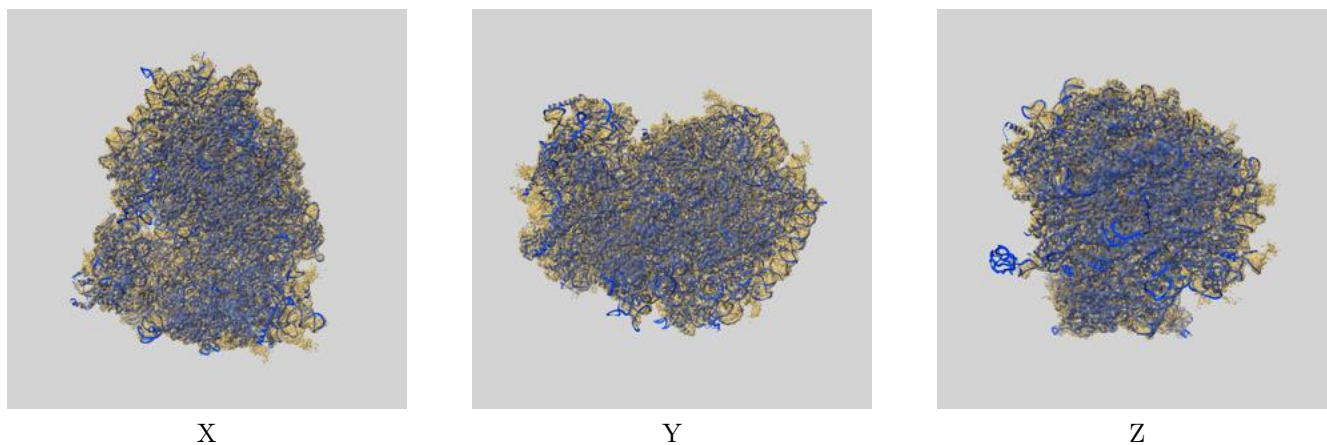
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.29 | - | - |
| Author-provided FSC curve | 2.28 | 2.81 | 2.33 |
| Unmasked-calculated* | 2.96 | 3.92 | 3.01 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.96 differs from the reported value 2.29 by more than 10 %

9 Map-model fit [i](#)

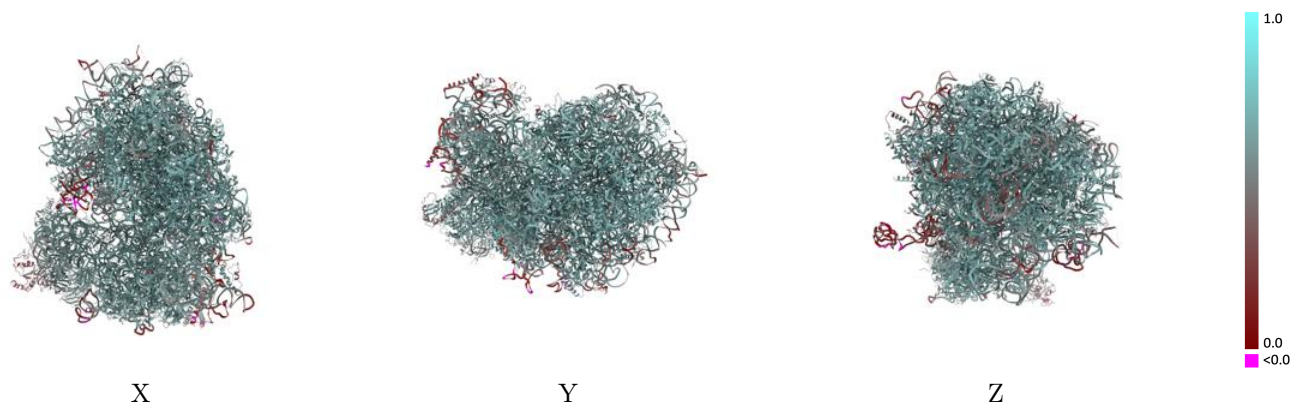
This section contains information regarding the fit between EMDB map EMD-29757 and PDB model 8G5Y. Per-residue inclusion information can be found in section 3 on page 28.

9.1 Map-model overlay [i](#)



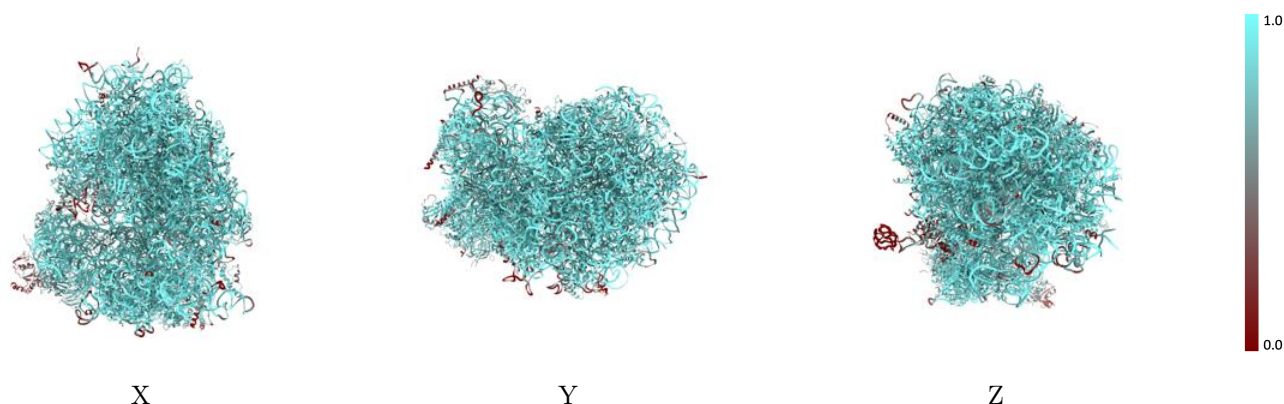
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



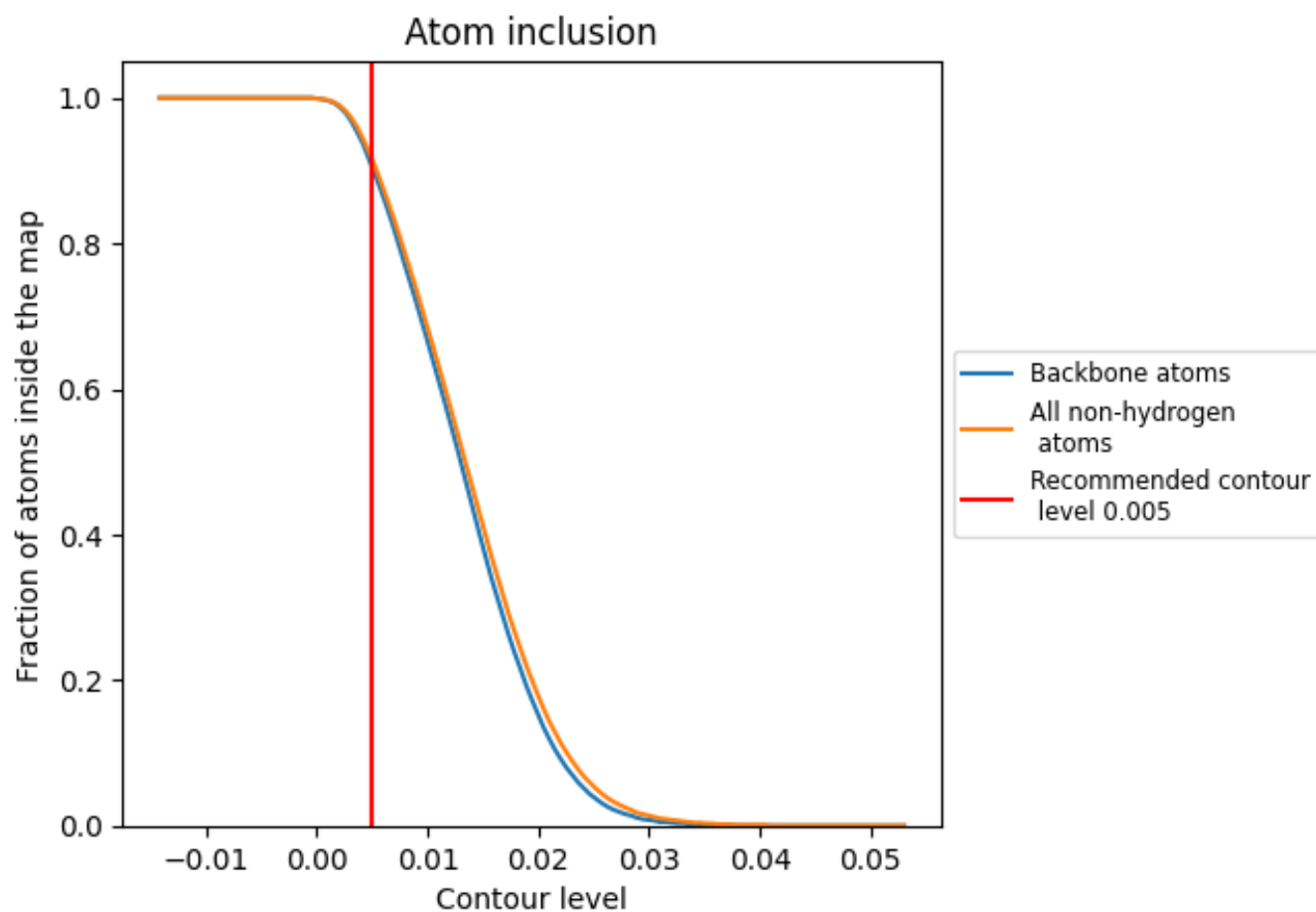
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 92% 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 (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9160 |  0.6050 |
| 5A |  0.5350 |  0.4730 |
| L5 |  0.9360 |  0.5990 |
| L7 |  0.9940 |  0.6520 |
| L8 |  0.9780 |  0.6360 |
| LA |  0.9730 |  0.6720 |
| LB |  0.9410 |  0.6550 |
| LC |  0.9530 |  0.6590 |
| LD |  0.9220 |  0.6310 |
| LE |  0.9180 |  0.6290 |
| LF |  0.9600 |  0.6610 |
| LG |  0.8380 |  0.5950 |
| LH |  0.9200 |  0.6300 |
| LI |  0.9480 |  0.6450 |
| LJ |  0.9110 |  0.6190 |
| LL |  0.9140 |  0.6320 |
| LM |  0.9500 |  0.6420 |
| LN |  0.9910 |  0.6740 |
| LO |  0.9590 |  0.6590 |
| LP |  0.9620 |  0.6700 |
| LQ |  0.9780 |  0.6750 |
| LR |  0.8830 |  0.6220 |
| LS |  0.9750 |  0.6590 |
| LT |  0.9380 |  0.6500 |
| LU |  0.8470 |  0.5820 |
| LV |  0.9540 |  0.6580 |
| LW |  0.6950 |  0.5080 |
| LX |  0.9400 |  0.6470 |
| LY |  0.9260 |  0.6400 |
| LZ |  0.9380 |  0.6400 |
| La |  0.9810 |  0.6760 |
| Lb |  0.8220 |  0.5910 |
| Lc |  0.9320 |  0.6460 |
| Ld |  0.9240 |  0.6330 |
| Le |  0.9800 |  0.6750 |

















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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Lf |  0.9680 |  0.6710 |
| Lg |  0.9020 |  0.6420 |
| Lh |  0.9280 |  0.6430 |
| Li |  0.9010 |  0.6210 |
| Lj |  0.9900 |  0.6780 |
| Lk |  0.8510 |  0.6130 |
| Ll |  0.9620 |  0.6510 |
| Lm |  0.9230 |  0.6360 |
| Ln |  0.9360 |  0.6470 |
| Lo |  0.9480 |  0.6490 |
| Lp |  0.9390 |  0.6600 |
| Lr |  0.9670 |  0.6610 |
| Lz |  0.2670 |  0.3690 |
| Pt |  0.9600 |  0.5990 |
| S2 |  0.9610 |  0.5960 |
| SA |  0.9030 |  0.6160 |
| SB |  0.8790 |  0.6200 |
| SC |  0.9160 |  0.6260 |
| SD |  0.8260 |  0.5680 |
| SE |  0.9010 |  0.6150 |
| SF |  0.8830 |  0.6050 |
| SG |  0.7700 |  0.5370 |
| SH |  0.7770 |  0.5500 |
| SI |  0.8900 |  0.6060 |
| SJ |  0.8850 |  0.5950 |
| SK |  0.8190 |  0.5380 |
| SL |  0.9120 |  0.6330 |
| SM |  0.2660 |  0.2970 |
| SN |  0.9370 |  0.6410 |
| SO |  0.9200 |  0.6320 |
| SP |  0.8220 |  0.5660 |
| SQ |  0.9090 |  0.6100 |
| SR |  0.8150 |  0.5660 |
| SS |  0.8920 |  0.6040 |
| ST |  0.8930 |  0.6030 |
| SU |  0.7750 |  0.5470 |
| SV |  0.9090 |  0.6230 |
| SW |  0.9680 |  0.6480 |
| SX |  0.9460 |  0.6390 |
| SY |  0.8040 |  0.5550 |
| SZ |  0.7920 |  0.5760 |
| Sa |  0.9420 |  0.6350 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Sb |  0.8420 |  0.6070 |
| Sc |  0.8070 |  0.5720 |
| Sd |  0.9570 |  0.6210 |
| Se |  0.8440 |  0.5940 |
| Sf |  0.4420 |  0.3830 |
| Sg |  0.7590 |  0.5360 |
| mR |  0.6110 |  0.5240 |