



wwPDB EM Validation Summary Report ⓘ

May 1, 2025 – 01:17 pm BST

PDB ID : 9G6J / pdb_00009g6j
EMDB ID : EMD-51103
Title : The structure of the *Candida albicans* ribosome with tRNA-fMet, mRNA, and compounds (GEN and MFQ) with strong density for the P-site tRNA
Authors : Kolosova, O.; Zgadzay, Y.; Jenner, L.B.; Guskov, A.; Yusupov, M.
Deposited on : 2024-07-18
Resolution : 2.15 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:

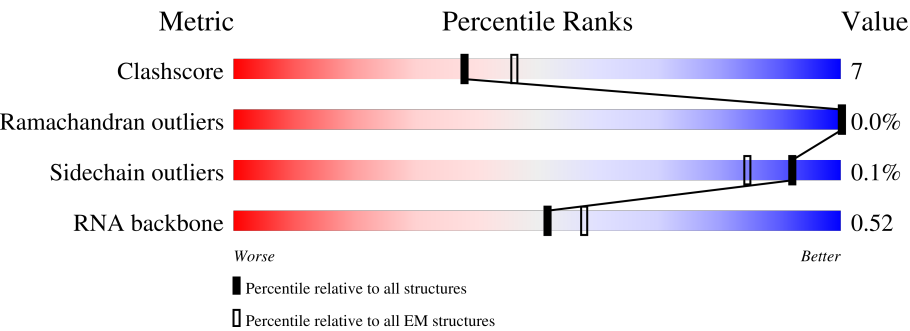
EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.15 Å.

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





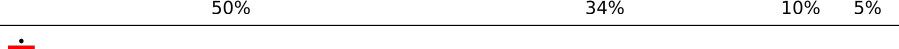
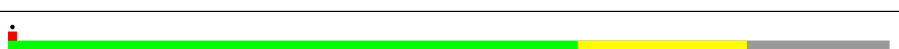



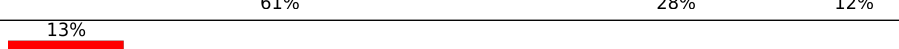



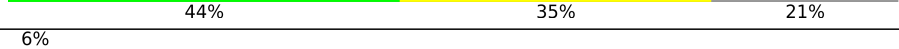

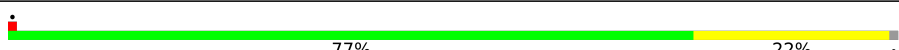


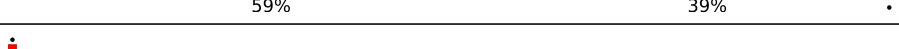







| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 | 0 | 172 | <div><div>85%15%.</div></div> |
| 2 | 1 | 3359 | <div><div>61%25%5%9%.</div></div> |
| 3 | 2 | 160 | <div><div>91%9%.</div></div> |
| 4 | 3 | 121 | <div><div>79%20%.</div></div> |
| 5 | 4 | 158 | <div><div>66%31%..</div></div> |
| 6 | 6 | 137 | <div><div>85%10%..</div></div> |
| 7 | 7 | 155 | <div><div>32%8%60%</div></div> |













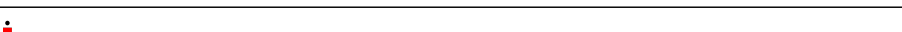

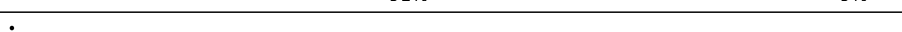

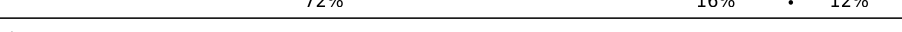








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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | 8 | 142 |  |
| 9 | 9 | 127 |  |
| 10 | A | 1787 |  |
| 11 | B | 261 |  |
| 12 | C | 256 |  |
| 13 | D | 249 |  |
| 14 | E | 251 |  |
| 15 | F | 262 |  |
| 16 | G | 225 |  |
| 17 | H | 236 |  |
| 18 | I | 186 |  |
| 19 | J | 206 |  |
| 20 | K | 189 |  |
| 21 | L | 118 |  |
| 22 | M | 155 |  |
| 23 | N | 143 |  |
| 24 | O | 151 |  |
| 25 | P | 132 |  |
| 26 | Q | 142 |  |
| 27 | T | 145 |  |
| 28 | R | 142 |  |
| 29 | S | 137 |  |
| 30 | U | 145 |  |
| 31 | V | 119 |  |
| 32 | W | 87 | |


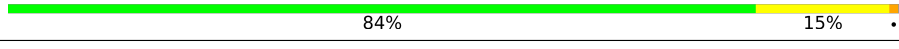
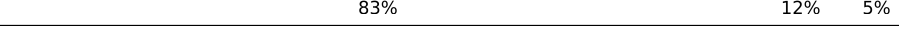
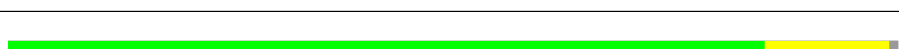



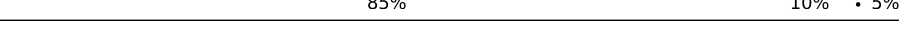



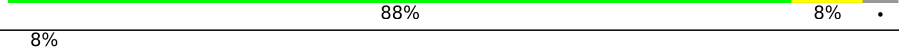











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 33 | X | 130 |  |
| 34 | Y | 145 |  |
| 35 | Z | 135 |  |
| 36 | a | 105 |  |
| 37 | b | 119 |  |
| 38 | c | 82 |  |
| 39 | d | 67 |  |
| 40 | e | 56 |  |
| 41 | f | 63 |  |
| 42 | g | 193 |  |
| 43 | h | 317 |  |
| 44 | j | 254 |  |
| 45 | k | 389 |  |
| 46 | l | 363 |  |
| 47 | m | 298 |  |
| 48 | n | 176 |  |
| 49 | o | 241 |  |
| 50 | p | 262 |  |
| 51 | q | 191 |  |
| 52 | r | 220 |  |
| 53 | s | 174 |  |
| 54 | t | 202 |  |
| 55 | u | 131 |  |
| 56 | v | 204 |  |
| 57 | w | 200 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 58 | x | 185 |  |
| 59 | y | 186 |  |
| 60 | z | 190 |  |
| 61 | AA | 136 |  |
| 62 | AB | 149 |  |
| 63 | AC | 63 |  |
| 64 | AD | 106 |  |
| 65 | AE | 112 |  |
| 66 | AF | 131 |  |
| 67 | AG | 107 |  |
| 68 | AH | 122 |  |
| 69 | AI | 120 |  |
| 70 | AJ | 99 |  |
| 71 | AK | 90 |  |
| 72 | AL | 78 |  |
| 73 | AM | 51 |  |
| 74 | AN | 52 |  |
| 75 | AO | 25 |  |
| 76 | AP | 106 |  |
| 77 | AQ | 92 |  |
| 78 | AT | 77 |  |
| 78 | PT | 77 |  |
| 79 | MR | 39 |  |

2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 197424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | 0 | 171 | Total | C | N | O | S | 2 | 0 |
| | | | 1442 | 933 | 262 | 244 | 3 | | |

- Molecule 2 is a RNA chain called 25S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 2 | 1 | 3066 | Total | C | N | O | P | 0 | 0 |
| | | | 65536 | 29280 | 11774 | 21416 | 3066 | | |

- Molecule 3 is a protein called Ribosomal 60S subunit protein L21A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | 2 | 159 | Total | C | N | O | S | 2 | 0 |
| | | | 1276 | 807 | 244 | 223 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4 | 3 | 121 | Total | C | N | O | P | 0 | 0 |
| | | | 2579 | 1153 | 463 | 842 | 121 | | |

- Molecule 5 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5 | 4 | 156 | Total | C | N | O | P | 0 | 0 |
| | | | 3313 | 1482 | 581 | 1094 | 156 | | |

- Molecule 6 is a protein called Ribosomal 60S subunit protein L23B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | 6 | 131 | Total | C | N | O | S | 1 | 0 |
| | | | 986 | 621 | 186 | 171 | 8 | | |

- Molecule 7 is a protein called Ribosomal 60S subunit protein L24A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 7 | 7 | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 516 | 328 | 102 | 85 | 1 | | |

- Molecule 8 is a protein called Ribosomal 60S subunit protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | 8 | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 974 | 622 | 175 | 176 | 1 | | |

- Molecule 9 is a protein called Ribosomal 60S subunit protein L26B.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 9 | 9 | 125 | Total | C | N | O | 0 | 0 |
| | | | 980 | 613 | 189 | 178 | | |

- Molecule 10 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 10 | A | 1692 | Total | C | N | O | P | 0 | 0 |
| | | | 36083 | 16130 | 6412 | 11849 | 1692 | | |

- Molecule 11 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11 | B | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1627 | 1041 | 284 | 297 | 5 | | |

- Molecule 12 is a protein called 40S ribosomal protein S1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | C | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1724 | 1094 | 313 | 313 | 4 | | |

- Molecule 13 is a protein called Ribosomal 40S subunit protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | D | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1620 | 1033 | 287 | 295 | 5 | | |

- Molecule 14 is a protein called Ribosomal 40S subunit protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | E | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1701 | 1084 | 310 | 303 | 4 | | |

- Molecule 15 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15 | F | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2055 | 1306 | 386 | 358 | 5 | | |

- Molecule 16 is a protein called Ribosomal 40S subunit protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | G | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1572 | 983 | 294 | 291 | 4 | | |

- Molecule 17 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17 | H | 226 | Total | C | N | O | S | 0 | 0 |
| | | | 1820 | 1133 | 351 | 330 | 6 | | |

- Molecule 18 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 18 | I | 182 | Total | C | N | O | | 0 | 0 |
| | | | 1466 | 939 | 264 | 263 | | | |

- Molecule 19 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | J | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1579 | 973 | 322 | 283 | 1 | | |

- Molecule 20 is a protein called Ribosomal 40S subunit protein S9B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | K | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1453 | 918 | 286 | 248 | 1 | | |

- Molecule 21 is a protein called Ribosomal 40S subunit protein S10A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | L | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 783 | 511 | 129 | 142 | 1 | | |

- Molecule 22 is a protein called Ribosomal 40S subunit protein S11A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | M | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 722 | 212 | 192 | 3 | | |

- Molecule 23 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23 | N | 71 | Total | C | N | O | S | 0 | 0 |
| | | | 539 | 341 | 95 | 99 | 4 | | |

- Molecule 24 is a protein called Ribosomal 40S subunit protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | O | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1187 | 757 | 219 | 210 | 1 | | |

- Molecule 25 is a protein called Ribosomal 40S subunit protein S14B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | P | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 579 | 186 | 174 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| P | 119 | IAS | ASP | conflict | UNP A0A1D8PDT3 |

- Molecule 26 is a protein called Ribosomal 40S subunit protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | Q | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 906 | 578 | 164 | 158 | 6 | | |

- Molecule 27 is a protein called Ribosomal 40S subunit protein S18B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | T | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1169 | 733 | 228 | 205 | 3 | | |

- Molecule 28 is a protein called Ribosomal 40S subunit protein S16A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | R | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1102 | 706 | 202 | 193 | 1 | | |

- Molecule 29 is a protein called Ribosomal 40S subunit protein S17B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | S | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 954 | 602 | 176 | 175 | 1 | | |

- Molecule 30 is a protein called Ribosomal 40S subunit protein S19A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | U | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1100 | 689 | 210 | 200 | 1 | | |

- Molecule 31 is a protein called Ribosomal 40S subunit protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | V | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 790 | 499 | 146 | 143 | 2 | | |

- Molecule 32 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | W | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 676 | 415 | 126 | 133 | 2 | | |

- Molecule 33 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | X | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 655 | 191 | 183 | 3 | | |

- Molecule 34 is a protein called Ribosomal 40S subunit protein S23B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | Y | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1110 | 701 | 219 | 188 | 2 | | |

- Molecule 35 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 35 | Z | 132 | Total | C | N | O | | 0 | 0 |
| | | | 1072 | 670 | 216 | 186 | | | |

- Molecule 36 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 36 | a | 72 | Total | C | N | O | | 0 | 0 |
| | | | 578 | 369 | 103 | 106 | | | |

- Molecule 37 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | b | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 779 | 482 | 163 | 128 | 6 | | |

- Molecule 38 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | c | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 614 | 383 | 110 | 114 | 7 | | |

- Molecule 39 is a protein called Ribosomal 40S subunit protein S28B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39 | d | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 487 | 299 | 98 | 88 | 2 | | |

- Molecule 40 is a protein called Ribosomal 40S subunit protein S29A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40 | e | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 454 | 281 | 94 | 75 | 4 | | |

- Molecule 41 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41 | f | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 461 | 289 | 93 | 77 | 2 | | |

- Molecule 42 is a protein called Ubiquitin-ribosomal 40S subunit protein S31 fusion protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42 | g | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 565 | 358 | 111 | 90 | 6 | | |

- Molecule 43 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43 | h | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1854 | 1176 | 319 | 355 | 4 | | |

- Molecule 44 is a protein called Ribosomal 60S subunit protein L2A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44 | j | 249 | Total | C | N | O | S | 1 | 0 |
| | | | 1894 | 1185 | 377 | 330 | 2 | | |

- Molecule 45 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45 | k | 386 | Total | C | N | O | S | 1 | 0 |
| | | | 3084 | 1955 | 584 | 538 | 7 | | |

- Molecule 46 is a protein called Ribosomal 60S subunit protein L4B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46 | l | 361 | Total | C | N | O | S | 0 | 0 |
| | | | 2751 | 1729 | 529 | 490 | 3 | | |

- Molecule 47 is a protein called Ribosomal 60S subunit protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47 | m | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2394 | 1526 | 416 | 450 | 2 | | |

- Molecule 48 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 48 | n | 155 | Total | C | N | O | 1 | 0 |
| | | | 1237 | 794 | 226 | 217 | | |

- Molecule 49 is a protein called Ribosomal 60S subunit protein L7A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49 | o | 230 | Total | C | N | O | S | 1 | 0 |
| | | | 1860 | 1193 | 343 | 323 | 1 | | |

- Molecule 50 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50 | p | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1795 | 1150 | 319 | 323 | 3 | | |

- Molecule 51 is a protein called Ribosomal 60S subunit protein L9B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | q | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 953 | 275 | 278 | 4 | | |

- Molecule 52 is a protein called Ribosomal 60S subunit protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52 | r | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1759 | 1110 | 336 | 305 | 8 | | |

- Molecule 53 is a protein called Ribosomal 60S subunit protein L11B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | s | 172 | Total | C | N | O | S | 1 | 0 |
| | | | 1385 | 864 | 262 | 255 | 4 | | |

- Molecule 54 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 54 | t | 195 | Total | C | N | O | 0 | 0 |
| | | | 1573 | 986 | 311 | 276 | | |

- Molecule 55 is a protein called Ribosomal 60S subunit protein L14B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55 | u | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1029 | 660 | 193 | 175 | 1 | | |

- Molecule 56 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56 | v | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1713 | 1075 | 356 | 280 | 2 | | |

- Molecule 57 is a protein called Ribosomal 60S subunit protein L16A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57 | w | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1590 | 1025 | 294 | 269 | 2 | | |

- Molecule 58 is a protein called Ribosomal 60S subunit protein L17B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 58 | x | 172 | Total | C | N | O | | 0 | 0 |
| | | | 1375 | 850 | 279 | 246 | | | |

- Molecule 59 is a protein called Ribosomal 60S subunit protein L18A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 59 | y | 185 | Total | C | N | O | | 3 | 0 |
| | | | 1478 | 930 | 302 | 246 | | | |

- Molecule 60 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60 | z | 180 | Total | C | N | O | S | 1 | 0 |
| | | | 1471 | 910 | 313 | 245 | 3 | | |

- Molecule 61 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61 | AA | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1087 | 705 | 197 | 183 | 2 | | |

- Molecule 62 is a protein called Ribosomal 60S subunit protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62 | AB | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1170 | 741 | 231 | 197 | 1 | | |

- Molecule 63 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 63 | AC | 60 | Total | C | N | O | S | 1 | 0 |
| | | | 489 | 305 | 105 | 78 | 1 | | |

- Molecule 64 is a protein called Ribosomal 60S subunit protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64 | AD | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 729 | 469 | 121 | 137 | 2 | | |

- Molecule 65 is a protein called Ribosomal 60S subunit protein L31B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65 | AE | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 881 | 558 | 166 | 155 | 2 | | |

- Molecule 66 is a protein called Ribosomal 60S subunit protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66 | AF | 125 | Total | C | N | O | S | 1 | 0 |
| | | | 1015 | 649 | 197 | 168 | 1 | | |

- Molecule 67 is a protein called Ribosomal 60S subunit protein L33A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67 | AG | 106 | Total | C | N | O | S | 3 | 0 |
| | | | 867 | 558 | 166 | 142 | 1 | | |

- Molecule 68 is a protein called Ribosomal 60S subunit protein L34B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68 | AH | 112 | Total | C | N | O | S | 4 | 0 |
| | | | 913 | 567 | 188 | 154 | 4 | | |

- Molecule 69 is a protein called Ribosomal 60S subunit protein L35A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 69 | AI | 119 | Total | C | N | O | 1 | 0 |
| | | | 990 | 629 | 195 | 166 | | |

- Molecule 70 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70 | AJ | 97 | Total | C | N | O | S | 1 | 0 |
| | | | 764 | 476 | 157 | 130 | 1 | | |

- Molecule 71 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71 | AK | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 677 | 413 | 148 | 110 | 6 | | |

- Molecule 72 is a protein called Ribosomal 60S subunit protein L38.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 72 | AL | 77 | Total | C | N | O | 1 | 0 |
| | | | 623 | 398 | 116 | 109 | | |

- Molecule 73 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 73 | AM | 50 | Total | C | N | O | 1 | 0 |
| | | | 446 | 280 | 100 | 66 | | |

- Molecule 74 is a protein called Rpl40bp.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 74 | AN | 52 | Total | C | N | O | S | 1 | 0 |
| | | | 427 | 265 | 89 | 67 | 6 | | |

- Molecule 75 is a protein called Small ribosomal subunit protein eS32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 75 | AO | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 236 | 144 | 63 | 28 | 1 | | |

- Molecule 76 is a protein called Ribosomal 60S subunit protein L42A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76 | AP | 105 | Total | C | N | O | S | 2 | 0 |
| | | | 863 | 547 | 171 | 140 | 5 | | |

- Molecule 77 is a protein called Ribosomal 60S subunit protein L43A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77 | AQ | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 698 | 430 | 140 | 124 | 4 | | |

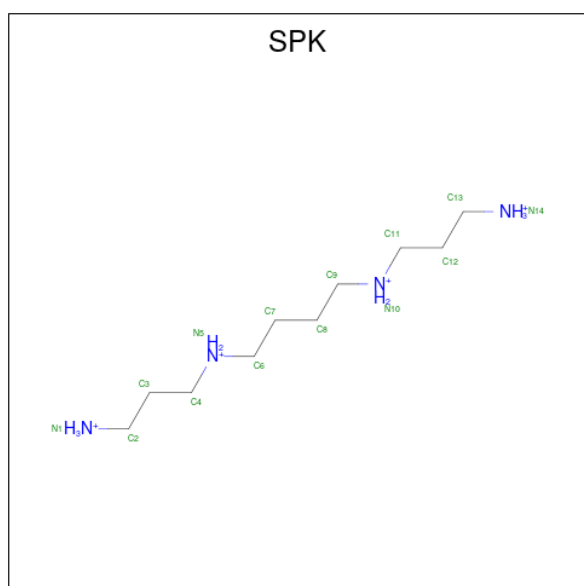
- Molecule 78 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 78 | PT | 76 | Total | C | N | O | P | 0 | 0 |
| | | | 1623 | 723 | 294 | 530 | 76 | | |
| 78 | AT | 76 | Total | C | N | O | P | 0 | 0 |
| | | | 1623 | 723 | 294 | 530 | 76 | | |

- Molecule 79 is a RNA chain called mRNA.

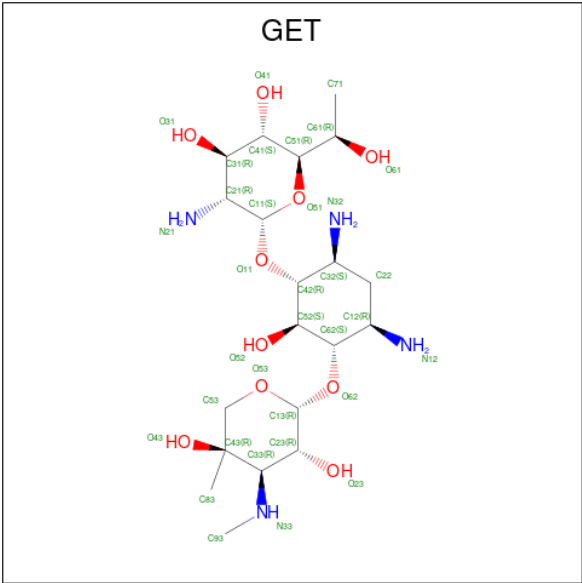
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 79 | MR | 11 | Total | C | N | O | P | 0 | 0 |
| | | | 229 | 103 | 36 | 79 | 11 | | |

- Molecule 80 is SPERMINE (FULLY PROTONATED FORM) (CCD ID: SPK) (formula: $C_{10}H_{30}N_4$).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 80 | 1 | 1 | Total | C | N | 0 |
| | | | 14 | 10 | 4 | |

- Molecule 81 is GENETICIN (CCD ID: GET) (formula: $C_{20}H_{40}N_4O_{10}$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | 1 | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | A | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | A | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | A | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |
| 81 | AT | 1 | Total | C | N | O | 0 |
| | | | 34 | 20 | 4 | 10 | |

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

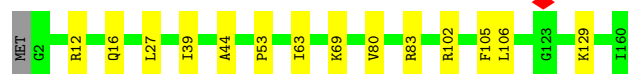
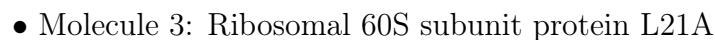
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 82 | b | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 82 | e | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 82 | AH | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 82 | AK | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 82 | AN | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 82 | AP | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 82 | AQ | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 83 is (11R,12S)- Mefloquine (CCD ID: YMZ) (formula: C₁₇H₁₆F₆N₂O) (labeled as "Ligand of Interest" by depositor).



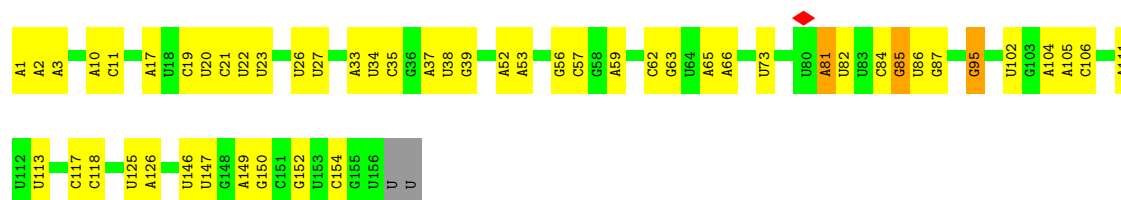
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 83 | AQ | 1 | Total 26 | C 17 | F 6 | N 2 | O 1 | 0 |





| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|--|----|----|-----|-----|-----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|--|------|------|------|------|--|------|
| G1 | G2 | U3 | U4 | | G7 | G8 | C19 | A20 | G21 | A22 | | A27 | C28 | U39 | | A42 | C48 | U54 | A55 | U59 | G60 | G65 | | C73 | | A76 | G89 | A90 | G91 | | A102 | G112 | C113 | U114 | | U121 |
|----|----|----|----|--|----|----|-----|-----|-----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|--|------|------|------|------|--|------|

Chain 4: 66% 31%



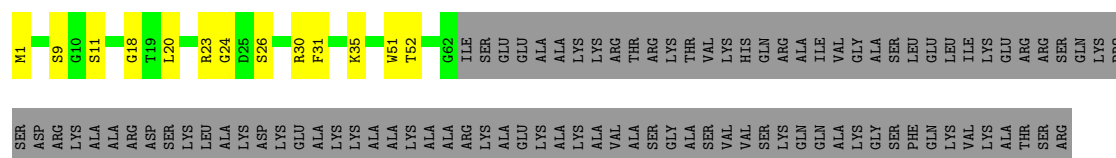
• Molecule 6: Ribosomal 60S subunit protein L23B

Chain 6: 85% 10% . .



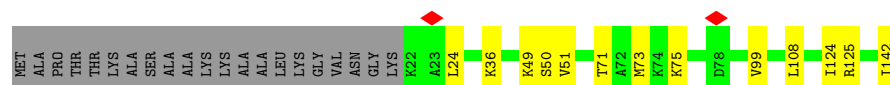
• Molecule 7: Ribosomal 60S subunit protein L24A

Chain 7: 32% 8% 60%



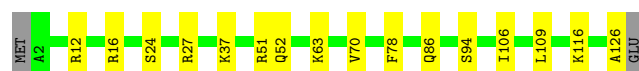
• Molecule 8: Ribosomal 60S subunit protein L25

Chain 8: 76% 9% 15%



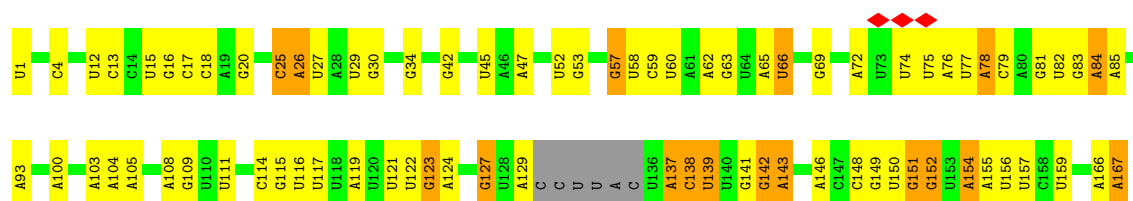
• Molecule 9: Ribosomal 60S subunit protein L26B

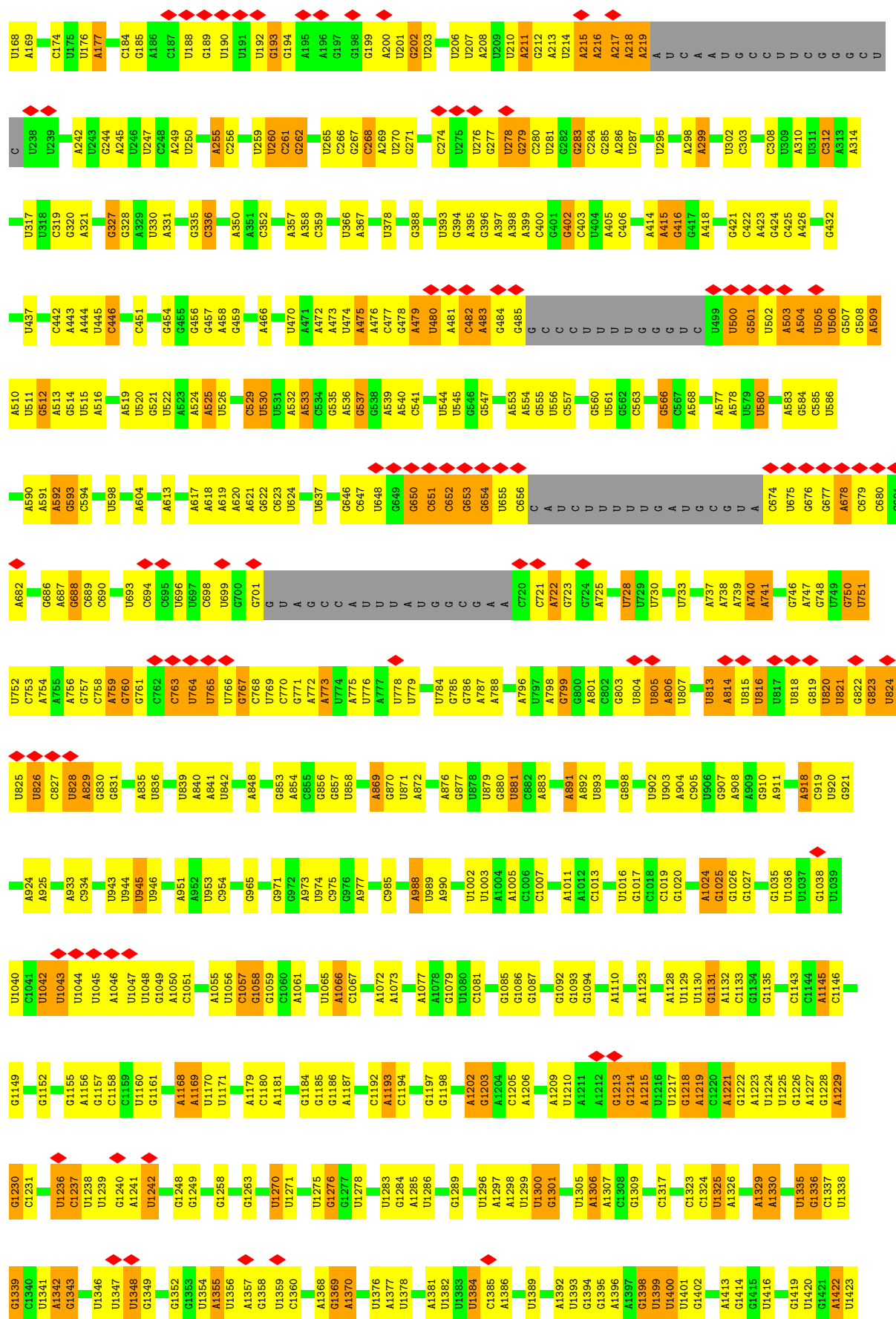
Chain 9: 86% 13% .

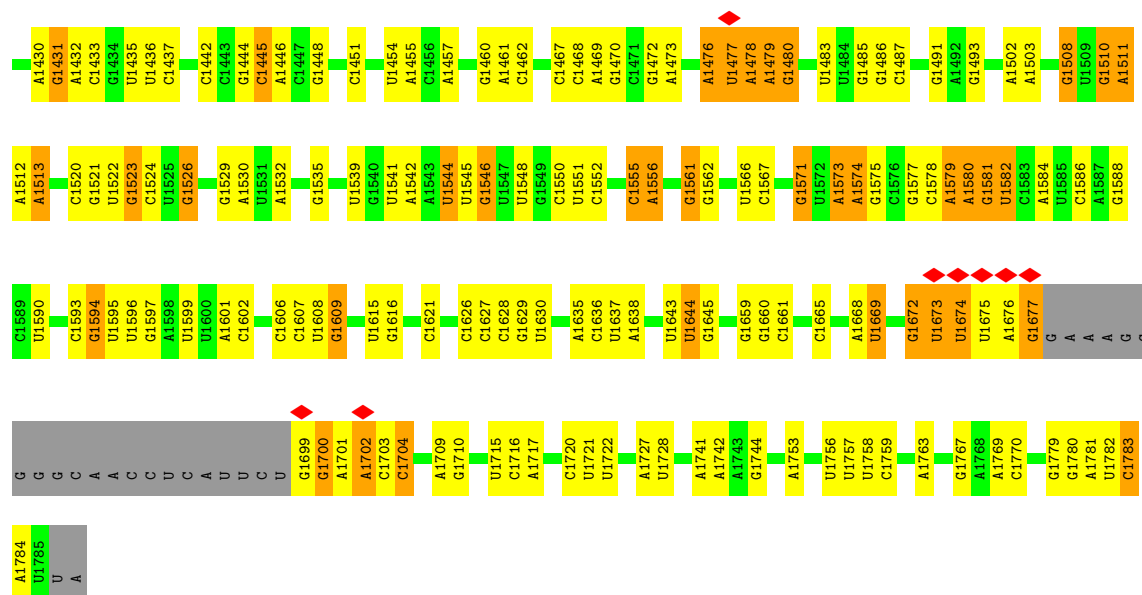


• Molecule 10: 18S rRNA

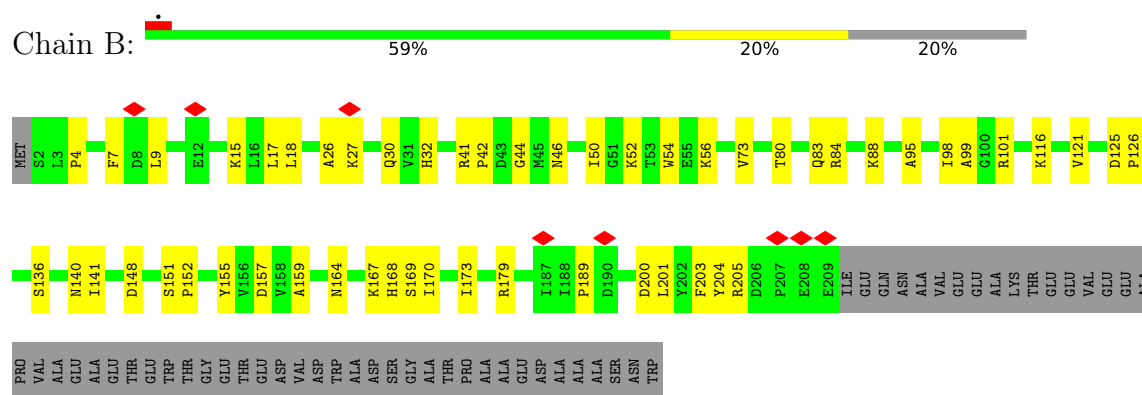
Chain A: 6% 50% 34% 10% 5%



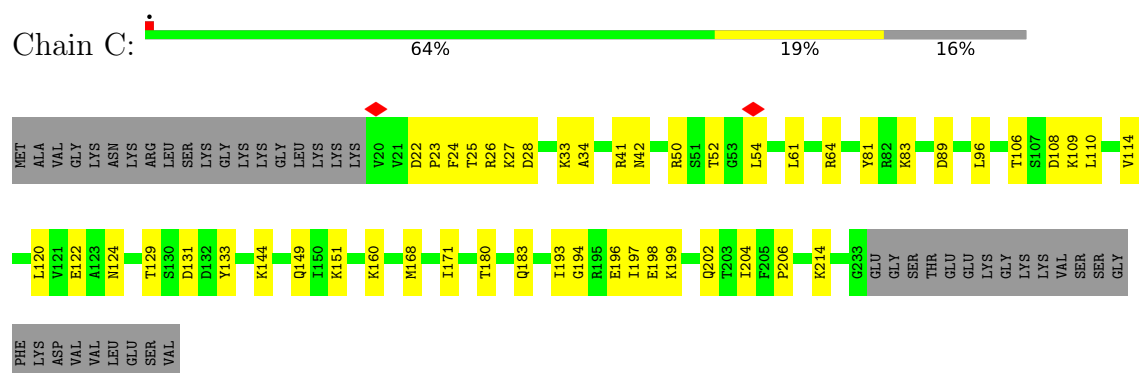




- Molecule 11: 40S ribosomal protein S0

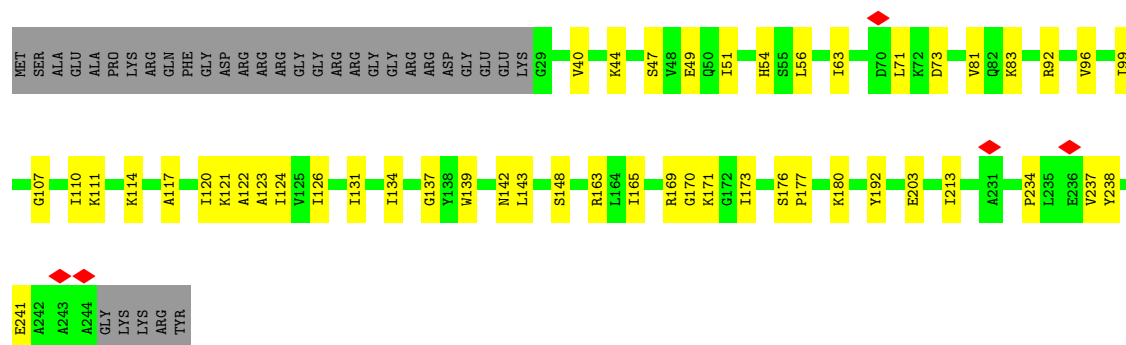


- Molecule 12: 40S ribosomal protein S1

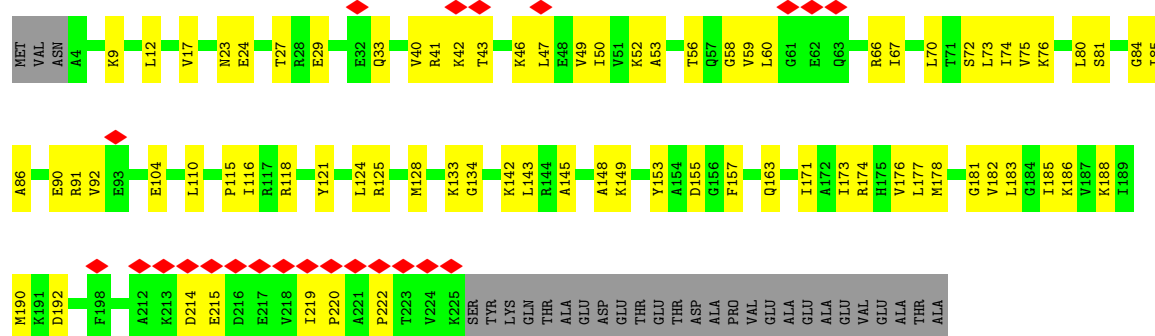


- Molecule 13: Ribosomal 40S subunit protein S2

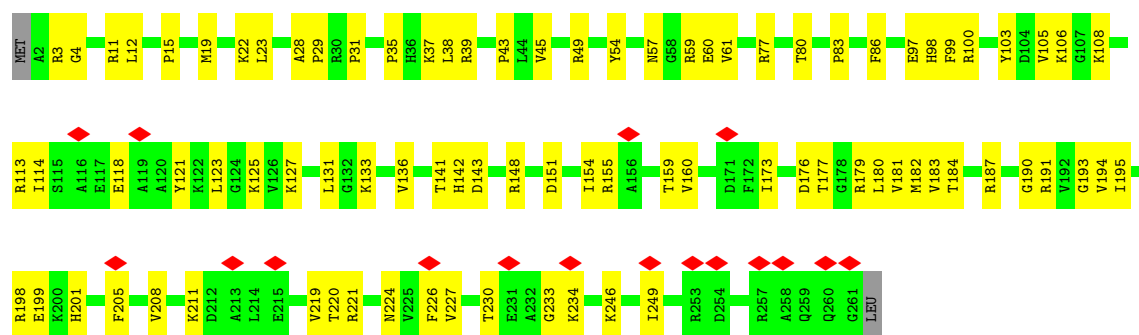




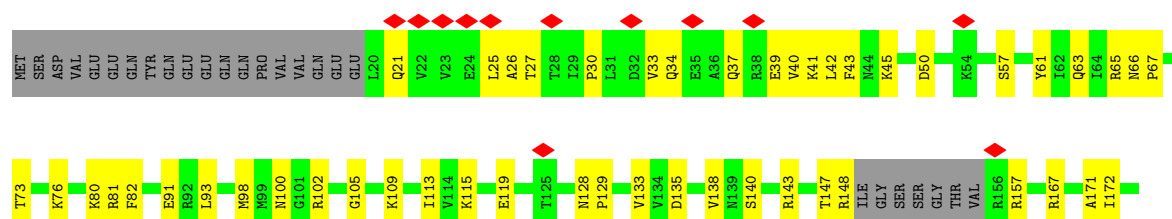
• Molecule 14: Ribosomal 40S subunit protein S3



• Molecule 15: 40S ribosomal protein S4

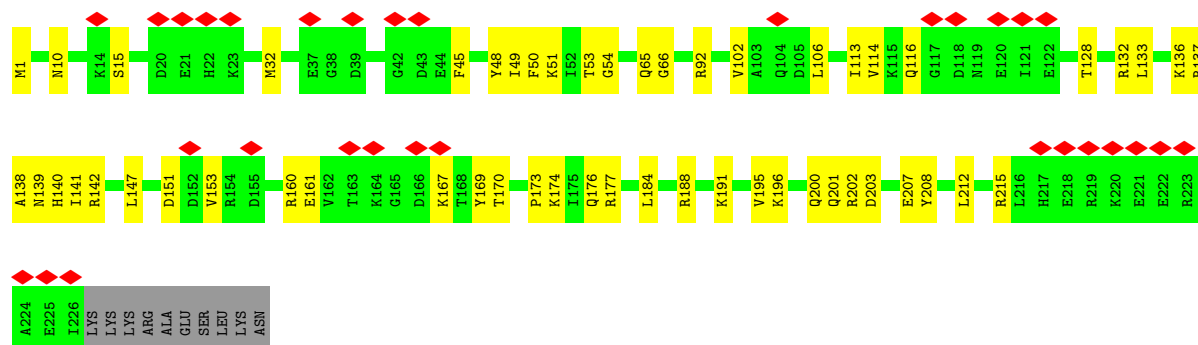
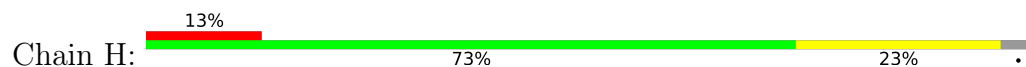


• Molecule 16: Ribosomal 40S subunit protein S5

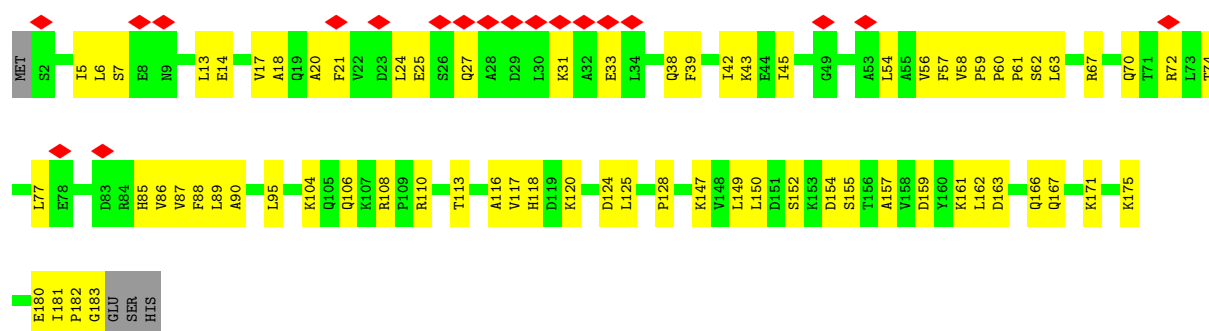




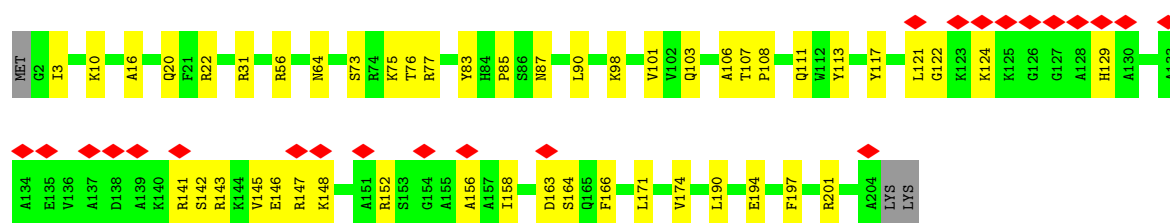
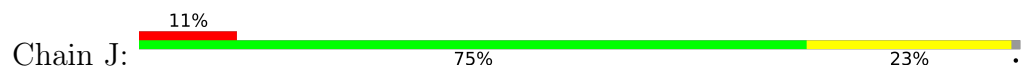
- Molecule 17: 40S ribosomal protein S6



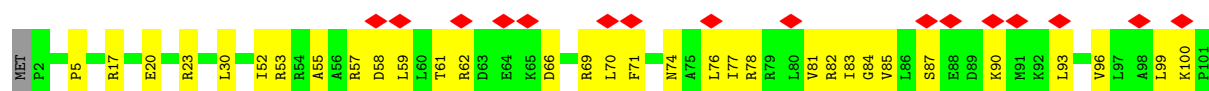
- Molecule 18: 40S ribosomal protein S7



- Molecule 19: 40S ribosomal protein S8

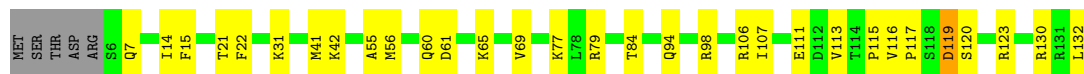


- Molecule 20: Ribosomal 40S subunit protein S9B



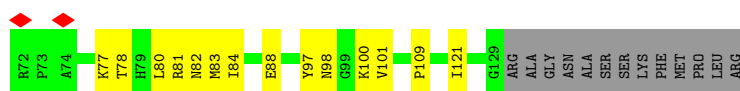
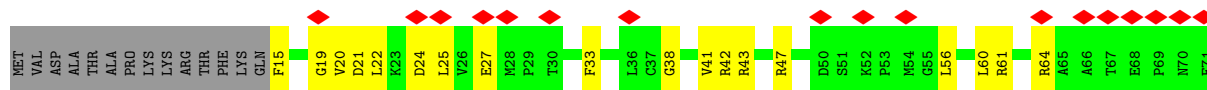
- Molecule 25: Ribosomal 40S subunit protein S14B

Chain P:  73% 23% . .



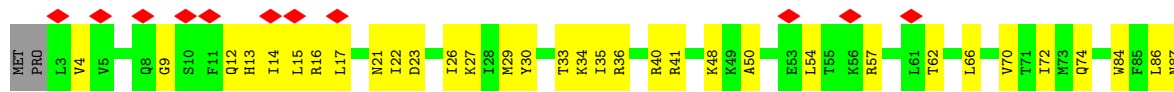
- Molecule 26: Ribosomal 40S subunit protein S15

Chain Q:  13% 58% 23% 19%



- Molecule 27: Ribosomal 40S subunit protein S18B

Chain T:  10% 59% 39% .



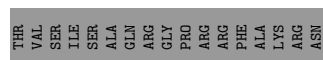
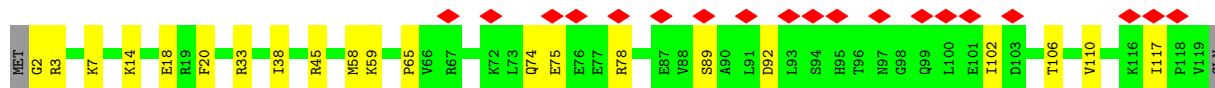
- Molecule 28: Ribosomal 40S subunit protein S16A

Chain R:  63% 36% .

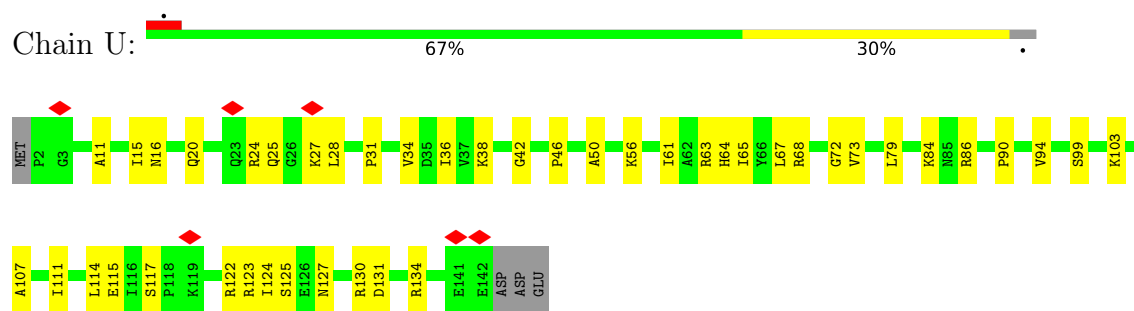


- Molecule 29: Ribosomal 40S subunit protein S17B

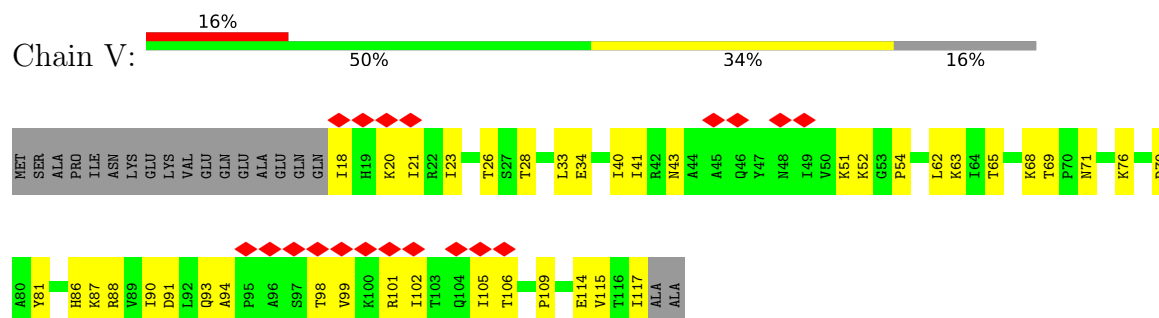
Chain S:  14% 71% 15% 14%



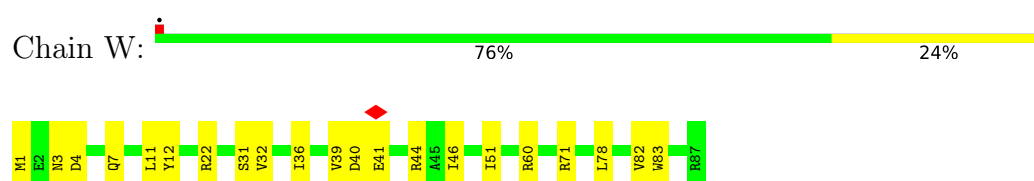
- Molecule 30: Ribosomal 40S subunit protein S19A



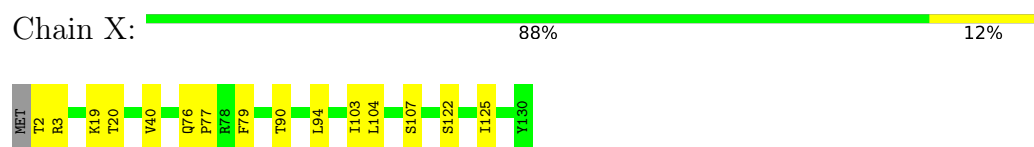
- Molecule 31: Ribosomal 40S subunit protein S20



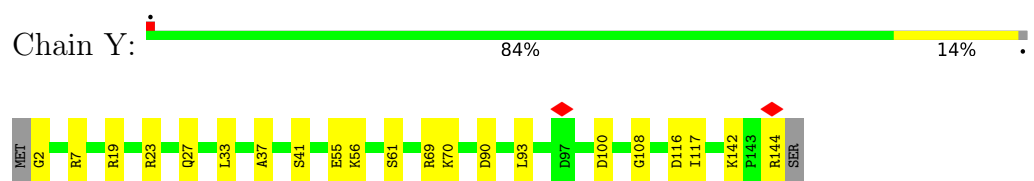
- Molecule 32: 40S ribosomal protein S21



- Molecule 33: 40S ribosomal protein S22-A

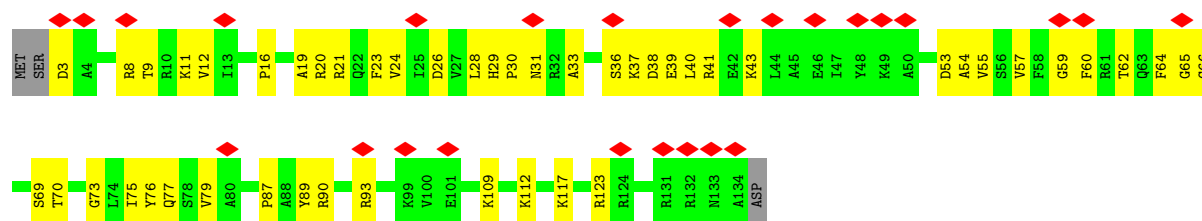


- Molecule 34: Ribosomal 40S subunit protein S23B

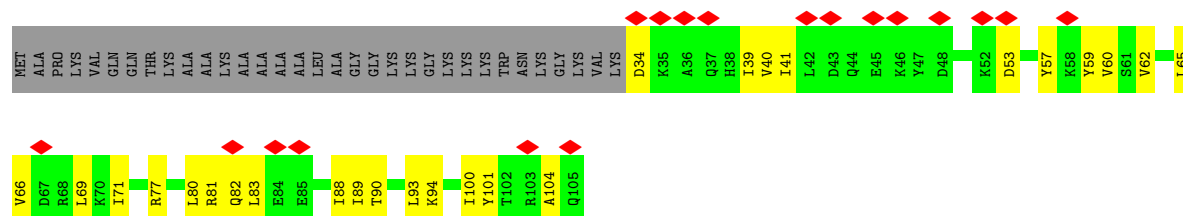
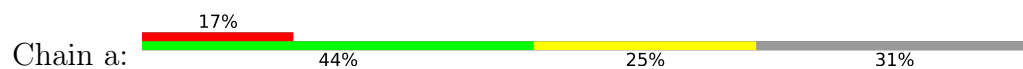


- Molecule 35: 40S ribosomal protein S24

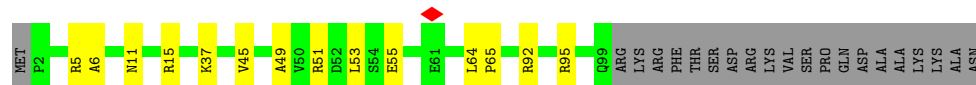




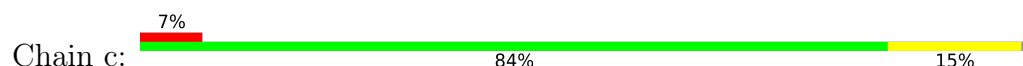
• Molecule 36: 40S ribosomal protein S25



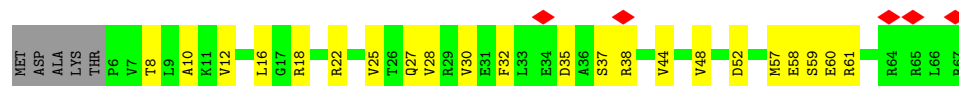
• Molecule 37: 40S ribosomal protein S26



• Molecule 38: 40S ribosomal protein S27



• Molecule 39: Ribosomal 40S subunit protein S28B



• Molecule 40: Ribosomal 40S subunit protein S29A



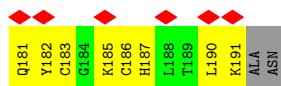
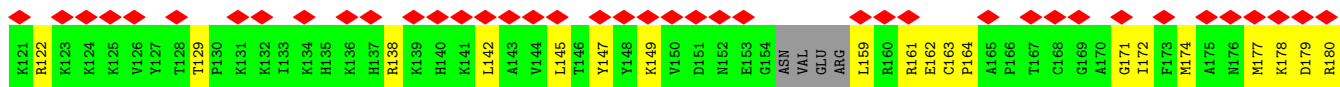
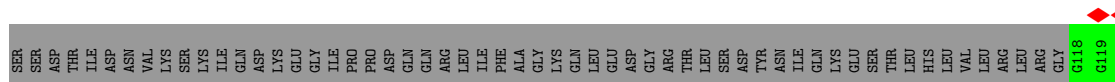
• Molecule 41: 40S ribosomal protein S30

Chain f: 



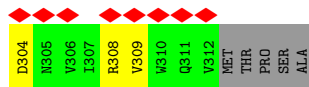
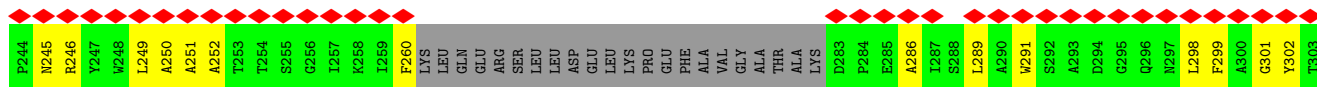
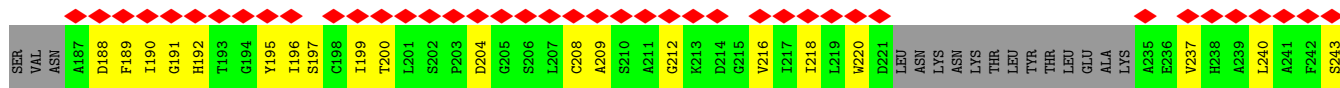
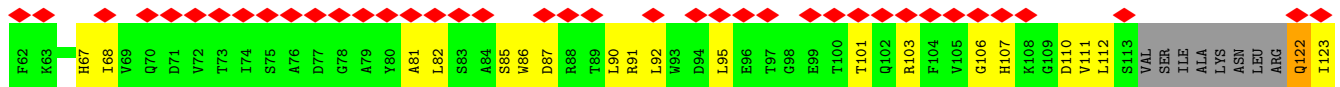
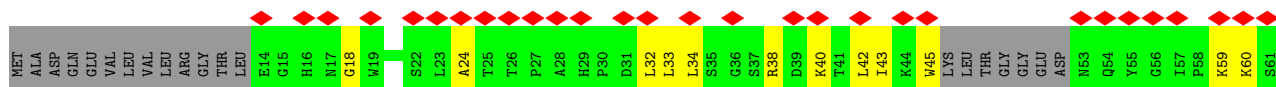
- Molecule 42: Ubiquitin-ribosomal 40S subunit protein S31 fusion protein

Chain g: 




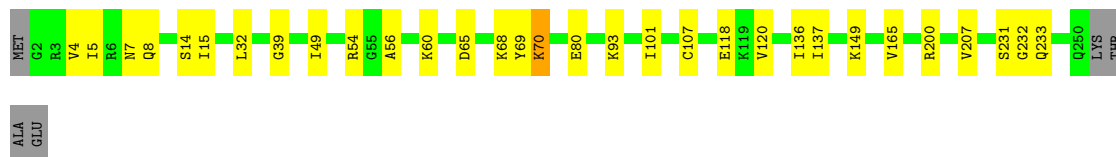
- Molecule 43: Guanine nucleotide-binding protein subunit beta-like protein

Chain h: 




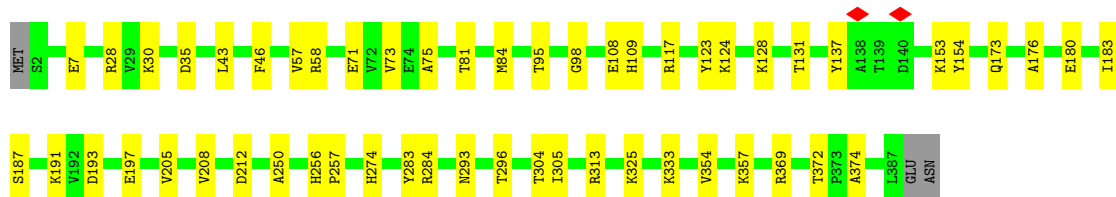
- Molecule 44: Ribosomal 60S subunit protein L2A

Chain j:  86% 12%




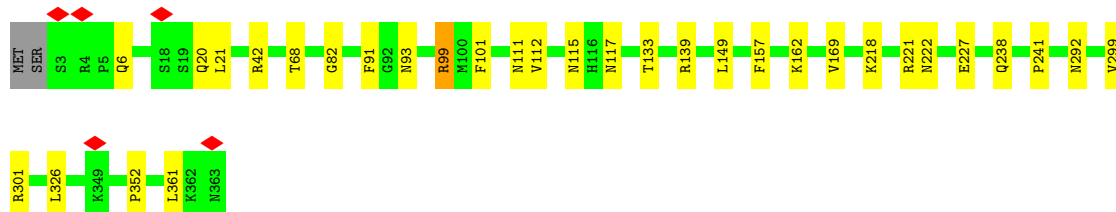
- Molecule 45: 60S ribosomal protein L3

Chain k:  85% 14%




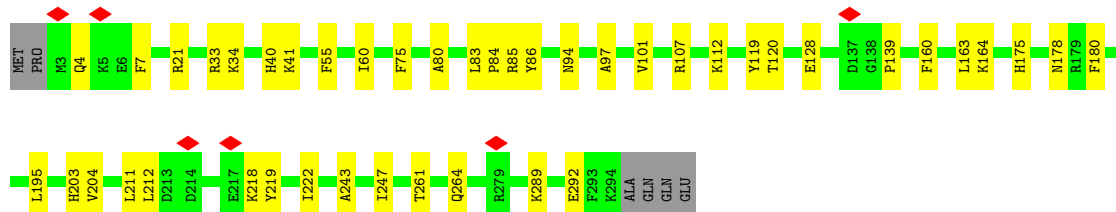
- Molecule 46: Ribosomal 60S subunit protein L4B

Chain l:  91% 9%



- Molecule 47: Ribosomal 60S subunit protein L5

Chain m:  83% 15%



- Molecule 48: 60S ribosomal protein L6

Chain n:  72% 16% 12%





- Molecule 49: Ribosomal 60S subunit protein L7A

Chain o: 86% 10% 5%



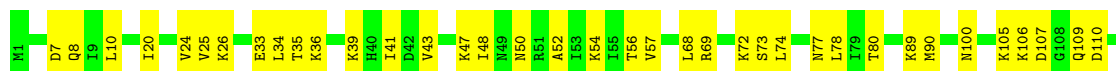
- Molecule 50: 60S ribosomal protein L8

Chain p: 77% 11% 12%



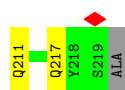
- Molecule 51: Ribosomal 60S subunit protein L9B

Chain q: 75% 24%



- Molecule 52: Ribosomal 60S subunit protein L10

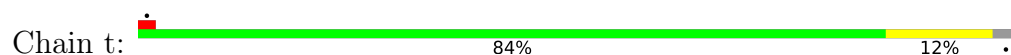
Chain r: 84% 15%



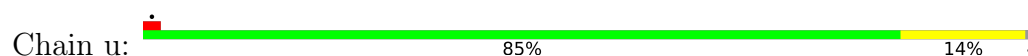
- Molecule 53: Ribosomal 60S subunit protein L11B

Chain s: 68% 31%

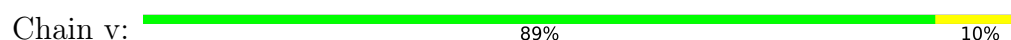
- Molecule 54: 60S ribosomal protein L13



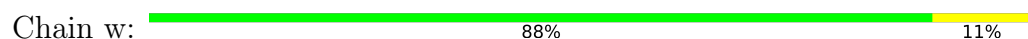
- Molecule 55: Ribosomal 60S subunit protein L14B



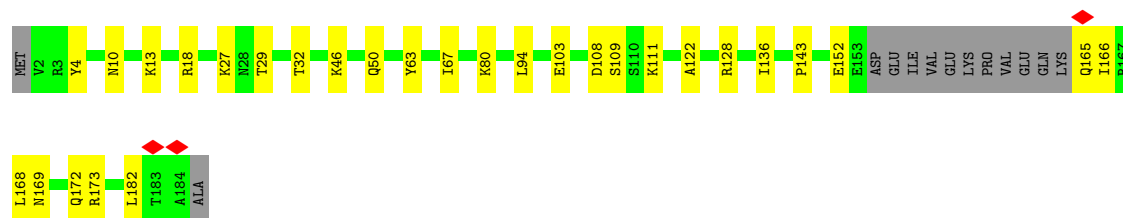
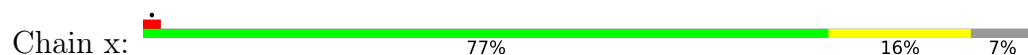
- Molecule 56: Ribosomal protein L15




- Molecule 57: Ribosomal 60S subunit protein L16A



- Molecule 58: Ribosomal 60S subunit protein L17B




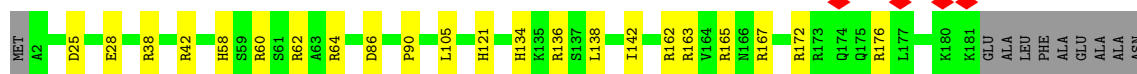
- Molecule 59: Ribosomal 60S subunit protein L18A

Chain y:  84% 15% ..




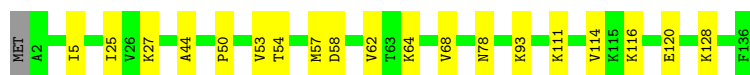
- Molecule 60: Ribosomal protein L19

Chain z:  83% 12% 5%




- Molecule 61: 60S ribosomal protein L27

Chain AA:  85% 14% .




- Molecule 62: Ribosomal 60S subunit protein L28

Chain AB:  85% 14% .




- Molecule 63: 60S ribosomal protein L29

Chain AC:  87% 8% 5%




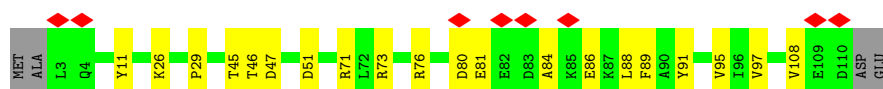
- Molecule 64: Ribosomal 60S subunit protein L30

Chain AD:  75% 15% 9%




- Molecule 65: Ribosomal 60S subunit protein L31B

Chain AE:  79% 18% .



- Molecule 66: Ribosomal 60S subunit protein L32

Chain AF:  85% 10% 5%



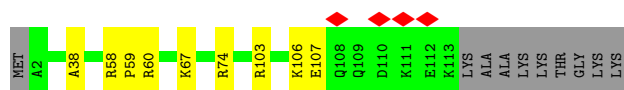
- Molecule 67: Ribosomal 60S subunit protein L33A

Chain AG:  89% 10% .




- Molecule 68: Ribosomal 60S subunit protein L34B

Chain AH:  84% 7% 8%



- Molecule 69: Ribosomal 60S subunit protein L35A

Chain AI:  83% 16% .



- Molecule 70: 60S ribosomal protein L36

Chain AJ:  75% 23% .




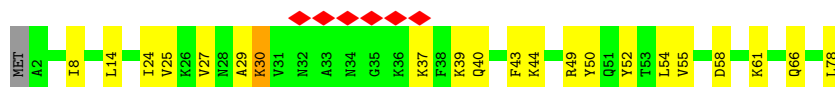
- Molecule 71: Ribosomal protein L37

Chain AK:  88% 8% .



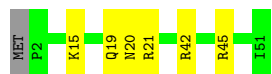
- Molecule 72: Ribosomal 60S subunit protein L38

Chain AL:  8% 72% 26% ..



- Molecule 73: 60S ribosomal protein L39

Chain AM:  86% 12% .




- Molecule 74: Rpl40bp

Chain AN:  90% 10% .




- Molecule 75: Small ribosomal subunit protein eS32

Chain AO:  72% 28% .




- Molecule 76: Ribosomal 60S subunit protein L42A

Chain AP:  83% 16% .



- Molecule 77: Ribosomal 60S subunit protein L43A

Chain AQ:  5% 89% 10% .



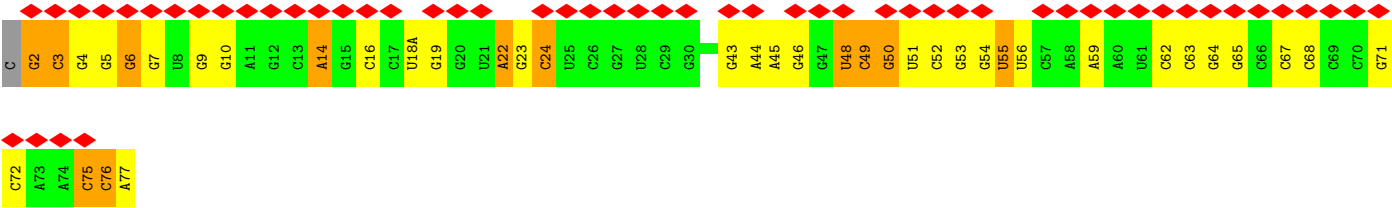
- Molecule 78: tRNA-fMet

Chain PT:  64% 32% . .



- Molecule 78: tRNA-fMet

Chain AT:  47% 71% 36% 16% .



● Molecule 79: mRNA



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 63238 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 29.7 | Depositor |
| Minimum defocus (nm) | 200 | Depositor |
| Maximum defocus (nm) | 1200 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 1.999 | Depositor |
| Minimum map value | -0.786 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.057 | Depositor |
| Recommended contour level | 0.174 | Depositor |
| Map size (Å) | 510.3, 510.3, 510.3 | wwPDB |
| Map dimensions | 700, 700, 700 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.729, 0.729, 0.729 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GET, SPK, MLZ, OMG, IAS, OMC, YMZ, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|---------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | 0 | 0.29 | 0/1483 | 0.46 | 0/1997 |
| 2 | 1 | 0.40 | 0/73296 | 0.41 | 0/114257 |
| 3 | 2 | 0.30 | 0/1305 | 0.40 | 0/1749 |
| 4 | 3 | 0.33 | 0/2884 | 0.33 | 0/4492 |
| 5 | 4 | 0.40 | 0/3702 | 0.40 | 0/5764 |
| 6 | 6 | 0.30 | 0/994 | 0.48 | 2/1339 (0.1%) |
| 7 | 7 | 0.31 | 0/528 | 0.45 | 0/701 |
| 8 | 8 | 0.31 | 0/990 | 0.44 | 0/1337 |
| 9 | 9 | 0.31 | 0/990 | 0.46 | 0/1322 |
| 10 | A | 0.32 | 0/40362 | 0.40 | 0/62888 |
| 11 | B | 0.26 | 0/1666 | 0.46 | 0/2273 |
| 12 | C | 0.27 | 0/1750 | 0.42 | 0/2354 |
| 13 | D | 0.28 | 0/1648 | 0.43 | 0/2237 |
| 14 | E | 0.24 | 0/1725 | 0.45 | 0/2316 |
| 15 | F | 0.24 | 0/2096 | 0.43 | 0/2822 |
| 16 | G | 0.24 | 0/1588 | 0.46 | 0/2139 |
| 17 | H | 0.22 | 0/1845 | 0.41 | 0/2464 |
| 18 | I | 0.25 | 0/1490 | 0.44 | 0/2004 |
| 19 | J | 0.26 | 0/1606 | 0.45 | 0/2150 |
| 20 | K | 0.23 | 0/1478 | 0.44 | 0/1978 |
| 21 | L | 0.21 | 0/801 | 0.52 | 0/1081 |
| 22 | M | 0.28 | 0/1154 | 0.44 | 0/1553 |
| 23 | N | 0.19 | 0/541 | 0.49 | 0/726 |
| 24 | O | 0.27 | 0/1210 | 0.43 | 0/1631 |
| 25 | P | 0.29 | 0/944 | 0.43 | 0/1265 |
| 26 | Q | 0.23 | 0/924 | 0.46 | 0/1243 |
| 27 | T | 0.24 | 0/1186 | 0.47 | 0/1590 |
| 28 | R | 0.25 | 0/1120 | 0.52 | 0/1500 |
| 29 | S | 0.24 | 0/966 | 0.46 | 0/1295 |
| 30 | U | 0.24 | 0/1120 | 0.46 | 0/1508 |
| 31 | V | 0.24 | 0/800 | 0.45 | 0/1082 |
| 32 | W | 0.28 | 0/683 | 0.49 | 0/918 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | X | 0.32 | 0/1049 | 0.44 | 0/1412 |
| 34 | Y | 0.25 | 0/1128 | 0.43 | 0/1505 |
| 35 | Z | 0.22 | 0/1086 | 0.46 | 0/1447 |
| 36 | a | 0.23 | 0/585 | 0.52 | 0/789 |
| 37 | b | 0.29 | 0/791 | 0.42 | 0/1060 |
| 38 | c | 0.25 | 0/624 | 0.40 | 0/843 |
| 39 | d | 0.25 | 0/489 | 0.45 | 0/654 |
| 40 | e | 0.23 | 0/466 | 0.44 | 0/620 |
| 41 | f | 0.24 | 0/469 | 0.52 | 0/626 |
| 42 | g | 0.23 | 0/575 | 0.58 | 0/760 |
| 43 | h | 0.19 | 0/1898 | 0.46 | 0/2584 |
| 44 | j | 0.35 | 0/1931 | 0.50 | 0/2592 |
| 45 | k | 0.33 | 0/3156 | 0.45 | 0/4246 |
| 46 | l | 0.30 | 0/2799 | 0.46 | 0/3777 |
| 47 | m | 0.26 | 0/2447 | 0.44 | 0/3294 |
| 48 | n | 0.28 | 0/1258 | 0.41 | 0/1696 |
| 49 | o | 0.30 | 0/1896 | 0.48 | 0/2544 |
| 50 | p | 0.30 | 0/1825 | 0.46 | 0/2458 |
| 51 | q | 0.27 | 0/1528 | 0.41 | 0/2055 |
| 52 | r | 0.26 | 0/1795 | 0.40 | 0/2411 |
| 53 | s | 0.25 | 0/1404 | 0.46 | 0/1880 |
| 54 | t | 0.31 | 0/1600 | 0.49 | 0/2147 |
| 55 | u | 0.30 | 0/1044 | 0.47 | 0/1407 |
| 56 | v | 0.34 | 0/1753 | 0.47 | 0/2347 |
| 57 | w | 0.31 | 0/1620 | 0.44 | 0/2167 |
| 58 | x | 0.32 | 0/1398 | 0.45 | 0/1879 |
| 59 | y | 0.30 | 0/1511 | 0.49 | 0/2022 |
| 60 | z | 0.29 | 0/1492 | 0.45 | 0/1983 |
| 61 | AA | 0.27 | 0/1112 | 0.38 | 0/1488 |
| 62 | AB | 0.32 | 0/1199 | 0.48 | 0/1607 |
| 63 | AC | 0.27 | 0/502 | 0.38 | 0/666 |
| 64 | AD | 0.27 | 0/738 | 0.36 | 0/994 |
| 65 | AE | 0.29 | 0/894 | 0.45 | 0/1201 |
| 66 | AF | 0.32 | 0/1039 | 0.46 | 0/1390 |
| 67 | AG | 0.32 | 0/895 | 0.40 | 0/1201 |
| 68 | AH | 0.30 | 0/934 | 0.48 | 0/1242 |
| 69 | AI | 0.30 | 0/1004 | 0.51 | 0/1337 |
| 70 | AJ | 0.27 | 0/772 | 0.42 | 0/1023 |
| 71 | AK | 0.36 | 0/690 | 0.51 | 0/916 |
| 72 | AL | 0.29 | 0/632 | 0.43 | 0/842 |
| 73 | AM | 0.32 | 0/458 | 0.43 | 0/609 |
| 74 | AN | 0.25 | 0/436 | 0.40 | 0/577 |
| 75 | AO | 0.27 | 0/237 | 0.65 | 0/304 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 76 | AP | 0.29 | 0/861 | 0.40 | 0/1136 |
| 77 | AQ | 0.30 | 0/705 | 0.44 | 0/940 |
| 78 | AT | 0.17 | 0/1813 | 0.35 | 0/2825 |
| 78 | PT | 0.24 | 0/1813 | 0.32 | 0/2825 |
| 79 | MR | 0.23 | 0/254 | 0.29 | 0/392 |
| All | All | 0.33 | 0/211480 | 0.42 | 2/310695 (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 |
|-----|-------|---------------------|---------------------|
| 25 | P | 0 | 1 |
| 28 | R | 0 | 1 |
| 46 | l | 0 | 1 |
| 48 | n | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 6 | 6 | 103 | VAL | CA-C-N | 5.17 | 135.64 | 120.97 |
| 6 | 6 | 103 | VAL | C-N-CA | 5.17 | 135.64 | 120.97 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 25 | P | 119 | IAS | Peptide |
| 28 | R | 39 | GLN | Peptide |
| 46 | l | 99 | ARG | Sidechain |
| 48 | n | 25 | ARG | Sidechain |

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 0 | 1442 | 0 | 1500 | 17 | 0 |
| 2 | 1 | 65536 | 0 | 32944 | 560 | 0 |
| 3 | 2 | 1276 | 0 | 1333 | 13 | 0 |
| 4 | 3 | 2579 | 0 | 1304 | 15 | 0 |
| 5 | 4 | 3313 | 0 | 1674 | 23 | 0 |
| 6 | 6 | 986 | 0 | 1040 | 10 | 0 |
| 7 | 7 | 516 | 0 | 534 | 13 | 0 |
| 8 | 8 | 974 | 0 | 1032 | 9 | 0 |
| 9 | 9 | 980 | 0 | 1058 | 12 | 0 |
| 10 | A | 36083 | 0 | 18151 | 561 | 0 |
| 11 | B | 1627 | 0 | 1644 | 44 | 0 |
| 12 | C | 1724 | 0 | 1805 | 36 | 0 |
| 13 | D | 1620 | 0 | 1715 | 33 | 0 |
| 14 | E | 1701 | 0 | 1802 | 61 | 0 |
| 15 | F | 2055 | 0 | 2137 | 70 | 0 |
| 16 | G | 1572 | 0 | 1644 | 48 | 0 |
| 17 | H | 1820 | 0 | 1896 | 46 | 0 |
| 18 | I | 1466 | 0 | 1561 | 49 | 0 |
| 19 | J | 1579 | 0 | 1602 | 39 | 0 |
| 20 | K | 1453 | 0 | 1532 | 61 | 0 |
| 21 | L | 783 | 0 | 799 | 41 | 0 |
| 22 | M | 1129 | 0 | 1183 | 17 | 0 |
| 23 | N | 539 | 0 | 573 | 21 | 0 |
| 24 | O | 1187 | 0 | 1249 | 22 | 0 |
| 25 | P | 942 | 0 | 980 | 21 | 0 |
| 26 | Q | 906 | 0 | 940 | 23 | 0 |
| 27 | T | 1169 | 0 | 1216 | 48 | 0 |
| 28 | R | 1102 | 0 | 1168 | 36 | 0 |
| 29 | S | 954 | 0 | 1008 | 21 | 0 |
| 30 | U | 1100 | 0 | 1114 | 35 | 0 |
| 31 | V | 790 | 0 | 855 | 33 | 0 |
| 32 | W | 676 | 0 | 677 | 21 | 0 |
| 33 | X | 1032 | 0 | 1066 | 13 | 0 |
| 34 | Y | 1110 | 0 | 1182 | 16 | 0 |
| 35 | Z | 1072 | 0 | 1123 | 38 | 0 |
| 36 | a | 578 | 0 | 613 | 21 | 0 |
| 37 | b | 779 | 0 | 832 | 15 | 0 |
| 38 | c | 614 | 0 | 630 | 8 | 0 |
| 39 | d | 487 | 0 | 523 | 20 | 0 |
| 40 | e | 454 | 0 | 430 | 12 | 0 |
| 41 | f | 461 | 0 | 499 | 15 | 0 |
| 42 | g | 565 | 0 | 605 | 23 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43 | h | 1854 | 0 | 1793 | 71 | 0 |
| 44 | j | 1894 | 0 | 1975 | 23 | 0 |
| 45 | k | 3084 | 0 | 3173 | 42 | 0 |
| 46 | l | 2751 | 0 | 2879 | 31 | 0 |
| 47 | m | 2394 | 0 | 2362 | 31 | 0 |
| 48 | n | 1237 | 0 | 1316 | 22 | 0 |
| 49 | o | 1860 | 0 | 1958 | 15 | 0 |
| 50 | p | 1795 | 0 | 1915 | 21 | 0 |
| 51 | q | 1510 | 0 | 1582 | 27 | 0 |
| 52 | r | 1759 | 0 | 1802 | 20 | 0 |
| 53 | s | 1385 | 0 | 1418 | 39 | 0 |
| 54 | t | 1573 | 0 | 1644 | 23 | 0 |
| 55 | u | 1029 | 0 | 1116 | 16 | 0 |
| 56 | v | 1713 | 0 | 1764 | 19 | 0 |
| 57 | w | 1590 | 0 | 1705 | 17 | 0 |
| 58 | x | 1375 | 0 | 1403 | 17 | 0 |
| 59 | y | 1478 | 0 | 1590 | 23 | 0 |
| 60 | z | 1471 | 0 | 1583 | 15 | 0 |
| 61 | AA | 1087 | 0 | 1154 | 14 | 0 |
| 62 | AB | 1170 | 0 | 1203 | 21 | 0 |
| 63 | AC | 489 | 0 | 522 | 4 | 0 |
| 64 | AD | 729 | 0 | 775 | 9 | 0 |
| 65 | AE | 881 | 0 | 932 | 13 | 0 |
| 66 | AF | 1015 | 0 | 1095 | 13 | 0 |
| 67 | AG | 867 | 0 | 932 | 8 | 0 |
| 68 | AH | 913 | 0 | 998 | 7 | 0 |
| 69 | AI | 990 | 0 | 1094 | 14 | 0 |
| 70 | AJ | 764 | 0 | 851 | 16 | 0 |
| 71 | AK | 677 | 0 | 697 | 5 | 0 |
| 72 | AL | 623 | 0 | 688 | 15 | 0 |
| 73 | AM | 446 | 0 | 488 | 4 | 0 |
| 74 | AN | 427 | 0 | 473 | 4 | 0 |
| 75 | AO | 236 | 0 | 285 | 6 | 0 |
| 76 | AP | 863 | 0 | 931 | 13 | 0 |
| 77 | AQ | 698 | 0 | 734 | 9 | 0 |
| 78 | AT | 1623 | 0 | 825 | 26 | 0 |
| 78 | PT | 1623 | 0 | 825 | 11 | 0 |
| 79 | MR | 229 | 0 | 117 | 0 | 0 |
| 80 | 1 | 14 | 0 | 30 | 3 | 0 |
| 81 | 1 | 408 | 0 | 480 | 20 | 0 |
| 81 | A | 102 | 0 | 120 | 5 | 0 |
| 81 | AT | 34 | 0 | 40 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 82 | AH | 1 | 0 | 0 | 0 | 0 |
| 82 | AK | 1 | 0 | 0 | 0 | 0 |
| 82 | AN | 1 | 0 | 0 | 0 | 0 |
| 82 | AP | 1 | 0 | 0 | 0 | 0 |
| 82 | AQ | 1 | 0 | 0 | 0 | 0 |
| 82 | b | 1 | 0 | 0 | 0 | 0 |
| 82 | e | 1 | 0 | 0 | 0 | 0 |
| 83 | AQ | 26 | 0 | 0 | 1 | 0 |
| All | All | 197424 | 0 | 146440 | 2458 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2458 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 78:AT:51:U:H3 | 78:AT:65:G:H1 | 1.05 | 1.01 |
| 2:1:437:G:H22 | 2:1:620:A:H61 | 1.13 | 0.96 |
| 46:l:139:ARG:HH21 | 46:l:241:PRO:HG2 | 1.33 | 0.94 |
| 10:A:1575:G:H1 | 10:A:1595:U:H3 | 0.94 | 0.91 |
| 10:A:1040:U:H3 | 10:A:1049:G:H1 | 1.16 | 0.91 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 0 | 171/172 (99%) | 169 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | 2 | 159/160 (99%) | 156 (98%) | 3 (2%) | 0 | 100 | 100 |
| 6 | 6 | 129/137 (94%) | 127 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 7 | 7 | 60/155 (39%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 8 | 8 | 119/142 (84%) | 117 (98%) | 2 (2%) | 0 | 100 | 100 |
| 9 | 9 | 123/127 (97%) | 120 (98%) | 3 (2%) | 0 | 100 | 100 |
| 11 | B | 206/261 (79%) | 192 (93%) | 14 (7%) | 0 | 100 | 100 |
| 12 | C | 212/256 (83%) | 203 (96%) | 9 (4%) | 0 | 100 | 100 |
| 13 | D | 214/249 (86%) | 209 (98%) | 5 (2%) | 0 | 100 | 100 |
| 14 | E | 220/251 (88%) | 211 (96%) | 9 (4%) | 0 | 100 | 100 |
| 15 | F | 258/262 (98%) | 240 (93%) | 18 (7%) | 0 | 100 | 100 |
| 16 | G | 195/225 (87%) | 187 (96%) | 8 (4%) | 0 | 100 | 100 |
| 17 | H | 224/236 (95%) | 212 (95%) | 12 (5%) | 0 | 100 | 100 |
| 18 | I | 180/186 (97%) | 170 (94%) | 10 (6%) | 0 | 100 | 100 |
| 19 | J | 201/206 (98%) | 193 (96%) | 8 (4%) | 0 | 100 | 100 |
| 20 | K | 176/189 (93%) | 163 (93%) | 13 (7%) | 0 | 100 | 100 |
| 21 | L | 91/118 (77%) | 84 (92%) | 7 (8%) | 0 | 100 | 100 |
| 22 | M | 139/155 (90%) | 132 (95%) | 7 (5%) | 0 | 100 | 100 |
| 23 | N | 65/143 (46%) | 53 (82%) | 12 (18%) | 0 | 100 | 100 |
| 24 | O | 148/151 (98%) | 145 (98%) | 3 (2%) | 0 | 100 | 100 |
| 25 | P | 124/132 (94%) | 122 (98%) | 2 (2%) | 0 | 100 | 100 |
| 26 | Q | 113/142 (80%) | 103 (91%) | 10 (9%) | 0 | 100 | 100 |
| 27 | T | 140/145 (97%) | 125 (89%) | 15 (11%) | 0 | 100 | 100 |
| 28 | R | 139/142 (98%) | 132 (95%) | 6 (4%) | 1 (1%) | 19 | 13 |
| 29 | S | 116/137 (85%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 30 | U | 139/145 (96%) | 135 (97%) | 4 (3%) | 0 | 100 | 100 |
| 31 | V | 98/119 (82%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 32 | W | 85/87 (98%) | 78 (92%) | 7 (8%) | 0 | 100 | 100 |
| 33 | X | 127/130 (98%) | 125 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | Y | 141/145 (97%) | 134 (95%) | 7 (5%) | 0 | 100 | 100 |
| 35 | Z | 130/135 (96%) | 118 (91%) | 12 (9%) | 0 | 100 | 100 |
| 36 | a | 70/105 (67%) | 62 (89%) | 8 (11%) | 0 | 100 | 100 |
| 37 | b | 96/119 (81%) | 92 (96%) | 4 (4%) | 0 | 100 | 100 |
| 38 | c | 79/82 (96%) | 70 (89%) | 9 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|----------|-------------|-----|
| 39 | d | 60/67 (90%) | 57 (95%) | 3 (5%) | 0 | 100 | 100 |
| 40 | e | 53/56 (95%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |
| 41 | f | 56/63 (89%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 42 | g | 66/193 (34%) | 51 (77%) | 15 (23%) | 0 | 100 | 100 |
| 43 | h | 229/317 (72%) | 198 (86%) | 31 (14%) | 0 | 100 | 100 |
| 44 | j | 248/254 (98%) | 239 (96%) | 9 (4%) | 0 | 100 | 100 |
| 45 | k | 385/389 (99%) | 376 (98%) | 9 (2%) | 0 | 100 | 100 |
| 46 | l | 359/363 (99%) | 349 (97%) | 10 (3%) | 0 | 100 | 100 |
| 47 | m | 290/298 (97%) | 278 (96%) | 12 (4%) | 0 | 100 | 100 |
| 48 | n | 152/176 (86%) | 147 (97%) | 5 (3%) | 0 | 100 | 100 |
| 49 | o | 229/241 (95%) | 224 (98%) | 5 (2%) | 0 | 100 | 100 |
| 50 | p | 229/262 (87%) | 222 (97%) | 7 (3%) | 0 | 100 | 100 |
| 51 | q | 187/191 (98%) | 181 (97%) | 6 (3%) | 0 | 100 | 100 |
| 52 | r | 216/220 (98%) | 212 (98%) | 4 (2%) | 0 | 100 | 100 |
| 53 | s | 171/174 (98%) | 170 (99%) | 1 (1%) | 0 | 100 | 100 |
| 54 | t | 193/202 (96%) | 183 (95%) | 8 (4%) | 2 (1%) | 13 | 8 |
| 55 | u | 128/131 (98%) | 124 (97%) | 4 (3%) | 0 | 100 | 100 |
| 56 | v | 201/204 (98%) | 195 (97%) | 6 (3%) | 0 | 100 | 100 |
| 57 | w | 197/200 (98%) | 194 (98%) | 3 (2%) | 0 | 100 | 100 |
| 58 | x | 168/185 (91%) | 162 (96%) | 6 (4%) | 0 | 100 | 100 |
| 59 | y | 186/186 (100%) | 180 (97%) | 6 (3%) | 0 | 100 | 100 |
| 60 | z | 179/190 (94%) | 177 (99%) | 2 (1%) | 0 | 100 | 100 |
| 61 | AA | 133/136 (98%) | 133 (100%) | 0 | 0 | 100 | 100 |
| 62 | AB | 146/149 (98%) | 142 (97%) | 4 (3%) | 0 | 100 | 100 |
| 63 | AC | 59/63 (94%) | 59 (100%) | 0 | 0 | 100 | 100 |
| 64 | AD | 94/106 (89%) | 93 (99%) | 1 (1%) | 0 | 100 | 100 |
| 65 | AE | 106/112 (95%) | 102 (96%) | 4 (4%) | 0 | 100 | 100 |
| 66 | AF | 124/131 (95%) | 124 (100%) | 0 | 0 | 100 | 100 |
| 67 | AG | 107/107 (100%) | 105 (98%) | 2 (2%) | 0 | 100 | 100 |
| 68 | AH | 114/122 (93%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 69 | AI | 118/120 (98%) | 114 (97%) | 4 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 70 | AJ | 96/99 (97%) | 95 (99%) | 1 (1%) | 0 | 100 | 100 |
| 71 | AK | 84/90 (93%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 72 | AL | 76/78 (97%) | 74 (97%) | 2 (3%) | 0 | 100 | 100 |
| 73 | AM | 49/51 (96%) | 47 (96%) | 2 (4%) | 0 | 100 | 100 |
| 74 | AN | 51/52 (98%) | 51 (100%) | 0 | 0 | 100 | 100 |
| 75 | AO | 23/25 (92%) | 21 (91%) | 1 (4%) | 1 (4%) | 2 | 0 |
| 76 | AP | 103/106 (97%) | 100 (97%) | 3 (3%) | 0 | 100 | 100 |
| 77 | AQ | 89/92 (97%) | 85 (96%) | 4 (4%) | 0 | 100 | 100 |
| All | All | 10641/11747 (91%) | 10202 (96%) | 435 (4%) | 4 (0%) | 100 | 100 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | R | 40 | PRO |
| 54 | t | 5 | LYS |
| 54 | t | 63 | VAL |
| 75 | AO | 3 | ASP |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | 0 | 158/157 (101%) | 158 (100%) | 0 | 100 | 100 |
| 3 | 2 | 135/134 (101%) | 135 (100%) | 0 | 100 | 100 |
| 6 | 6 | 101/103 (98%) | 101 (100%) | 0 | 100 | 100 |
| 7 | 7 | 56/127 (44%) | 56 (100%) | 0 | 100 | 100 |
| 8 | 8 | 108/121 (89%) | 108 (100%) | 0 | 100 | 100 |
| 9 | 9 | 110/112 (98%) | 110 (100%) | 0 | 100 | 100 |
| 11 | B | 176/215 (82%) | 176 (100%) | 0 | 100 | 100 |
| 12 | C | 194/229 (85%) | 194 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 13 | D | 174/198 (88%) | 174 (100%) | 0 | 100 | 100 |
| 14 | E | 173/196 (88%) | 173 (100%) | 0 | 100 | 100 |
| 15 | F | 218/220 (99%) | 218 (100%) | 0 | 100 | 100 |
| 16 | G | 173/197 (88%) | 173 (100%) | 0 | 100 | 100 |
| 17 | H | 195/204 (96%) | 195 (100%) | 0 | 100 | 100 |
| 18 | I | 163/167 (98%) | 163 (100%) | 0 | 100 | 100 |
| 19 | J | 157/160 (98%) | 157 (100%) | 0 | 100 | 100 |
| 20 | K | 153/160 (96%) | 153 (100%) | 0 | 100 | 100 |
| 21 | L | 87/104 (84%) | 87 (100%) | 0 | 100 | 100 |
| 22 | M | 122/134 (91%) | 122 (100%) | 0 | 100 | 100 |
| 23 | N | 60/123 (49%) | 60 (100%) | 0 | 100 | 100 |
| 24 | O | 129/130 (99%) | 129 (100%) | 0 | 100 | 100 |
| 25 | P | 96/101 (95%) | 96 (100%) | 0 | 100 | 100 |
| 26 | Q | 99/121 (82%) | 99 (100%) | 0 | 100 | 100 |
| 27 | T | 126/129 (98%) | 126 (100%) | 0 | 100 | 100 |
| 28 | R | 115/116 (99%) | 115 (100%) | 0 | 100 | 100 |
| 29 | S | 106/122 (87%) | 106 (100%) | 0 | 100 | 100 |
| 30 | U | 113/117 (97%) | 113 (100%) | 0 | 100 | 100 |
| 31 | V | 90/105 (86%) | 90 (100%) | 0 | 100 | 100 |
| 32 | W | 71/71 (100%) | 71 (100%) | 0 | 100 | 100 |
| 33 | X | 112/113 (99%) | 112 (100%) | 0 | 100 | 100 |
| 34 | Y | 116/118 (98%) | 116 (100%) | 0 | 100 | 100 |
| 35 | Z | 109/112 (97%) | 109 (100%) | 0 | 100 | 100 |
| 36 | a | 64/85 (75%) | 64 (100%) | 0 | 100 | 100 |
| 37 | b | 84/102 (82%) | 84 (100%) | 0 | 100 | 100 |
| 38 | c | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| 39 | d | 54/58 (93%) | 54 (100%) | 0 | 100 | 100 |
| 40 | e | 47/48 (98%) | 47 (100%) | 0 | 100 | 100 |
| 41 | f | 50/54 (93%) | 50 (100%) | 0 | 100 | 100 |
| 42 | g | 60/175 (34%) | 60 (100%) | 0 | 100 | 100 |
| 43 | h | 199/263 (76%) | 198 (100%) | 1 (0%) | 86 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 44 | j | 191/194 (98%) | 189 (99%) | 2 (1%) | 73 | 78 |
| 45 | k | 326/328 (99%) | 326 (100%) | 0 | 100 | 100 |
| 46 | l | 290/292 (99%) | 290 (100%) | 0 | 100 | 100 |
| 47 | m | 247/252 (98%) | 247 (100%) | 0 | 100 | 100 |
| 48 | n | 135/154 (88%) | 135 (100%) | 0 | 100 | 100 |
| 49 | o | 195/204 (96%) | 195 (100%) | 0 | 100 | 100 |
| 50 | p | 193/216 (89%) | 193 (100%) | 0 | 100 | 100 |
| 51 | q | 168/170 (99%) | 168 (100%) | 0 | 100 | 100 |
| 52 | r | 185/186 (100%) | 185 (100%) | 0 | 100 | 100 |
| 53 | s | 148/149 (99%) | 148 (100%) | 0 | 100 | 100 |
| 54 | t | 163/168 (97%) | 163 (100%) | 0 | 100 | 100 |
| 55 | u | 108/109 (99%) | 108 (100%) | 0 | 100 | 100 |
| 56 | v | 177/178 (99%) | 177 (100%) | 0 | 100 | 100 |
| 57 | w | 166/167 (99%) | 166 (100%) | 0 | 100 | 100 |
| 58 | x | 142/154 (92%) | 142 (100%) | 0 | 100 | 100 |
| 59 | y | 156/154 (101%) | 154 (99%) | 2 (1%) | 65 | 71 |
| 60 | z | 148/153 (97%) | 148 (100%) | 0 | 100 | 100 |
| 61 | AA | 117/118 (99%) | 117 (100%) | 0 | 100 | 100 |
| 62 | AB | 120/121 (99%) | 120 (100%) | 0 | 100 | 100 |
| 63 | AC | 48/49 (98%) | 46 (96%) | 2 (4%) | 25 | 24 |
| 64 | AD | 81/90 (90%) | 81 (100%) | 0 | 100 | 100 |
| 65 | AE | 97/100 (97%) | 97 (100%) | 0 | 100 | 100 |
| 66 | AF | 111/115 (96%) | 109 (98%) | 2 (2%) | 54 | 59 |
| 67 | AG | 94/92 (102%) | 94 (100%) | 0 | 100 | 100 |
| 68 | AH | 99/102 (97%) | 99 (100%) | 0 | 100 | 100 |
| 69 | AI | 106/106 (100%) | 106 (100%) | 0 | 100 | 100 |
| 70 | AJ | 78/79 (99%) | 78 (100%) | 0 | 100 | 100 |
| 71 | AK | 70/73 (96%) | 70 (100%) | 0 | 100 | 100 |
| 72 | AL | 69/69 (100%) | 67 (97%) | 2 (3%) | 37 | 38 |
| 73 | AM | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 74 | AN | 48/47 (102%) | 48 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 75 | AO | 24/24 (100%) | 24 (100%) | 0 | 100 | 100 |
| 76 | AP | 90/89 (101%) | 90 (100%) | 0 | 100 | 100 |
| 77 | AQ | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| All | All | 9134/9896 (92%) | 9123 (100%) | 11 (0%) | 92 | 95 |

5 of 11 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 66 | AF | 17[A] | LYS |
| 66 | AF | 17[B] | LYS |
| 72 | AL | 30[B] | LYS |
| 72 | AL | 30[A] | LYS |
| 59 | y | 31[B] | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | l | 176 | HIS |
| 57 | w | 51 | ASN |
| 46 | l | 321 | ASN |
| 51 | q | 77 | ASN |
| 58 | x | 137 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10 | A | 1685/1787 (94%) | 385 (22%) | 26 (1%) |
| 2 | 1 | 3060/3359 (91%) | 467 (15%) | 34 (1%) |
| 4 | 3 | 120/121 (99%) | 9 (7%) | 0 |
| 5 | 4 | 155/158 (98%) | 20 (12%) | 1 (0%) |
| 78 | AT | 76/77 (98%) | 21 (27%) | 1 (1%) |
| 78 | PT | 75/77 (97%) | 14 (18%) | 0 |
| 79 | MR | 10/39 (25%) | 0 | 0 |
| All | All | 5181/5618 (92%) | 916 (17%) | 62 (1%) |

5 of 916 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 1 | 5 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 1 | 25 | A |
| 2 | 1 | 39 | A |
| 2 | 1 | 42 | A |
| 2 | 1 | 48 | A |

5 of 62 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | 1 | 3234 | U |
| 10 | A | 1467 | C |
| 10 | A | 25 | C |
| 10 | A | 1398 | G |
| 10 | A | 1579 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 25 | IAS | P | 119 | 25 | 6,7,8 | 1.19 | 0 | 5,8,10 | 1.44 | 1 (20%) |
| 2 | OMC | 1 | 2808 | 2 | 19,22,23 | 2.84 | 8 (42%) | 26,31,34 | 1.13 | 2 (7%) |
| 76 | MLZ | AP | 40 | 76 | 8,9,10 | 0.80 | 0 | 4,9,11 | 0.62 | 0 |
| 2 | OMG | 1 | 2765 | 2 | 18,26,27 | 2.34 | 8 (44%) | 19,38,41 | 1.53 | 4 (21%) |
| 6 | MLZ | 6 | 110 | 6 | 8,9,10 | 0.77 | 0 | 4,9,11 | 0.56 | 0 |
| 76 | MLZ | AP | 55 | 76 | 8,9,10 | 0.71 | 0 | 4,9,11 | 0.64 | 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 |
|-----|------|-------|------|------|---------|-----------|---------|
| 25 | IAS | P | 119 | 25 | - | 2/5/6/8 | - |
| 2 | OMC | 1 | 2808 | 2 | - | 2/9/27/28 | 0/2/2/2 |
| 76 | MLZ | AP | 40 | 76 | - | 3/7/8/10 | - |
| 2 | OMG | 1 | 2765 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 6 | MLZ | 6 | 110 | 6 | - | 2/7/8/10 | - |
| 76 | MLZ | AP | 55 | 76 | - | 1/7/8/10 | - |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | 1 | 2808 | OMC | C2-N3 | 5.76 | 1.48 | 1.36 |
| 2 | 1 | 2808 | OMC | C6-C5 | 5.61 | 1.48 | 1.35 |
| 2 | 1 | 2765 | OMG | C2-N3 | 4.96 | 1.45 | 1.33 |
| 2 | 1 | 2808 | OMC | C2-N1 | 4.57 | 1.49 | 1.40 |
| 2 | 1 | 2808 | OMC | C4-N4 | 4.56 | 1.44 | 1.33 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2 | 1 | 2765 | OMG | C5-C6-N1 | 3.68 | 120.45 | 113.95 |
| 2 | 1 | 2808 | OMC | O2-C2-N3 | -3.18 | 117.15 | 122.33 |
| 2 | 1 | 2765 | OMG | C2-N1-C6 | -2.85 | 119.84 | 125.10 |
| 2 | 1 | 2765 | OMG | C8-N7-C5 | 2.51 | 107.78 | 102.99 |
| 25 | P | 119 | IAS | CA-CB-CG | -2.43 | 98.55 | 113.74 |

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 2 | 1 | 2808 | OMC | O4'-C1'-N1-C2 |
| 2 | 1 | 2808 | OMC | O4'-C1'-N1-C6 |
| 25 | P | 119 | IAS | C-CA-CB-CG |
| 76 | AP | 40 | MLZ | CG-CD-CE-NZ |
| 6 | 6 | 110 | MLZ | CE-CD-CG-CB |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | 1 | 2808 | OMC | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 7 are monoatomic - leaving 18 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 |
| 81 | GET | A | 1801 | - | 33,36,36 | 0.46 | 0 | 43,55,55 | 0.84 | 3 (6%) |
| 81 | GET | 1 | 3412 | - | 33,36,36 | 0.53 | 0 | 43,55,55 | 0.63 | 0 |
| 81 | GET | 1 | 3403 | - | 33,36,36 | 0.56 | 0 | 43,55,55 | 0.92 | 2 (4%) |
| 80 | SPK | 1 | 3401 | - | 13,13,13 | 0.39 | 0 | 12,12,12 | 0.90 | 0 |
| 81 | GET | 1 | 3402 | - | 33,36,36 | 0.44 | 0 | 43,55,55 | 0.63 | 1 (2%) |
| 81 | GET | A | 1803 | - | 33,36,36 | 0.47 | 0 | 43,55,55 | 0.81 | 2 (4%) |
| 83 | YMZ | AQ | 301 | - | 28,28,28 | 1.20 | 1 (3%) | 41,43,43 | 1.47 | 5 (12%) |
| 81 | GET | 1 | 3413 | - | 33,36,36 | 0.44 | 0 | 43,55,55 | 0.98 | 2 (4%) |
| 81 | GET | 1 | 3409 | - | 33,36,36 | 0.50 | 0 | 43,55,55 | 0.78 | 1 (2%) |
| 81 | GET | AT | 101 | - | 33,36,36 | 0.49 | 0 | 43,55,55 | 0.64 | 1 (2%) |
| 81 | GET | 1 | 3404 | - | 33,36,36 | 0.55 | 0 | 43,55,55 | 0.88 | 2 (4%) |
| 81 | GET | A | 1802 | - | 33,36,36 | 0.44 | 0 | 43,55,55 | 0.87 | 2 (4%) |
| 81 | GET | 1 | 3407 | - | 33,36,36 | 0.45 | 0 | 43,55,55 | 0.77 | 2 (4%) |
| 81 | GET | 1 | 3410 | - | 33,36,36 | 0.42 | 0 | 43,55,55 | 0.71 | 1 (2%) |
| 81 | GET | 1 | 3411 | - | 33,36,36 | 0.46 | 0 | 43,55,55 | 0.77 | 2 (4%) |
| 81 | GET | 1 | 3405 | - | 33,36,36 | 0.43 | 0 | 43,55,55 | 0.80 | 1 (2%) |
| 81 | GET | 1 | 3406 | - | 33,36,36 | 0.49 | 0 | 43,55,55 | 0.92 | 1 (2%) |
| 81 | GET | 1 | 3408 | - | 33,36,36 | 0.42 | 0 | 43,55,55 | 0.69 | 1 (2%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 81 | GET | A | 1801 | - | - | 1/13/74/74 | 1/3/3/3 |
| 81 | GET | 1 | 3412 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3403 | - | - | 7/13/74/74 | 1/3/3/3 |
| 80 | SPK | 1 | 3401 | - | - | 6/11/11/11 | - |
| 81 | GET | 1 | 3402 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | A | 1803 | - | - | 7/13/74/74 | 0/3/3/3 |
| 83 | YMZ | AQ | 301 | - | - | 7/20/28/28 | 0/3/3/3 |
| 81 | GET | 1 | 3413 | - | - | 3/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3409 | - | - | 3/13/74/74 | 1/3/3/3 |
| 81 | GET | AT | 101 | - | - | 2/13/74/74 | 1/3/3/3 |
| 81 | GET | 1 | 3404 | - | - | 3/13/74/74 | 1/3/3/3 |
| 81 | GET | A | 1802 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3407 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3410 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3411 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3405 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3406 | - | - | 1/13/74/74 | 0/3/3/3 |
| 81 | GET | 1 | 3408 | - | - | 1/13/74/74 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 83 | AQ | 301 | YMZ | CAW-CAX | 5.17 | 1.60 | 1.53 |

The worst 5 of 29 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 83 | AQ | 301 | YMZ | CAK-CAR-NAP | 4.54 | 128.32 | 125.50 |
| 81 | 1 | 3405 | GET | O11-C11-C21 | 4.33 | 115.67 | 108.22 |
| 81 | 1 | 3406 | GET | O11-C11-C21 | 4.02 | 115.14 | 108.22 |
| 81 | A | 1802 | GET | O11-C11-C21 | 3.63 | 114.47 | 108.22 |
| 81 | 1 | 3413 | GET | O11-C11-C21 | 3.60 | 114.41 | 108.22 |

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 81 | 1 | 3402 | GET | C23-C33-N33-C93 |
| 81 | 1 | 3403 | GET | C21-C11-O11-C42 |
| 81 | 1 | 3403 | GET | C41-C51-C61-O61 |
| 81 | 1 | 3403 | GET | C41-C51-C61-C71 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 81 | 1 | 3403 | GET | O51-C51-C61-C71 |

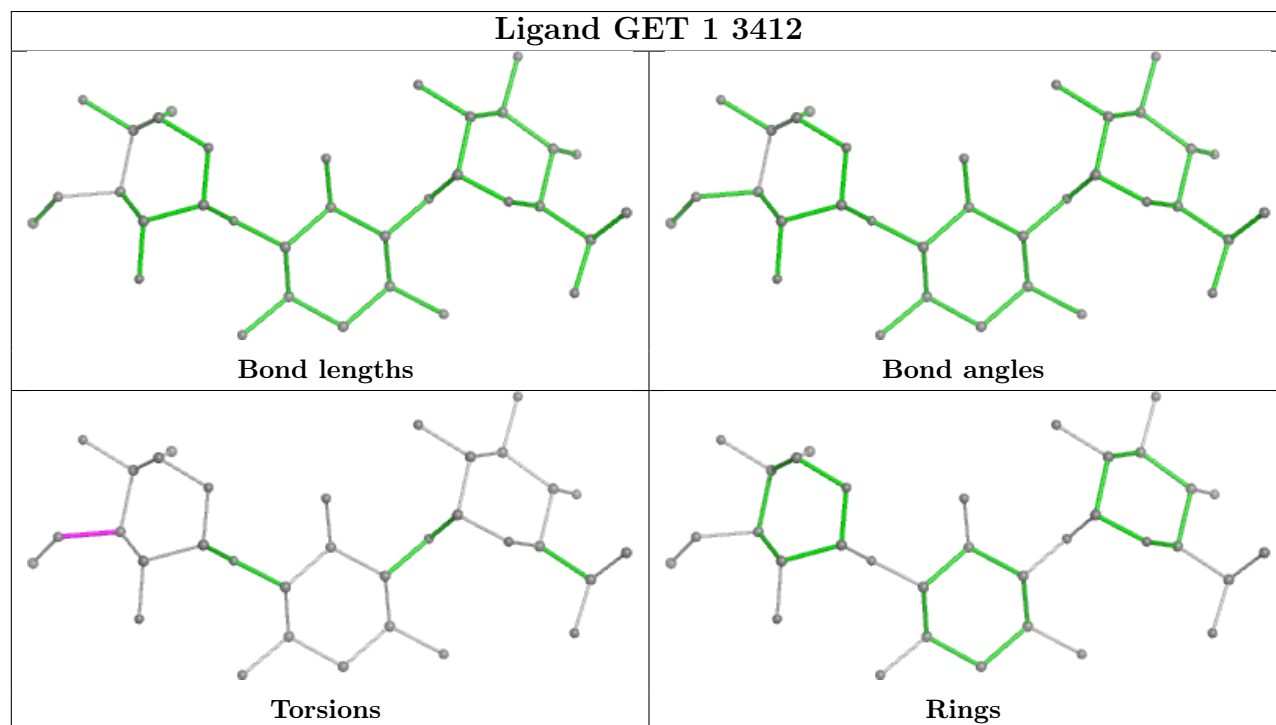
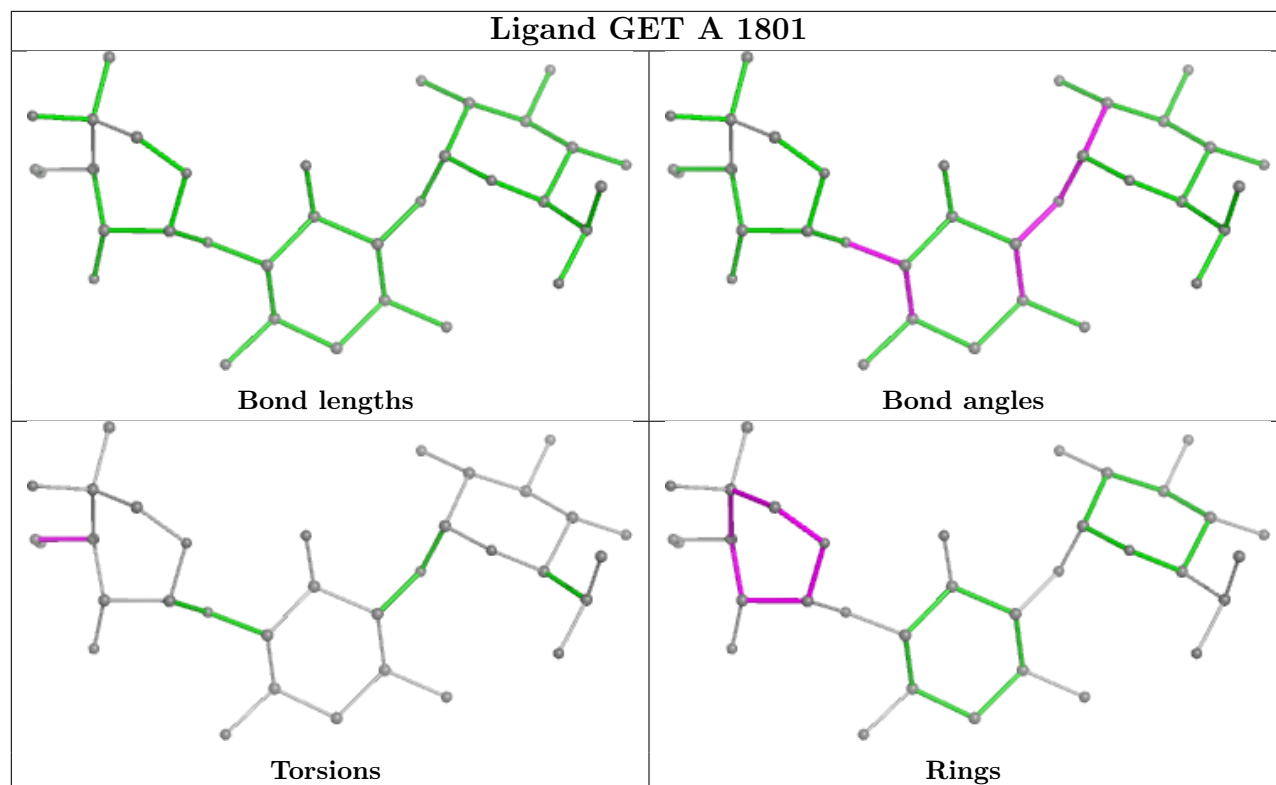
All (5) ring outliers are listed below:

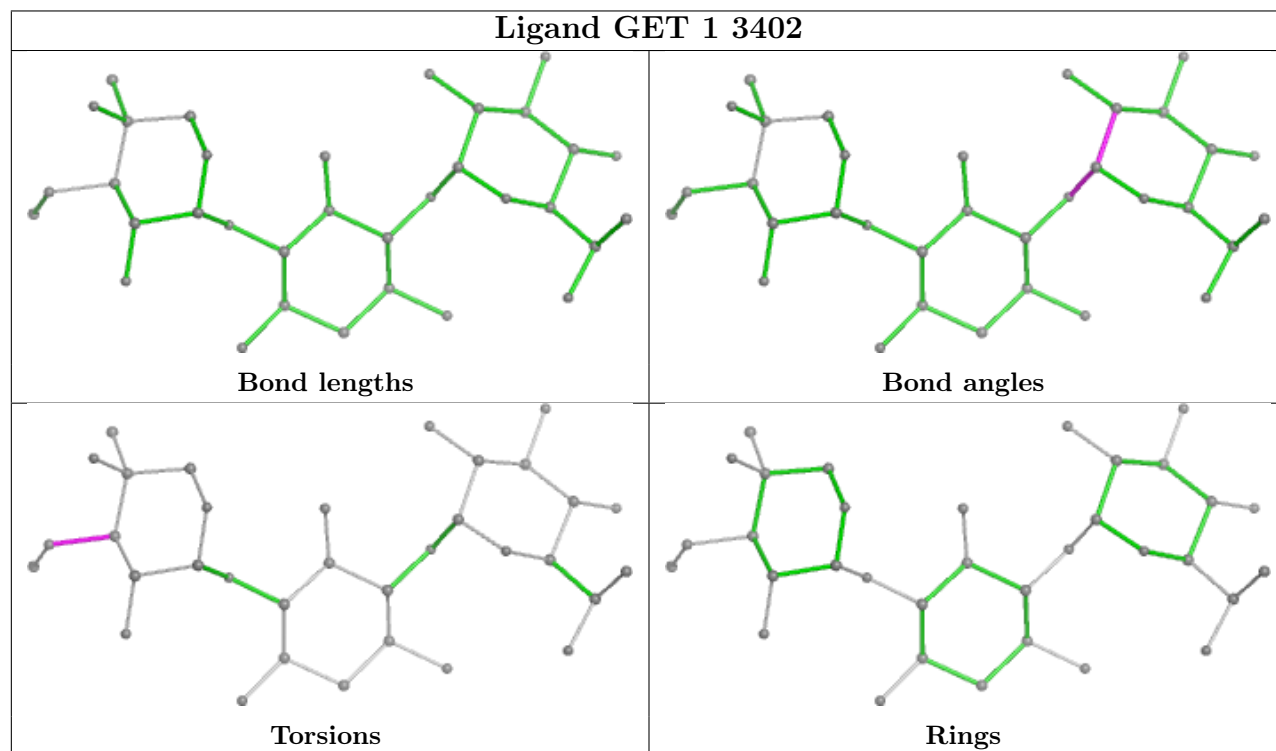
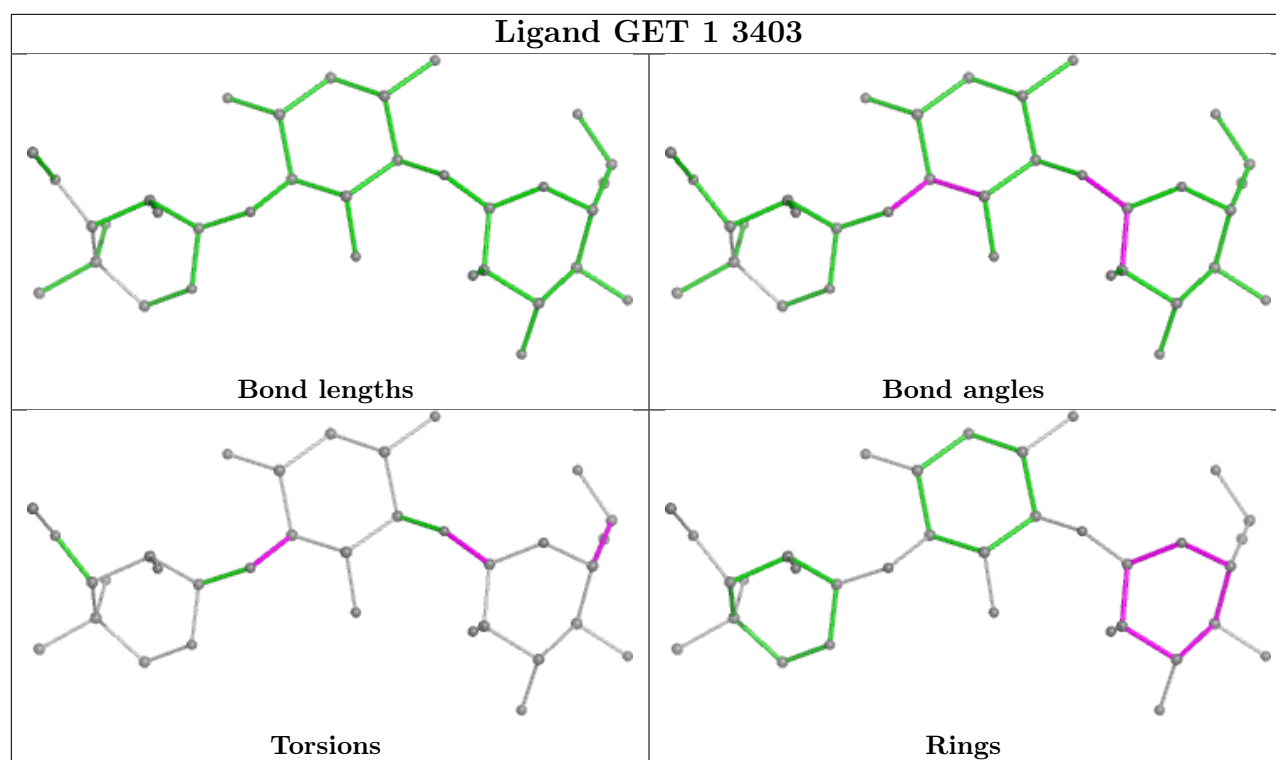
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------------------|
| 81 | 1 | 3403 | GET | C11-C21-C31-C41-C51-O51 |
| 81 | 1 | 3409 | GET | C13-C23-C33-C43-C53-O53 |
| 81 | 1 | 3404 | GET | C13-C23-C33-C43-C53-O53 |
| 81 | A | 1801 | GET | C13-C23-C33-C43-C53-O53 |
| 81 | AT | 101 | GET | C11-C21-C31-C41-C51-O51 |

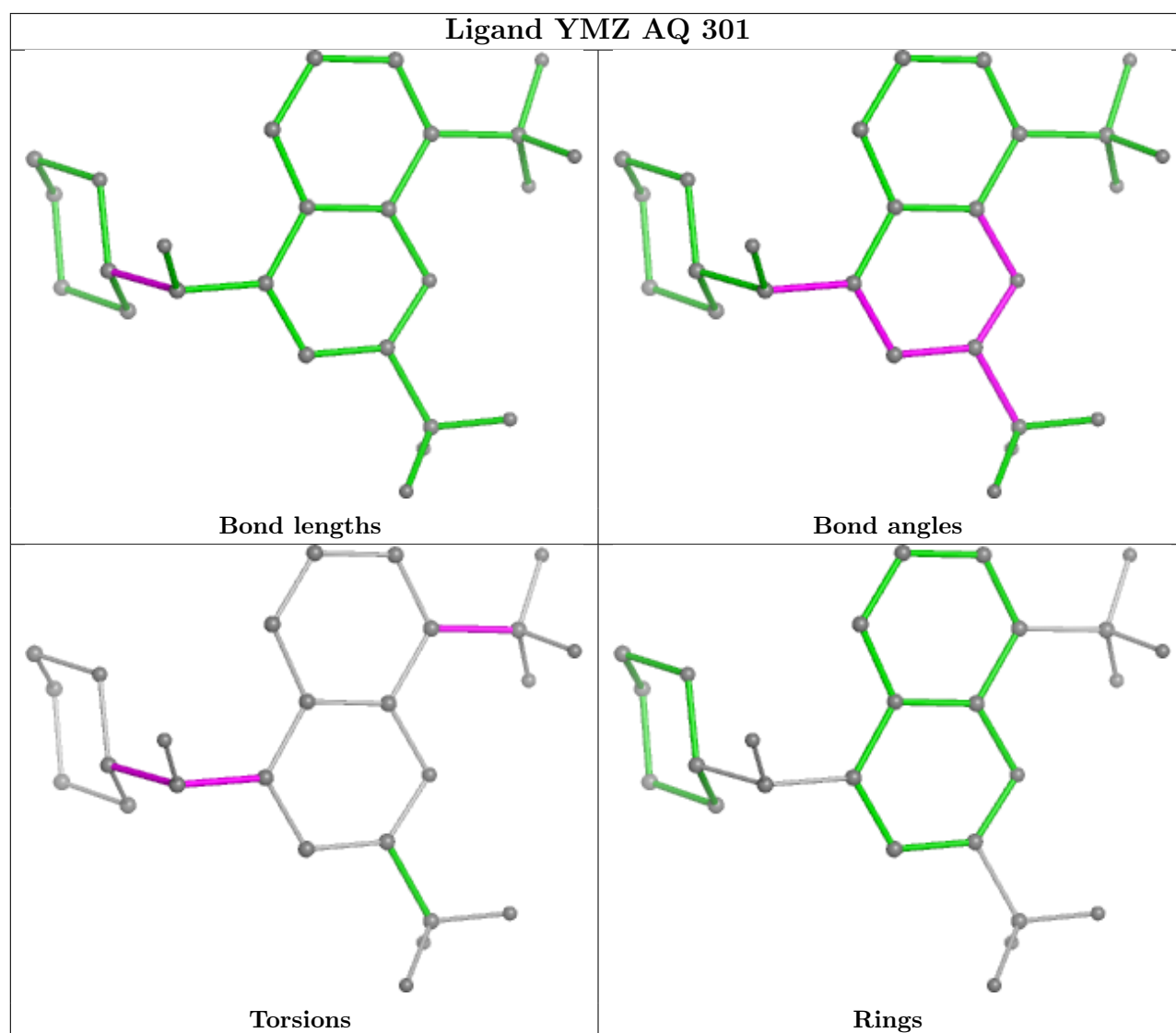
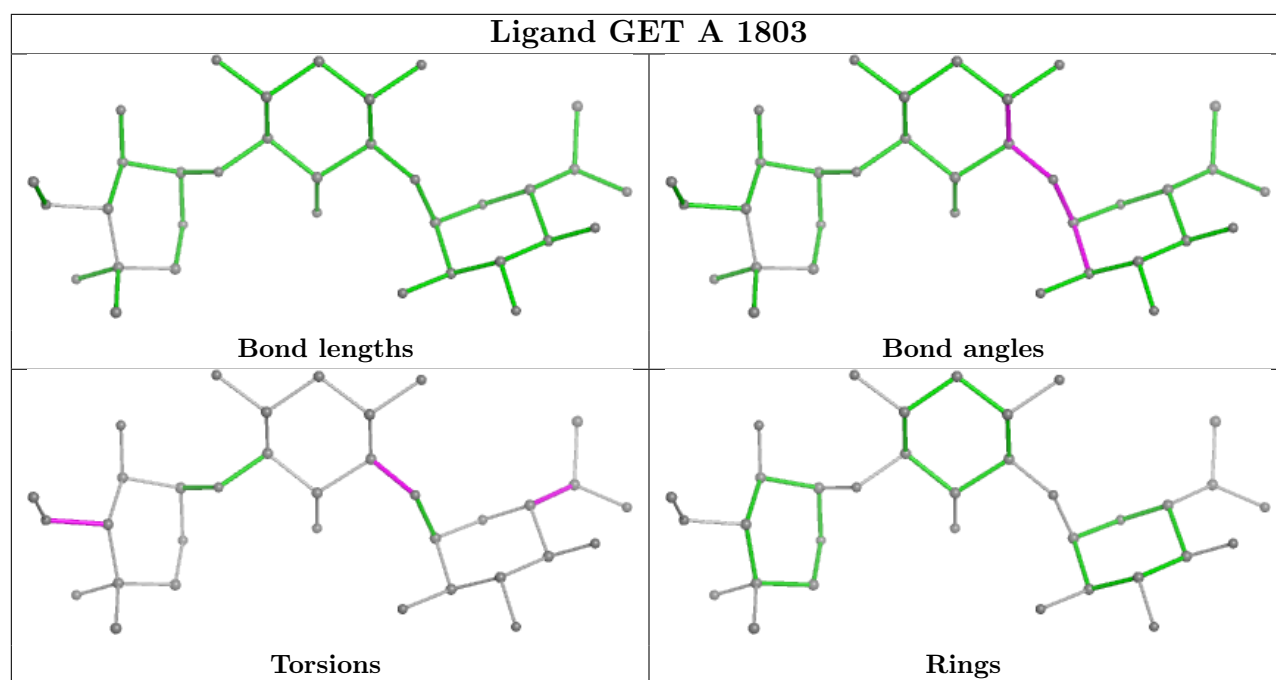
16 monomers are involved in 30 short contacts:

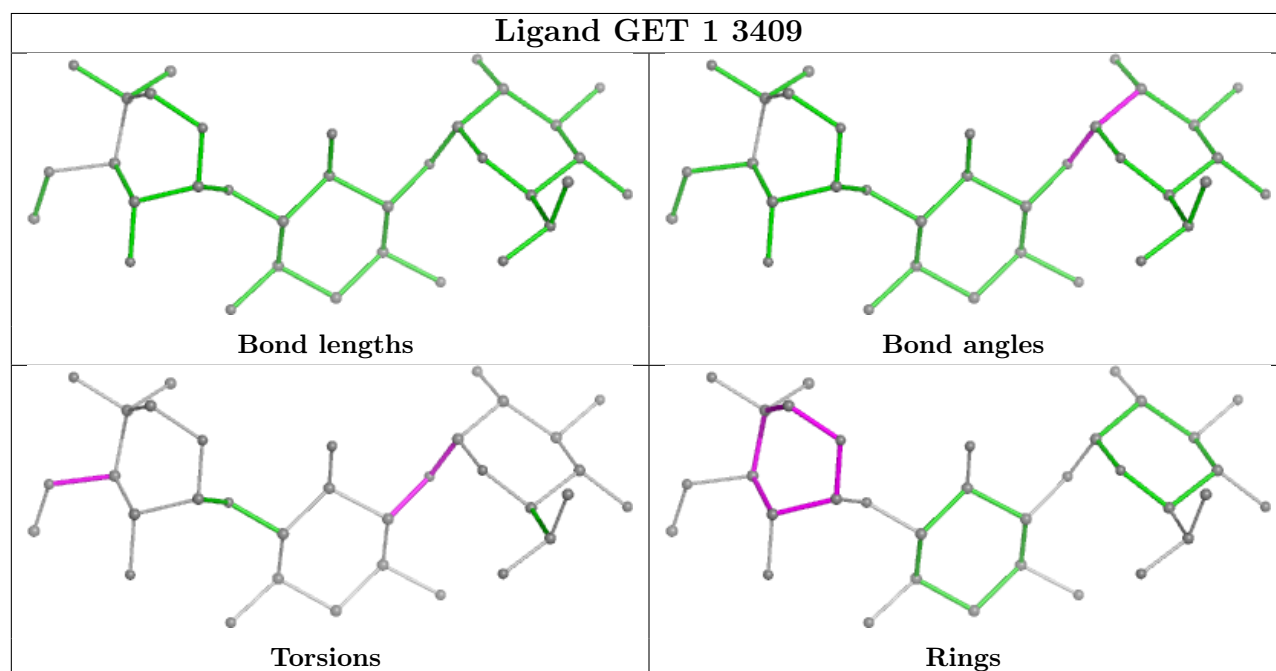
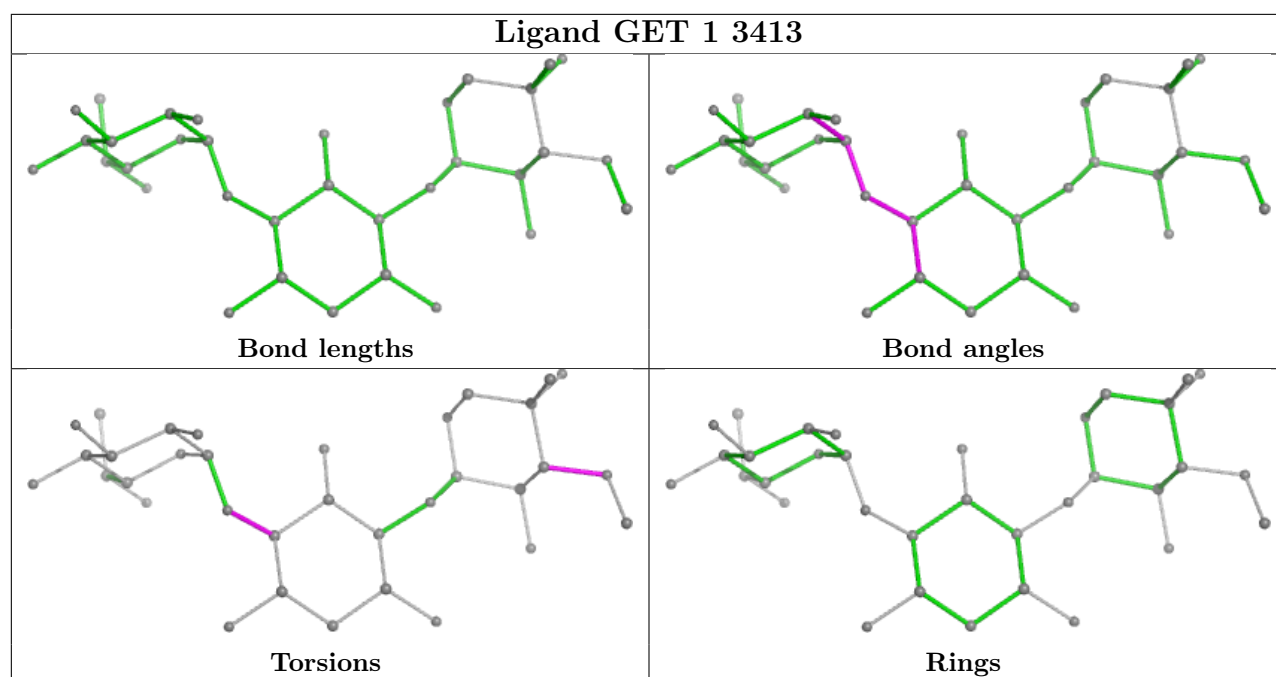
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 81 | A | 1801 | GET | 2 | 0 |
| 81 | 1 | 3412 | GET | 6 | 0 |
| 81 | 1 | 3403 | GET | 3 | 0 |
| 80 | 1 | 3401 | SPK | 3 | 0 |
| 81 | A | 1803 | GET | 2 | 0 |
| 83 | AQ | 301 | YMZ | 1 | 0 |
| 81 | 1 | 3413 | GET | 2 | 0 |
| 81 | 1 | 3409 | GET | 2 | 0 |
| 81 | AT | 101 | GET | 1 | 0 |
| 81 | 1 | 3404 | GET | 1 | 0 |
| 81 | A | 1802 | GET | 1 | 0 |
| 81 | 1 | 3407 | GET | 2 | 0 |
| 81 | 1 | 3410 | GET | 1 | 0 |
| 81 | 1 | 3405 | GET | 1 | 0 |
| 81 | 1 | 3406 | GET | 1 | 0 |
| 81 | 1 | 3408 | GET | 1 | 0 |

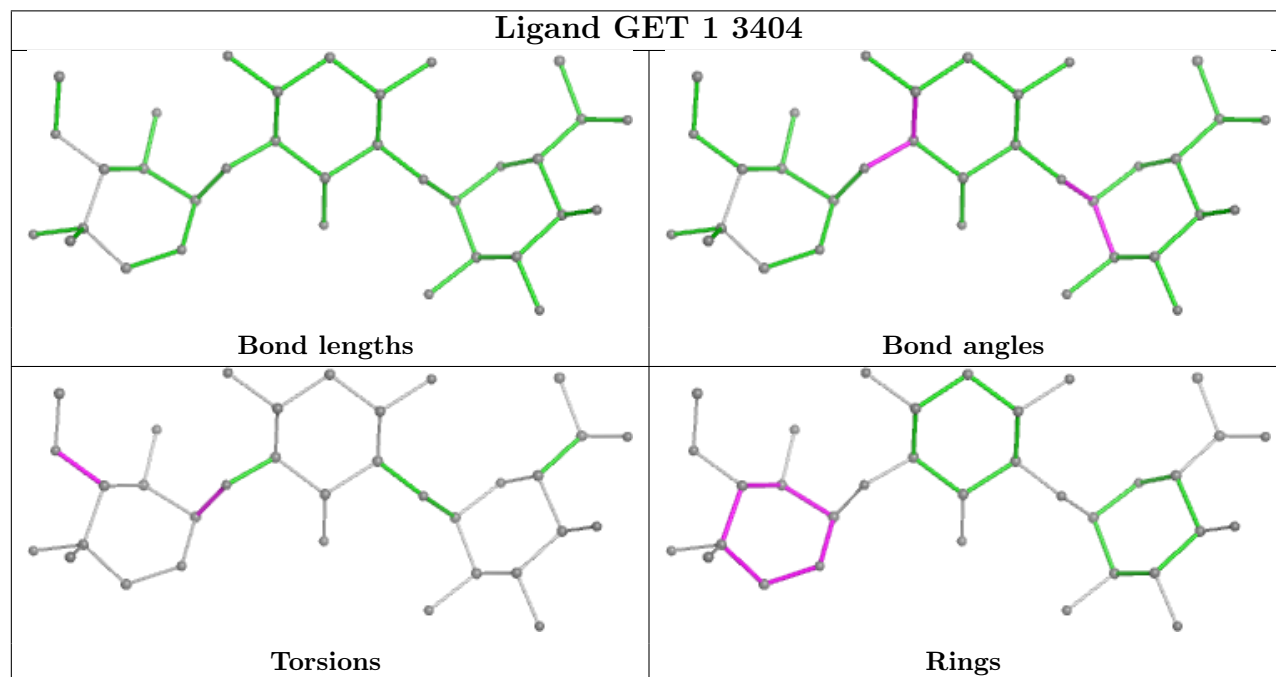
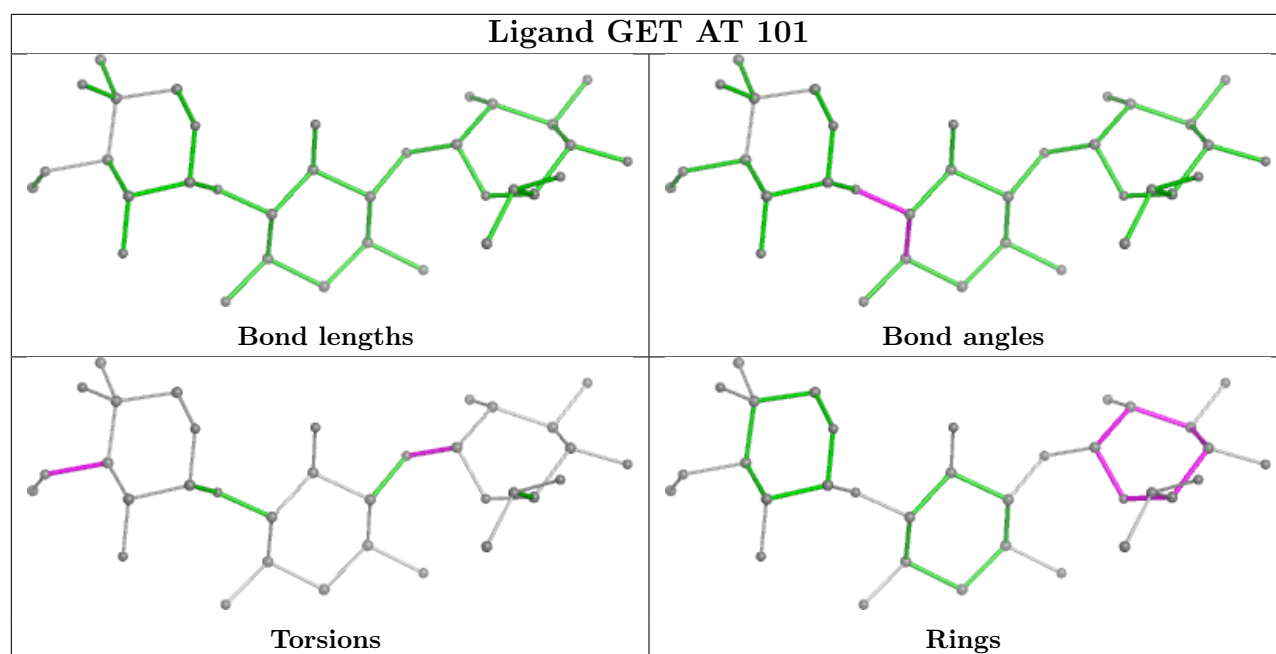
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

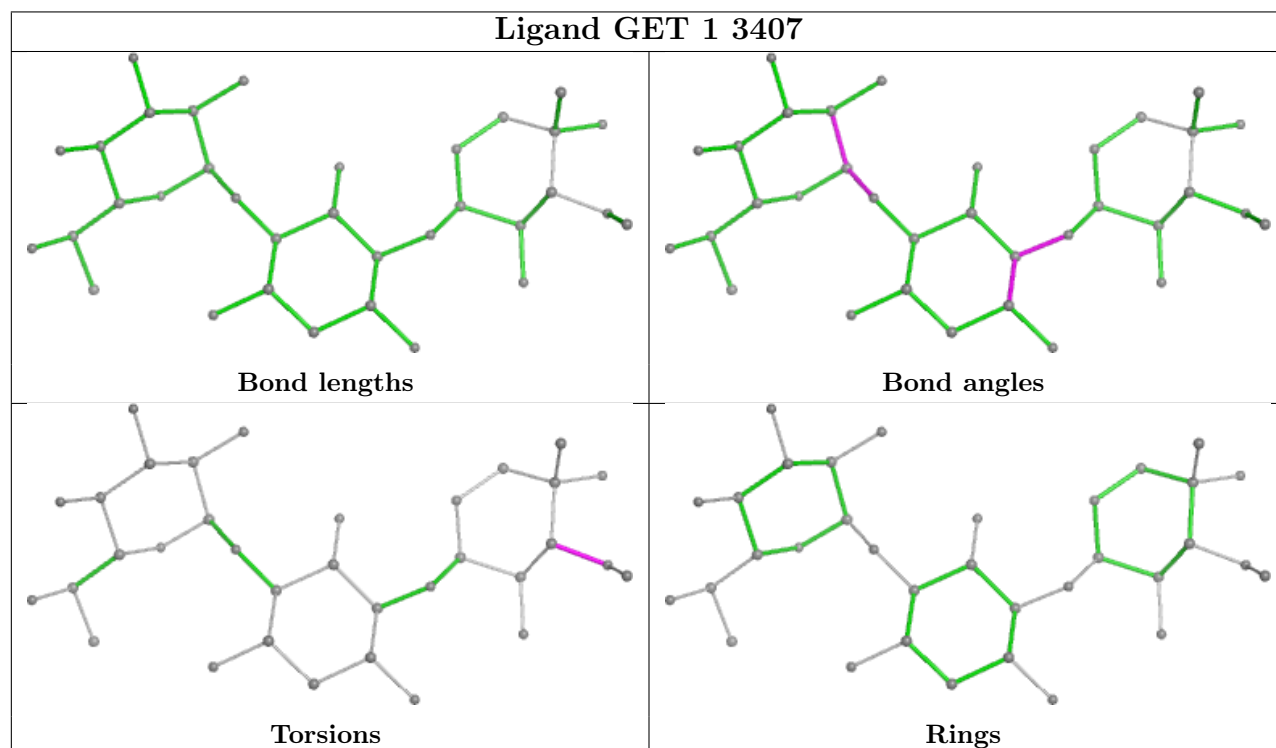
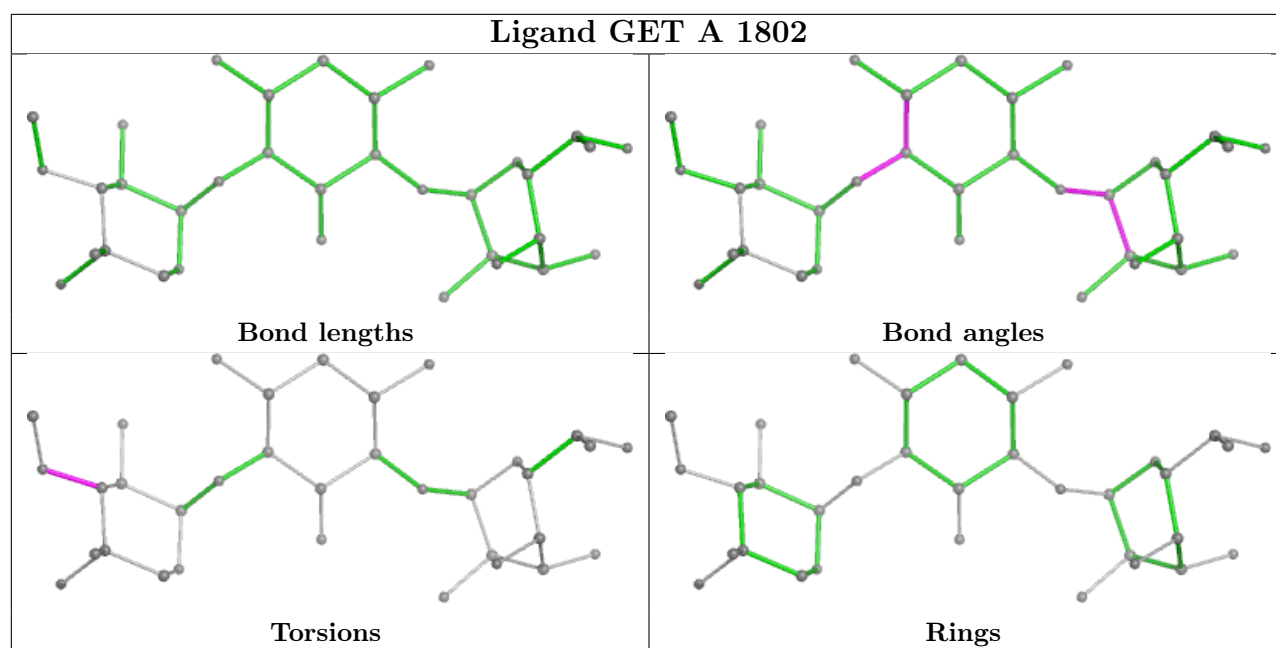


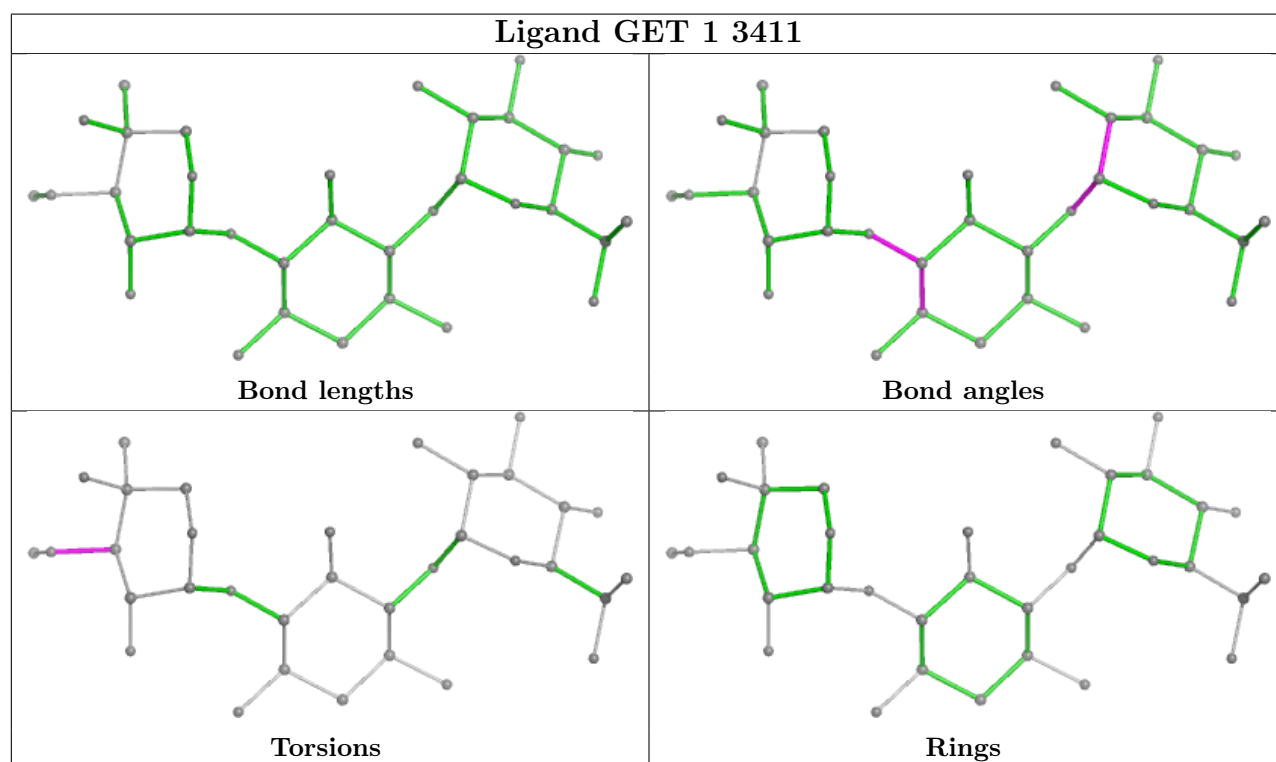
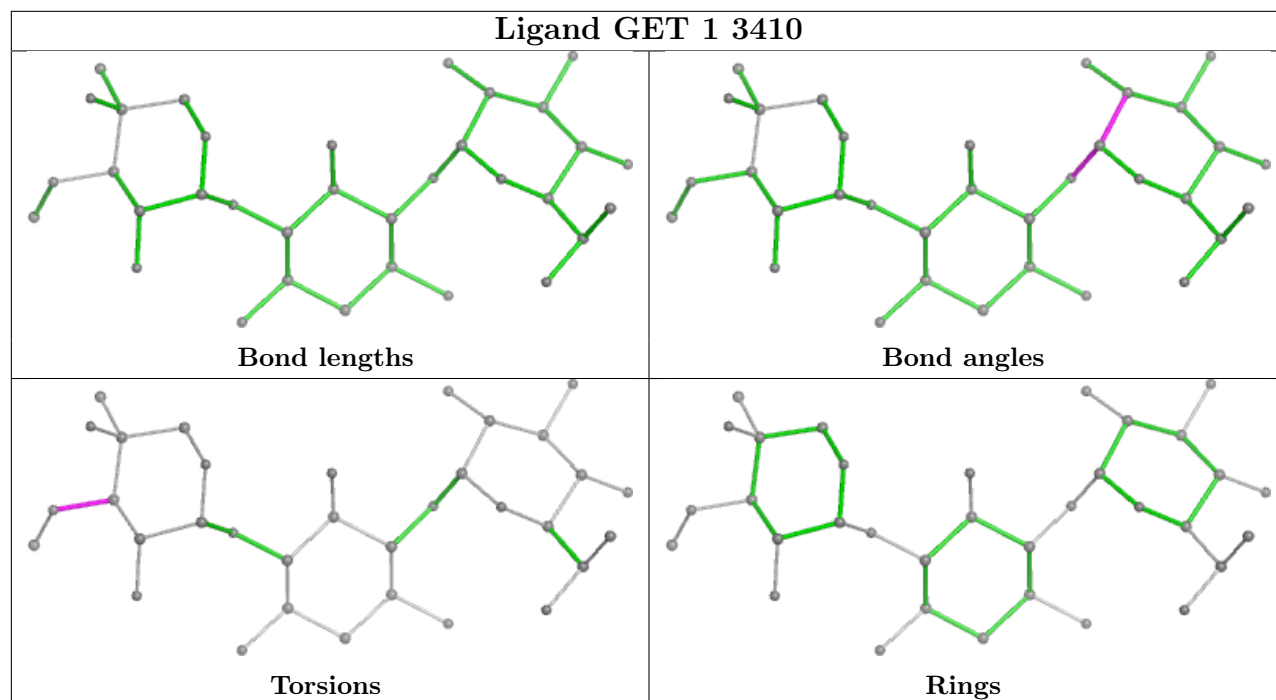


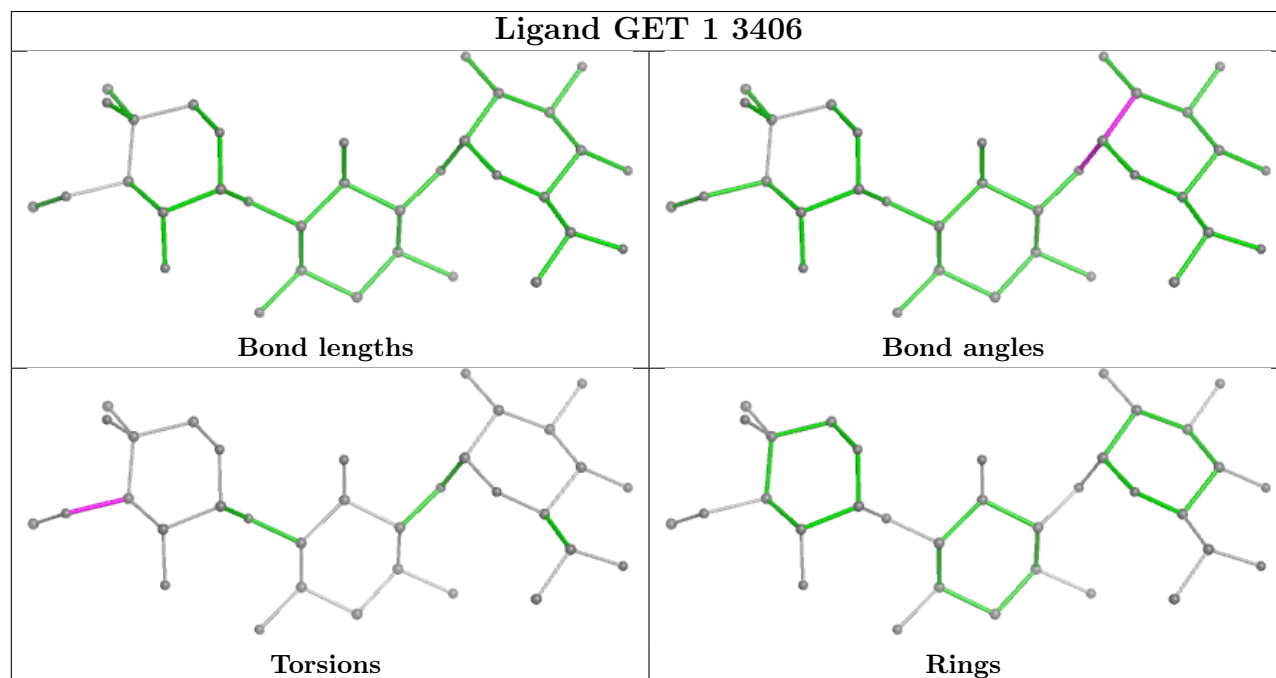
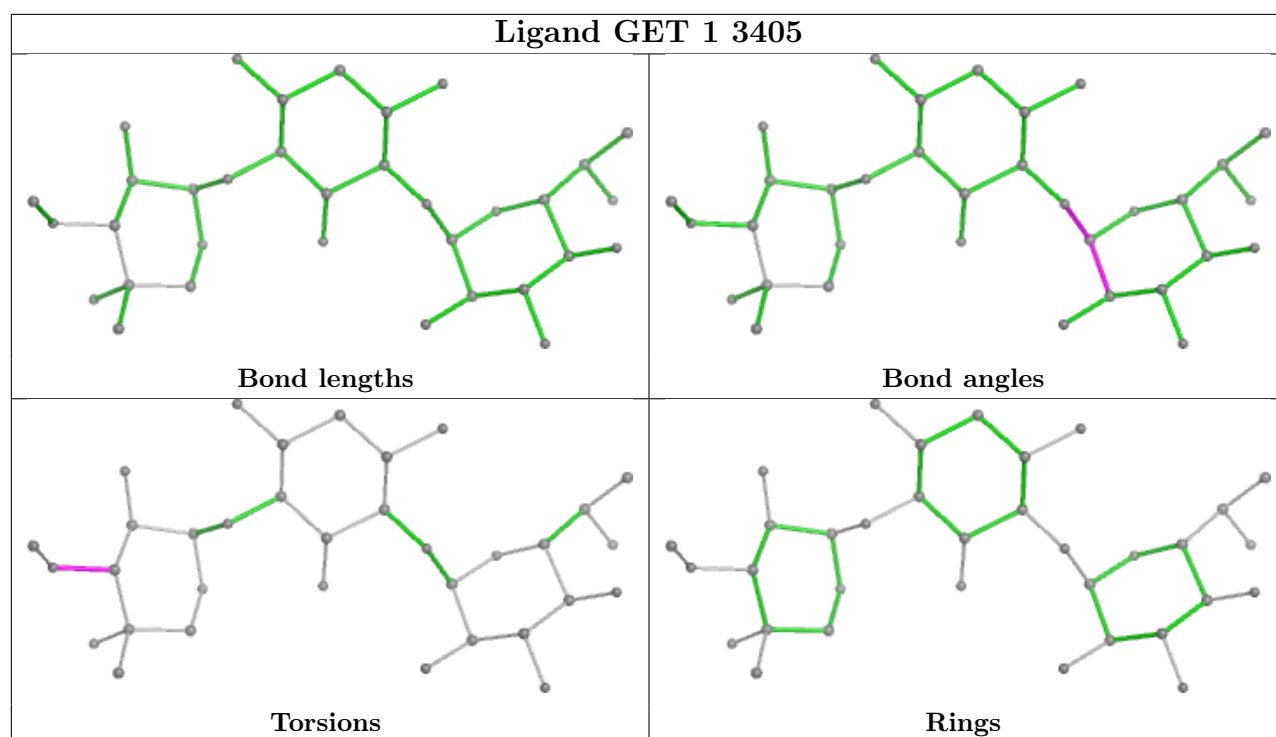


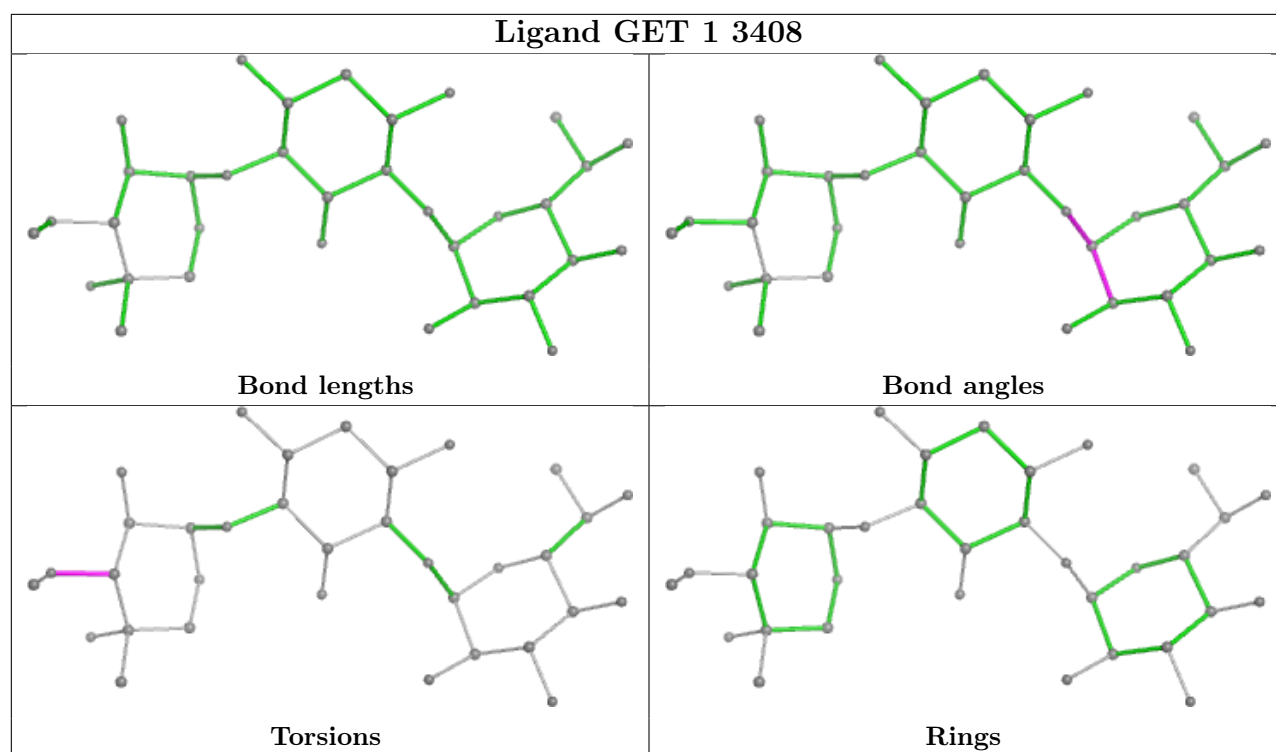












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

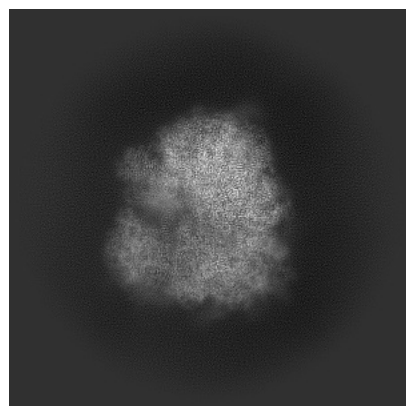
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51103. These allow visual inspection of the internal detail of the map and identification of artifacts.

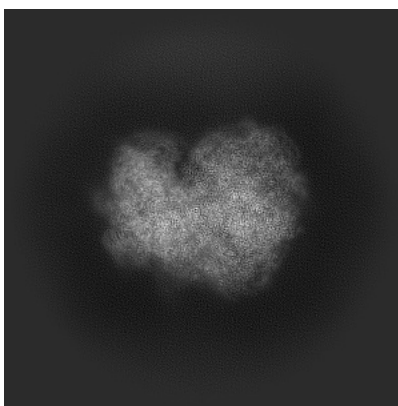
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

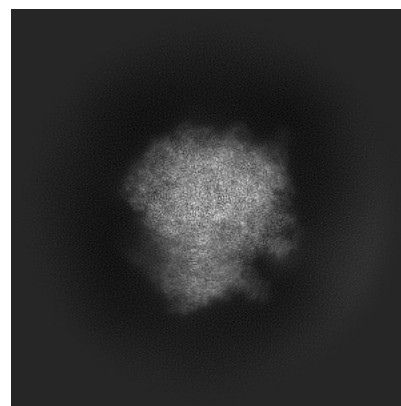
6.1.1 Primary map



X

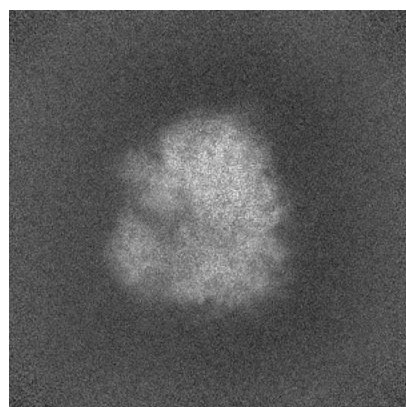


Y

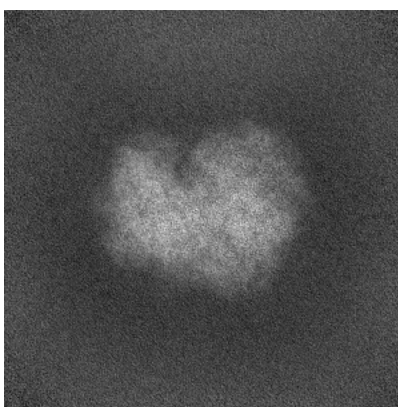


Z

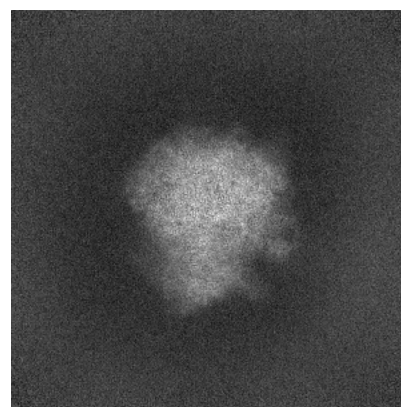
6.1.2 Raw map



X



Y

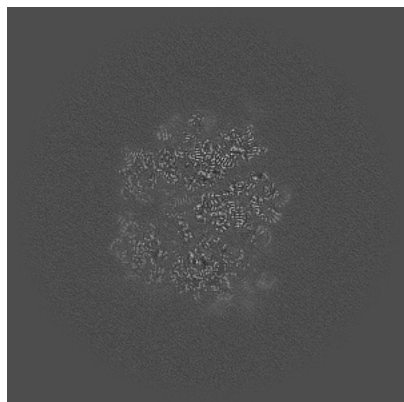


Z

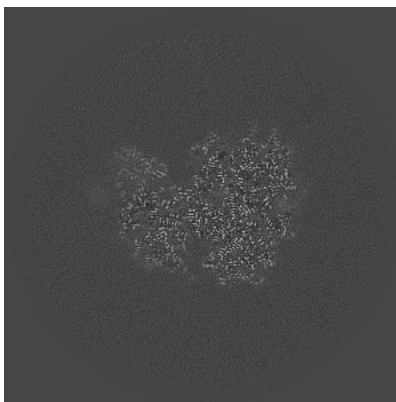
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

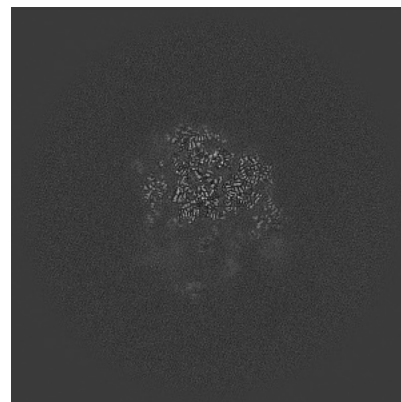
6.2.1 Primary map



X Index: 350

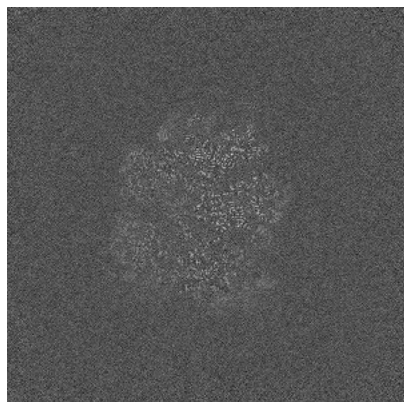


Y Index: 350

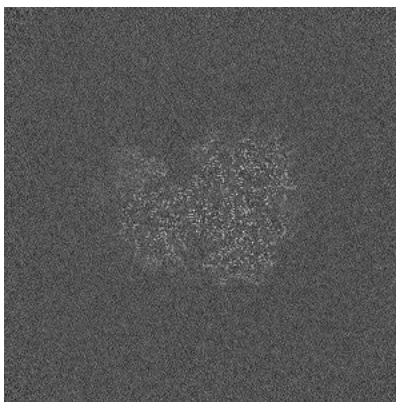


Z Index: 350

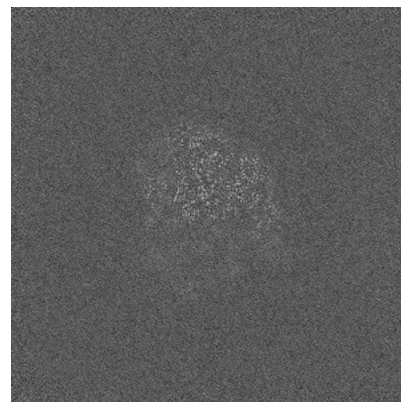
6.2.2 Raw map



X Index: 350



Y Index: 350

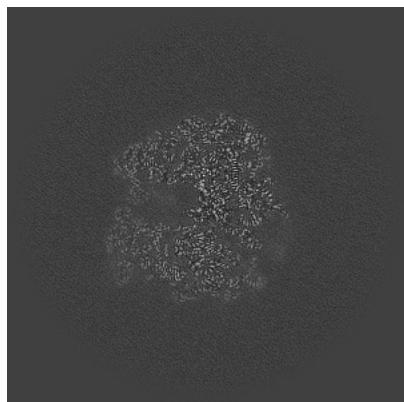


Z Index: 350

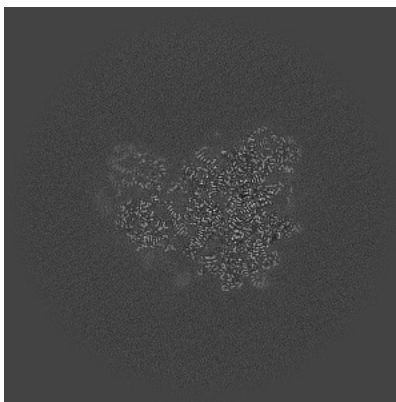
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

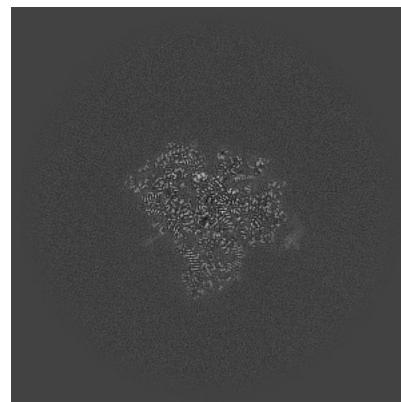
6.3.1 Primary map



X Index: 324

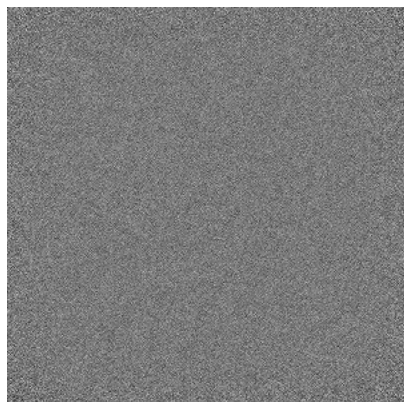


Y Index: 363

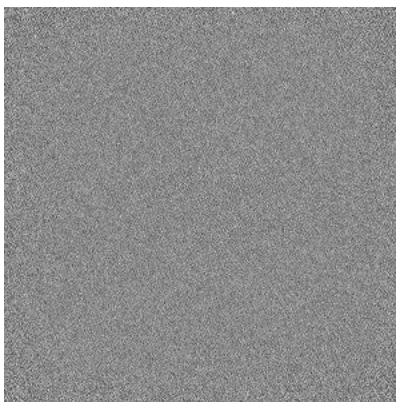


Z Index: 423

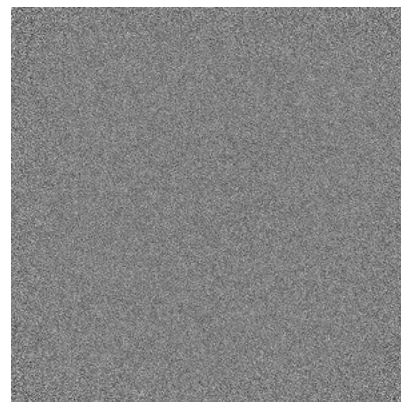
6.3.2 Raw map



X Index: 0



Y Index: 0

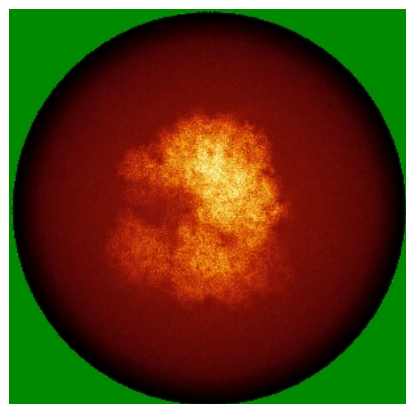


Z Index: 0

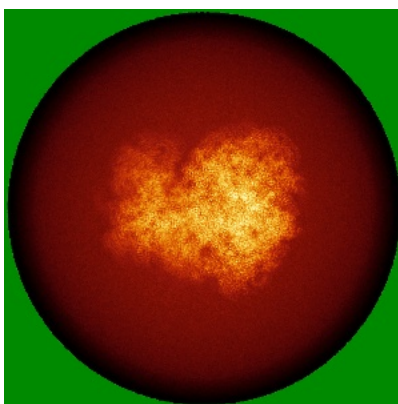
The images above show the largest variance slices of the map in three orthogonal directions.

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

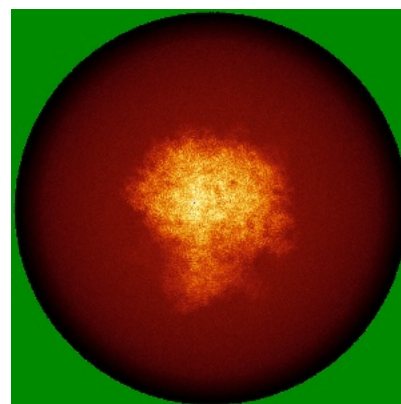
6.4.1 Primary map



X

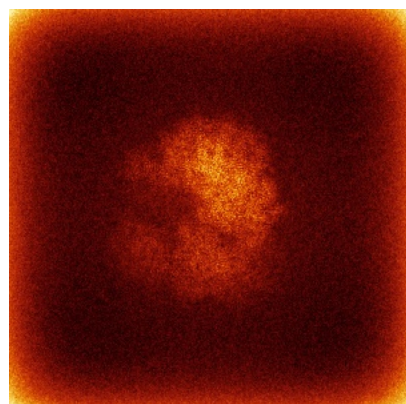


Y

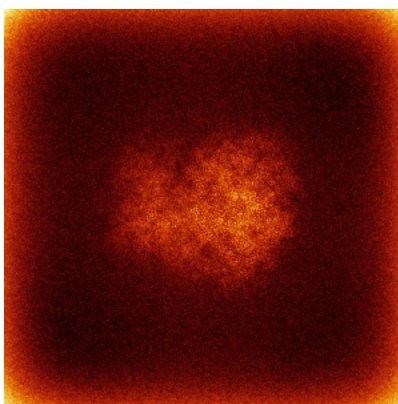


Z

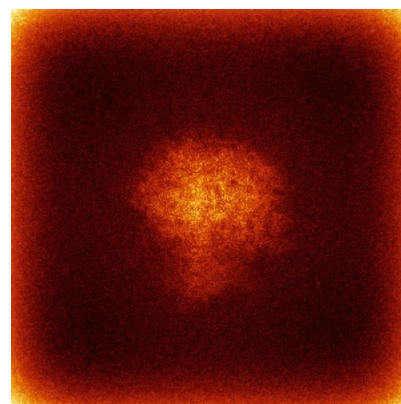
6.4.2 Raw map



X



Y

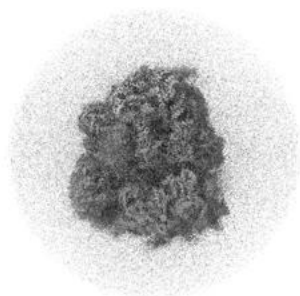


Z

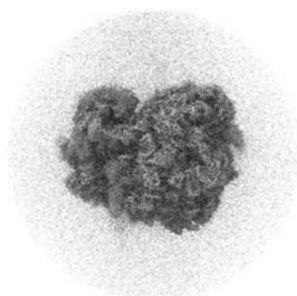
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

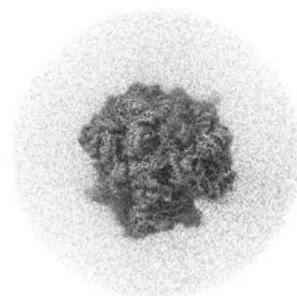
6.5.1 Primary map



X



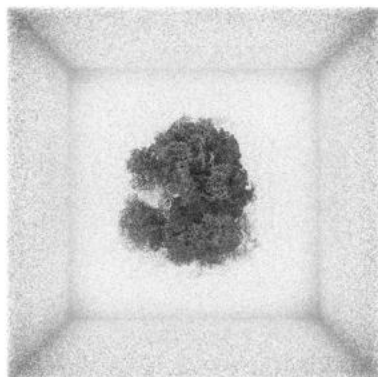
Y



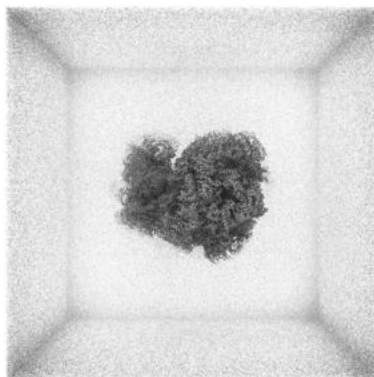
Z

The images above show the 3D surface view of the map at the recommended contour level 0.174. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

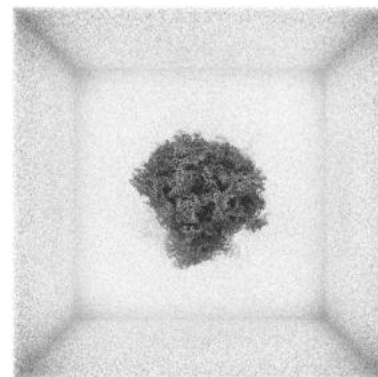
6.5.2 Raw map



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.

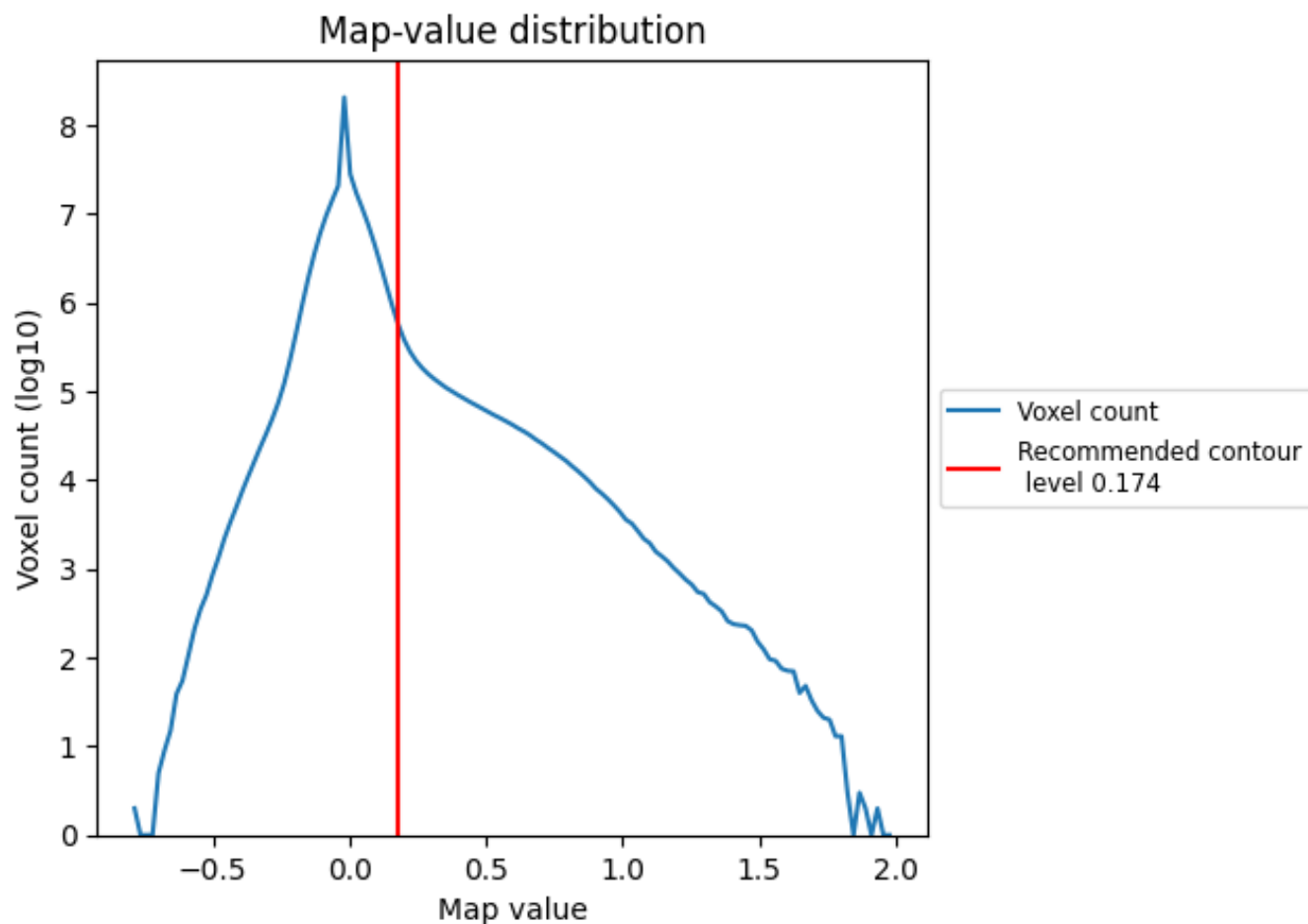
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

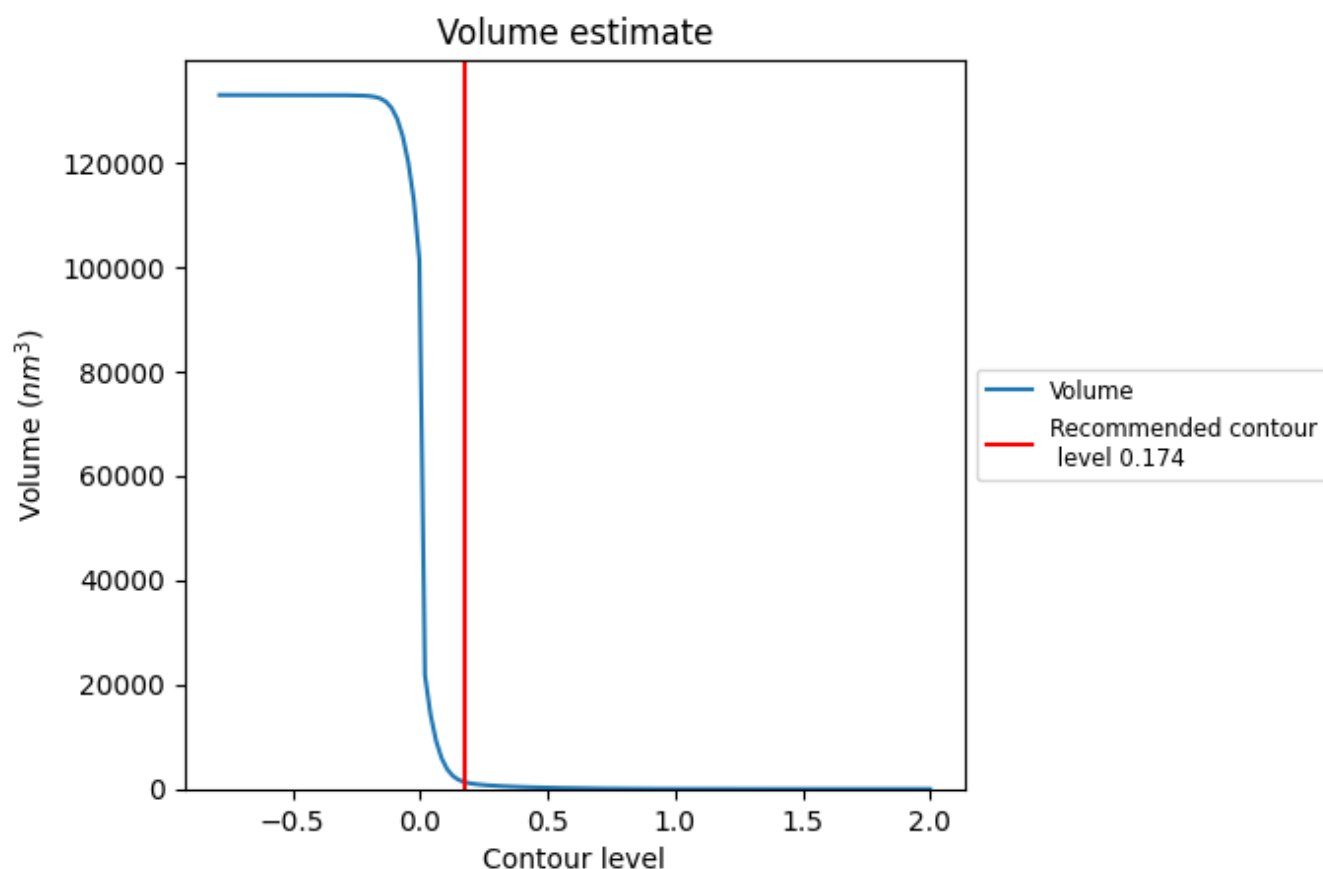
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

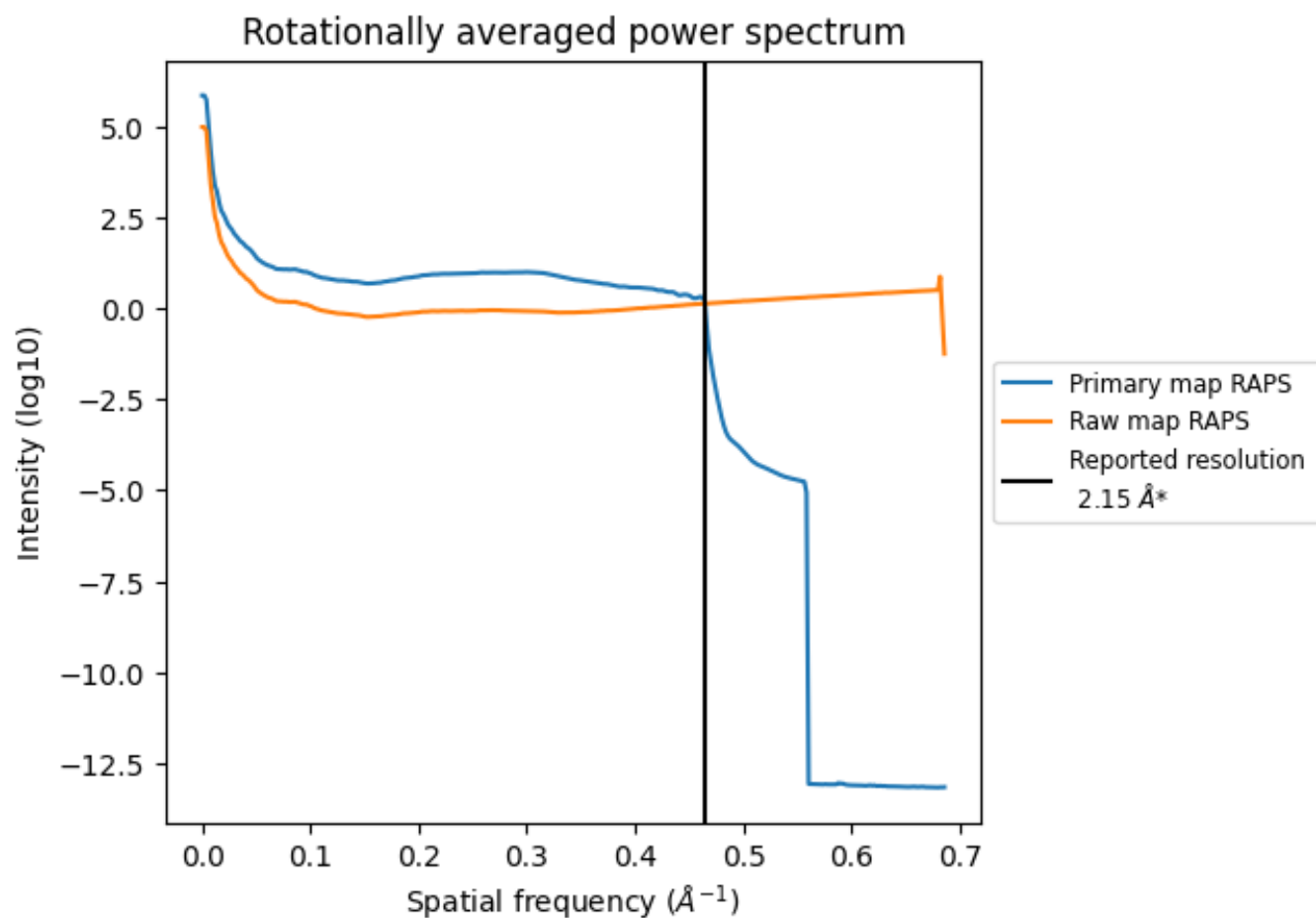
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1328 nm³; this corresponds to an approximate mass of 1200 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

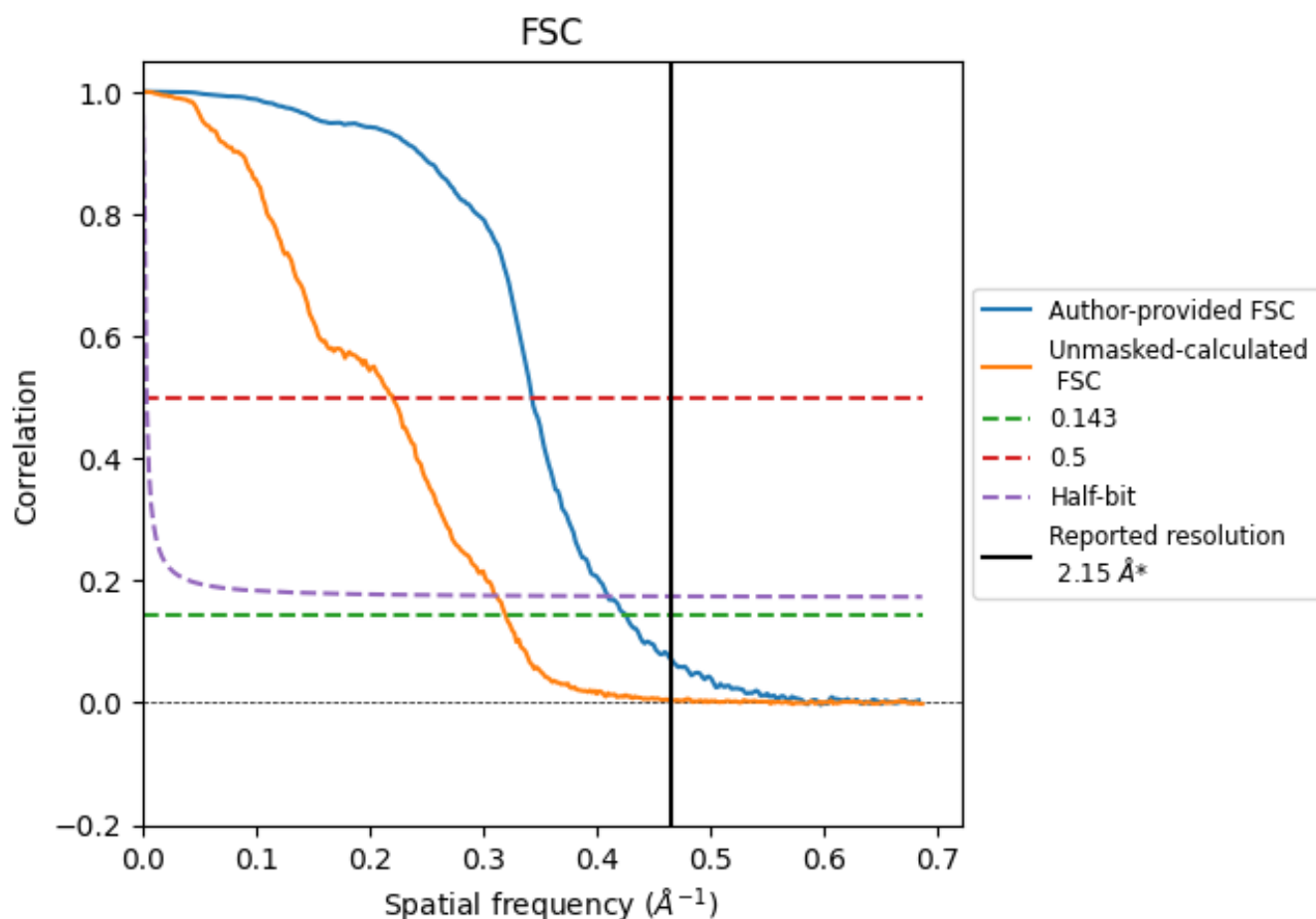


*Reported resolution corresponds to spatial frequency of 0.465 Å⁻¹

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 0.465 \AA^{-1}

8.2 Resolution estimates [i](#)

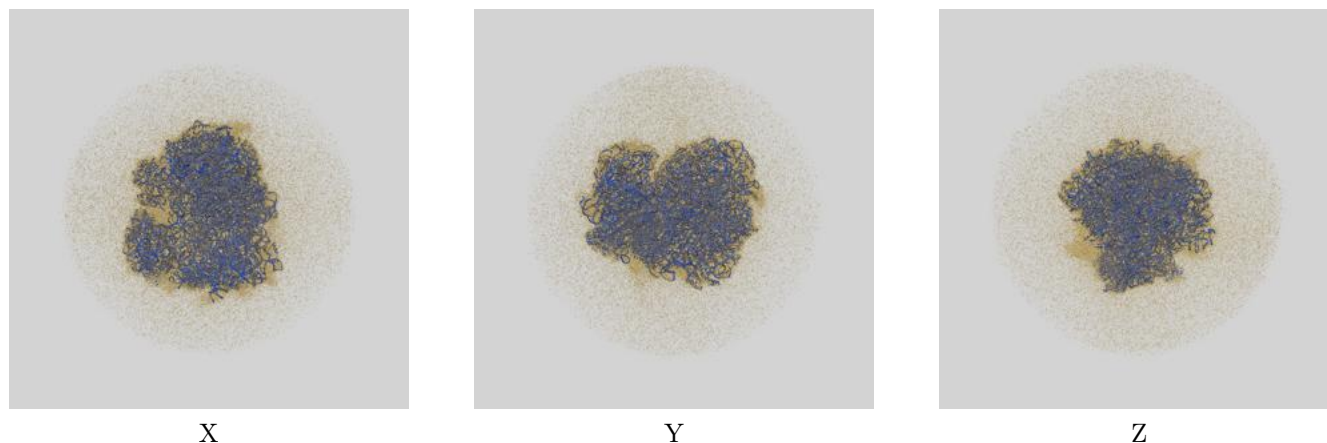
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.15 | - | - |
| Author-provided FSC curve | 2.35 | 2.92 | 2.44 |
| Unmasked-calculated* | 3.13 | 4.54 | 3.21 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.15 by more than 10 %

9 Map-model fit [i](#)

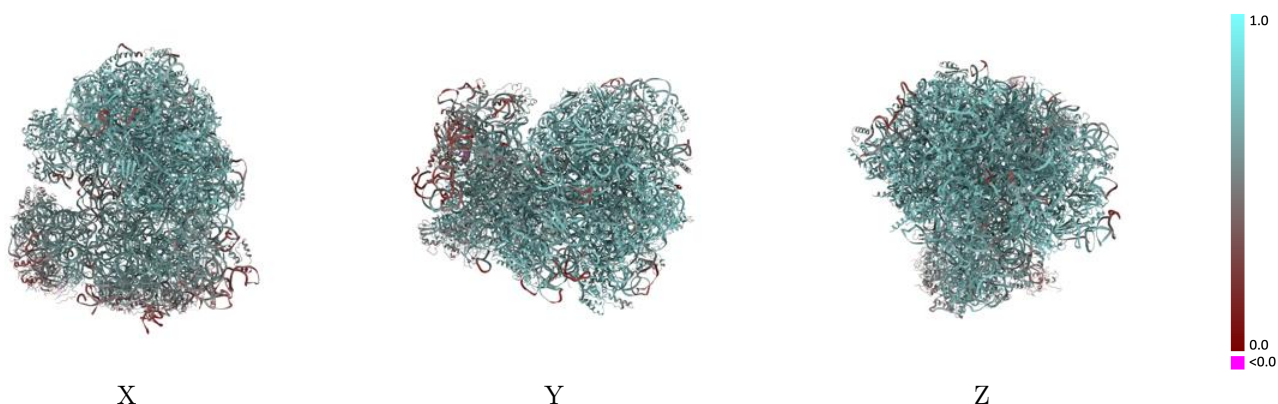
This section contains information regarding the fit between EMDB map EMD-51103 and PDB model 9G6J. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



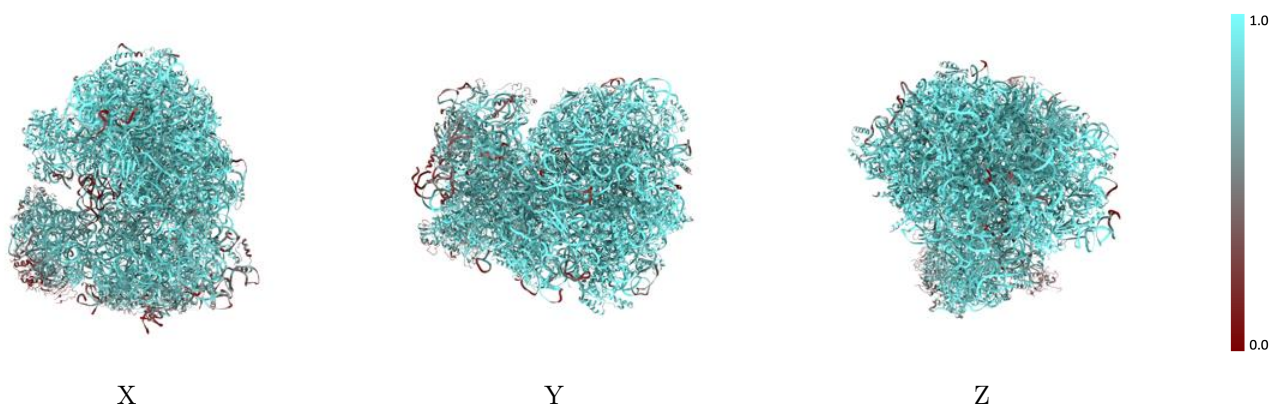
The images above show the 3D surface view of the map at the recommended contour level 0.174 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



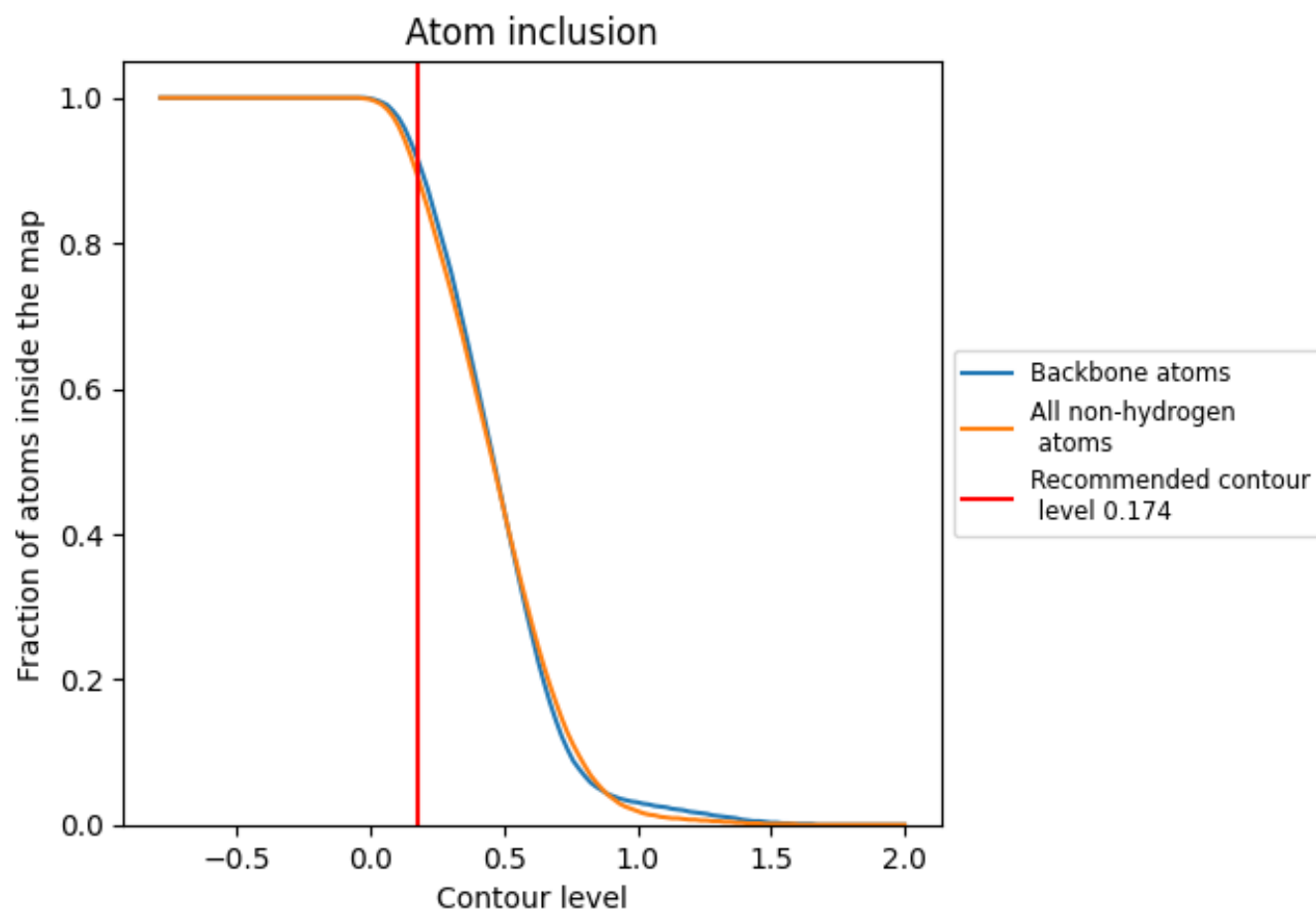
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.174).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.174) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8950 |  0.6390 |
| 0 |  0.9620 |  0.6990 |
| 1 |  0.9580 |  0.6800 |
| 2 |  0.9310 |  0.6870 |
| 3 |  0.9860 |  0.6790 |
| 4 |  0.9750 |  0.6880 |
| 6 |  0.9680 |  0.7110 |
| 7 |  0.9560 |  0.7010 |
| 8 |  0.9570 |  0.6950 |
| 9 |  0.9450 |  0.6940 |
| A |  0.8870 |  0.5980 |
| AA |  0.9270 |  0.6730 |
| AB |  0.9780 |  0.7240 |
| AC |  0.9190 |  0.6710 |
| AD |  0.9360 |  0.6800 |
| AE |  0.9040 |  0.6790 |
| AF |  0.9610 |  0.7080 |
| AG |  0.9770 |  0.7170 |
| AH |  0.9280 |  0.6880 |
| AI |  0.9400 |  0.6750 |
| AJ |  0.9140 |  0.6570 |
| AK |  0.9860 |  0.7250 |
| AL |  0.8020 |  0.6000 |
| AM |  0.9620 |  0.6940 |
| AN |  0.9210 |  0.6730 |
| AO |  0.7440 |  0.6170 |
| AP |  0.9150 |  0.6830 |
| AQ |  0.8930 |  0.6780 |
| AT |  0.2820 |  0.4020 |
| B |  0.8530 |  0.6000 |
| C |  0.9060 |  0.6490 |
| D |  0.9310 |  0.6590 |
| E |  0.7600 |  0.5540 |
| F |  0.7410 |  0.4980 |
| G |  0.8000 |  0.5790 |










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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| H |  0.7030 |  0.5070 |
| I |  0.7310 |  0.5470 |
| J |  0.8130 |  0.5820 |
| K |  0.6390 |  0.4360 |
| L |  0.6160 |  0.4630 |
| M |  0.8750 |  0.6210 |
| MR |  0.8080 |  0.5800 |
| N |  0.2060 |  0.3150 |
| O |  0.9300 |  0.6550 |
| P |  0.9510 |  0.6710 |
| PT |  0.8480 |  0.5940 |
| Q |  0.6670 |  0.5060 |
| R |  0.8150 |  0.5850 |
| S |  0.7050 |  0.5240 |
| T |  0.7210 |  0.5210 |
| U |  0.7790 |  0.5500 |
| V |  0.6990 |  0.5040 |
| W |  0.8740 |  0.6260 |
| X |  0.9630 |  0.6990 |
| Y |  0.8980 |  0.6320 |
| Z |  0.6050 |  0.4280 |
| a |  0.5830 |  0.4750 |
| b |  0.9330 |  0.6720 |
| c |  0.8620 |  0.6260 |
| d |  0.7520 |  0.5520 |
| e |  0.9250 |  0.6320 |
| f |  0.5950 |  0.4550 |
| g |  0.3290 |  0.3560 |
| h |  0.2570 |  0.3990 |
| j |  0.9780 |  0.7280 |
| k |  0.9680 |  0.7140 |
| l |  0.9450 |  0.6960 |
| m |  0.8840 |  0.6410 |
| n |  0.9080 |  0.6450 |
| o |  0.9450 |  0.6970 |
| p |  0.9320 |  0.6730 |
| q |  0.9170 |  0.6610 |
| r |  0.9270 |  0.6700 |
| s |  0.8280 |  0.5810 |
| t |  0.9280 |  0.6860 |
| u |  0.9490 |  0.6810 |
| v |  0.9930 |  0.7330 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| w |  0.9600 |  0.7090 |
| x |  0.9560 |  0.7060 |
| y |  0.9770 |  0.7140 |
| z |  0.9130 |  0.6680 |