# wwPDB EM Validation Summary Report

Mar 8, 2026 – 12:16 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 8OVA / pdb_00008ova |
| EMDB ID | : | EMD-17208 |
| Title | : | CRYO-EM STRUCTURE OF TRYPANOSOMA BRUCEI PROCYCLIC FORM 80S RIBOSOME : PARENTAL STRAIN |
| Authors | : | Rajan, K.S.; Yonath, A. |
| Deposited on | : | 2023-04-25 |
| Resolution | : | 2.47 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:

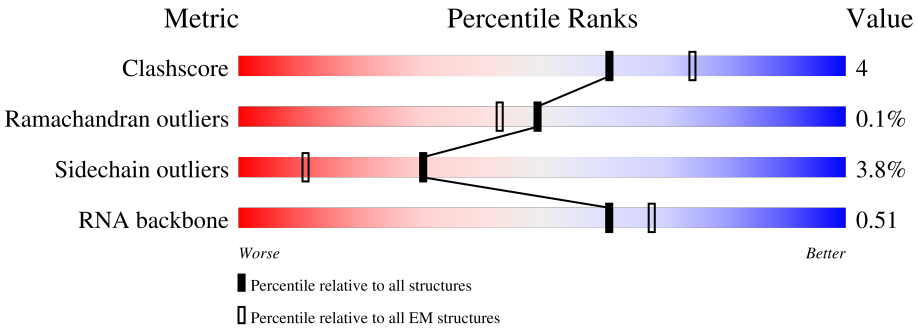
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using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

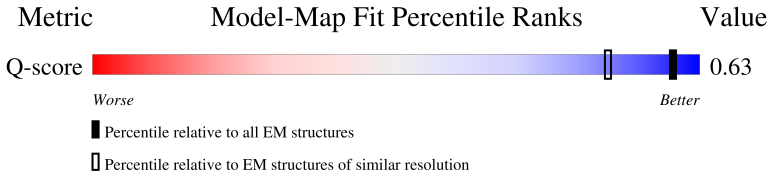
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.47 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| RNA backbone | 8273 | 3508 | - |
| Q-score | - | 25397 | 6086 ( 1.98 - 2.97 ) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | BA | 1920 | 56% 23% • 16% |
| 2 | AA | 2282 | 51% 25% 7% 16% |
| 3 | BB | 1536 | 49% 20% 5% 27% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | BH | 136 | 53% 27% 7% 12% |
| 5 | BG | 183 | 68% 25% 7% |
| 6 | BF | 78 | 55% 19% 14% 12% |
| 7 | BE | 216 | 53% 21% 12% 13% |
| 8 | BD | 119 | 70% 24% 6% |
| 9 | BC | 209 | 54% 21% 23% |
| 10 | AB | 19 | 37% 53% 11% |
| 11 | AQ | 117 | 68% 16% 15% |
| 12 | A8 | 57 | 88% 11% |
| 13 | A9 | 153 | 42% 54% |
| 14 | Az | 279 | 6% 23% 11% 64% |
| 15 | AH | 144 | 80% 12% 7% |
| 16 | AI | 152 | 70% 9% 22% |
| 17 | AJ | 130 | 91% 8% |
| 18 | AK | 149 | 83% 12% 5% |
| 19 | AM | 153 | 78% 14% 8% |
| 20 | AO | 167 | 82% 10% 8% |
| 21 | AP | 266 | 71% 10% 18% |
| 22 | AR | 194 | 41% 54% |
| 23 | AS | 143 | 85% 13% |
| 24 | AT | 137 | 79% 15% 6% |
| 25 | AU | 113 | 54% 11% 35% |
| 26 | AV | 111 | 84% 9% 7% |
| 27 | AW | 86 | 81% 17% |
| 28 | AX | 214 | 86% 10% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | AY | 66 | 79% 5% 17% |
| 30 | AZ | 103 | 50% 6% 44% |
| 31 | AL | 142 | 75% 10% 14% |
| 32 | A0 | 256 | 79% 7% 14% |
| 33 | A1 | 273 | 83% 12% |
| 34 | A2 | 190 | 88% 8% |
| 35 | A3 | 250 | 81% 13% 5% |
| 36 | A4 | 202 | 78% 18% |
| 37 | A5 | 220 | 75% 9% 15% |
| 38 | A6 | 190 | 87% 7% 6% |
| 39 | A7 | 318 | 80% 16% |
| 40 | AC | 277 | 64% 11% 25% |
| 41 | AD | 172 | 49% 8% 42% |
| 42 | AE | 174 | 76% 11% 12% |
| 43 | AG | 151 | 91% 7% |
| 44 | Bh | 188 | 70% 13% 17% |
| 45 | Ba | 133 | 77% 21% |
| 46 | Bb | 145 | 88% 10% |
| 47 | Bc | 146 | 86% 12% |
| 48 | Bd | 71 | 92% 6% |
| 49 | Be | 260 | 90% 8% |
| 50 | Bz | 34 | 91% 6% |
| 51 | Bg | 105 | 82% 6% 12% |
| 52 | Bf | 429 | 85% 7% 8% |
| 53 | BI | 193 | 89% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 54 | Bj | 170 | 61% 8% 32% |
| 55 | BK | 213 | 77% 14% 9% |
| 56 | Bk | 127 | 85% 12% |
| 57 | BL | 194 | 68% 18% 14% |
| 58 | Bl | 149 | 83% 12% |
| 59 | Bm | 109 | 83% 7% 10% |
| 60 | BN | 218 | 90% 8% |
| 61 | Bn | 84 | 89% 6% 5% |
| 62 | BO | 222 | 95% 5% |
| 63 | Bo | 93 | 84% 12% |
| 64 | Bp | 82 | 74% 17% 6% |
| 65 | Bq | 51 | 90% 8% |
| 66 | BQ | 221 | 86% 6% 8% |
| 67 | BR | 166 | 87% 9% |
| 68 | Br | 374 | 92% 6% |
| 69 | BS | 179 | 89% 10% |
| 70 | Bs | 128 | 33% 6% 61% |
| 71 | BT | 260 | 67% 8% 25% |
| 72 | Bt | 106 | 81% 8% 8% |
| 73 | BU | 159 | 81% 16% |
| 74 | Bu | 308 | 64% 15% 20% |
| 75 | BV | 130 | 71% 21% 6% |
| 76 | Bv | 192 | 60% 14% 26% |
| 77 | BW | 139 | 83% 14% |
| 78 | BX | 164 | 67% 5% 27% |

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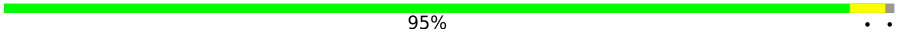
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 79 | Bw | 257 | |
| 80 | Bx | 276 | |
| 81 | BY | 125 | |
| 82 | By | 189 | |
| 83 | BZ | 143 | |
| 84 | Bi | 132 |   |
| 85 | BP | 189 | |
| 86 | AF | 144 | |

# 2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 209127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called LSUa rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | BA | 1604 | 34346 | 15345 | 6216 | 11181 | 1604 | 0 | 0 |

- Molecule 2 is a RNA chain called SSU rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | AA | 1919 | 40964 | 18316 | 7328 | 13401 | 1919 | 0 | 0 |

- Molecule 3 is a RNA chain called LSUb rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | BB | 1119 | 23918 | 10699 | 4282 | 7818 | 1119 | 0 | 0 |

- Molecule 4 is a RNA chain called SrRNA-4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | BH | 119 | 2538 | 1131 | 451 | 837 | 119 | 0 | 0 |

- Molecule 5 is a RNA chain called SrRNA-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | BG | 183 | 3919 | 1746 | 708 | 1282 | 183 | 0 | 0 |

- Molecule 6 is a RNA chain called SrRNA-6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | BF | 69 | 1444 | 646 | 239 | 490 | 69 | 0 | 0 |

- Molecule 7 is a RNA chain called SrRNA-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | BE | 188 | Total | C | N | O | P | 0 | 0 |
| | | | 3981 | 1780 | 692 | 1321 | 188 | | |

- Molecule 8 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | BD | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2533 | 1131 | 449 | 835 | 118 | | |

- Molecule 9 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | BC | 160 | Total | C | N | O | P | 0 | 0 |
| | | | 3411 | 1529 | 610 | 1113 | 159 | | |

- Molecule 10 is a RNA chain called E-SITE TRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | AB | 19 | Total | C | N | O | P | 0 | 0 |
| | | | 404 | 181 | 76 | 129 | 18 | | |

- Molecule 11 is a protein called Ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | AQ | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 800 | 501 | 152 | 144 | 3 | | |

- Molecule 12 is a protein called uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | A8 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 461 | 284 | 97 | 75 | 5 | | |

- Molecule 13 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | A9 | 70 | Total | C | N | O | S | 0 | 1 |
| | | | 569 | 361 | 109 | 92 | 7 | | |

- Molecule 14 is a protein called RNA-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | Az | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 807 | 504 | 154 | 148 | 1 | | |

- Molecule 15 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | AH | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 992 | 607 | 193 | 183 | 9 | | |

- Molecule 16 is a protein called 40S ribosomal protein S15, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | AI | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 966 | 614 | 188 | 161 | 3 | | |

- Molecule 17 is a protein called 40S ribosomal protein S15a, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | AJ | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1018 | 645 | 191 | 174 | 8 | | |

- Molecule 18 is a protein called 40S ribosomal protein S16, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | AK | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1140 | 728 | 215 | 194 | 3 | | |

- Molecule 19 is a protein called 40S ribosomal protein S18, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | AM | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1143 | 713 | 227 | 198 | 5 | | |

- Molecule 20 is a protein called Ribosomal protein S19, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | AO | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1220 | 770 | 242 | 199 | 9 | | |

- Molecule 21 is a protein called 40S ribosomal protein S2, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | AP | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1688 | 1078 | 298 | 303 | 9 | | |

- Molecule 22 is a protein called 40S ribosomal protein S21, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | AR | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 666 | 415 | 119 | 129 | 3 | | |

- Molecule 23 is a protein called 40S ribosomal protein S23, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | AS | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1096 | 696 | 213 | 185 | 2 | | |

- Molecule 24 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | AT | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1034 | 659 | 202 | 170 | 3 | | |

- Molecule 25 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | AU | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 575 | 365 | 105 | 100 | 5 | | |

- Molecule 26 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | AV | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 830 | 512 | 175 | 135 | 8 | | |

- Molecule 27 is a protein called 40S ribosomal protein S27, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | AW | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 660 | 411 | 124 | 116 | 9 | | |

- Molecule 28 is a protein called 40S ribosomal protein S3, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | AX | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1652 | 1036 | 310 | 294 | 12 | | |

- Molecule 29 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | AY | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 448 | 283 | 93 | 71 | 1 | | |

- Molecule 30 is a protein called 40S ribosomal protein S33, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | AZ | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 271 | 94 | 80 | 4 | | |

- Molecule 31 is a protein called 40S ribosomal protein S17, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | AL | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 945 | 600 | 184 | 156 | 5 | | |

- Molecule 32 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | A0 | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1789 | 1129 | 336 | 316 | 8 | | |

- Molecule 33 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | A1 | 262 | Total | C | N | O | S | 0 | 0 |
| | | | 2062 | 1306 | 388 | 359 | 9 | | |

- Molecule 34 is a protein called 40S ribosomal protein S5, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | A2 | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1464 | 915 | 282 | 262 | 5 | | |

- Molecule 35 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | A3 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1871 | 1161 | 383 | 323 | 4 | | |

- Molecule 36 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | A4 | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1602 | 1023 | 308 | 266 | 5 | | |

- Molecule 37 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | A5 | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1471 | 927 | 291 | 251 | 2 | | |

- Molecule 38 is a protein called Probable 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | A6 | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1477 | 929 | 297 | 243 | 8 | | |

- Molecule 39 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | A7 | 309 | Total | C | N | O | S | 0 | 0 |
| | | | 2371 | 1483 | 418 | 458 | 12 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | AC | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1648 | 1049 | 297 | 291 | 11 | | |

- Molecule 41 is a protein called 40S ribosomal protein S10, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | AD | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 531 | 140 | 139 | 4 | | |

- Molecule 42 is a protein called 40S ribosomal proteins S11, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | AE | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1249 | 782 | 253 | 209 | 5 | | |

- Molecule 43 is a protein called 40S ribosomal protein S13, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | AG | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1203 | 756 | 236 | 203 | 8 | | |

- Molecule 44 is a protein called 60S ribosomal subunit protein L31, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | Bh | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1249 | 785 | 253 | 207 | 4 | | |

- Molecule 45 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | Ba | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1085 | 688 | 219 | 175 | 3 | | |

- Molecule 46 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | Bb | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1137 | 717 | 228 | 186 | 6 | | |

- Molecule 47 is a protein called 60S ribosomal protein L28, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | Bc | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 723 | 234 | 197 | 8 | | |

- Molecule 48 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | Bd | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 547 | 335 | 123 | 88 | 1 | | |

- Molecule 49 is a protein called 60S ribosomal protein L2, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | Be | 254 | Total | C | N | O | S | 1 | 0 |
| | | | 1907 | 1189 | 394 | 312 | 12 | | |

- Molecule 50 is a protein called Ribosomal protein L41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | Bz | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 284 | 172 | 74 | 36 | 2 | | |

- Molecule 51 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | Bg | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 708 | 441 | 128 | 134 | 5 | | |

- Molecule 52 is a protein called Ribosomal protein L3, mitochondrial, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | Bf | 396 | Total | C | N | O | S | 0 | 0 |
| | | | 3174 | 2001 | 626 | 534 | 13 | | |

- Molecule 53 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | BI | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1517 | 950 | 313 | 246 | 8 | | |

- Molecule 54 is a protein called 60S ribosomal protein L34, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | Bj | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 959 | 593 | 214 | 148 | 4 | | |

- Molecule 55 is a protein called 60S ribosomal protein L10, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | BK | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1588 | 1002 | 314 | 260 | 12 | | |

- Molecule 56 is a protein called 60S ribosomal protein L35, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | Bk | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 1010 | 634 | 217 | 156 | 3 | | |

- Molecule 57 is a protein called 60S ribosomal protein L11, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | BL | 166 | Total | C | N | O | S | 0 | 0 |
| | | | 1325 | 836 | 247 | 235 | 7 | | |

- Molecule 58 is a protein called 60S ribosomal protein L35A, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | Bl | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1163 | 728 | 239 | 193 | 3 | | |

- Molecule 59 is a protein called Ribosomal protein L36, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | Bm | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 493 | 164 | 127 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | BN | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1762 | 1097 | 365 | 294 | 6 | | |

- Molecule 61 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | Bn | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 676 | 410 | 157 | 103 | 6 | | |

- Molecule 62 is a protein called 60S ribosomal protein L13a, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | BO | 221 | Total | C | N | O | S | 0 | 0 |
| | | | 1801 | 1141 | 364 | 289 | 7 | | |

- Molecule 63 is a protein called 60S ribosomal protein L37a, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | Bo | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 699 | 434 | 144 | 115 | 6 | | |

- Molecule 64 is a protein called 60S ribosomal protein L38, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | Bp | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 626 | 393 | 125 | 104 | 4 | | |

- Molecule 65 is a protein called 60S ribosomal protein L39, putative.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 65 | Bq | 50 | Total | C | N | O | 0 | 0 |
| | | | 457 | 297 | 98 | 62 | | |

- Molecule 66 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | BQ | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1716 | 1077 | 370 | 264 | 5 | | |

- Molecule 67 is a protein called 60S ribosomal protein L17, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | BR | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1219 | 767 | 242 | 202 | 8 | | |

- Molecule 68 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | Br | 367 | Total | C | N | O | S | 0 | 0 |
| | | | 2882 | 1802 | 575 | 488 | 17 | | |

- Molecule 69 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | BS | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1465 | 926 | 289 | 243 | 7 | | |

- Molecule 70 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | Bs | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 394 | 247 | 80 | 60 | 7 | | |

- Molecule 71 is a protein called 60S ribosomal protein L19, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | BT | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1590 | 974 | 349 | 259 | 8 | | |

- Molecule 72 is a protein called 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | Bt | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 801 | 507 | 159 | 130 | 5 | | |

- Molecule 73 is a protein called 60S ribosomal protein L21E, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | BU | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1247 | 793 | 245 | 203 | 6 | | |

- Molecule 74 is a protein called 60S ribosomal protein L5, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | Bu | 247 | Total | C | N | O | S | 0 | 0 |
| | | | 1964 | 1234 | 378 | 347 | 5 | | |

- Molecule 75 is a protein called 60S ribosomal protein L22, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | BV | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 629 | 179 | 168 | 3 | | |

- Molecule 76 is a protein called 60S ribosomal protein L6, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | Bv | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1101 | 699 | 202 | 197 | 3 | | |

- Molecule 77 is a protein called 60S ribosomal protein L23, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | BW | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1029 | 651 | 195 | 178 | 5 | | |

- Molecule 78 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | BX | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 982 | 624 | 185 | 171 | 2 | | |

- Molecule 79 is a protein called 60S ribosomal protein L7, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 79 | Bw | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1872 | 1190 | 362 | 312 | 8 | | |

- Molecule 80 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 80 | Bx | 235 | Total | C | N | O | S | 0 | 0 |
| | | | 1874 | 1178 | 369 | 321 | 6 | | |

- Molecule 81 is a protein called 60S ribosomal protein L24, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 81 | BY | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 550 | 358 | 108 | 79 | 5 | | |

- Molecule 82 is a protein called 60S ribosomal protein L9, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 82 | By | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1515 | 961 | 281 | 269 | 4 | | |

- Molecule 83 is a protein called 60S ribosomal protein L26, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 83 | BZ | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 993 | 614 | 210 | 164 | 5 | | |

- Molecule 84 is a protein called 60S ribosomal protein L32, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 84 | Bi | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1075 | 678 | 217 | 176 | 4 | | |

- Molecule 85 is a protein called 40S ribosomal protein L14, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 85 | BP | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1237 | 784 | 240 | 209 | 4 | | |

- Molecule 86 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 86 | AF | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 868 | 531 | 156 | 173 | 8 | | |

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

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 87 | BA | 67 | Total | Mg | 0 |
| | | | 67 | 67 | |
| 87 | AA | 88 | Total | Mg | 0 |
| | | | 88 | 88 | |
| 87 | BB | 61 | Total | Mg | 0 |
| | | | 61 | 61 | |
| 87 | BG | 5 | Total | Mg | 0 |
| | | | 5 | 5 | |
| 87 | BE | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 87 | BD | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 87 | BC | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 87 | AH | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 87 | AO | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 87 | A0 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 87 | Be | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 87 | Bf | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 87 | BN | 1 | Total Mg<br>1 1 | 0 |
| 87 | BR | 1 | Total Mg<br>1 1 | 0 |
| 87 | BW | 1 | Total Mg<br>1 1 | 0 |

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 88 | BA | 8 | Total K<br>8 8 | 0 |
| 88 | AA | 25 | Total K<br>25 25 | 0 |
| 88 | BB | 12 | Total K<br>12 12 | 0 |
| 88 | AH | 1 | Total K<br>1 1 | 0 |
| 88 | BZ | 1 | Total K<br>1 1 | 0 |

- Molecule 89 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 89 | BA | 10 | Total Na<br>10 10 | 0 |
| 89 | AA | 14 | Total Na<br>14 14 | 0 |
| 89 | BB | 14 | Total Na<br>14 14 | 0 |
| 89 | A3 | 1 | Total Na<br>1 1 | 0 |
| 89 | BK | 1 | Total Na<br>1 1 | 0 |

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 90 | A9 | 1 | Total Zn<br>1 1 | 0 |
| 90 | Bn | 1 | Total Zn<br>1 1 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 90 | Bo | 1 | Total Zn<br>1 1 | 0 |
| 90 | Bs | 1 | Total Zn<br>1 1 | 0 |

- Molecule 91 is water.

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 91 | BA | 53 | Total O<br>53 53 | 0 |
| 91 | AA | 40 | Total O<br>40 40 | 0 |
| 91 | BB | 61 | Total O<br>61 61 | 0 |
| 91 | BH | 2 | Total O<br>2 2 | 0 |
| 91 | BG | 4 | Total O<br>4 4 | 0 |
| 91 | BE | 1 | Total O<br>1 1 | 0 |
| 91 | BC | 1 | Total O<br>1 1 | 0 |
| 91 | A8 | 1 | Total O<br>1 1 | 0 |
| 91 | AH | 1 | Total O<br>1 1 | 0 |
| 91 | AK | 1 | Total O<br>1 1 | 0 |
| 91 | AV | 3 | Total O<br>3 3 | 0 |
| 91 | A2 | 1 | Total O<br>1 1 | 0 |
| 91 | AG | 1 | Total O<br>1 1 | 0 |
| 91 | Bb | 3 | Total O<br>3 3 | 0 |
| 91 | Bd | 1 | Total O<br>1 1 | 0 |
| 91 | Be | 7 | Total O<br>7 7 | 0 |
| 91 | Bj | 1 | Total O<br>1 1 | 0 |

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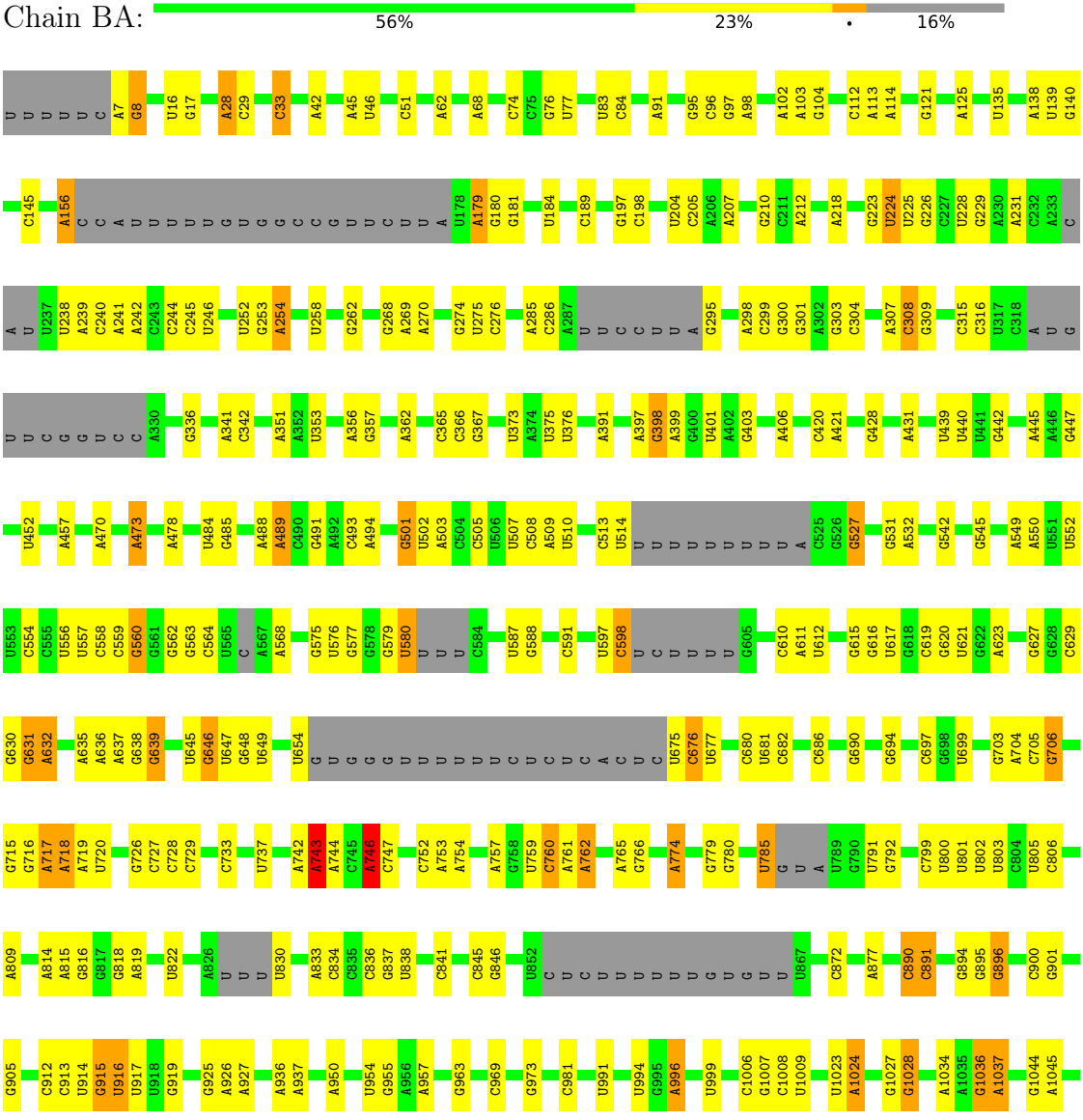
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 91 | BK | 1 | Total O<br>1 1 | 0 |
| 91 | BN | 1 | Total O<br>1 1 | 0 |
| 91 | Bn | 1 | Total O<br>1 1 | 0 |
| 91 | BQ | 2 | Total O<br>2 2 | 0 |
| 91 | Br | 1 | Total O<br>1 1 | 0 |
| 91 | Bi | 1 | Total O<br>1 1 | 0 |

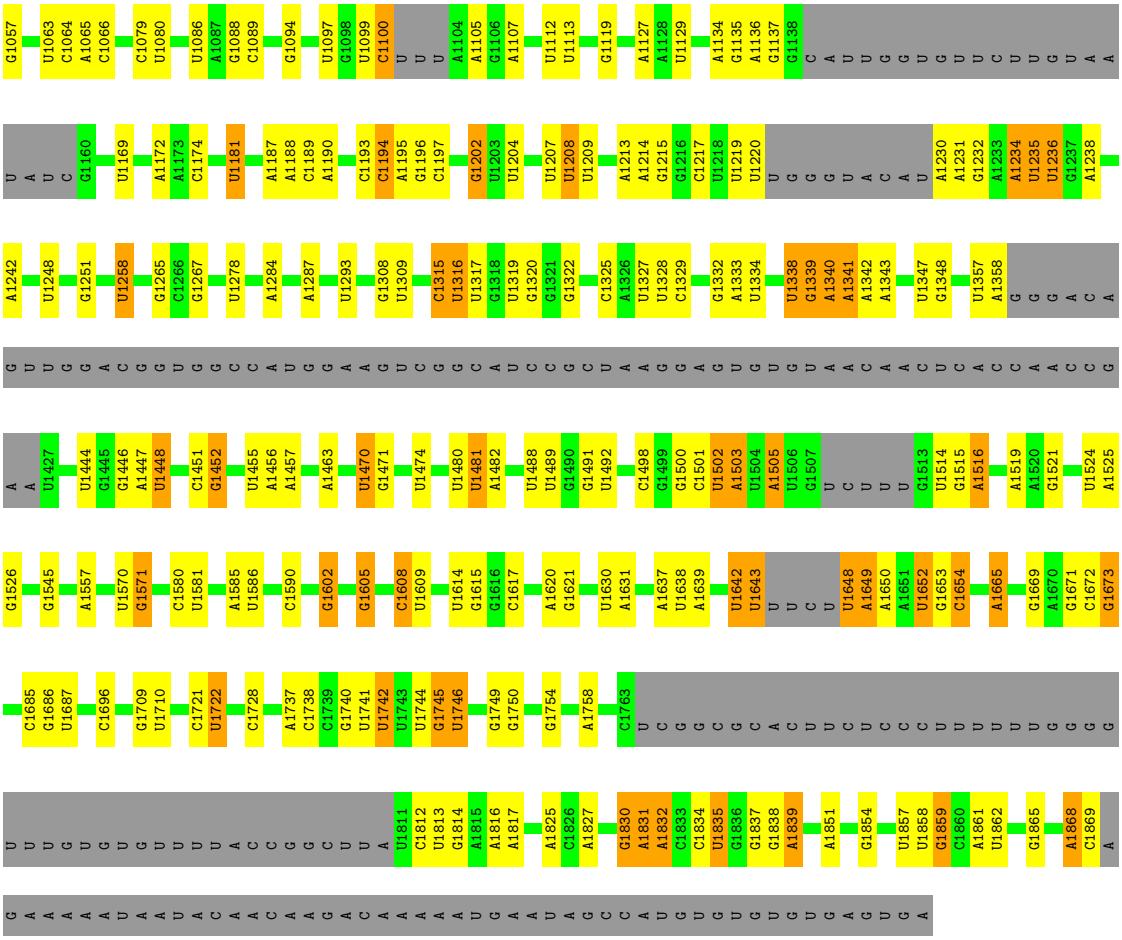
# 3 Residue-property plots (i)

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

- Molecule 1: LSUa rRNA

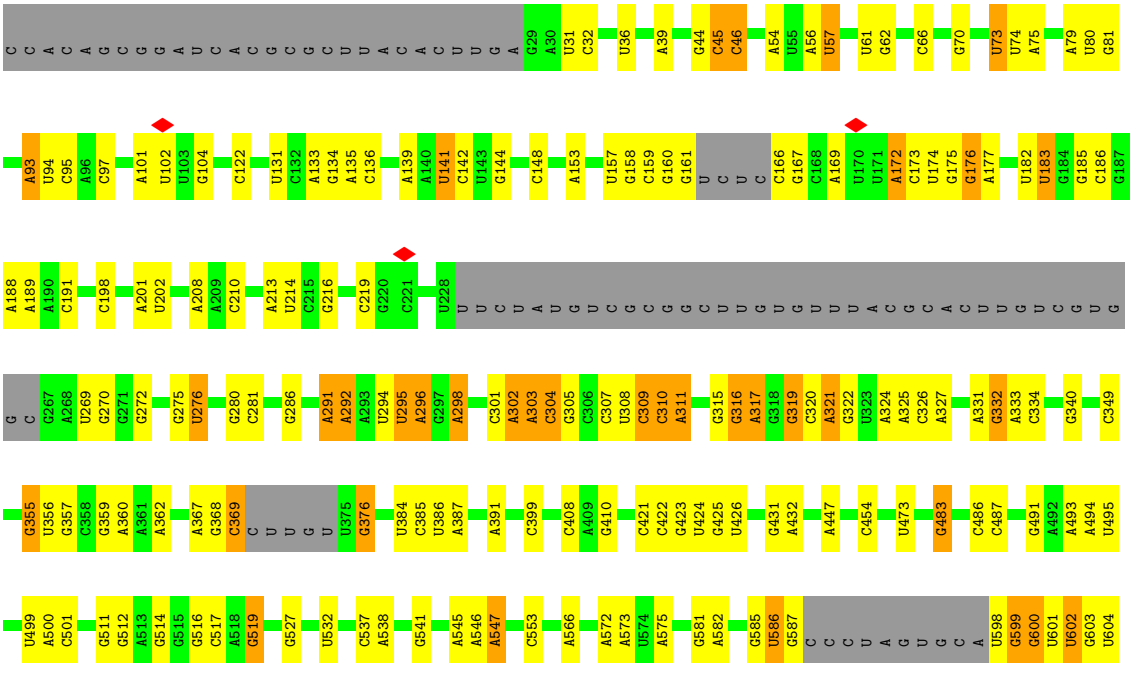
Chain BA:

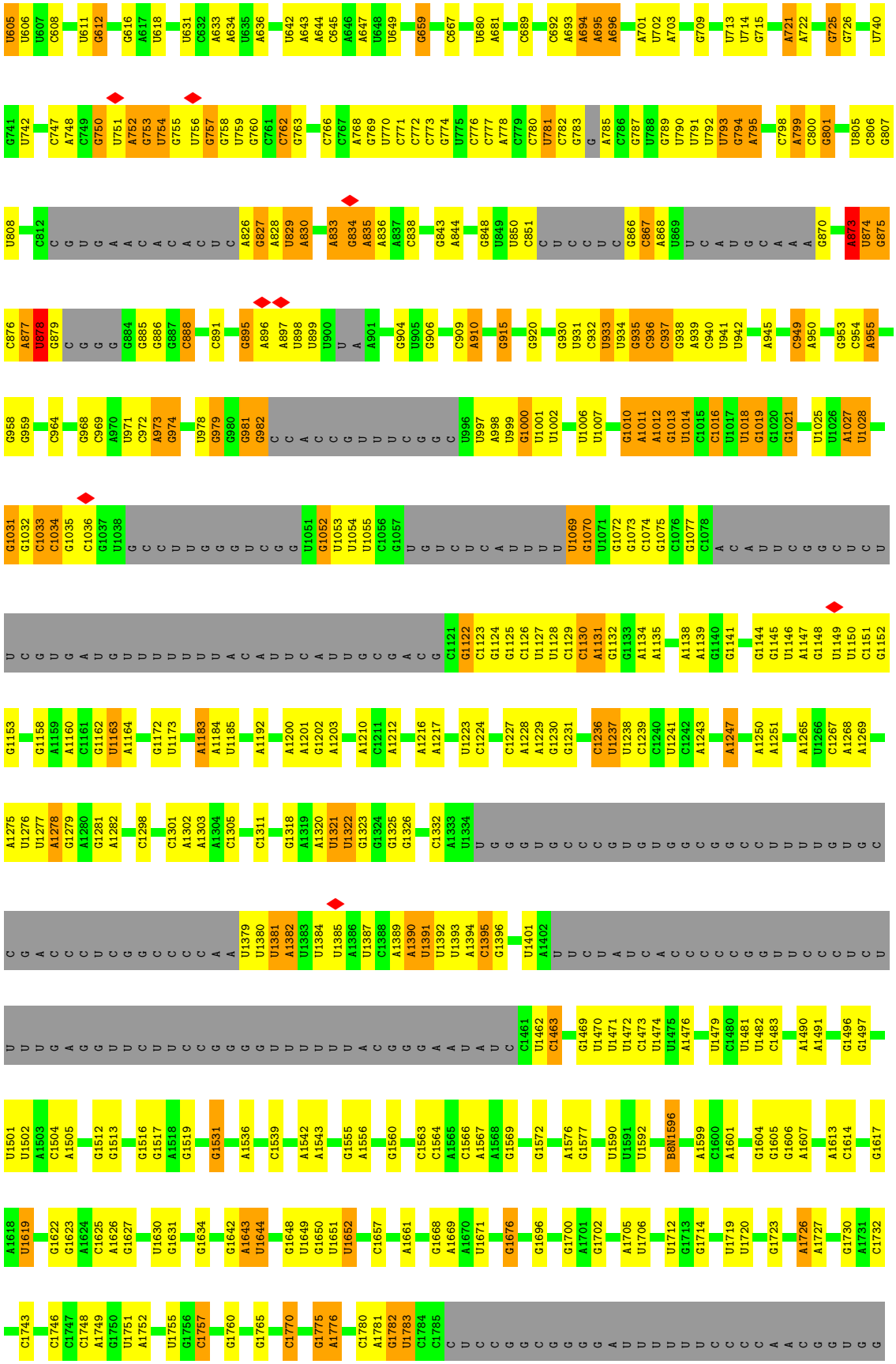


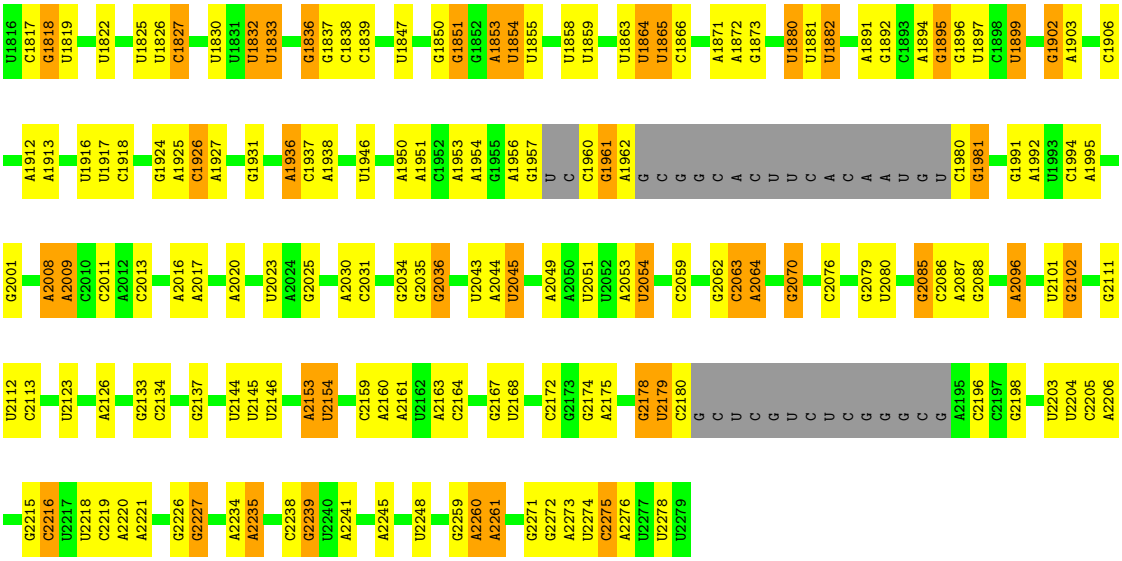


• Molecule 2: SSU rRNA

Chain AA:

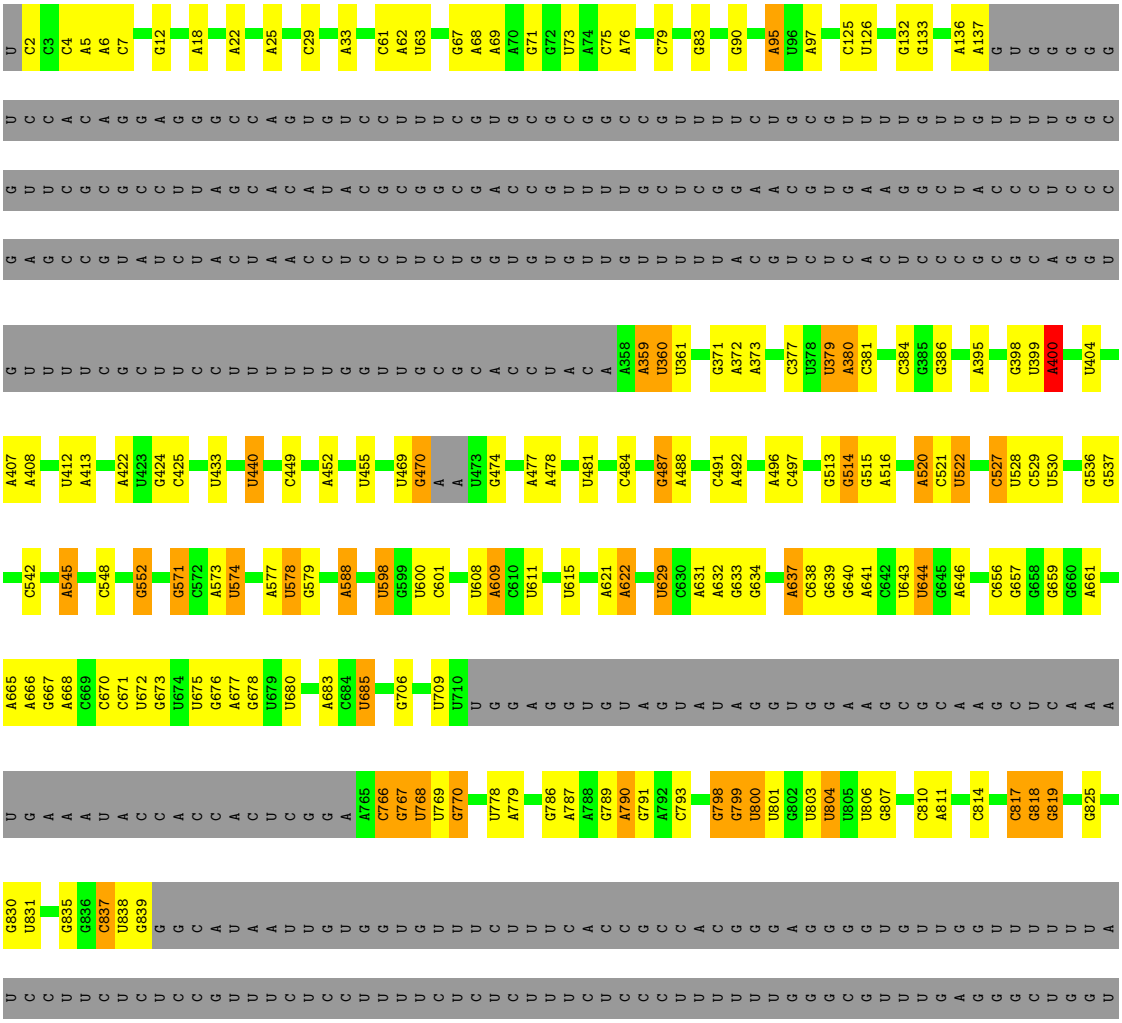


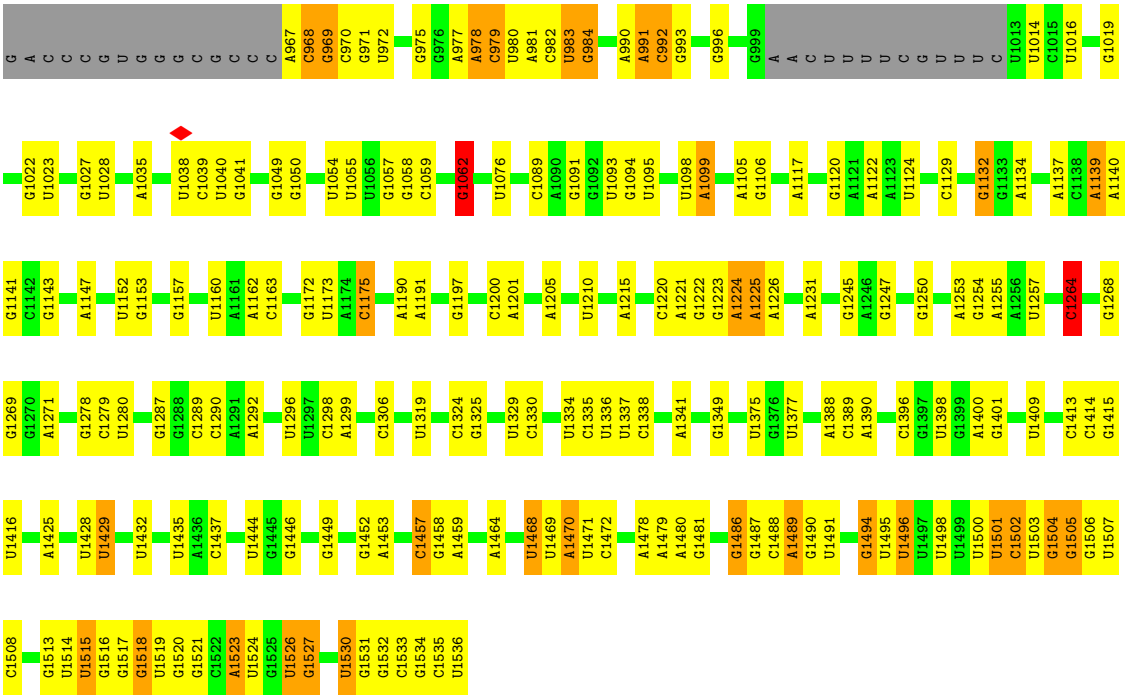




• Molecule 3: LSUb rRNA

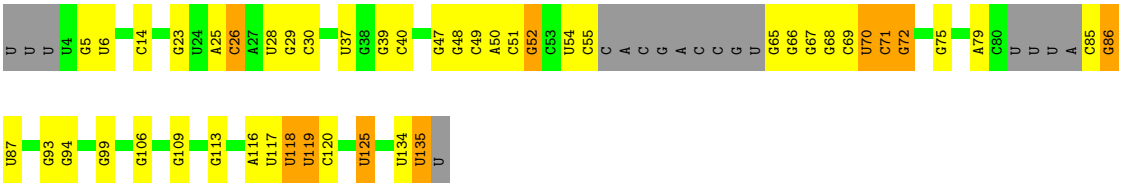
Chain BB:





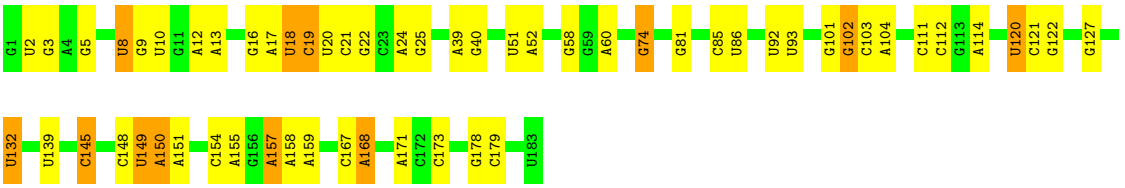
• Molecule 4: SrRNA-4

Chain BH:



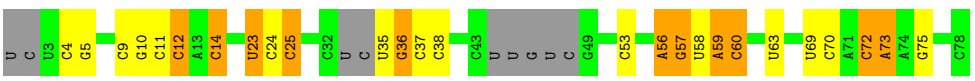
• Molecule 5: SrRNA-2

Chain BG:



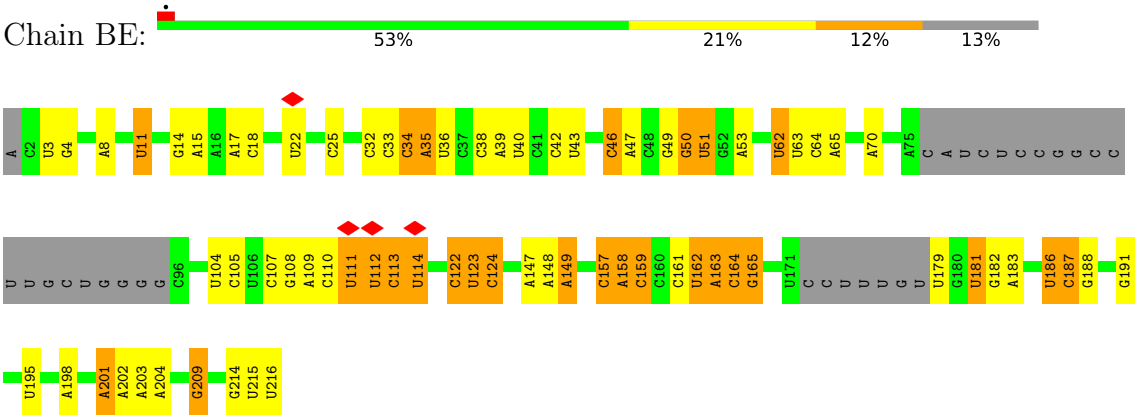
• Molecule 6: SrRNA-6

Chain BF:



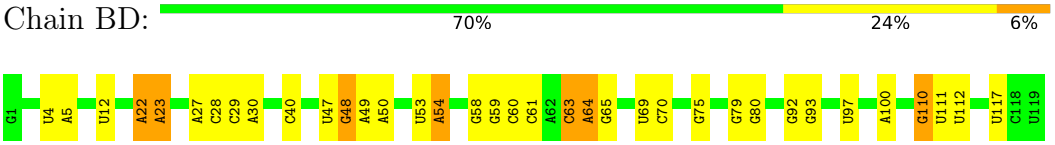
• Molecule 7: SrRNA-1

Chain BE:



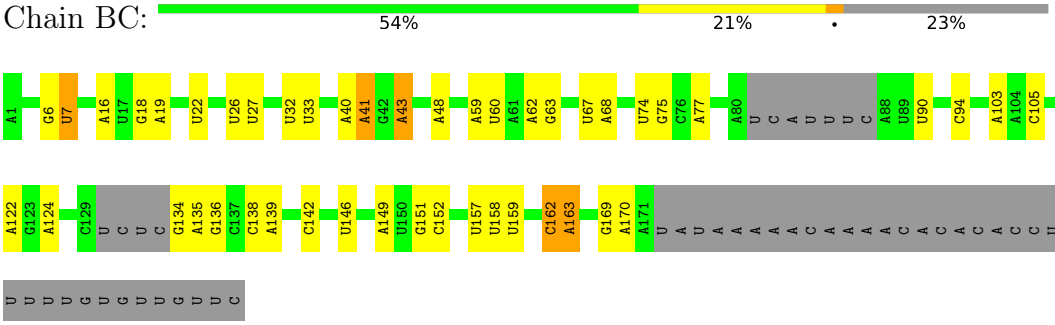

• Molecule 8: 5S rRNA

Chain BD:




• Molecule 9: 5.8S rRNA

Chain BC:

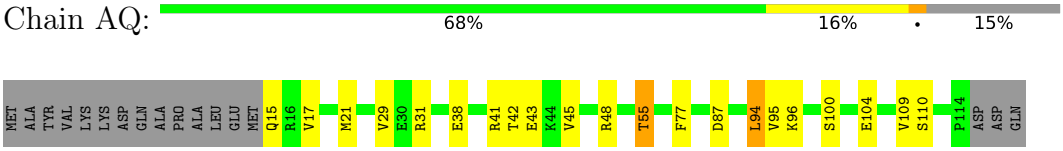



• Molecule 10: E-SITE TRNA

Chain AB:

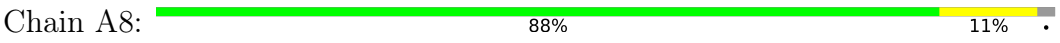
• Molecule 11: Ribosomal protein S10

Chain AQ:



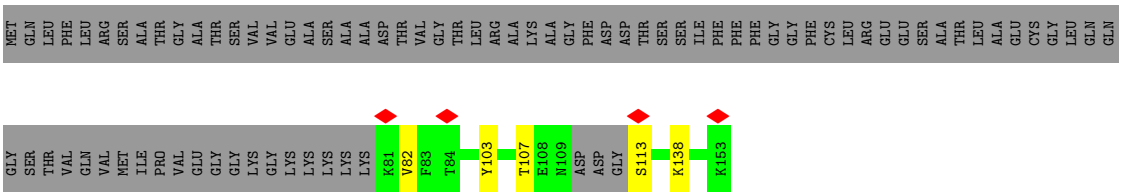

• Molecule 12: uS14

Chain A8:



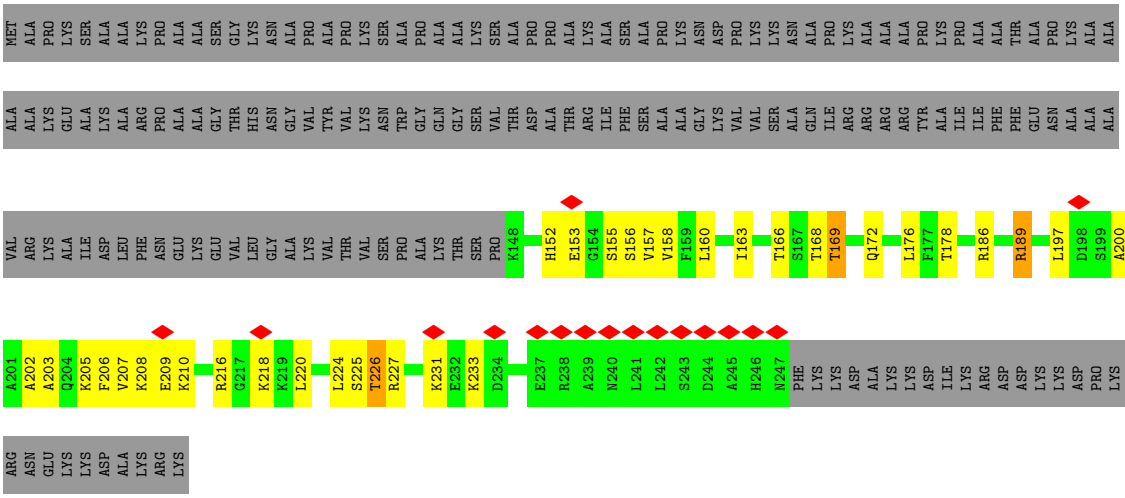
• Molecule 13: Ubiquitin-60S ribosomal protein L40

Chain A9:



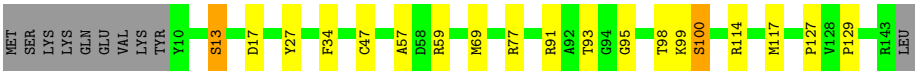

• Molecule 14: RNA-binding protein

Chain Az:



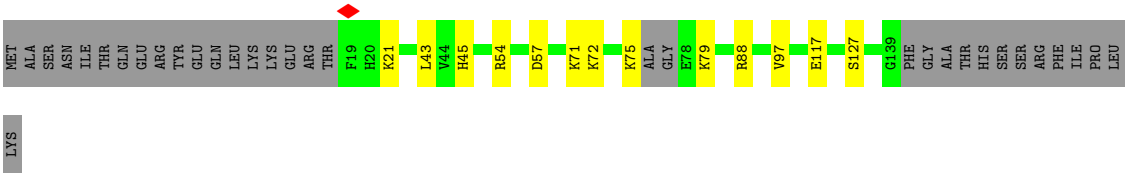

• Molecule 15: 40S ribosomal protein S14

Chain AH:



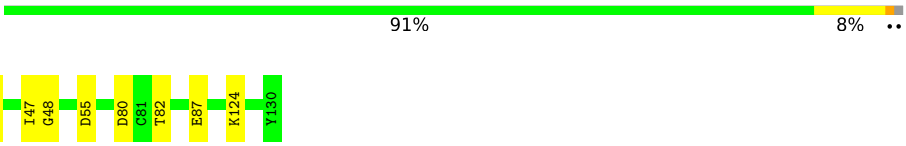

• Molecule 16: 40S ribosomal protein S15, putative

Chain AI:



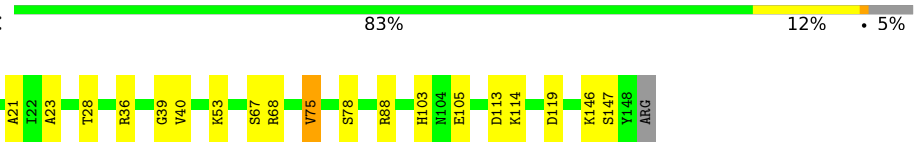

• Molecule 17: 40S ribosomal protein S15a, putative

Chain AJ:



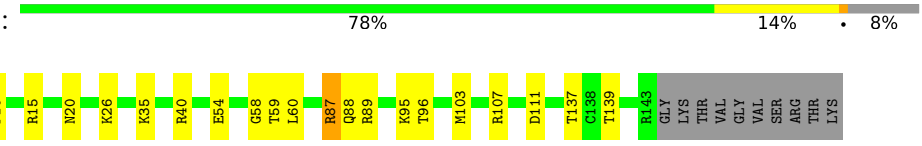

• Molecule 18: 40S ribosomal protein S16, putative

Chain AK:



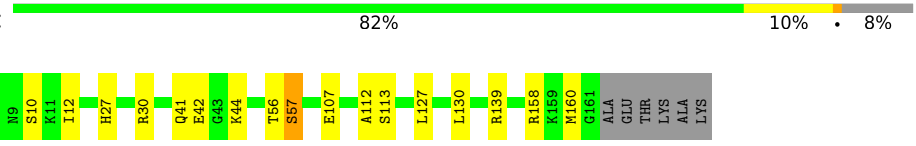

• Molecule 19: 40S ribosomal protein S18, putative

Chain AM:



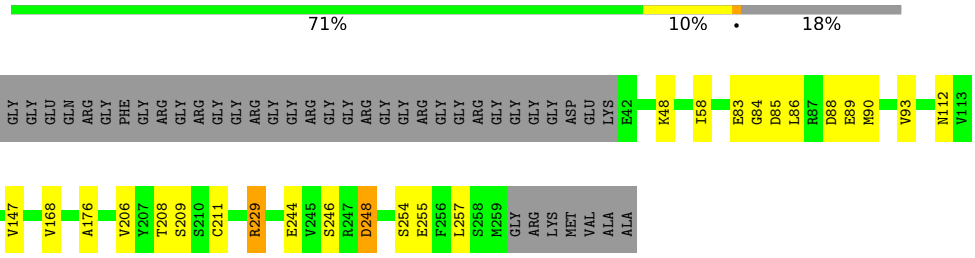

• Molecule 20: Ribosomal protein S19, putative

Chain AO:



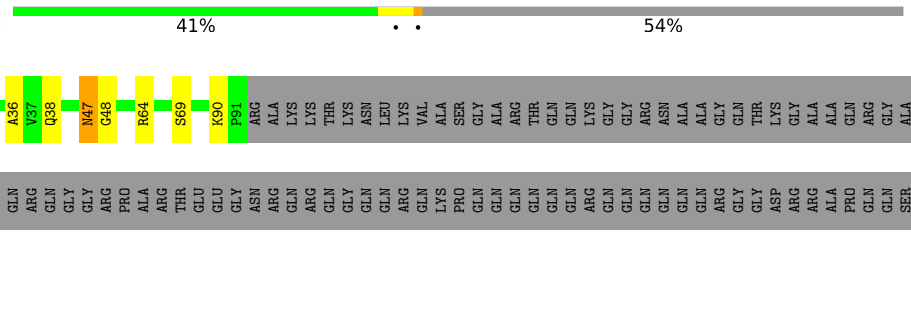

• Molecule 21: 40S ribosomal protein S2, putative

Chain AP:



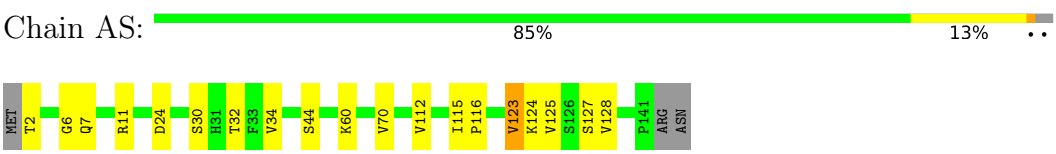

• Molecule 22: 40S ribosomal protein S21, putative

Chain AR:



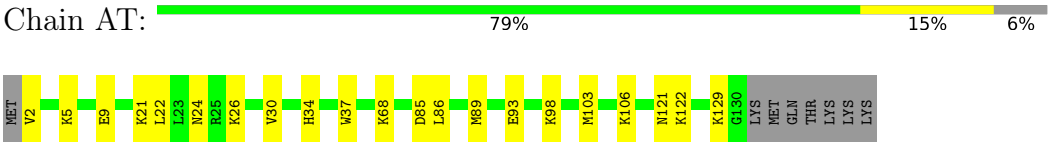

• Molecule 23: 40S ribosomal protein S23, putative

Chain AS:



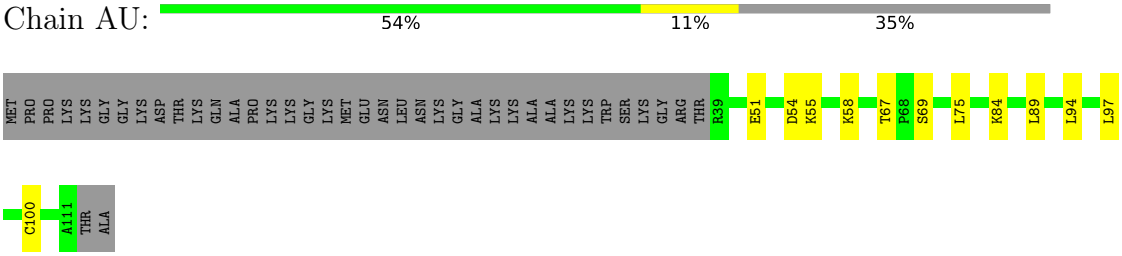

• Molecule 24: 40S ribosomal protein S24

Chain AT:



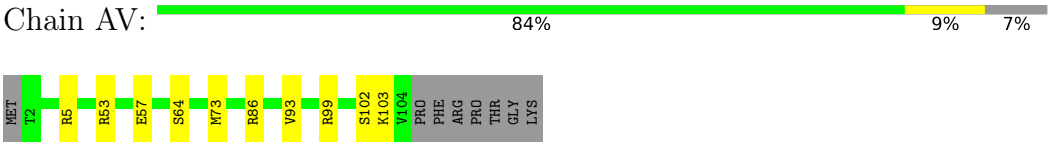

• Molecule 25: 40S ribosomal protein S25

Chain AU:



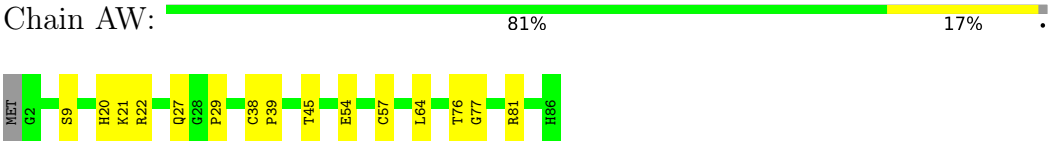

• Molecule 26: 40S ribosomal protein S26

Chain AV:



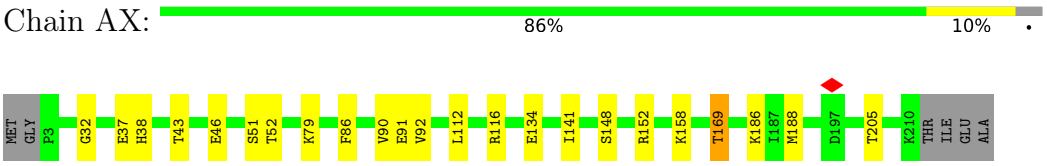

• Molecule 27: 40S ribosomal protein S27, putative

Chain AW:



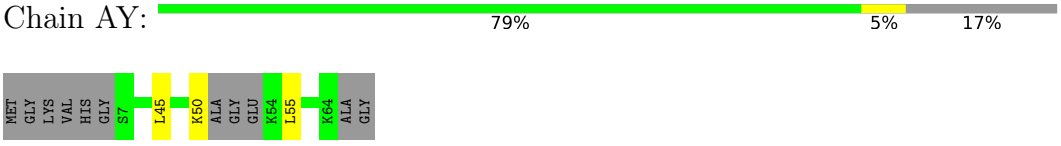

• Molecule 28: 40S ribosomal protein S3, putative

Chain AX:



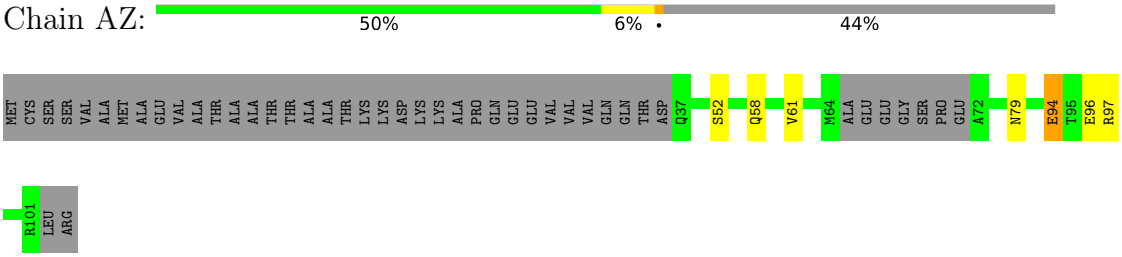

• Molecule 29: 40S ribosomal protein S30

Chain AY:



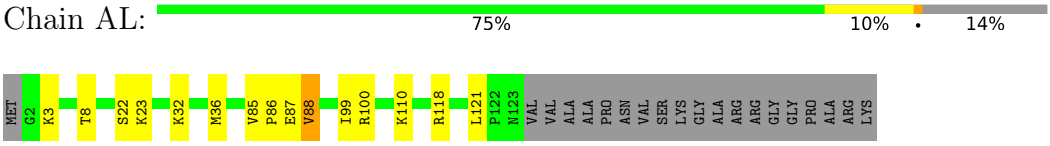
• Molecule 30: 40S ribosomal protein S33, putative

Chain AZ:



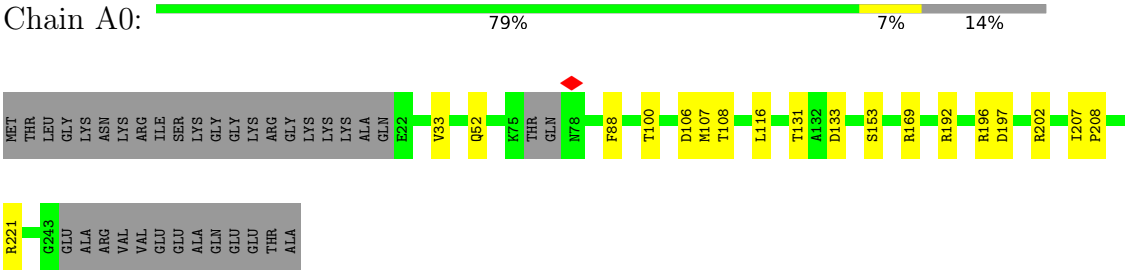

• Molecule 31: 40S ribosomal protein S17, putative

Chain AL:



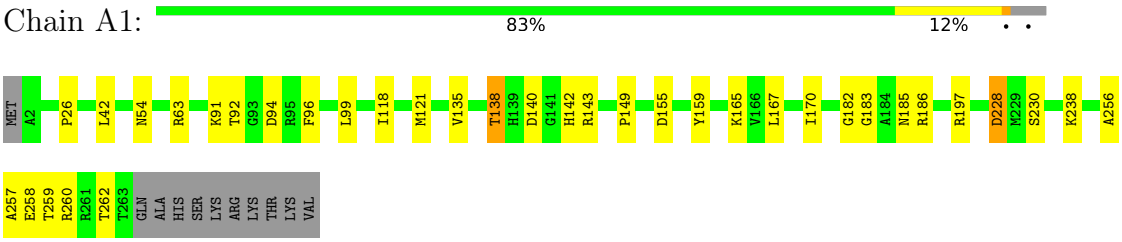

• Molecule 32: 40S ribosomal protein S3a

Chain A0:



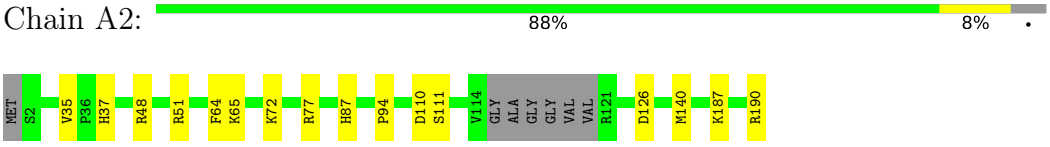

• Molecule 33: 40S ribosomal protein S4

Chain A1:



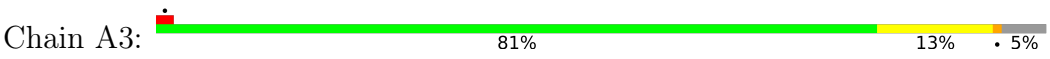

• Molecule 34: 40S ribosomal protein S5, putative

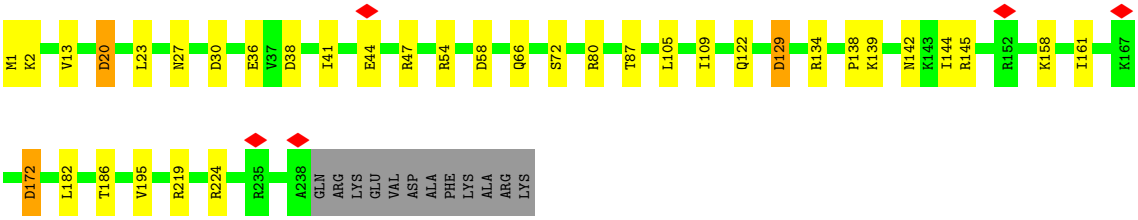
Chain A2:



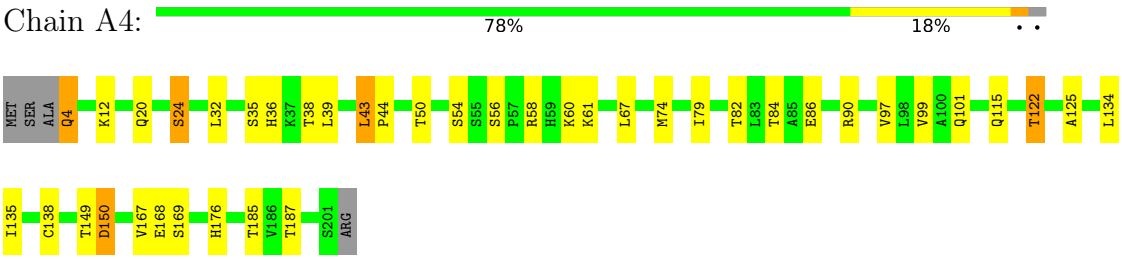

• Molecule 35: 40S ribosomal protein S6

Chain A3:

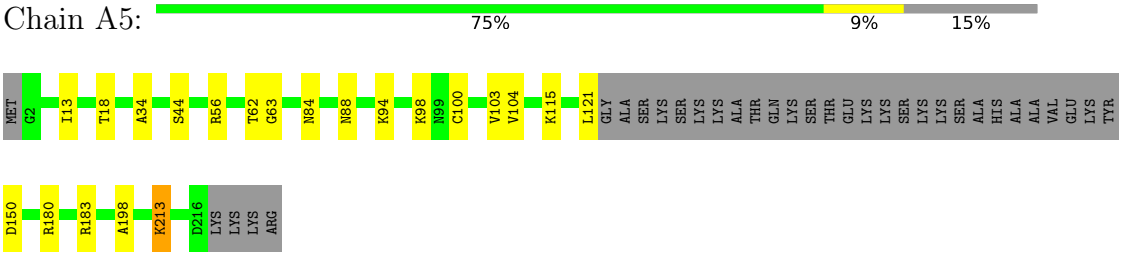




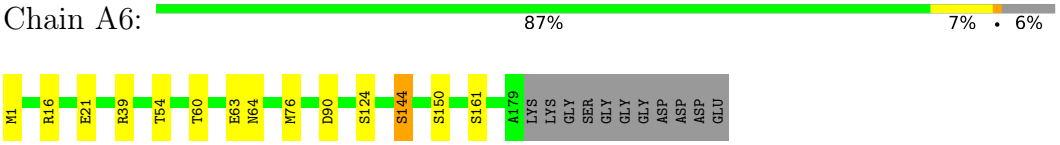

• Molecule 36: 40S ribosomal protein S7



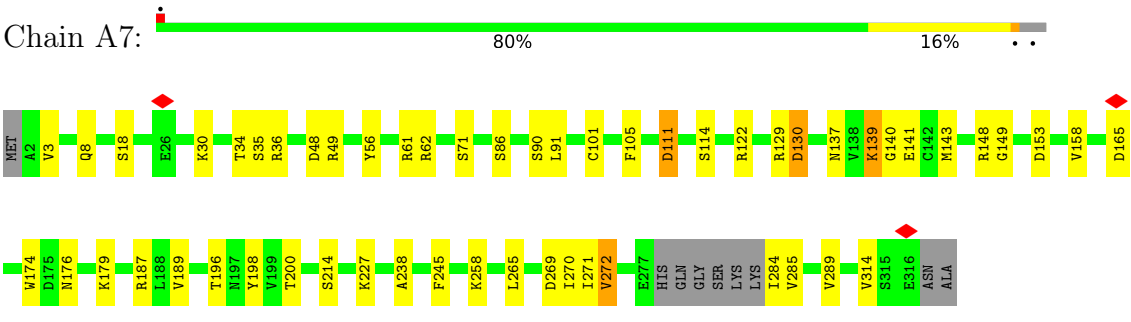

• Molecule 37: 40S ribosomal protein S8



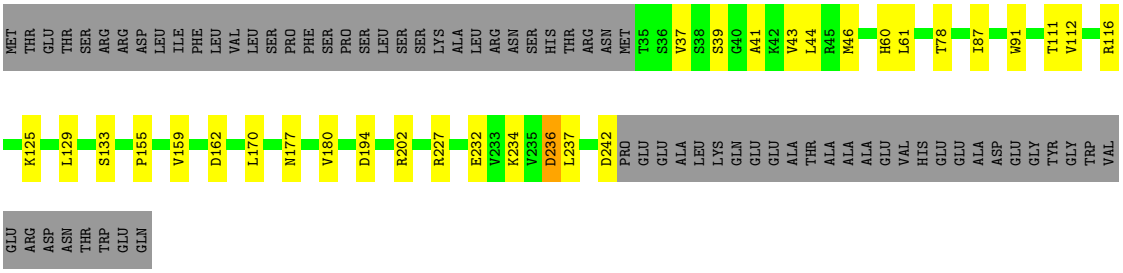

• Molecule 38: Probable 40S ribosomal protein S9




• Molecule 39: Guanine nucleotide-binding protein subunit beta-like protein

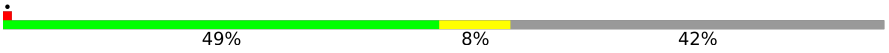


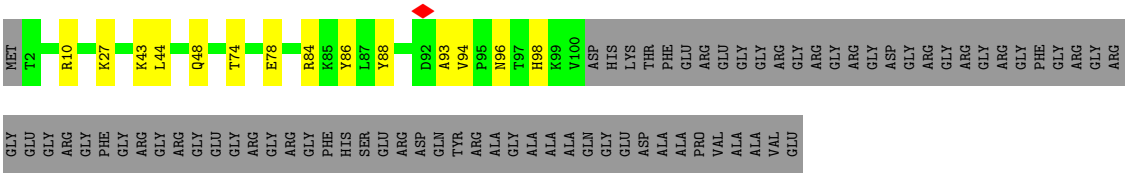

• Molecule 40: 40S ribosomal protein SA



• Molecule 41: 40S ribosomal protein S10, putative

Chain AD:



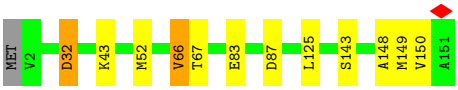



• Molecule 42: 40S ribosomal proteins S11, putative

Chain AE:

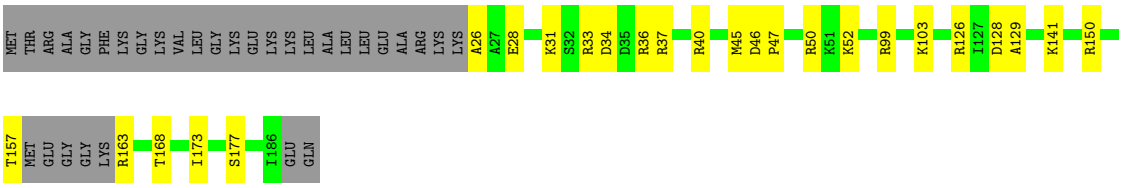
• Molecule 43: 40S ribosomal protein S13, putative

Chain AG:



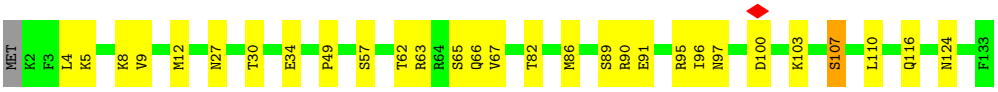
• Molecule 44: 60S ribosomal subunit protein L31, putative

Chain Bh:



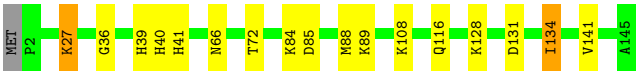
• Molecule 45: 60S ribosomal protein L27

Chain Ba:



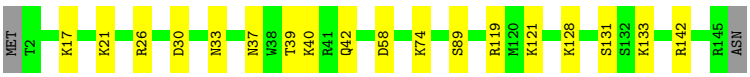
• Molecule 46: 60S ribosomal protein L27a

Chain Bb:



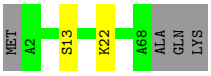

• Molecule 47: 60S ribosomal protein L28, putative

Chain Bc:




• Molecule 48: 60S ribosomal protein L29

Chain Bd:

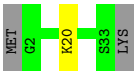



• Molecule 49: 60S ribosomal protein L2, putative

Chain Be:

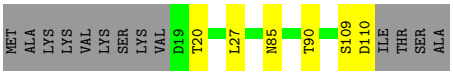
• Molecule 50: Ribosomal protein L41

Chain Bz:




• Molecule 51: 60S ribosomal protein L30

Chain Bg:

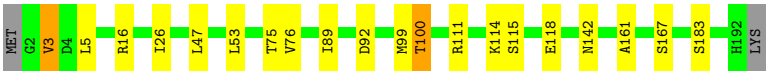



• Molecule 52: Ribosomal protein L3, mitochondrial, putative

Chain Bf:

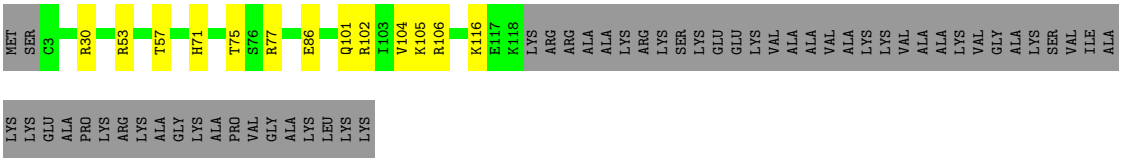
• Molecule 53: 60S ribosomal protein L18

Chain BI:



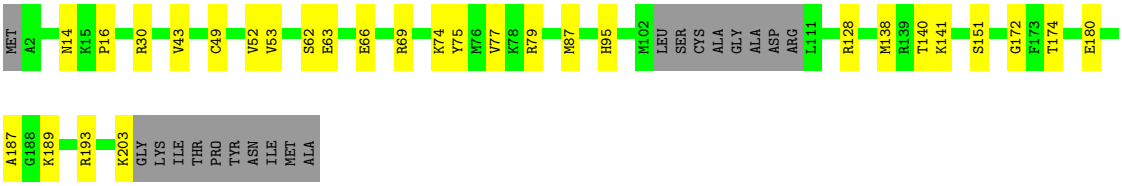

• Molecule 54: 60S ribosomal protein L34, putative

Chain Bj:



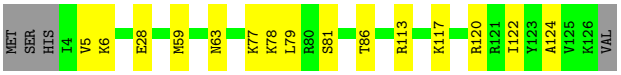

• Molecule 55: 60S ribosomal protein L10, putative

Chain BK:



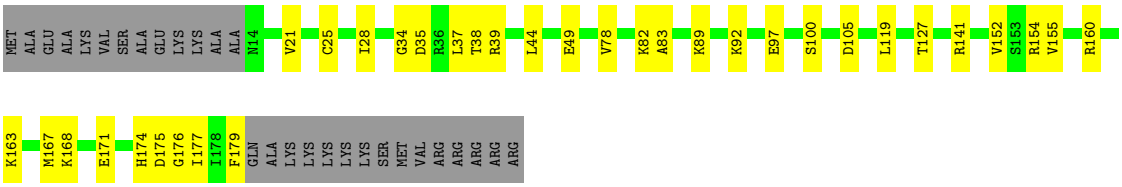

• Molecule 56: 60S ribosomal protein L35, putative

Chain Bk:



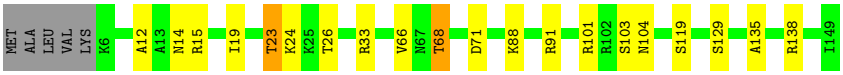

• Molecule 57: 60S ribosomal protein L11, putative

Chain BL:



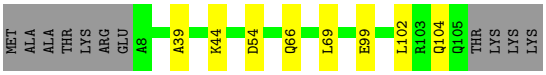

• Molecule 58: 60S ribosomal protein L35A, putative

Chain Bl:




• Molecule 59: Ribosomal protein L36, putative

Chain Bm:

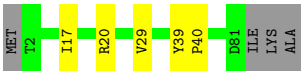



• Molecule 60: 60S ribosomal protein L13

Chain BN:

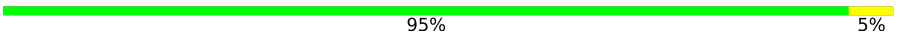
• Molecule 61: Ribosomal protein L37

Chain Bn:



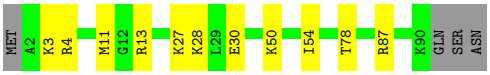

• Molecule 62: 60S ribosomal protein L13a, putative

Chain BO:



• Molecule 63: 60S ribosomal protein L37a, putative

Chain Bo:

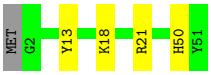



• Molecule 64: 60S ribosomal protein L38, putative

Chain Bp:

• Molecule 65: 60S ribosomal protein L39, putative

Chain Bq:

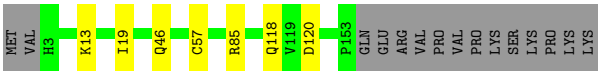



• Molecule 66: Ribosomal protein L15

Chain BQ:

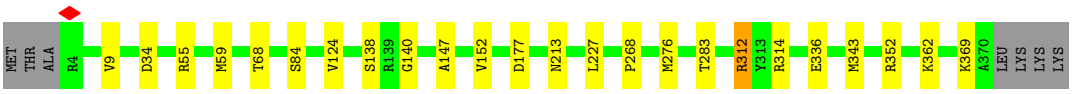
• Molecule 67: 60S ribosomal protein L17, putative

Chain BR:




• Molecule 68: 60S ribosomal protein L4

Chain Br:

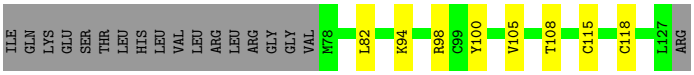



• Molecule 69: 60S ribosomal protein L18a

Chain BS:

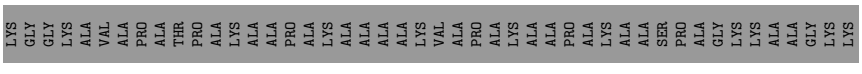
• Molecule 70: Ubiquitin-60S ribosomal protein L40

Chain Bs:



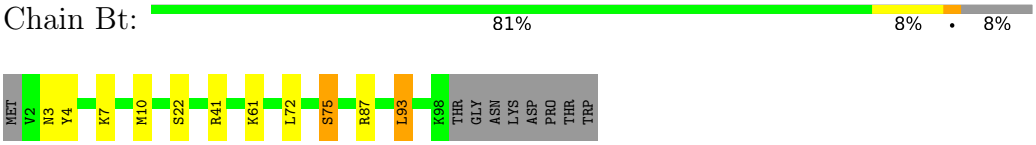

• Molecule 71: 60S ribosomal protein L19, putative

Chain BT:



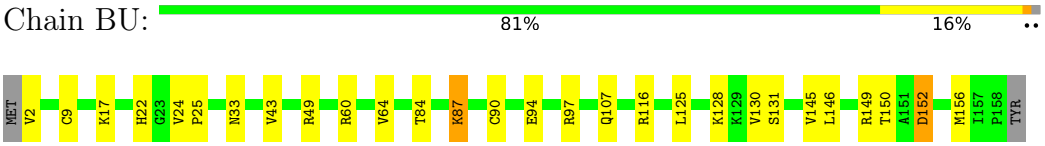
• Molecule 72: 60S ribosomal protein L44

Chain Bt:



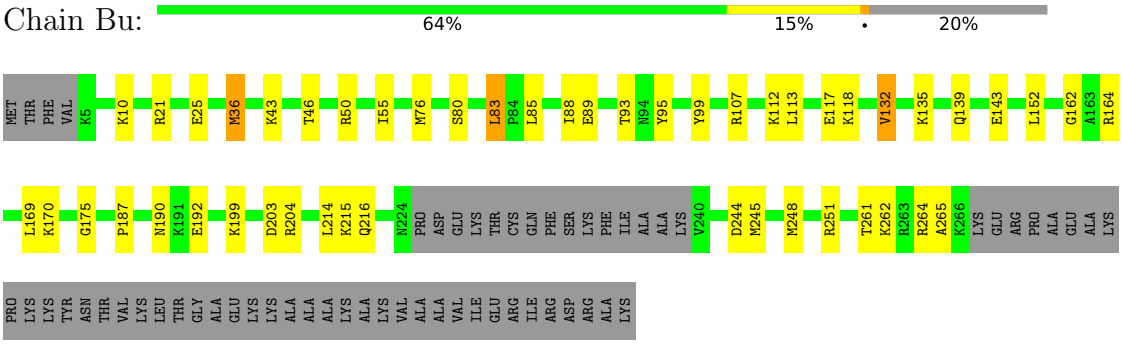

• Molecule 73: 60S ribosomal protein L21E, putative

Chain BU:



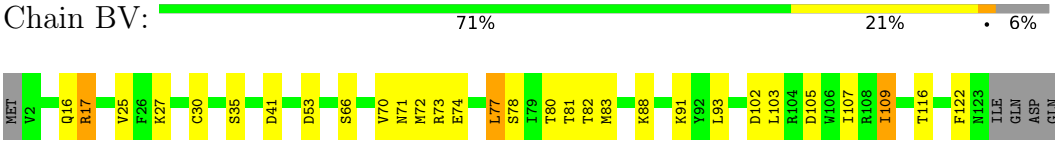

• Molecule 74: 60S ribosomal protein L5, putative

Chain Bu:



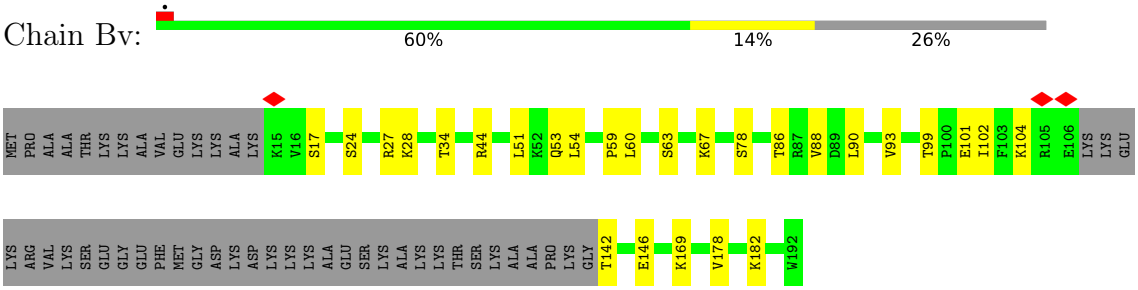

• Molecule 75: 60S ribosomal protein L22, putative

Chain BV:



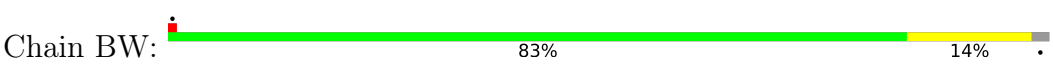

• Molecule 76: 60S ribosomal protein L6, putative

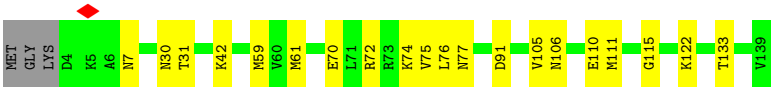
Chain Bv:




• Molecule 77: 60S ribosomal protein L23, putative

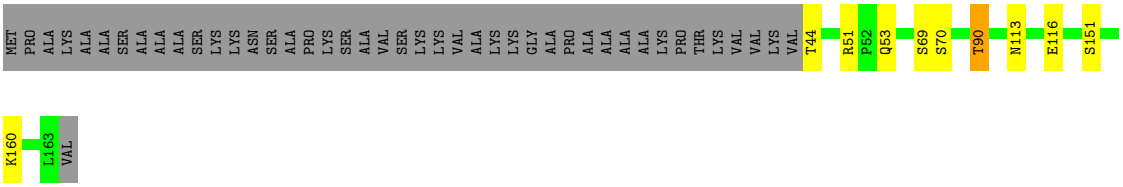
Chain BW:





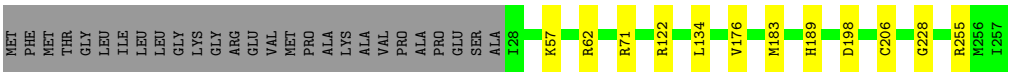

• Molecule 78: 60S ribosomal protein L23a

Chain BX:



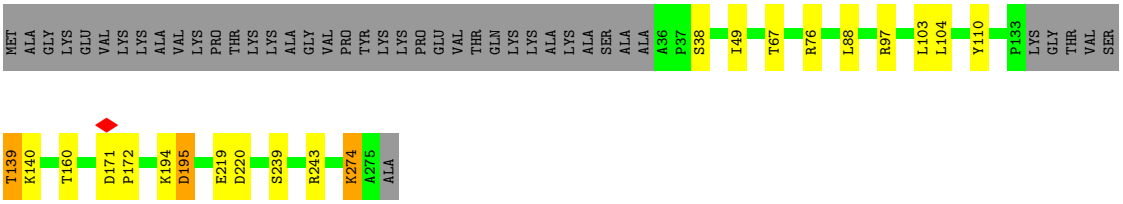

• Molecule 79: 60S ribosomal protein L7, putative

Chain Bw:



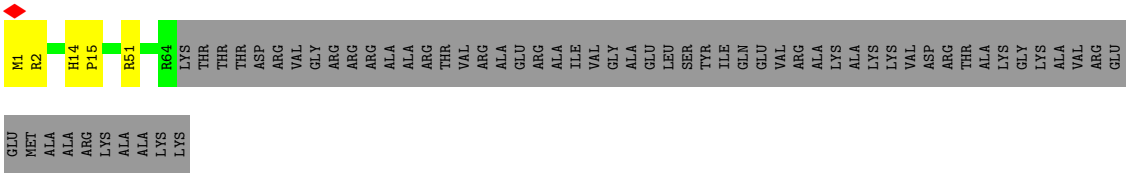

• Molecule 80: 60S ribosomal protein L7a

Chain Bx:



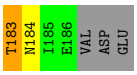

• Molecule 81: 60S ribosomal protein L24, putative

Chain BY:



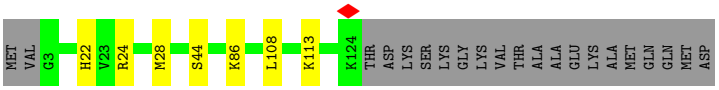

• Molecule 82: 60S ribosomal protein L9, putative

Chain By:



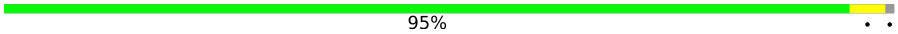

• Molecule 83: 60S ribosomal protein L26, putative

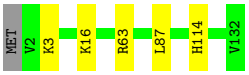
Chain BZ:




• Molecule 84: 60S ribosomal protein L32, putative

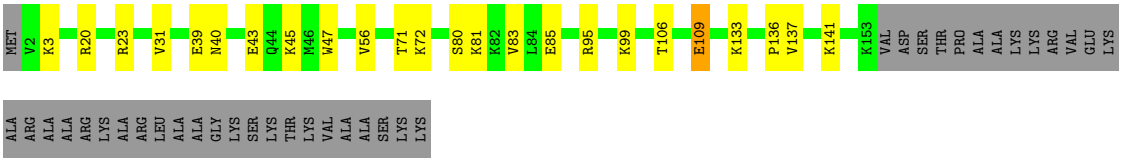
Chain Bi:



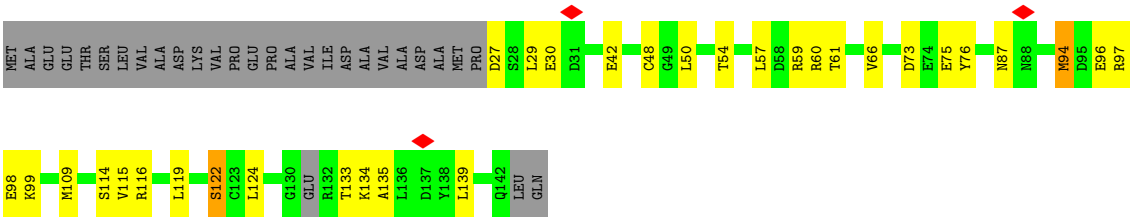

• Molecule 85: 40S ribosomal protein L14, putative

Chain BP:




• Molecule 86: 40S ribosomal protein S12

Chain AF:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 459985 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 1.17 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 1500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.188 | Depositor |
| Minimum map value | -0.056 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.005 | Depositor |
| Recommended contour level | 0.01 | Depositor |
| Map size (Å) | 408.0, 408.0, 408.0 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.85, 0.85, 0.85 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 1MA, MG, K, NA, 5MC, ZN, OMU, OMG, PSU, A2M, B8N, OMC, 7MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | BA | 0.21 | 1/37519 (0.0%) | 0.32 | 0/58462 |
| 2 | AA | 0.24 | 0/44961 | 0.35 | 8/70031 (0.0%) |
| 3 | BB | 0.24 | 1/25592 (0.0%) | 0.34 | 7/39885 (0.0%) |
| 4 | BH | 0.18 | 0/2833 | 0.30 | 0/4410 |
| 5 | BG | 0.19 | 0/4383 | 0.30 | 0/6835 |
| 6 | BF | 0.17 | 0/1604 | 0.33 | 0/2487 |
| 7 | BE | 0.19 | 0/4442 | 0.33 | 0/6910 |
| 8 | BD | 0.16 | 0/2830 | 0.24 | 0/4410 |
| 9 | BC | 0.23 | 0/3662 | 0.26 | 0/5700 |
| 10 | AB | 0.20 | 0/450 | 0.35 | 0/698 |
| 11 | AQ | 0.17 | 0/809 | 0.36 | 0/1091 |
| 12 | A8 | 0.17 | 0/468 | 0.29 | 0/619 |
| 13 | A9 | 0.17 | 0/582 | 0.42 | 0/773 |
| 14 | Az | 0.17 | 0/820 | 0.48 | 0/1100 |
| 15 | AH | 0.18 | 0/1006 | 0.38 | 0/1349 |
| 16 | AI | 0.15 | 0/986 | 0.25 | 0/1321 |
| 17 | AJ | 0.18 | 0/1035 | 0.29 | 0/1386 |
| 18 | AK | 0.18 | 0/1161 | 0.34 | 0/1561 |
| 19 | AM | 0.15 | 0/1161 | 0.27 | 0/1554 |
| 20 | AO | 0.17 | 0/1245 | 0.30 | 0/1665 |
| 21 | AP | 0.20 | 0/1723 | 0.32 | 0/2328 |
| 22 | AR | 0.16 | 0/676 | 0.27 | 0/919 |
| 23 | AS | 0.19 | 0/1117 | 0.38 | 0/1495 |
| 24 | AT | 0.16 | 0/1050 | 0.31 | 0/1395 |
| 25 | AU | 0.16 | 0/581 | 0.29 | 0/776 |
| 26 | AV | 0.25 | 0/846 | 0.39 | 0/1132 |
| 27 | AW | 0.17 | 0/674 | 0.41 | 0/904 |
| 28 | AX | 0.15 | 0/1674 | 0.28 | 0/2236 |
| 29 | AY | 0.17 | 0/453 | 0.31 | 0/596 |
| 30 | AZ | 0.19 | 0/448 | 0.35 | 0/595 |
| 31 | AL | 0.15 | 0/957 | 0.27 | 0/1282 |
| 32 | A0 | 0.17 | 0/1815 | 0.29 | 0/2440 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 33 | A1 | 0.18 | 0/2096 | 0.34 | 0/2819 |
| 34 | A2 | 0.16 | 0/1486 | 0.26 | 0/1997 |
| 35 | A3 | 0.16 | 0/1893 | 0.32 | 0/2533 |
| 36 | A4 | 0.16 | 0/1634 | 0.30 | 0/2208 |
| 37 | A5 | 0.18 | 0/1494 | 0.32 | 0/2004 |
| 38 | A6 | 0.17 | 0/1507 | 0.29 | 0/2023 |
| 39 | A7 | 0.14 | 0/2428 | 0.31 | 0/3311 |
| 40 | AC | 0.20 | 0/1682 | 0.27 | 0/2275 |
| 41 | AD | 0.17 | 0/837 | 0.34 | 0/1129 |
| 42 | AE | 0.17 | 0/1274 | 0.28 | 0/1714 |
| 43 | AG | 0.18 | 0/1225 | 0.28 | 0/1642 |
| 44 | Bh | 0.15 | 0/1270 | 0.30 | 0/1696 |
| 45 | Ba | 0.17 | 0/1105 | 0.28 | 0/1472 |
| 46 | Bb | 0.16 | 0/1165 | 0.32 | 0/1554 |
| 47 | Bc | 0.13 | 0/1179 | 0.26 | 0/1573 |
| 48 | Bd | 0.15 | 0/558 | 0.27 | 0/747 |
| 49 | Be | 0.18 | 0/1948 | 0.31 | 0/2621 |
| 50 | Bz | 0.22 | 0/288 | 0.37 | 0/374 |
| 51 | Bg | 0.16 | 0/718 | 0.23 | 0/969 |
| 52 | Bf | 0.15 | 0/3244 | 0.27 | 0/4360 |
| 53 | BI | 0.15 | 0/1543 | 0.27 | 0/2059 |
| 54 | Bj | 0.16 | 0/977 | 0.31 | 0/1304 |
| 55 | BK | 0.15 | 0/1620 | 0.27 | 0/2171 |
| 56 | Bk | 0.15 | 0/1018 | 0.33 | 0/1346 |
| 57 | BL | 0.15 | 0/1346 | 0.29 | 0/1800 |
| 58 | Bl | 0.15 | 0/1187 | 0.33 | 0/1592 |
| 59 | Bm | 0.14 | 0/796 | 0.28 | 0/1057 |
| 60 | BN | 0.15 | 0/1793 | 0.30 | 0/2391 |
| 61 | Bn | 0.16 | 0/690 | 0.30 | 0/920 |
| 62 | BO | 0.14 | 0/1832 | 0.26 | 0/2446 |
| 63 | Bo | 0.20 | 0/711 | 0.30 | 0/946 |
| 64 | Bp | 0.16 | 0/635 | 0.40 | 0/844 |
| 65 | Bq | 0.14 | 0/471 | 0.24 | 0/626 |
| 66 | BQ | 0.16 | 0/1755 | 0.28 | 0/2346 |
| 67 | BR | 0.15 | 0/1244 | 0.29 | 0/1669 |
| 68 | Br | 0.13 | 0/2936 | 0.27 | 0/3941 |
| 69 | BS | 0.15 | 0/1500 | 0.29 | 0/2018 |
| 70 | Bs | 0.17 | 0/400 | 0.35 | 0/531 |
| 71 | BT | 0.16 | 0/1607 | 0.33 | 0/2130 |
| 72 | Bt | 0.17 | 0/815 | 0.36 | 0/1077 |
| 73 | BU | 0.15 | 0/1276 | 0.32 | 0/1716 |
| 74 | Bu | 0.15 | 0/1999 | 0.31 | 0/2684 |
| 75 | BV | 0.18 | 0/995 | 0.40 | 0/1329 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | Bv | 0.14 | 0/1120 | 0.28 | 0/1511 |
| 77 | BW | 0.17 | 0/1046 | 0.34 | 0/1408 |
| 78 | BX | 0.14 | 0/999 | 0.29 | 0/1343 |
| 79 | Bw | 0.15 | 0/1907 | 0.26 | 0/2556 |
| 80 | Bx | 0.14 | 0/1901 | 0.27 | 0/2557 |
| 81 | BY | 0.17 | 0/570 | 0.34 | 0/766 |
| 82 | By | 0.15 | 0/1536 | 0.33 | 0/2065 |
| 83 | BZ | 0.14 | 0/1006 | 0.29 | 0/1340 |
| 84 | Bi | 0.14 | 0/1097 | 0.27 | 0/1468 |
| 85 | BP | 0.14 | 0/1256 | 0.28 | 0/1683 |
| 86 | AF | 0.15 | 0/870 | 0.36 | 0/1169 |
| All | All | 0.20 | 2/221048 (0.0%) | 0.32 | 15/324175 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | BB | 545 | A2M | O3'-P | 5.02 | 1.61 | 1.56 |
| 1 | BA | 743 | A2M | O3'-P | 5.00 | 1.61 | 1.56 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | BB | 515 | G | P-O3'-C3' | -8.07 | 108.09 | 120.20 |
| 3 | BB | 528 | U | P-O3'-C3' | -8.06 | 108.11 | 120.20 |
| 2 | AA | 878 | U | P-O3'-C3' | -7.99 | 108.21 | 120.20 |
| 3 | BB | 514 | G | P-O3'-C3' | -7.48 | 108.98 | 120.20 |
| 2 | AA | 874 | U | P-O3'-C3' | -7.30 | 109.25 | 120.20 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | BA | 34346 | 0 | 17349 | 210 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | AA | 40964 | 0 | 20713 | 365 | 0 |
| 3 | BB | 23918 | 0 | 12111 | 169 | 0 |
| 4 | BH | 2538 | 0 | 1286 | 29 | 0 |
| 5 | BG | 3919 | 0 | 1975 | 34 | 0 |
| 6 | BF | 1444 | 0 | 744 | 20 | 0 |
| 7 | BE | 3981 | 0 | 2023 | 43 | 0 |
| 8 | BD | 2533 | 0 | 1283 | 22 | 0 |
| 9 | BC | 3411 | 0 | 1736 | 21 | 0 |
| 10 | AB | 404 | 0 | 211 | 6 | 0 |
| 11 | AQ | 800 | 0 | 856 | 12 | 0 |
| 12 | A8 | 461 | 0 | 471 | 4 | 0 |
| 13 | A9 | 569 | 0 | 582 | 1 | 0 |
| 14 | Az | 807 | 0 | 820 | 24 | 0 |
| 15 | AH | 992 | 0 | 1004 | 13 | 0 |
| 16 | AI | 966 | 0 | 999 | 11 | 0 |
| 17 | AJ | 1018 | 0 | 1050 | 7 | 0 |
| 18 | AK | 1140 | 0 | 1198 | 10 | 0 |
| 19 | AM | 1143 | 0 | 1192 | 14 | 0 |
| 20 | AO | 1220 | 0 | 1286 | 10 | 0 |
| 21 | AP | 1688 | 0 | 1734 | 13 | 0 |
| 22 | AR | 666 | 0 | 670 | 7 | 0 |
| 23 | AS | 1096 | 0 | 1151 | 10 | 0 |
| 24 | AT | 1034 | 0 | 1117 | 13 | 0 |
| 25 | AU | 575 | 0 | 622 | 7 | 0 |
| 26 | AV | 830 | 0 | 868 | 8 | 0 |
| 27 | AW | 660 | 0 | 666 | 9 | 0 |
| 28 | AX | 1652 | 0 | 1721 | 9 | 0 |
| 29 | AY | 448 | 0 | 502 | 1 | 0 |
| 30 | AZ | 449 | 0 | 483 | 6 | 0 |
| 31 | AL | 945 | 0 | 996 | 12 | 0 |
| 32 | A0 | 1789 | 0 | 1859 | 12 | 0 |
| 33 | A1 | 2062 | 0 | 2181 | 19 | 0 |
| 34 | A2 | 1464 | 0 | 1524 | 10 | 0 |
| 35 | A3 | 1871 | 0 | 1960 | 22 | 0 |
| 36 | A4 | 1602 | 0 | 1664 | 25 | 0 |
| 37 | A5 | 1471 | 0 | 1532 | 10 | 0 |
| 38 | A6 | 1477 | 0 | 1536 | 8 | 0 |
| 39 | A7 | 2371 | 0 | 2283 | 26 | 0 |
| 40 | AC | 1648 | 0 | 1687 | 19 | 0 |
| 41 | AD | 814 | 0 | 819 | 10 | 0 |
| 42 | AE | 1249 | 0 | 1296 | 11 | 0 |
| 43 | AG | 1203 | 0 | 1281 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 44 | Bh | 1249 | 0 | 1319 | 20 | 0 |
| 45 | Ba | 1085 | 0 | 1151 | 14 | 0 |
| 46 | Bb | 1137 | 0 | 1174 | 13 | 0 |
| 47 | Bc | 1162 | 0 | 1246 | 12 | 0 |
| 48 | Bd | 547 | 0 | 570 | 1 | 0 |
| 49 | Be | 1907 | 0 | 1967 | 13 | 0 |
| 50 | Bz | 284 | 0 | 323 | 1 | 0 |
| 51 | Bg | 708 | 0 | 726 | 3 | 0 |
| 52 | Bf | 3174 | 0 | 3300 | 20 | 0 |
| 53 | BI | 1517 | 0 | 1633 | 10 | 0 |
| 54 | Bj | 959 | 0 | 1026 | 11 | 0 |
| 55 | BK | 1588 | 0 | 1651 | 13 | 0 |
| 56 | Bk | 1010 | 0 | 1126 | 10 | 0 |
| 57 | BL | 1325 | 0 | 1355 | 19 | 0 |
| 58 | Bl | 1163 | 0 | 1221 | 14 | 0 |
| 59 | Bm | 786 | 0 | 865 | 6 | 0 |
| 60 | BN | 1762 | 0 | 1864 | 15 | 0 |
| 61 | Bn | 676 | 0 | 685 | 3 | 0 |
| 62 | BO | 1801 | 0 | 1952 | 6 | 0 |
| 63 | Bo | 699 | 0 | 726 | 8 | 0 |
| 64 | Bp | 626 | 0 | 685 | 10 | 0 |
| 65 | Bq | 457 | 0 | 495 | 3 | 0 |
| 66 | BQ | 1716 | 0 | 1796 | 5 | 0 |
| 67 | BR | 1219 | 0 | 1278 | 3 | 0 |
| 68 | Br | 2882 | 0 | 3011 | 14 | 0 |
| 69 | BS | 1465 | 0 | 1500 | 11 | 0 |
| 70 | Bs | 394 | 0 | 417 | 3 | 0 |
| 71 | BT | 1590 | 0 | 1662 | 16 | 0 |
| 72 | Bt | 801 | 0 | 865 | 5 | 0 |
| 73 | BU | 1247 | 0 | 1306 | 16 | 0 |
| 74 | Bu | 1964 | 0 | 2002 | 32 | 0 |
| 75 | BV | 979 | 0 | 1002 | 17 | 0 |
| 76 | Bv | 1101 | 0 | 1158 | 14 | 0 |
| 77 | BW | 1029 | 0 | 1090 | 12 | 0 |
| 78 | BX | 982 | 0 | 1050 | 6 | 0 |
| 79 | Bw | 1872 | 0 | 1966 | 7 | 0 |
| 80 | Bx | 1874 | 0 | 2008 | 11 | 0 |
| 81 | BY | 550 | 0 | 558 | 4 | 0 |
| 82 | By | 1515 | 0 | 1589 | 22 | 0 |
| 83 | BZ | 993 | 0 | 1071 | 4 | 0 |
| 84 | Bi | 1075 | 0 | 1135 | 4 | 0 |
| 85 | BP | 1237 | 0 | 1320 | 13 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 86 | AF | 868 | 0 | 879 | 23 | 0 |
| 87 | A0 | 1 | 0 | 0 | 0 | 0 |
| 87 | AA | 88 | 0 | 0 | 0 | 0 |
| 87 | AH | 1 | 0 | 0 | 0 | 0 |
| 87 | AO | 2 | 0 | 0 | 0 | 0 |
| 87 | BA | 67 | 0 | 0 | 0 | 0 |
| 87 | BB | 61 | 0 | 0 | 0 | 0 |
| 87 | BC | 1 | 0 | 0 | 0 | 0 |
| 87 | BD | 1 | 0 | 0 | 0 | 0 |
| 87 | BE | 1 | 0 | 0 | 0 | 0 |
| 87 | BG | 5 | 0 | 0 | 0 | 0 |
| 87 | BN | 1 | 0 | 0 | 0 | 0 |
| 87 | BR | 1 | 0 | 0 | 0 | 0 |
| 87 | BW | 1 | 0 | 0 | 0 | 0 |
| 87 | Be | 2 | 0 | 0 | 0 | 0 |
| 87 | Bf | 1 | 0 | 0 | 0 | 0 |
| 88 | AA | 25 | 0 | 0 | 0 | 0 |
| 88 | AH | 1 | 0 | 0 | 0 | 0 |
| 88 | BA | 8 | 0 | 0 | 0 | 0 |
| 88 | BB | 12 | 0 | 0 | 0 | 0 |
| 88 | BZ | 1 | 0 | 0 | 0 | 0 |
| 89 | A3 | 1 | 0 | 0 | 0 | 0 |
| 89 | AA | 14 | 0 | 0 | 0 | 0 |
| 89 | BA | 10 | 0 | 0 | 0 | 0 |
| 89 | BB | 14 | 0 | 0 | 0 | 0 |
| 89 | BK | 1 | 0 | 0 | 0 | 0 |
| 90 | A9 | 1 | 0 | 0 | 0 | 0 |
| 90 | Bn | 1 | 0 | 0 | 0 | 0 |
| 90 | Bo | 1 | 0 | 0 | 0 | 0 |
| 90 | Bs | 1 | 0 | 0 | 0 | 0 |
| 91 | A2 | 1 | 0 | 0 | 0 | 0 |
| 91 | A8 | 1 | 0 | 0 | 0 | 0 |
| 91 | AA | 40 | 0 | 0 | 0 | 0 |
| 91 | AG | 1 | 0 | 0 | 0 | 0 |
| 91 | AH | 1 | 0 | 0 | 0 | 0 |
| 91 | AK | 1 | 0 | 0 | 1 | 0 |
| 91 | AV | 3 | 0 | 0 | 0 | 0 |
| 91 | BA | 53 | 0 | 0 | 0 | 0 |
| 91 | BB | 61 | 0 | 0 | 0 | 0 |
| 91 | BC | 1 | 0 | 0 | 0 | 0 |
| 91 | BE | 1 | 0 | 0 | 0 | 0 |
| 91 | BG | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 91 | BH | 2 | 0 | 0 | 0 | 0 |
| 91 | BK | 1 | 0 | 0 | 0 | 0 |
| 91 | BN | 1 | 0 | 0 | 0 | 0 |
| 91 | BQ | 2 | 0 | 0 | 0 | 0 |
| 91 | Bb | 3 | 0 | 0 | 0 | 0 |
| 91 | Bd | 1 | 0 | 0 | 0 | 0 |
| 91 | Be | 7 | 0 | 0 | 0 | 0 |
| 91 | Bi | 1 | 0 | 0 | 0 | 0 |
| 91 | Bj | 1 | 0 | 0 | 0 | 0 |
| 91 | Bn | 1 | 0 | 0 | 0 | 0 |
| 91 | Br | 1 | 0 | 0 | 0 | 0 |
| All | All | 209127 | 0 | 154764 | 1580 | 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 4.

The worst 5 of 1580 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) |
|---|---|---|---|
| 2:AA:770:U:H3 | 2:AA:780:C:N4 | 1.56 | 1.03 |
| 2:AA:758:G:H1 | 2:AA:791:U:H3 | 1.10 | 0.99 |
| 36:A4:4:GLN:N | 36:A4:4:GLN:HE21 | 1.60 | 0.98 |
| 4:BH:79:A:H2 | 4:BH:86:G:H1 | 1.05 | 0.95 |
| 3:BB:996:G:H1 | 3:BB:1016:U:H3 | 1.12 | 0.95 |

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 |
|---|---|---|---|---|---|---|
| 11 | AQ | 98/117 (84%) | 96 (98%) | 2 (2%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 12 | A8 | 54/57 (95%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 13 | A9 | 66/153 (43%) | 61 (92%) | 5 (8%) | 0 | 100 | 100 |
| 14 | Az | 98/279 (35%) | 84 (86%) | 13 (13%) | 1 (1%) | 12 | 22 |
| 15 | AH | 132/144 (92%) | 118 (89%) | 14 (11%) | 0 | 100 | 100 |
| 16 | AI | 115/152 (76%) | 112 (97%) | 3 (3%) | 0 | 100 | 100 |
| 17 | AJ | 127/130 (98%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |
| 18 | AK | 140/149 (94%) | 134 (96%) | 6 (4%) | 0 | 100 | 100 |
| 19 | AM | 139/153 (91%) | 134 (96%) | 5 (4%) | 0 | 100 | 100 |
| 20 | AO | 152/167 (91%) | 147 (97%) | 5 (3%) | 0 | 100 | 100 |
| 21 | AP | 216/266 (81%) | 203 (94%) | 12 (6%) | 1 (0%) | 24 | 40 |
| 22 | AR | 87/194 (45%) | 85 (98%) | 2 (2%) | 0 | 100 | 100 |
| 23 | AS | 138/143 (96%) | 128 (93%) | 10 (7%) | 0 | 100 | 100 |
| 24 | AT | 127/137 (93%) | 118 (93%) | 9 (7%) | 0 | 100 | 100 |
| 25 | AU | 71/113 (63%) | 67 (94%) | 4 (6%) | 0 | 100 | 100 |
| 26 | AV | 101/111 (91%) | 94 (93%) | 7 (7%) | 0 | 100 | 100 |
| 27 | AW | 83/86 (96%) | 80 (96%) | 3 (4%) | 0 | 100 | 100 |
| 28 | AX | 206/214 (96%) | 196 (95%) | 10 (5%) | 0 | 100 | 100 |
| 29 | AY | 51/66 (77%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | AZ | 54/103 (52%) | 52 (96%) | 2 (4%) | 0 | 100 | 100 |
| 31 | AL | 120/142 (84%) | 115 (96%) | 5 (4%) | 0 | 100 | 100 |
| 32 | A0 | 216/256 (84%) | 211 (98%) | 5 (2%) | 0 | 100 | 100 |
| 33 | A1 | 260/273 (95%) | 245 (94%) | 15 (6%) | 0 | 100 | 100 |
| 34 | A2 | 179/190 (94%) | 177 (99%) | 2 (1%) | 0 | 100 | 100 |
| 35 | A3 | 236/250 (94%) | 228 (97%) | 8 (3%) | 0 | 100 | 100 |
| 36 | A4 | 196/202 (97%) | 187 (95%) | 9 (5%) | 0 | 100 | 100 |
| 37 | A5 | 183/220 (83%) | 176 (96%) | 7 (4%) | 0 | 100 | 100 |
| 38 | A6 | 177/190 (93%) | 173 (98%) | 4 (2%) | 0 | 100 | 100 |
| 39 | A7 | 305/318 (96%) | 294 (96%) | 11 (4%) | 0 | 100 | 100 |
| 40 | AC | 206/277 (74%) | 200 (97%) | 6 (3%) | 0 | 100 | 100 |
| 41 | AD | 97/172 (56%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 42 | AE | 151/174 (87%) | 143 (95%) | 8 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 43 | AG | 148/151 (98%) | 144 (97%) | 4 (3%) | 0 | 100 | 100 |
| 44 | Bh | 152/188 (81%) | 142 (93%) | 10 (7%) | 0 | 100 | 100 |
| 45 | Ba | 130/133 (98%) | 129 (99%) | 1 (1%) | 0 | 100 | 100 |
| 46 | Bb | 142/145 (98%) | 136 (96%) | 6 (4%) | 0 | 100 | 100 |
| 47 | Bc | 142/146 (97%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 48 | Bd | 65/71 (92%) | 63 (97%) | 2 (3%) | 0 | 100 | 100 |
| 49 | Be | 253/260 (97%) | 247 (98%) | 6 (2%) | 0 | 100 | 100 |
| 50 | Bz | 30/34 (88%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 51 | Bg | 90/105 (86%) | 90 (100%) | 0 | 0 | 100 | 100 |
| 52 | Bf | 394/429 (92%) | 388 (98%) | 6 (2%) | 0 | 100 | 100 |
| 53 | BI | 189/193 (98%) | 183 (97%) | 6 (3%) | 0 | 100 | 100 |
| 54 | Bj | 114/170 (67%) | 111 (97%) | 3 (3%) | 0 | 100 | 100 |
| 55 | BK | 190/213 (89%) | 182 (96%) | 8 (4%) | 0 | 100 | 100 |
| 56 | Bk | 121/127 (95%) | 115 (95%) | 5 (4%) | 1 (1%) | 16 | 28 |
| 57 | BL | 164/194 (84%) | 155 (94%) | 9 (6%) | 0 | 100 | 100 |
| 58 | Bl | 142/149 (95%) | 136 (96%) | 6 (4%) | 0 | 100 | 100 |
| 59 | Bm | 96/109 (88%) | 95 (99%) | 1 (1%) | 0 | 100 | 100 |
| 60 | BN | 213/218 (98%) | 202 (95%) | 11 (5%) | 0 | 100 | 100 |
| 61 | Bn | 78/84 (93%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 62 | BO | 219/222 (99%) | 218 (100%) | 1 (0%) | 0 | 100 | 100 |
| 63 | Bo | 87/93 (94%) | 83 (95%) | 4 (5%) | 0 | 100 | 100 |
| 64 | Bp | 75/82 (92%) | 71 (95%) | 4 (5%) | 0 | 100 | 100 |
| 65 | Bq | 48/51 (94%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 66 | BQ | 201/221 (91%) | 197 (98%) | 4 (2%) | 0 | 100 | 100 |
| 67 | BR | 149/166 (90%) | 147 (99%) | 2 (1%) | 0 | 100 | 100 |
| 68 | Br | 365/374 (98%) | 352 (96%) | 13 (4%) | 0 | 100 | 100 |
| 69 | BS | 176/179 (98%) | 170 (97%) | 6 (3%) | 0 | 100 | 100 |
| 70 | Bs | 48/128 (38%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 71 | BT | 194/260 (75%) | 186 (96%) | 8 (4%) | 0 | 100 | 100 |
| 72 | Bt | 95/106 (90%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 73 | BU | 155/159 (98%) | 143 (92%) | 11 (7%) | 1 (1%) | 21 | 35 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 74 | Bu | 243/308 (79%) | 234 (96%) | 9 (4%) | 0 | 100 100 |
| 75 | BV | 120/130 (92%) | 111 (92%) | 8 (7%) | 1 (1%) | 16 28 |
| 76 | Bv | 139/192 (72%) | 134 (96%) | 5 (4%) | 0 | 100 100 |
| 77 | BW | 134/139 (96%) | 132 (98%) | 2 (2%) | 0 | 100 100 |
| 78 | BX | 118/164 (72%) | 114 (97%) | 4 (3%) | 0 | 100 100 |
| 79 | Bw | 228/257 (89%) | 223 (98%) | 5 (2%) | 0 | 100 100 |
| 80 | Bx | 231/276 (84%) | 220 (95%) | 11 (5%) | 0 | 100 100 |
| 81 | BY | 62/125 (50%) | 60 (97%) | 2 (3%) | 0 | 100 100 |
| 82 | By | 184/189 (97%) | 175 (95%) | 9 (5%) | 0 | 100 100 |
| 83 | BZ | 120/143 (84%) | 118 (98%) | 2 (2%) | 0 | 100 100 |
| 84 | Bi | 129/132 (98%) | 125 (97%) | 4 (3%) | 0 | 100 100 |
| 85 | BP | 150/189 (79%) | 144 (96%) | 6 (4%) | 0 | 100 100 |
| 86 | AF | 111/144 (77%) | 107 (96%) | 3 (3%) | 1 (1%) | 14 25 |
| All | All | 11215/13146 (85%) | 10789 (96%) | 420 (4%) | 6 (0%) | 49 66 |

5 of 6 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | Az | 169 | THR |
| 56 | Bk | 6 | LYS |
| 73 | BU | 33 | ASN |
| 75 | BV | 17 | ARG |
| 86 | AF | 122 | SER |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 11 | AQ | 90/104 (86%) | 83 (92%) | 7 (8%) | 11 22 |
| 12 | A8 | 49/50 (98%) | 47 (96%) | 2 (4%) | 27 50 |
| 13 | A9 | 62/126 (49%) | 58 (94%) | 4 (6%) | 15 30 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 14 | Az | 86/216 (40%) | 81 (94%) | 5 (6%) | 18 35 |
| 15 | AH | 101/112 (90%) | 97 (96%) | 4 (4%) | 28 51 |
| 16 | AI | 100/128 (78%) | 100 (100%) | 0 | 100 100 |
| 17 | AJ | 108/109 (99%) | 105 (97%) | 3 (3%) | 38 63 |
| 18 | AK | 117/124 (94%) | 113 (97%) | 4 (3%) | 32 57 |
| 19 | AM | 123/133 (92%) | 118 (96%) | 5 (4%) | 27 50 |
| 20 | AO | 127/137 (93%) | 123 (97%) | 4 (3%) | 35 60 |
| 21 | AP | 181/204 (89%) | 171 (94%) | 10 (6%) | 19 37 |
| 22 | AR | 73/150 (49%) | 71 (97%) | 2 (3%) | 39 64 |
| 23 | AS | 115/118 (98%) | 108 (94%) | 7 (6%) | 17 33 |
| 24 | AT | 108/116 (93%) | 103 (95%) | 5 (5%) | 24 45 |
| 25 | AU | 64/94 (68%) | 60 (94%) | 4 (6%) | 16 31 |
| 26 | AV | 90/97 (93%) | 89 (99%) | 1 (1%) | 65 83 |
| 27 | AW | 74/75 (99%) | 71 (96%) | 3 (4%) | 27 50 |
| 28 | AX | 176/180 (98%) | 166 (94%) | 10 (6%) | 18 36 |
| 29 | AY | 47/53 (89%) | 45 (96%) | 2 (4%) | 26 48 |
| 30 | AZ | 49/84 (58%) | 47 (96%) | 2 (4%) | 27 50 |
| 31 | AL | 96/122 (79%) | 92 (96%) | 4 (4%) | 26 49 |
| 32 | A0 | 190/218 (87%) | 187 (98%) | 3 (2%) | 55 77 |
| 33 | A1 | 221/231 (96%) | 212 (96%) | 9 (4%) | 27 50 |
| 34 | A2 | 157/160 (98%) | 154 (98%) | 3 (2%) | 50 73 |
| 35 | A3 | 191/207 (92%) | 180 (94%) | 11 (6%) | 18 35 |
| 36 | A4 | 173/187 (92%) | 157 (91%) | 16 (9%) | 8 17 |
| 37 | A5 | 147/180 (82%) | 136 (92%) | 11 (8%) | 12 24 |
| 38 | A6 | 159/166 (96%) | 154 (97%) | 5 (3%) | 35 60 |
| 39 | A7 | 260/267 (97%) | 241 (93%) | 19 (7%) | 13 25 |
| 40 | AC | 183/243 (75%) | 177 (97%) | 6 (3%) | 33 58 |
| 41 | AD | 87/131 (66%) | 85 (98%) | 2 (2%) | 44 69 |
| 42 | AE | 137/156 (88%) | 133 (97%) | 4 (3%) | 37 62 |
| 43 | AG | 130/131 (99%) | 126 (97%) | 4 (3%) | 35 60 |
| 44 | Bh | 133/162 (82%) | 129 (97%) | 4 (3%) | 36 61 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 45 | Ba | 115/117 (98%) | 107 (93%) | 8 (7%) | 14 27 |
| 46 | Bb | 115/116 (99%) | 113 (98%) | 2 (2%) | 53 75 |
| 47 | Bc | 128/130 (98%) | 126 (98%) | 2 (2%) | 55 77 |
| 48 | Bd | 56/59 (95%) | 55 (98%) | 1 (2%) | 51 74 |
| 49 | Be | 191/204 (94%) | 186 (97%) | 5 (3%) | 40 65 |
| 50 | Bz | 29/31 (94%) | 29 (100%) | 0 | 100 100 |
| 51 | Bg | 81/92 (88%) | 79 (98%) | 2 (2%) | 42 66 |
| 52 | Bf | 337/360 (94%) | 331 (98%) | 6 (2%) | 51 74 |
| 53 | BI | 163/165 (99%) | 155 (95%) | 8 (5%) | 22 42 |
| 54 | Bj | 99/137 (72%) | 98 (99%) | 1 (1%) | 68 84 |
| 55 | BK | 169/185 (91%) | 161 (95%) | 8 (5%) | 23 44 |
| 56 | Bk | 104/114 (91%) | 100 (96%) | 4 (4%) | 29 53 |
| 57 | BL | 142/167 (85%) | 135 (95%) | 7 (5%) | 22 42 |
| 58 | Bl | 122/126 (97%) | 118 (97%) | 4 (3%) | 33 58 |
| 59 | Bm | 81/90 (90%) | 81 (100%) | 0 | 100 100 |
| 60 | BN | 185/188 (98%) | 184 (100%) | 1 (0%) | 81 91 |
| 61 | Bn | 68/71 (96%) | 68 (100%) | 0 | 100 100 |
| 62 | BO | 194/195 (100%) | 193 (100%) | 1 (0%) | 81 91 |
| 63 | Bo | 72/76 (95%) | 71 (99%) | 1 (1%) | 59 79 |
| 64 | Bp | 72/77 (94%) | 66 (92%) | 6 (8%) | 10 20 |
| 65 | Bq | 46/47 (98%) | 46 (100%) | 0 | 100 100 |
| 66 | BQ | 176/193 (91%) | 171 (97%) | 5 (3%) | 38 63 |
| 67 | BR | 129/144 (90%) | 126 (98%) | 3 (2%) | 44 69 |
| 68 | Br | 304/310 (98%) | 296 (97%) | 8 (3%) | 40 65 |
| 69 | BS | 159/160 (99%) | 155 (98%) | 4 (2%) | 42 66 |
| 70 | Bs | 41/111 (37%) | 38 (93%) | 3 (7%) | 13 25 |
| 71 | BT | 153/198 (77%) | 149 (97%) | 4 (3%) | 40 65 |
| 72 | Bt | 87/95 (92%) | 82 (94%) | 5 (6%) | 18 36 |
| 73 | BU | 132/134 (98%) | 122 (92%) | 10 (8%) | 12 23 |
| 74 | Bu | 199/247 (81%) | 190 (96%) | 9 (4%) | 24 46 |
| 75 | BV | 100/116 (86%) | 89 (89%) | 11 (11%) | 6 11 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 76 | Bv | 119/160 (74%) | 110 (92%) | 9 (8%) | 12 23 |
| 77 | BW | 106/108 (98%) | 102 (96%) | 4 (4%) | 29 53 |
| 78 | BX | 107/136 (79%) | 102 (95%) | 5 (5%) | 23 44 |
| 79 | Bw | 193/213 (91%) | 190 (98%) | 3 (2%) | 55 77 |
| 80 | Bx | 199/229 (87%) | 190 (96%) | 9 (4%) | 24 46 |
| 81 | BY | 57/102 (56%) | 57 (100%) | 0 | 100 100 |
| 82 | By | 169/172 (98%) | 160 (95%) | 9 (5%) | 20 39 |
| 83 | BZ | 108/125 (86%) | 107 (99%) | 1 (1%) | 70 86 |
| 84 | Bi | 116/117 (99%) | 115 (99%) | 1 (1%) | 70 86 |
| 85 | BP | 132/158 (84%) | 125 (95%) | 7 (5%) | 20 39 |
| 86 | AF | 93/120 (78%) | 89 (96%) | 4 (4%) | 26 48 |
| All | All | 9652/11066 (87%) | 9286 (96%) | 366 (4%) | 30 53 |

5 of 366 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 56 | Bk | 122 | ILE |
| 73 | BU | 60 | ARG |
| 57 | BL | 177 | ILE |
| 68 | Br | 68 | THR |
| 74 | Bu | 214 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 69 | BS | 107 | GLN |
| 83 | BZ | 78 | HIS |
| 72 | Bt | 94 | ASN |
| 79 | Bw | 140 | ASN |
| 85 | BP | 34 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | BA | 1585/1920 (82%) | 300 (18%) | 9 (0%) |
| 10 | AB | 17/19 (89%) | 7 (41%) | 1 (5%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 2 | AA | 1902/2282 (83%) | 426 (22%) | 13 (0%) |
| 3 | BB | 1113/1536 (72%) | 209 (18%) | 5 (0%) |
| 4 | BH | 116/136 (85%) | 27 (23%) | 0 |
| 5 | BG | 182/183 (99%) | 30 (16%) | 1 (0%) |
| 6 | BF | 66/78 (84%) | 17 (25%) | 1 (1%) |
| 7 | BE | 185/216 (85%) | 47 (25%) | 4 (2%) |
| 8 | BD | 118/119 (99%) | 15 (12%) | 0 |
| 9 | BC | 157/209 (75%) | 22 (14%) | 0 |
| All | All | 5441/6698 (81%) | 1100 (20%) | 34 (0%) |

5 of 1100 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BA | 8 | G |
| 1 | BA | 28 | A |
| 1 | BA | 33 | C |
| 1 | BA | 42 | A |
| 1 | BA | 45 | A |

5 of 34 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | BF | 56 | A |
| 7 | BE | 123 | U |
| 7 | BE | 186 | U |
| 2 | AA | 324 | A |
| 2 | AA | 291 | A |

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

125 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 | $\#\|Z\|>2$ |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | PSU | AA | 131 | 2 | 18,21,22 | 4.57 | 7 (38%) | 21,30,33 | 1.87 | 3 (14%) |
| 3 | PSU | BB | 455 | 87,88,3 | 18,21,22 | 4.58 | 7 (38%) | 21,30,33 | 1.99 | 5 (23%) |
| 3 | OMG | BB | 659 | 3 | 23,26,27 | 2.40 | 9 (39%) | 32,38,41 | 2.47 | 12 (37%) |
| 3 | OMC | BB | 1264 | 3 | 19,22,23 | 2.96 | 8 (42%) | 25,31,34 | 0.83 | 0 |
| 3 | OMU | BB | 1435 | 3 | 19,22,23 | 3.03 | 8 (42%) | 25,31,34 | 1.83 | 5 (20%) |
| 3 | A2M | BB | 545 | 87,3 | 22,25,26 | 3.24 | 10 (45%) | 30,36,39 | 3.27 | 14 (46%) |
| 3 | PSU | BB | 1160 | 3 | 18,21,22 | 4.63 | 7 (38%) | 21,30,33 | 1.97 | 5 (23%) |
| 9 | A2M | BC | 163 | 1,9 | 22,25,26 | 3.20 | 9 (40%) | 30,36,39 | 3.08 | 11 (36%) |
| 1 | OMC | BA | 1329 | 1 | 19,22,23 | 3.05 | 8 (42%) | 25,31,34 | 0.79 | 0 |
| 1 | OMU | BA | 1181 | 1 | 19,22,23 | 3.02 | 8 (42%) | 25,31,34 | 1.91 | 5 (20%) |
| 3 | OMG | BB | 673 | 3 | 23,26,27 | 2.41 | 9 (39%) | 32,38,41 | 2.60 | 10 (31%) |
| 9 | PSU | BC | 74 | 9 | 18,21,22 | 4.66 | 7 (38%) | 21,30,33 | 2.03 | 5 (23%) |
| 1 | PSU | BA | 1248 | 1 | 18,21,22 | 4.61 | 7 (38%) | 21,30,33 | 1.99 | 6 (28%) |
| 2 | OMC | AA | 2134 | 2 | 19,22,23 | 2.85 | 8 (42%) | 25,31,34 | 0.73 | 0 |
| 3 | A2M | BB | 588 | 1,3 | 22,25,26 | 3.23 | 10 (45%) | 30,36,39 | 3.14 | 13 (43%) |
| 3 | A2M | BB | 400 | 3 | 22,25,26 | 3.25 | 10 (45%) | 30,36,39 | 3.01 | 12 (40%) |
| 1 | A2M | BA | 762 | 1 | 22,25,26 | 3.23 | 10 (45%) | 30,36,39 | 2.97 | 11 (36%) |
| 2 | PSU | AA | 1276 | 2 | 18,21,22 | 4.53 | 7 (38%) | 21,30,33 | 2.03 | 5 (23%) |
| 3 | PSU | BB | 1429 | 3 | 18,21,22 | 4.53 | 7 (38%) | 21,30,33 | 2.02 | 5 (23%) |
| 1 | A2M | BA | 743 | 1,3 | 22,25,26 | 3.20 | 9 (40%) | 30,36,39 | 3.16 | 11 (36%) |
| 3 | OMG | BB | 1062 | 3 | 23,26,27 | 2.41 | 9 (39%) | 32,38,41 | 2.61 | 10 (31%) |
| 3 | OMC | BB | 1175 | 3 | 19,22,23 | 2.96 | 8 (42%) | 25,31,34 | 0.79 | 0 |
| 3 | A2M | BB | 646 | 3 | 22,25,26 | 3.24 | 10 (45%) | 30,36,39 | 3.09 | 11 (36%) |
| 3 | OMG | BB | 1245 | 3 | 23,26,27 | 2.41 | 9 (39%) | 32,38,41 | 2.55 | 10 (31%) |
| 3 | 5MC | BB | 1324 | 3 | 19,22,23 | 3.75 | 8 (42%) | 26,32,35 | 1.10 | 1 (3%) |
| 1 | PSU | BA | 737 | 1,87 | 18,21,22 | 4.55 | 7 (38%) | 21,30,33 | 1.92 | 5 (23%) |
| 9 | A2M | BC | 43 | 9 | 22,25,26 | 3.21 | 9 (40%) | 30,36,39 | 3.07 | 11 (36%) |
| 2 | OMC | AA | 66 | 2 | 19,22,23 | 2.94 | 8 (42%) | 25,31,34 | 0.78 | 0 |
| 2 | OMG | AA | 1895 | 2,87 | 23,26,27 | 2.40 | 9 (39%) | 32,38,41 | 2.55 | 10 (31%) |
| 1 | PSU | BA | 1129 | 1 | 18,21,22 | 4.60 | 7 (38%) | 21,30,33 | 1.96 | 5 (23%) |
| 1 | PSU | BA | 1009 | 1 | 18,21,22 | 4.56 | 7 (38%) | 21,30,33 | 2.00 | 5 (23%) |
| 2 | OMG | AA | 1700 | 2 | 23,26,27 | 2.36 | 9 (39%) | 32,38,41 | 2.50 | 14 (43%) |
| 3 | A2M | BB | 609 | 3 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.01 | 12 (40%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | A2M | BB | 1400 | 87,3 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.10 | 12 (40%) |
| 3 | PSU | BB | 1409 | 3 | 18,21,22 | 4.64 | 7 (38%) | 21,30,33 | 1.89 | 5 (23%) |
| 1 | 1MA | BA | 742 | 1,87 | 21,25,26 | 2.85 | 5 (23%) | 30,37,40 | 1.81 | 6 (20%) |
| 3 | OMU | BB | 1375 | 3 | 19,22,23 | 3.01 | 8 (42%) | 25,31,34 | 1.82 | 5 (20%) |
| 3 | A2M | BB | 95 | 3 | 22,25,26 | 3.21 | 9 (40%) | 30,36,39 | 3.01 | 12 (40%) |
| 1 | OMU | BA | 1448 | 1 | 19,22,23 | 3.02 | 8 (42%) | 25,31,34 | 1.85 | 5 (20%) |
| 3 | PSU | BB | 1280 | 3 | 18,21,22 | 4.57 | 8 (44%) | 21,30,33 | 2.01 | 6 (28%) |
| 2 | OMG | AA | 1531 | 2 | 23,26,27 | 2.35 | 9 (39%) | 32,38,41 | 2.53 | 10 (31%) |
| 2 | PSU | AA | 2045 | 2 | 18,21,22 | 4.56 | 7 (38%) | 21,30,33 | 1.96 | 5 (23%) |
| 1 | OMG | BA | 915 | 1 | 23,26,27 | 2.39 | 9 (39%) | 32,38,41 | 2.53 | 10 (31%) |
| 1 | A2M | BA | 1024 | 1 | 22,25,26 | 3.20 | 10 (45%) | 30,36,39 | 3.04 | 11 (36%) |
| 3 | OMU | BB | 578 | 89,3 | 19,22,23 | 3.00 | 8 (42%) | 25,31,34 | 1.84 | 4 (16%) |
| 3 | OMG | BB | 1269 | 3 | 23,26,27 | 2.38 | 9 (39%) | 32,38,41 | 2.56 | 11 (34%) |
| 1 | OMG | BA | 1267 | 1 | 23,26,27 | 2.38 | 9 (39%) | 32,38,41 | 2.42 | 13 (40%) |
| 1 | PSU | BA | 1614 | 1,3 | 18,21,22 | 4.59 | 7 (38%) | 21,30,33 | 1.94 | 6 (28%) |
| 2 | OMU | AA | 714 | 2 | 19,22,23 | 2.98 | 8 (42%) | 25,31,34 | 1.82 | 5 (20%) |
| 1 | A2M | BA | 996 | 1,89 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.04 | 11 (36%) |
| 2 | OMU | AA | 2154 | 2 | 19,22,23 | 3.03 | 8 (42%) | 25,31,34 | 1.85 | 5 (20%) |
| 3 | OMC | BB | 1413 | 3 | 19,22,23 | 2.93 | 8 (42%) | 25,31,34 | 0.77 | 0 |
| 3 | OMU | BB | 73 | 3 | 19,22,23 | 3.01 | 8 (42%) | 25,31,34 | 1.80 | 5 (20%) |
| 3 | OMC | BB | 601 | 3 | 19,22,23 | 2.92 | 8 (42%) | 25,31,34 | 0.72 | 0 |
| 1 | PSU | BA | 1258 | 1 | 18,21,22 | 4.57 | 7 (38%) | 21,30,33 | 1.98 | 5 (23%) |
| 3 | PSU | BB | 644 | 3 | 18,21,22 | 4.57 | 7 (38%) | 21,30,33 | 1.96 | 5 (23%) |
| 2 | OMU | AA | 1652 | 2 | 19,22,23 | 3.04 | 8 (42%) | 25,31,34 | 1.82 | 5 (20%) |
| 3 | A2M | BB | 1388 | 3 | 22,25,26 | 3.26 | 10 (45%) | 30,36,39 | 3.13 | 11 (36%) |
| 3 | OMG | BB | 71 | 3 | 23,26,27 | 2.41 | 9 (39%) | 32,38,41 | 2.55 | 10 (31%) |
| 2 | PSU | AA | 1592 | 2 | 18,21,22 | 4.56 | 7 (38%) | 21,30,33 | 2.00 | 5 (23%) |
| 9 | A2M | BC | 41 | 9 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.07 | 11 (36%) |
| 1 | PSU | BA | 1169 | 1 | 18,21,22 | 4.59 | 7 (38%) | 21,30,33 | 2.02 | 5 (23%) |
| 1 | PSU | BA | 452 | 1 | 18,21,22 | 4.63 | 7 (38%) | 21,30,33 | 1.92 | 5 (23%) |
| 9 | OMG | BC | 75 | 9 | 23,26,27 | 2.43 | 9 (39%) | 32,38,41 | 2.55 | 10 (31%) |
| 1 | A2M | BA | 254 | 1 | 22,25,26 | 3.22 | 9 (40%) | 30,36,39 | 3.05 | 11 (36%) |
| 9 | OMU | BC | 7 | 1,9 | 19,22,23 | 3.04 | 8 (42%) | 25,31,34 | 1.83 | 5 (20%) |
| 3 | PSU | BB | 1319 | 3 | 18,21,22 | 4.62 | 8 (44%) | 21,30,33 | 1.98 | 6 (28%) |
| 1 | OMG | BA | 1709 | 1 | 23,26,27 | 2.42 | 9 (39%) | 32,38,41 | 2.58 | 10 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | PSU | BB | 522 | 3 | 18,21,22 | 4.59 | 7 (38%) | 21,30,33 | 1.91 | 5 (23%) |
| 1 | A2M | BA | 746 | 1 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.05 | 11 (36%) |
| 3 | 5MC | BB | 542 | 87,3 | 19,22,23 | 3.66 | 8 (42%) | 26,32,35 | 1.07 | 2 (7%) |
| 1 | OMG | BA | 1605 | 1 | 23,26,27 | 2.41 | 9 (39%) | 32,38,41 | 2.61 | 10 (31%) |
| 1 | OMC | BA | 1608 | 1 | 19,22,23 | 2.96 | 8 (42%) | 25,31,34 | 0.98 | 2 (8%) |
| 2 | OMG | AA | 1676 | 2,88 | 23,26,27 | 2.41 | 9 (39%) | 32,38,41 | 2.65 | 10 (31%) |
| 1 | PSU | BA | 1609 | 1 | 18,21,22 | 4.61 | 7 (38%) | 21,30,33 | 1.99 | 6 (28%) |
| 1 | OMC | BA | 1006 | 1 | 19,22,23 | 2.93 | 8 (42%) | 25,31,34 | 0.75 | 0 |
| 2 | A2M | AA | 56 | 2,89 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.05 | 11 (36%) |
| 2 | PSU | AA | 2146 | 2 | 18,21,22 | 4.55 | 7 (38%) | 21,30,33 | 1.84 | 4 (19%) |
| 2 | OMU | AA | 2054 | 2 | 19,22,23 | 3.02 | 8 (42%) | 25,31,34 | 1.84 | 4 (16%) |
| 2 | A2M | AA | 2153 | 2 | 22,25,26 | 3.25 | 10 (45%) | 30,36,39 | 3.21 | 12 (40%) |
| 1 | OMU | BA | 1742 | 1 | 19,22,23 | 3.01 | 8 (42%) | 25,31,34 | 1.82 | 4 (16%) |
| 3 | PSU | BB | 680 | 87,3 | 18,21,22 | 4.56 | 7 (38%) | 21,30,33 | 1.97 | 5 (23%) |
| 3 | OMU | BB | 1093 | 3 | 19,22,23 | 3.05 | 8 (42%) | 25,31,34 | 1.84 | 5 (20%) |
| 2 | A2M | AA | 721 | 2,87 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.14 | 11 (36%) |
| 3 | PSU | BB | 629 | 3 | 18,21,22 | 4.56 | 7 (38%) | 21,30,33 | 1.93 | 5 (23%) |
| 1 | PSU | BA | 1086 | 1,88,87 | 18,21,22 | 4.55 | 7 (38%) | 21,30,33 | 1.98 | 5 (23%) |
| 1 | OMG | BA | 925 | 1 | 23,26,27 | 2.39 | 9 (39%) | 32,38,41 | 2.54 | 11 (34%) |
| 2 | OMC | AA | 46 | 2 | 19,22,23 | 2.87 | 8 (42%) | 25,31,34 | 0.77 | 0 |
| 2 | OMU | AA | 2123 | 2 | 19,22,23 | 2.91 | 7 (36%) | 25,31,34 | 1.93 | 4 (16%) |
| 3 | PSU | BB | 1076 | 3 | 18,21,22 | 4.57 | 7 (38%) | 21,30,33 | 2.10 | 5 (23%) |
| 3 | OMG | BB | 1247 | 3 | 23,26,27 | 2.42 | 9 (39%) | 32,38,41 | 2.58 | 10 (31%) |
| 2 | PSU | AA | 942 | 2 | 18,21,22 | 4.58 | 7 (38%) | 21,30,33 | 1.81 | 5 (23%) |
| 3 | PSU | BB | 615 | 3 | 18,21,22 | 4.58 | 7 (38%) | 21,30,33 | 1.97 | 5 (23%) |
| 3 | A2M | BB | 1201 | 3 | 22,25,26 | 3.22 | 9 (40%) | 30,36,39 | 3.10 | 12 (40%) |
| 3 | OMG | BB | 1094 | 3 | 23,26,27 | 2.39 | 9 (39%) | 32,38,41 | 2.46 | 13 (40%) |
| 1 | OMG | BA | 1621 | 1,3 | 23,26,27 | 2.37 | 9 (39%) | 32,38,41 | 2.53 | 11 (34%) |
| 2 | PSU | AA | 1619 | 2 | 18,21,22 | 4.55 | 8 (44%) | 21,30,33 | 1.76 | 4 (19%) |
| 1 | PSU | BA | 258 | 1 | 18,21,22 | 4.66 | 7 (38%) | 21,30,33 | 1.92 | 5 (23%) |
| 3 | PSU | BB | 1334 | 3 | 18,21,22 | 4.55 | 7 (38%) | 21,30,33 | 1.94 | 6 (28%) |
| 2 | MA6 | AA | 2260 | 2 | 23,26,27 | 1.52 | 4 (17%) | 33,38,41 | 2.96 | 11 (33%) |
| 2 | B8N | AA | 1596 | 2 | 25,29,30 | 3.35 | 8 (32%) | 28,42,45 | 1.98 | 7 (25%) |
| 1 | A2M | BA | 927 | 1 | 22,25,26 | 3.22 | 9 (40%) | 30,36,39 | 3.09 | 14 (46%) |
| 2 | OMU | AA | 36 | 2 | 19,22,23 | 3.00 | 8 (42%) | 25,31,34 | 1.97 | 5 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | OMG | AA | 2227 | 2 | 23,26,27 | 2.40 | 9 (39%) | 32,38,41 | 2.60 | 10 (31%) |
| 3 | OMU | BB | 685 | 3 | 19,22,23 | 3.02 | 8 (42%) | 25,31,34 | 1.84 | 5 (20%) |
| 3 | PSU | BB | 1210 | 3 | 18,21,22 | 4.62 | 7 (38%) | 21,30,33 | 1.92 | 5 (23%) |
| 3 | OMC | BB | 377 | 3 | 19,22,23 | 2.99 | 8 (42%) | 25,31,34 | 0.72 | 0 |
| 2 | OMU | AA | 1899 | 2 | 19,22,23 | 3.05 | 8 (42%) | 25,31,34 | 1.88 | 5 (20%) |
| 2 | MA6 | AA | 2261 | 2 | 23,26,27 | 1.57 | 5 (21%) | 33,38,41 | 2.90 | 13 (39%) |
| 3 | OMG | BB | 552 | 3 | 23,26,27 | 2.37 | 9 (39%) | 32,38,41 | 2.52 | 10 (31%) |
| 2 | PSU | AA | 61 | 2 | 18,21,22 | 4.63 | 7 (38%) | 21,30,33 | 2.01 | 5 (23%) |
| 2 | OMG | AA | 1931 | 2,89 | 23,26,27 | 2.40 | 9 (39%) | 32,38,41 | 2.50 | 11 (34%) |
| 3 | PSU | BB | 1398 | 87,3 | 18,21,22 | 4.57 | 8 (44%) | 21,30,33 | 2.01 | 6 (28%) |
| 1 | OMG | BA | 1028 | 1 | 23,26,27 | 2.41 | 9 (39%) | 32,38,41 | 2.67 | 10 (31%) |
| 1 | A2M | BA | 1665 | 1,3 | 22,25,26 | 3.22 | 9 (40%) | 30,36,39 | 3.05 | 11 (36%) |
| 3 | PSU | BB | 611 | 3 | 18,21,22 | 4.53 | 8 (44%) | 21,30,33 | 1.78 | 4 (19%) |
| 1 | OMC | BA | 760 | 1 | 19,22,23 | 2.93 | 8 (42%) | 25,31,34 | 0.72 | 0 |
| 1 | OMU | BA | 916 | 1 | 19,22,23 | 3.01 | 8 (42%) | 25,31,34 | 1.88 | 5 (20%) |
| 1 | OMU | BA | 46 | 1 | 19,22,23 | 3.00 | 8 (42%) | 25,31,34 | 1.89 | 5 (20%) |
| 2 | OMG | AA | 1517 | 2 | 23,26,27 | 2.43 | 9 (39%) | 32,38,41 | 2.65 | 10 (31%) |
| 3 | A2M | BB | 622 | 1,3 | 22,25,26 | 3.21 | 9 (40%) | 30,36,39 | 3.05 | 11 (36%) |
| 1 | A2M | BA | 1620 | 1,3,87 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.04 | 11 (36%) |
| 2 | OMU | AA | 57 | 2 | 19,22,23 | 3.00 | 8 (42%) | 25,31,34 | 1.83 | 5 (20%) |
| 2 | 7MG | AA | 2070 | 2 | 23,26,27 | 3.82 | 10 (43%) | 27,39,42 | 2.19 | 9 (33%) |
| 2 | A2M | AA | 2096 | 2 | 22,25,26 | 3.23 | 9 (40%) | 30,36,39 | 3.12 | 12 (40%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | PSU | AA | 131 | 2 | - | 2/7/25/26 | 0/2/2/2 |
| 3 | PSU | BB | 455 | 87,88,3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMG | BB | 659 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | OMC | BB | 1264 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | OMU | BB | 1435 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | A2M | BB | 545 | 87,3 | - | 2/9/27/28 | 0/3/3/3 |
| 3 | PSU | BB | 1160 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 9 | A2M | BC | 163 | 1,9 | - | 1/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | OMC | BA | 1329 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 1 | OMU | BA | 1181 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMG | BB | 673 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 9 | PSU | BC | 74 | 9 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | BA | 1248 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | AA | 2134 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | A2M | BB | 588 | 1,3 | - | 4/9/27/28 | 0/3/3/3 |
| 3 | A2M | BB | 400 | 3 | - | 2/9/27/28 | 0/3/3/3 |
| 1 | A2M | BA | 762 | 1 | - | 1/9/27/28 | 0/3/3/3 |
| 2 | PSU | AA | 1276 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | BB | 1429 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | A2M | BA | 743 | 1,3 | - | 1/9/27/28 | 0/3/3/3 |
| 3 | OMG | BB | 1062 | 3 | - | 3/9/27/28 | 0/3/3/3 |
| 3 | OMC | BB | 1175 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | A2M | BB | 646 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | OMG | BB | 1245 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | 5MC | BB | 1324 | 3 | - | 4/7/25/26 | 0/2/2/2 |
| 1 | PSU | BA | 737 | 1,87 | - | 0/7/25/26 | 0/2/2/2 |
| 9 | A2M | BC | 43 | 9 | - | 1/9/27/28 | 0/3/3/3 |
| 2 | OMC | AA | 66 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | AA | 1895 | 2,87 | - | 1/9/27/28 | 0/3/3/3 |
| 1 | PSU | BA | 1129 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | BA | 1009 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | AA | 1700 | 2 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | A2M | BB | 609 | 3 | - | 1/9/27/28 | 0/3/3/3 |
| 3 | A2M | BB | 1400 | 87,3 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | PSU | BB | 1409 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 1MA | BA | 742 | 1,87 | - | 1/7/25/26 | 0/3/3/3 |
| 3 | OMU | BB | 1375 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | A2M | BB | 95 | 3 | - | 1/9/27/28 | 0/3/3/3 |
| 1 | OMU | BA | 1448 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 3 | PSU | BB | 1280 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | AA | 1531 | 2 | - | 1/9/27/28 | 0/3/3/3 |
| 2 | PSU | AA | 2045 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | BA | 915 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | A2M | BA | 1024 | 1 | - | 1/9/27/28 | 0/3/3/3 |
| 3 | OMU | BB | 578 | 89,3 | - | 5/9/27/28 | 0/2/2/2 |
| 3 | OMG | BB | 1269 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | OMG | BA | 1267 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | BA | 1614 | 1,3 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | OMU | AA | 714 | 2 | - | 0/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | A2M | BA | 996 | 1,89 | - | 1/9/27/28 | 0/3/3/3 |
| 2 | OMU | AA | 2154 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | OMC | BB | 1413 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMU | BB | 73 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | OMC | BB | 601 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | BA | 1258 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 3 | PSU | BB | 644 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | AA | 1652 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | A2M | BB | 1388 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | OMG | BB | 71 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | PSU | AA | 1592 | 2 | - | 2/7/25/26 | 0/2/2/2 |
| 9 | A2M | BC | 41 | 9 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | BA | 1169 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | BA | 452 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 9 | OMG | BC | 75 | 9 | - | 1/9/27/28 | 0/3/3/3 |
| 1 | A2M | BA | 254 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 9 | OMU | BC | 7 | 1,9 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | BB | 1319 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | BA | 1709 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | PSU | BB | 522 | 3 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | A2M | BA | 746 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | 5MC | BB | 542 | 87,3 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | OMG | BA | 1605 | 1 | - | 2/9/27/28 | 0/3/3/3 |
| 1 | OMC | BA | 1608 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | OMG | AA | 1676 | 2,88 | - | 1/9/27/28 | 0/3/3/3 |
| 1 | PSU | BA | 1609 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | BA | 1006 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | A2M | AA | 56 | 2,89 | - | 1/9/27/28 | 0/3/3/3 |
| 2 | PSU | AA | 2146 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | AA | 2054 | 2 | - | 2/9/27/28 | 0/2/2/2 |
| 2 | A2M | AA | 2153 | 2 | - | 1/9/27/28 | 0/3/3/3 |
| 1 | OMU | BA | 1742 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | BB | 680 | 87,3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMU | BB | 1093 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | A2M | AA | 721 | 2,87 | - | 6/9/27/28 | 0/3/3/3 |
| 3 | PSU | BB | 629 | 3 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | BA | 1086 | 1,88,87 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | BA | 925 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | OMC | AA | 46 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMU | AA | 2123 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 3 | PSU | BB | 1076 | 3 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | OMG | BB | 1247 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | PSU | AA | 942 | 2 | - | 3/7/25/26 | 0/2/2/2 |
| 3 | PSU | BB | 615 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | A2M | BB | 1201 | 3 | - | 3/9/27/28 | 0/3/3/3 |
| 3 | OMG | BB | 1094 | 3 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | OMG | BA | 1621 | 1,3 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | PSU | AA | 1619 | 2 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | BA | 258 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | PSU | BB | 1334 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | MA6 | AA | 2260 | 2 | - | 2/11/29/30 | 0/3/3/3 |
| 2 | B8N | AA | 1596 | 2 | - | 5/16/34/35 | 0/2/2/2 |
| 1 | A2M | BA | 927 | 1 | - | 1/9/27/28 | 0/3/3/3 |
| 2 | OMU | AA | 36 | 2 | - | 6/9/27/28 | 0/2/2/2 |
| 2 | OMG | AA | 2227 | 2 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | OMU | BB | 685 | 3 | - | 1/9/27/28 | 0/2/2/2 |
| 3 | PSU | BB | 1210 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | OMC | BB | 377 | 3 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMU | AA | 1899 | 2 | - | 3/9/27/28 | 0/2/2/2 |
| 2 | MA6 | AA | 2261 | 2 | - | 1/11/29/30 | 0/3/3/3 |
| 3 | OMG | BB | 552 | 3 | - | 2/9/27/28 | 0/3/3/3 |
| 2 | PSU | AA | 61 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | AA | 1931 | 2,89 | - | 0/9/27/28 | 0/3/3/3 |
| 3 | PSU | BB | 1398 | 87,3 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | OMG | BA | 1028 | 1 | - | 2/9/27/28 | 0/3/3/3 |
| 1 | A2M | BA | 1665 | 1,3 | - | 3/9/27/28 | 0/3/3/3 |
| 3 | PSU | BB | 611 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | BA | 760 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 1 | OMU | BA | 916 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMU | BA | 46 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | AA | 1517 | 2 | - | 1/9/27/28 | 0/3/3/3 |
| 3 | A2M | BB | 622 | 1,3 | - | 1/9/27/28 | 0/3/3/3 |
| 1 | A2M | BA | 1620 | 1,3,87 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | OMU | AA | 57 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | 7MG | AA | 2070 | 2 | - | 1/7/37/38 | 0/3/3/3 |
| 2 | A2M | AA | 2096 | 2 | - | 2/9/27/28 | 0/3/3/3 |

The worst 5 of 1018 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | BA | 258 | PSU | C6-C5 | 12.28 | 1.48 | 1.35 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | BB | 1409 | PSU | C6-C5 | 12.23 | 1.48 | 1.35 |
| 1 | BA | 452 | PSU | C6-C5 | 12.22 | 1.48 | 1.35 |
| 9 | BC | 74 | PSU | C6-C5 | 12.18 | 1.48 | 1.35 |
| 3 | BB | 1160 | PSU | C6-C5 | 12.18 | 1.48 | 1.35 |

The worst 5 of 886 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | AA | 2260 | MA6 | N1-C6-N6 | -10.72 | 103.80 | 116.86 |
| 2 | AA | 2261 | MA6 | N1-C6-N6 | -9.85 | 104.85 | 116.86 |
| 1 | BA | 1028 | OMG | C1'-N9-C8 | -8.25 | 103.30 | 126.73 |
| 2 | AA | 1676 | OMG | C1'-N9-C8 | -8.03 | 103.92 | 126.73 |
| 2 | AA | 1517 | OMG | C1'-N9-C8 | -7.91 | 104.25 | 126.73 |

There are no chirality outliers.

5 of 110 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 9 | BC | 7 | OMU | C1'-C2'-O2'-CM2 |
| 9 | BC | 43 | A2M | C1'-C2'-O2'-CM' |
| 9 | BC | 163 | A2M | C1'-C2'-O2'-CM' |
| 1 | BA | 743 | A2M | C1'-C2'-O2'-CM' |
| 1 | BA | 760 | OMC | C1'-C2'-O2'-CM2 |

There are no ring outliers.

38 monomers are involved in 50 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | BB | 1264 | OMC | 1 | 0 |
| 9 | BC | 163 | A2M | 2 | 0 |
| 1 | BA | 1181 | OMU | 1 | 0 |
| 3 | BB | 588 | A2M | 1 | 0 |
| 3 | BB | 400 | A2M | 2 | 0 |
| 1 | BA | 762 | A2M | 3 | 0 |
| 3 | BB | 1429 | PSU | 1 | 0 |
| 1 | BA | 743 | A2M | 2 | 0 |
| 3 | BB | 1062 | OMG | 1 | 0 |
| 3 | BB | 1175 | OMC | 1 | 0 |
| 9 | BC | 43 | A2M | 1 | 0 |
| 3 | BB | 609 | A2M | 3 | 0 |
| 3 | BB | 95 | A2M | 1 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | AA | 1531 | OMG | 1 | 0 |
| 2 | AA | 2045 | PSU | 2 | 0 |
| 1 | BA | 915 | OMG | 1 | 0 |
| 1 | BA | 1024 | A2M | 2 | 0 |
| 3 | BB | 578 | OMU | 1 | 0 |
| 1 | BA | 996 | A2M | 1 | 0 |
| 2 | AA | 2154 | OMU | 1 | 0 |
| 3 | BB | 644 | PSU | 1 | 0 |
| 2 | AA | 1652 | OMU | 1 | 0 |
| 9 | BC | 41 | A2M | 1 | 0 |
| 1 | BA | 254 | A2M | 1 | 0 |
| 9 | BC | 7 | OMU | 2 | 0 |
| 1 | BA | 746 | A2M | 1 | 0 |
| 2 | AA | 1676 | OMG | 1 | 0 |
| 2 | AA | 2153 | A2M | 1 | 0 |
| 1 | BA | 1742 | OMU | 1 | 0 |
| 2 | AA | 46 | OMC | 1 | 0 |
| 2 | AA | 2260 | MA6 | 2 | 0 |
| 2 | AA | 2227 | OMG | 1 | 0 |
| 3 | BB | 685 | OMU | 1 | 0 |
| 1 | BA | 1665 | A2M | 1 | 0 |
| 1 | BA | 760 | OMC | 2 | 0 |
| 1 | BA | 916 | OMU | 1 | 0 |
| 3 | BB | 622 | A2M | 2 | 0 |
| 2 | AA | 57 | OMU | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 325 ligands modelled in this entry, 325 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 10 | AB | 1 |
| 2 | AA | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | AB | 7:A | O3' | 65:G | P | 16.03 |
| 1 | AA | 1596:B8N | O3' | 1597:C | P | 4.10 |

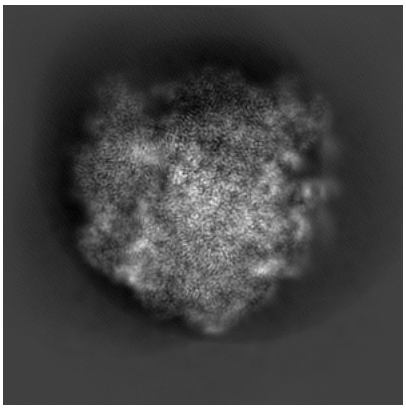
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17208. These allow visual inspection of the internal detail of the map and identification of artifacts.

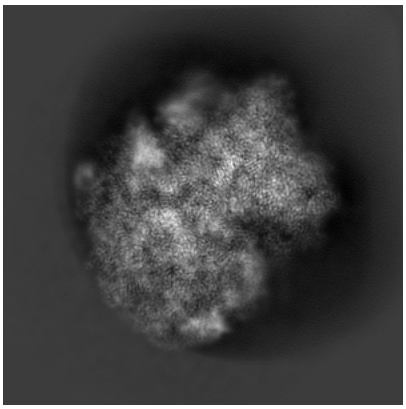
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

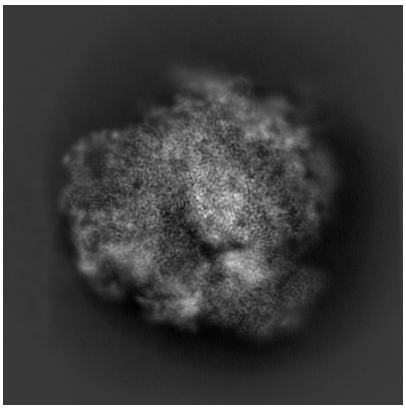
### 6.1.1 Primary map



X

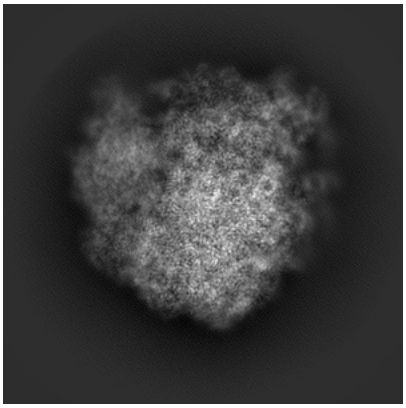


Y

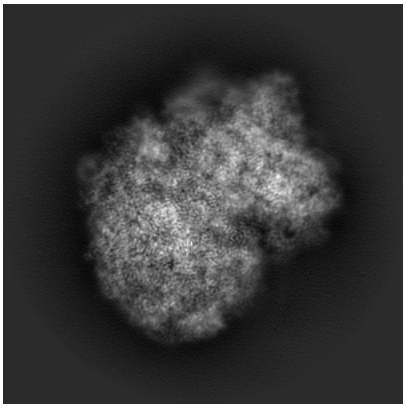


Z

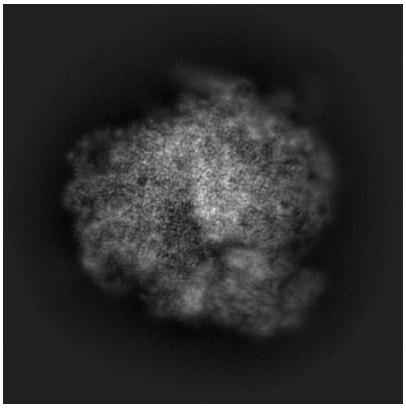
### 6.1.2 Raw map



X



Y

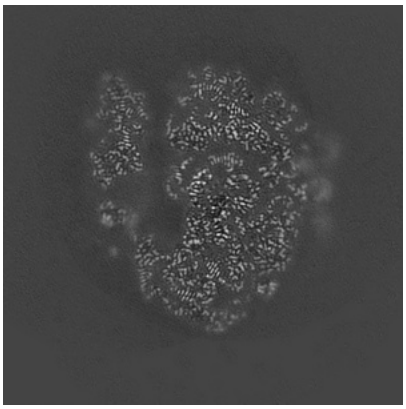


Z

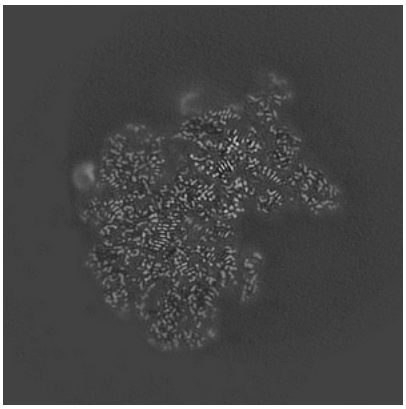
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

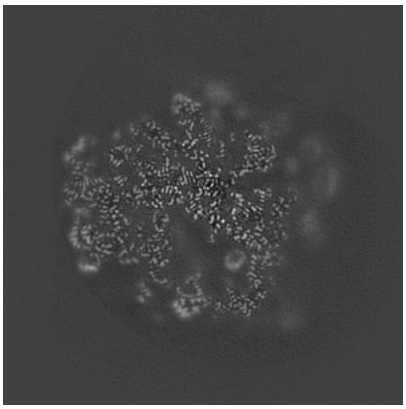
### 6.2.1 Primary map



X Index: 240

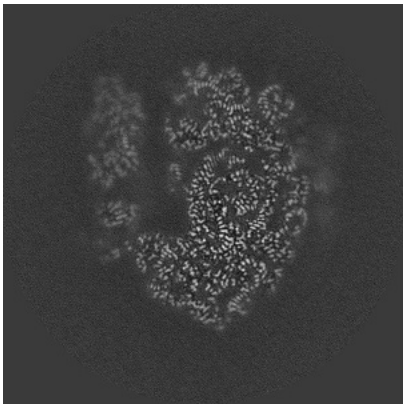


Y Index: 240

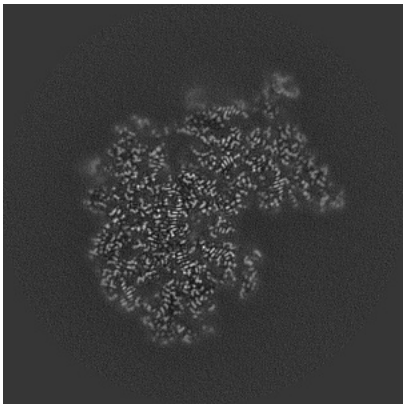


Z Index: 240

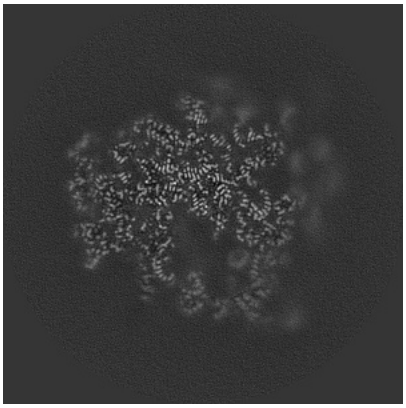
### 6.2.2 Raw map



X Index: 240



Y Index: 240

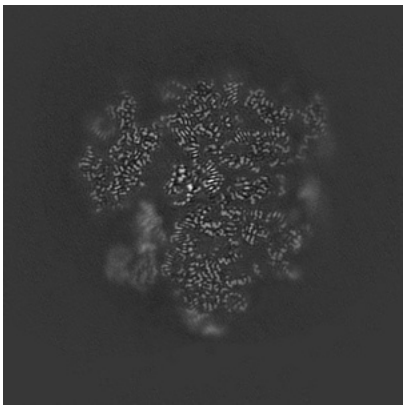


Z Index: 240

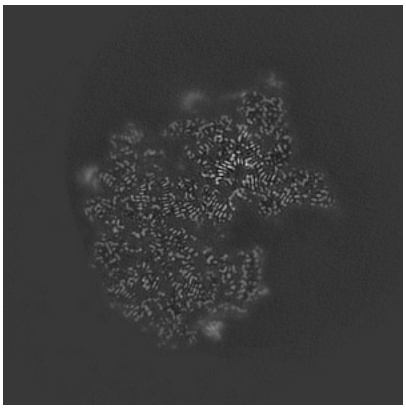
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

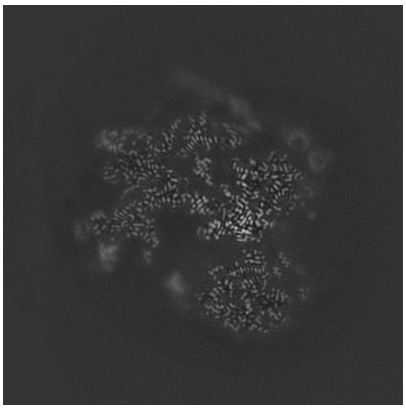
### 6.3.1 Primary map



X Index: 269

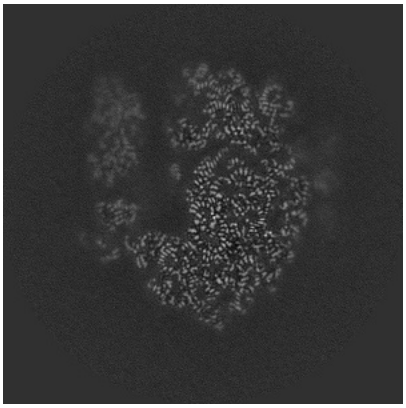


Y Index: 230

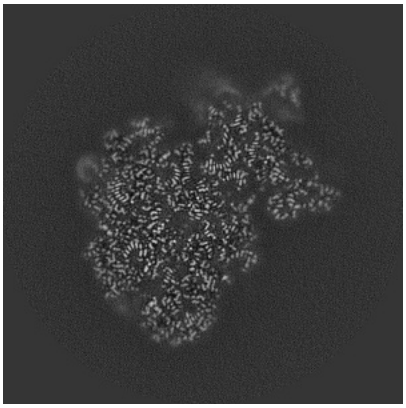


Z Index: 274

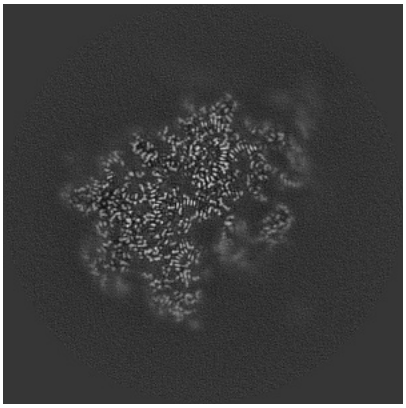
### 6.3.2 Raw map



X Index: 238



Y Index: 252

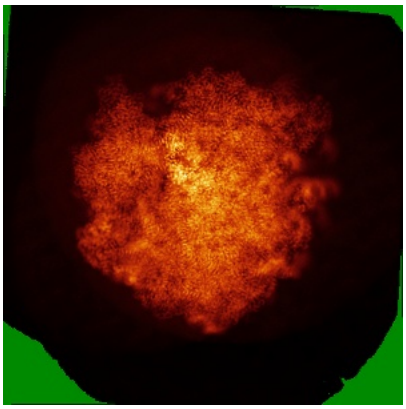


Z Index: 206

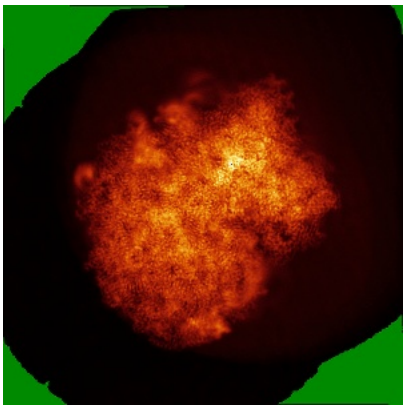
The images above show the largest variance slices of the map in three orthogonal directions.

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

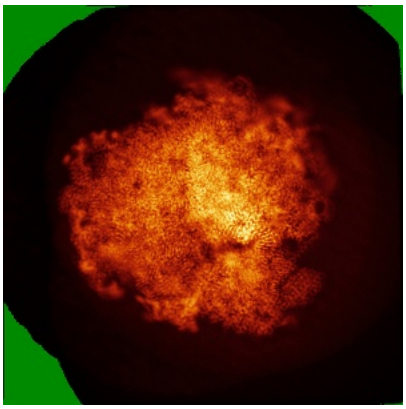
### 6.4.1 Primary map



X

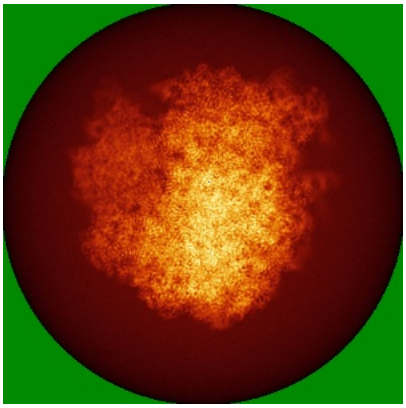


Y

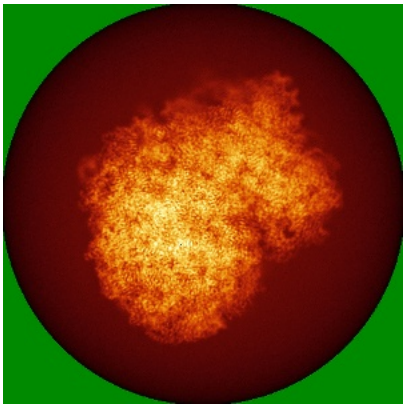


Z

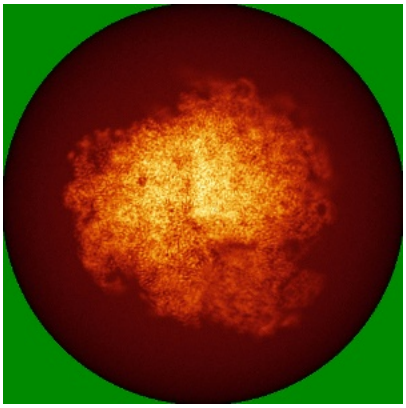
### 6.4.2 Raw map



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.

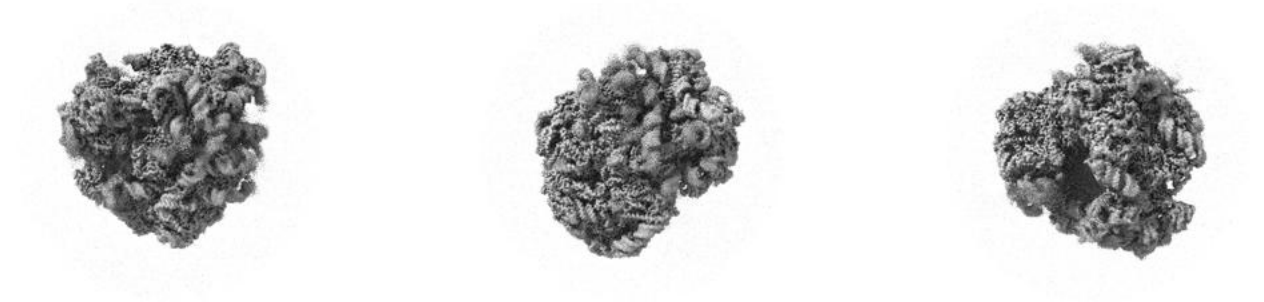
## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

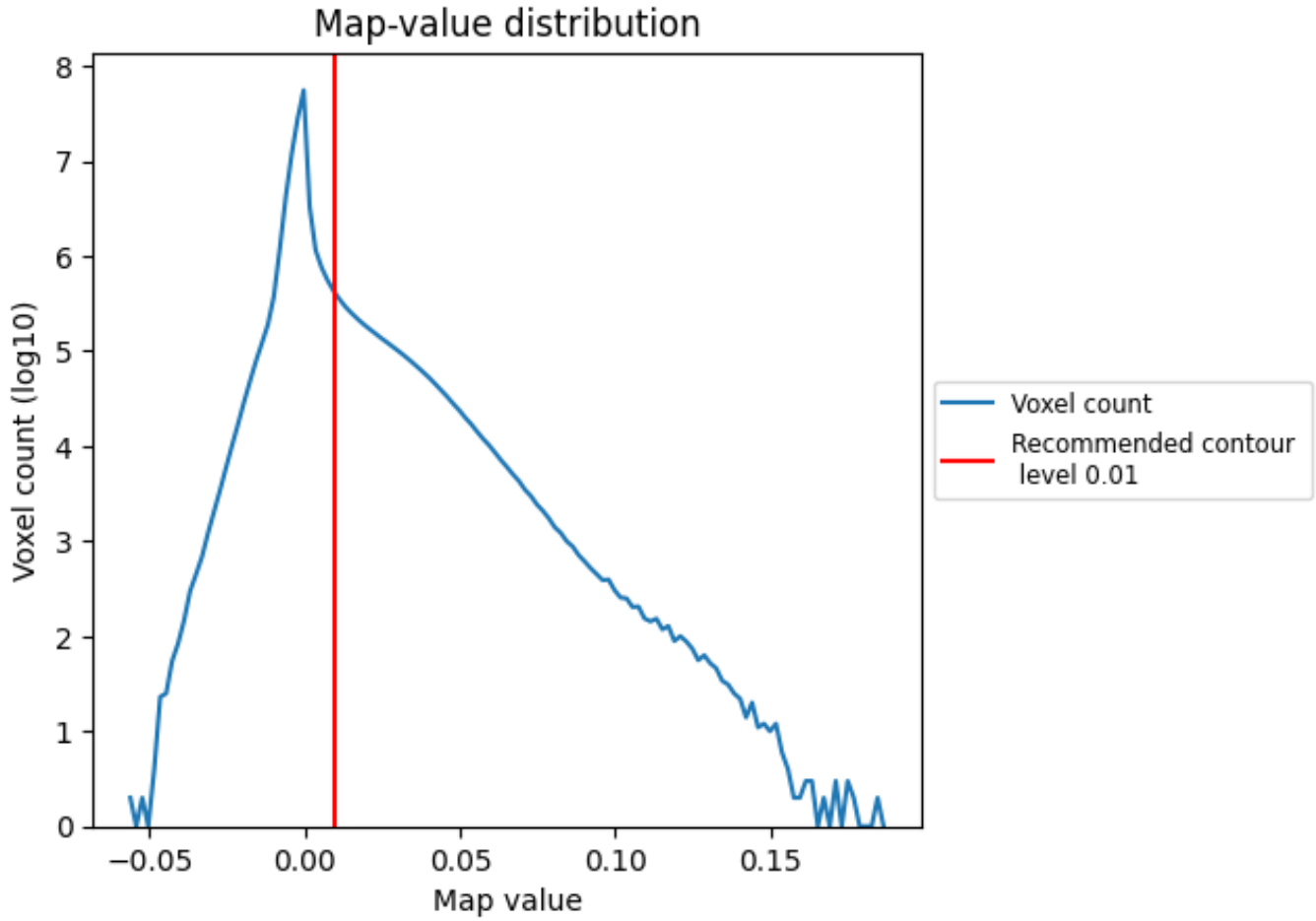
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

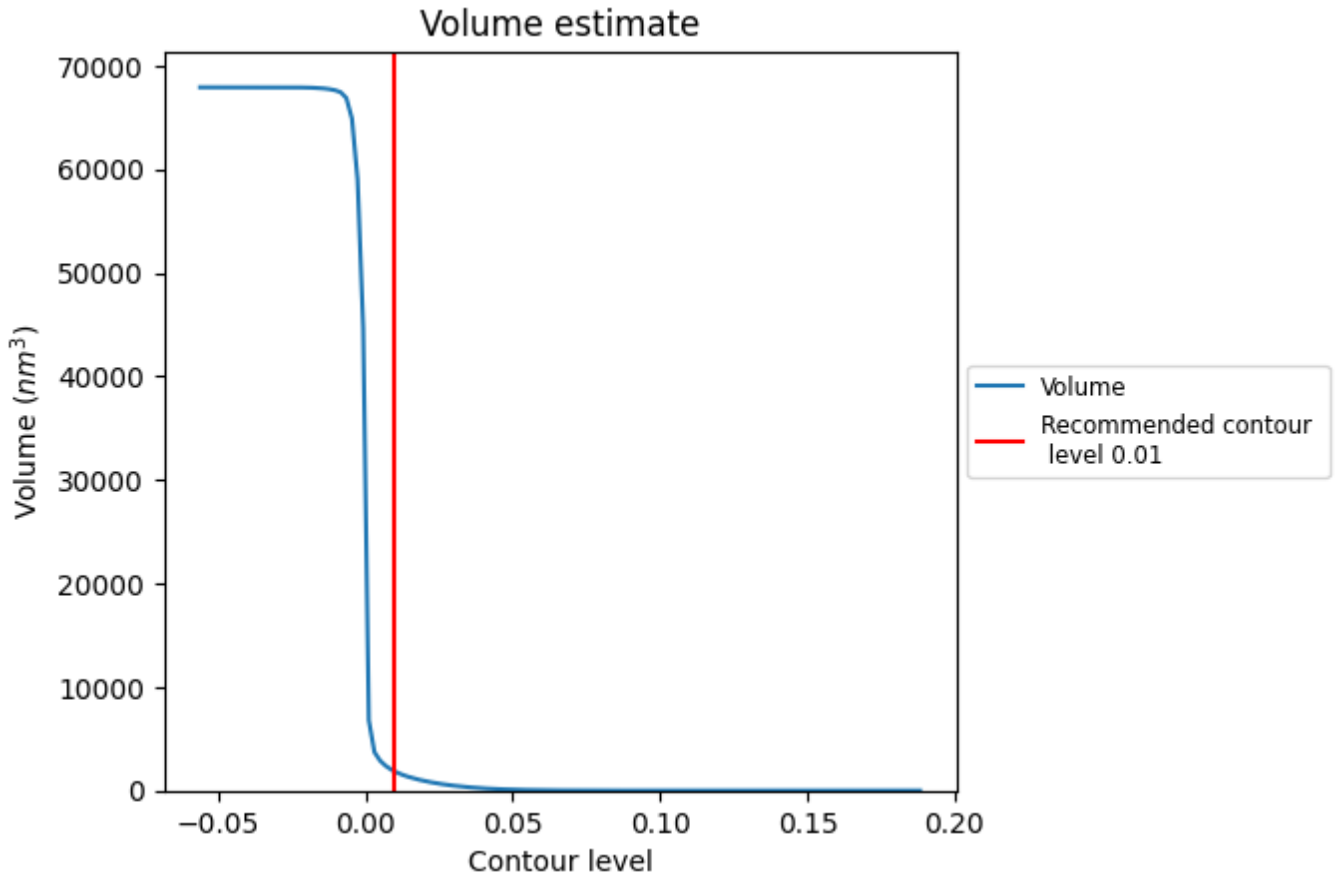
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

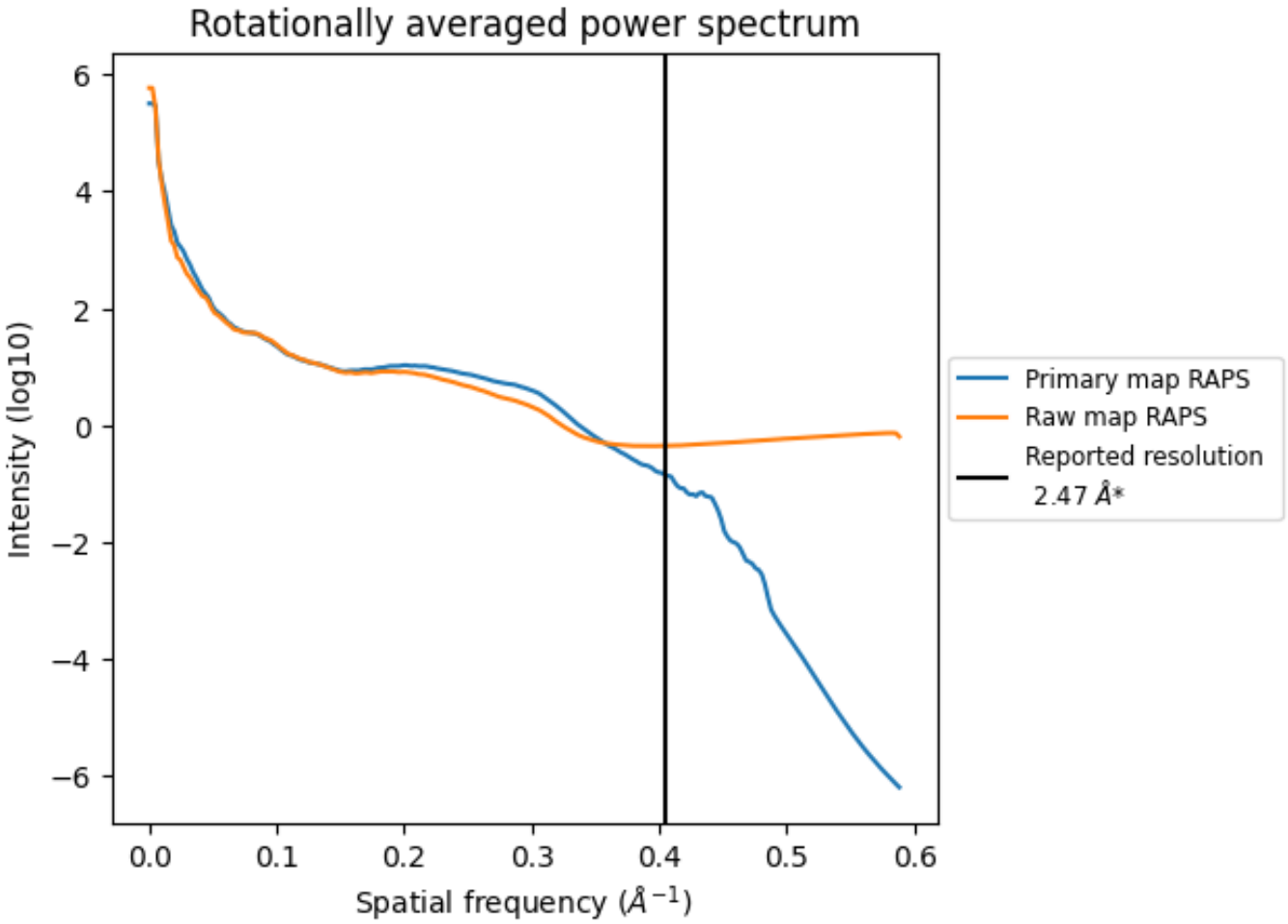
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1853 $nm^3$; this corresponds to an approximate mass of 1674 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)

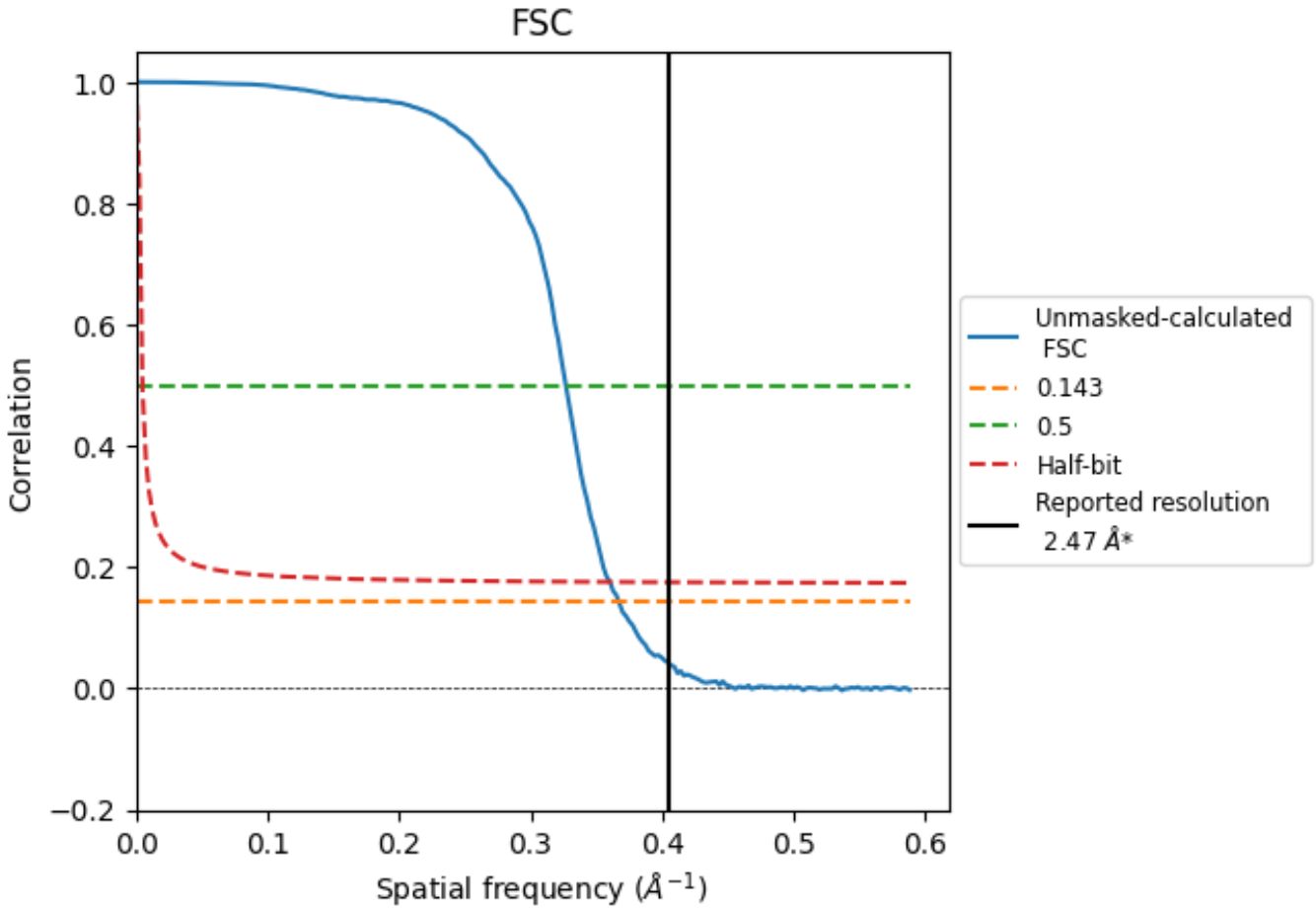



*Reported resolution corresponds to spatial frequency of 0.405 Å$^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.405 Å$^{-1}$

## 8.2 Resolution estimates (i)

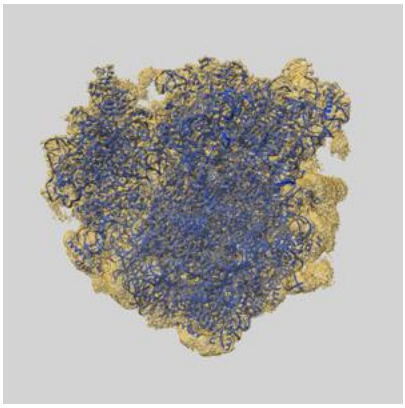
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.47 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 2.72 | 3.06 | 2.77 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.72 differs from the reported value 2.47 by more than 10 %

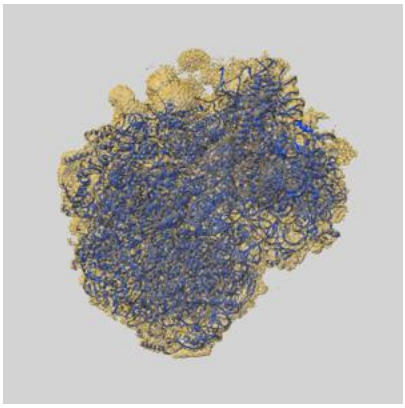
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17208 and PDB model 8OVA. Per-residue inclusion information can be found in section 3 on page 23.

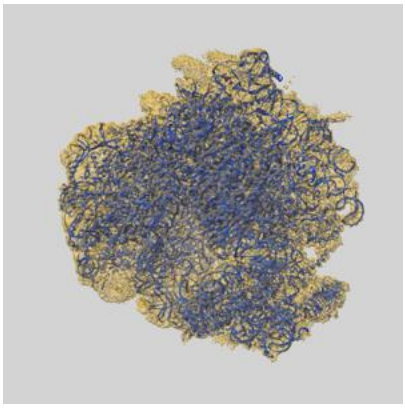
## 9.1 Map-model overlay



X



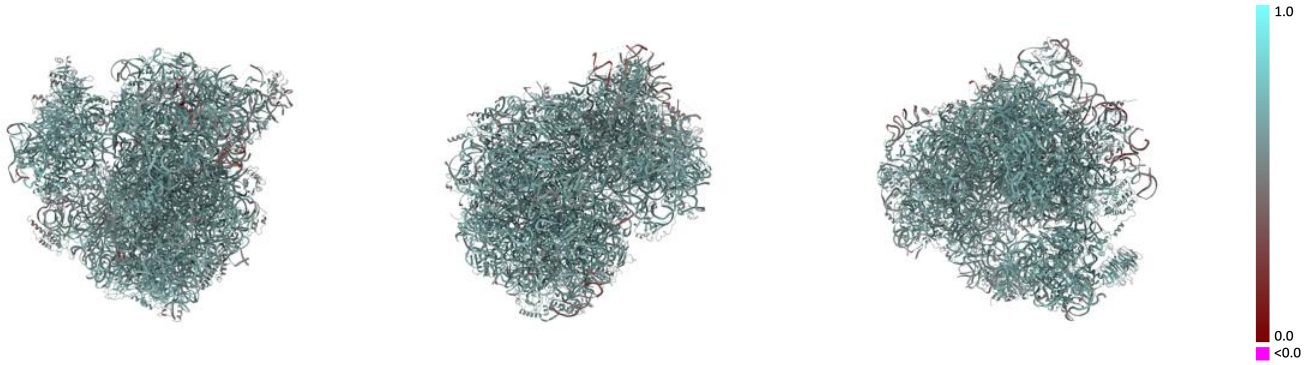
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

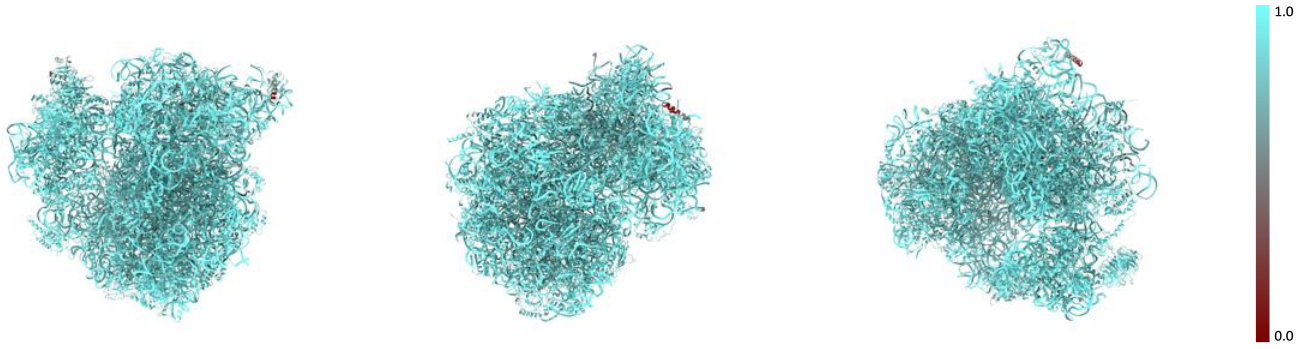
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

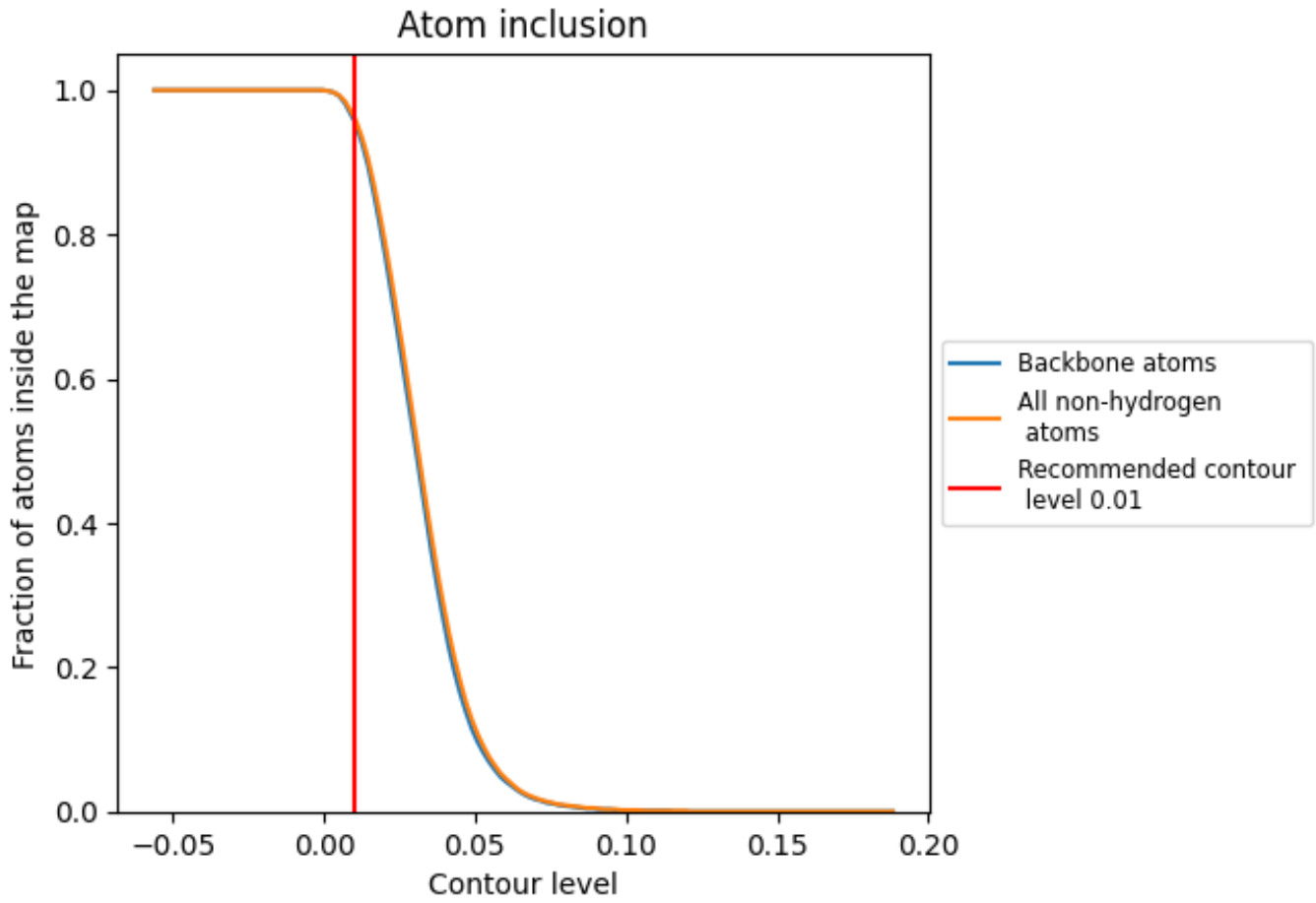
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

## 9.4 Atom inclusion (i)




At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9630 | 0.6300 |
| A0 | 0.9530 | 0.6360 |
| A1 | 0.9380 | 0.6390 |
| A2 | 0.9490 | 0.6370 |
| A3 | 0.8860 | 0.5930 |
| A4 | 0.9350 | 0.6190 |
| A5 | 0.9400 | 0.6270 |
| A6 | 0.9510 | 0.6410 |
| A7 | 0.9040 | 0.6060 |
| A8 | 0.9780 | 0.6660 |
| A9 | 0.8290 | 0.5920 |
| AA | 0.9700 | 0.6190 |
| AB | 0.9850 | 0.5040 |
| AC | 0.9780 | 0.6320 |
| AD | 0.9370 | 0.6330 |
| AE | 0.9410 | 0.6400 |
| AF | 0.7780 | 0.5560 |
| AG | 0.9420 | 0.6350 |
| AH | 0.9500 | 0.6270 |
| AI | 0.9170 | 0.6370 |
| AJ | 0.9720 | 0.6620 |
| AK | 0.9760 | 0.6510 |
| AL | 0.9550 | 0.6070 |
| AM | 0.9380 | 0.6370 |
| AO | 0.9760 | 0.6570 |
| AP | 0.9500 | 0.6400 |
| AQ | 0.9130 | 0.6050 |
| AR | 0.9620 | 0.6350 |
| AS | 0.9550 | 0.6450 |
| AT | 0.9200 | 0.6320 |
| AU | 0.9290 | 0.6250 |
| AV | 0.9670 | 0.6390 |
| AW | 0.9320 | 0.6250 |
| AX | 0.9150 | 0.6210 |
| AY | 0.9260 | 0.6300 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| AZ | 0.9330 | 0.6060 |
| Az | 0.7110 | 0.5290 |
| BA | 0.9880 | 0.6470 |
| BB | 0.9900 | 0.6330 |
| BC | 0.9930 | 0.6420 |
| BD | 0.9990 | 0.5970 |
| BE | 0.9640 | 0.6100 |
| BF | 0.9800 | 0.5970 |
| BG | 0.9920 | 0.6440 |
| BH | 0.9820 | 0.6030 |
| BI | 0.9530 | 0.6640 |
| BK | 0.9420 | 0.6330 |
| BL | 0.9540 | 0.5200 |
| BN | 0.9370 | 0.6370 |
| BO | 0.9390 | 0.6590 |
| BP | 0.9490 | 0.6080 |
| BQ | 0.9850 | 0.6790 |
| BR | 0.9720 | 0.6770 |
| BS | 0.9390 | 0.6500 |
| BT | 0.9270 | 0.6060 |
| BU | 0.9370 | 0.6250 |
| BV | 0.9690 | 0.5600 |
| BW | 0.9470 | 0.6400 |
| BX | 0.9230 | 0.6370 |
| BY | 0.9700 | 0.6290 |
| BZ | 0.9240 | 0.6390 |
| Ba | 0.9650 | 0.5990 |
| Bb | 0.9590 | 0.6620 |
| Bc | 0.9410 | 0.6400 |
| Bd | 0.9620 | 0.6640 |
| Be | 0.9840 | 0.6710 |
| Bf | 0.9540 | 0.6600 |
| Bg | 0.9580 | 0.6290 |
| Bh | 0.9460 | 0.6030 |
| Bi | 0.9370 | 0.6640 |
| Bj | 0.9510 | 0.6420 |
| Bk | 0.9550 | 0.5850 |
| Bl | 0.9610 | 0.6600 |
| Bm | 0.9190 | 0.6290 |
| Bn | 0.9870 | 0.6890 |
| Bo | 0.9690 | 0.6490 |
| Bp | 0.9660 | 0.5790 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| Bq | 0.9450 | 0.6610 |
| Br | 0.9400 | 0.6560 |
| Bs | 0.9870 | 0.6110 |
| Bt | 0.9480 | 0.6500 |
| Bu | 0.9700 | 0.5640 |
| Bv | 0.8800 | 0.6030 |
| Bw | 0.9530 | 0.6580 |
| Bx | 0.9360 | 0.6210 |
| By | 0.9470 | 0.6100 |
| Bz | 0.9730 | 0.6500 |