# wwPDB EM Validation Summary Report (i)

May 5, 2024 – 01:51 AM JST

| | | |
|---|---|---|
| PDB ID | : | 8IP8 |
| EMDB ID | : | EMD-35634 |
| Title | : | Wheat 80S ribosome stalled on AUG-Stop boron dependently |
| Authors | : | Yokoyama, T.; Tanaka, M.; Saito, H.; Nishimoto, M.; Tsuda, K.; Sotta, N.; Shigematsu, H.; Shirouzu, M.; Iwasaki, S.; Ito, T.; Fujiwara, T. |
| Deposited on | : | 2023-03-14 |
| Resolution | : | 2.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

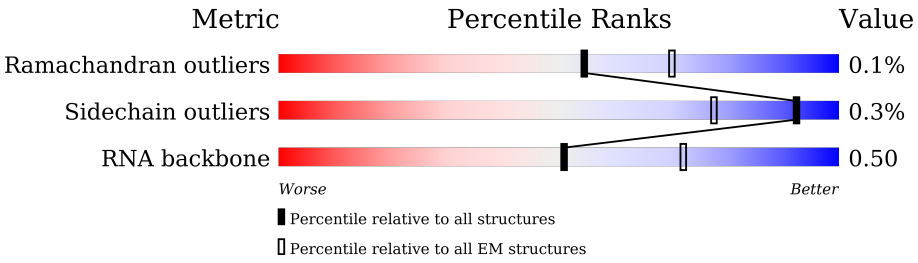
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 2.90 Å.

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




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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | aa | 1810 | 19% 67% 25% · 6% |
| 2 | ba | 137 | 53% 81% · 18% |
| 3 | ca | 225 | 16% 79% 21% |
| 4 | da | 188 | 35% 43% 57% |
| 5 | ga | 142 | 7% 97% · |
| 6 | ha | 332 | 92% 97% · |
| 7 | ia | 227 | 54% 94% 6% |
| 8 | ja | 265 | 33% 98% · |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | ka | 200 | 41% 96% |
| 10 | la | 149 | 43% 93% 6% |
| 11 | ma | 127 | 50% 81% 19% |
| 12 | na | 151 | 21% 81% 17% |
| 13 | oa | 152 | 56% 89% 11% |
| 14 | pa | 151 | 15% 99% |
| 15 | qa | 143 | 58% 83% 17% |
| 16 | ra | 155 | 43% 87% 13% |
| 17 | sa | 154 | 55% 65% 35% |
| 18 | ta | 108 | 64% 69% 29% |
| 19 | ua | 86 | 38% 74% 26% |
| 20 | va | 129 | 14% 96% |
| 21 | wa | 56 | 5% 68% 30% |
| 22 | xa | 86 | 33% 80% 19% |
| 23 | ya | 62 | 24% 63% 37% |
| 24 | za | 308 | 23% 66% 34% |
| 25 | bb | 263 | 36% 79% 20% |
| 26 | cb | 82 | 28% 93% 7% |
| 27 | db | 156 | 9% 61% 39% |
| 28 | eb | 195 | 29% 92% 7% |
| 29 | fb | 274 | 9% 78% 22% |
| 30 | gb | 250 | 44% 60% 40% |
| 31 | hb | 192 | 63% 87% 12% |
| 32 | ib | 159 | 11% 91% 9% |
| 33 | AA | 258 | 33% 88% 11% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | BA | 164 | 10% 95% 5% |
| 35 | CA | 137 | 25% 99% |
| 36 | DA | 261 | 96% |
| 37 | EA | 180 | 29% 91% 9% |
| 38 | FA | 189 | 21% 98% |
| 39 | GA | 140 | 91% 8% |
| 40 | HA | 204 | 100% |
| 41 | IA | 145 | 7% 99% |
| 42 | JA | 187 | 99% |
| 43 | KA | 301 | 22% 91% 9% |
| 44 | LA | 213 | 12% 80% 20% |
| 45 | MA | 170 | 7% 90% 9% |
| 46 | NA | 152 | 12% 76% 24% |
| 47 | OA | 162 | 37% 62% |
| 48 | PA | 157 | 6% 83% 17% |
| 49 | QA | 147 | 18% 96% |
| 50 | RA | 112 | 12% 87% 12% |
| 51 | SA | 123 | 18% 87% 13% |
| 52 | TA | 133 | 95% 5% |
| 53 | UA | 93 | 86% 14% |
| 54 | VA | 76 | 66% 34% |
| 55 | WA | 105 | 5% 93% 7% |
| 56 | XA | 135 | 26% 98% |
| 57 | YA | 178 | 10% 99% |
| 58 | ZA | 130 | 55% 77% 22% |

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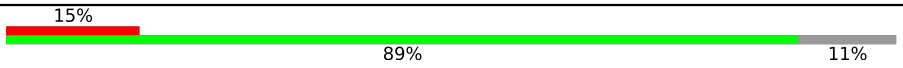
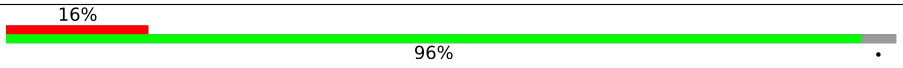
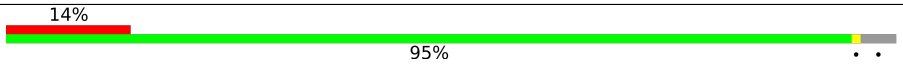
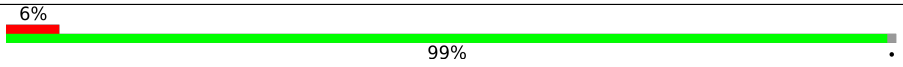
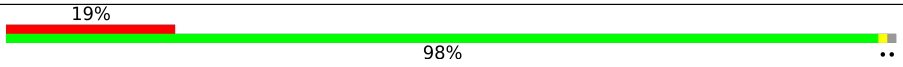
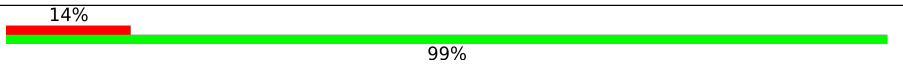
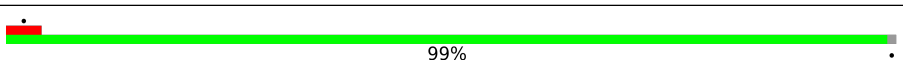
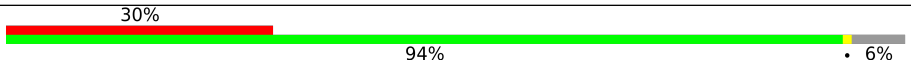
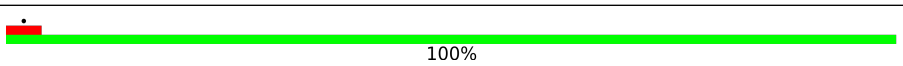
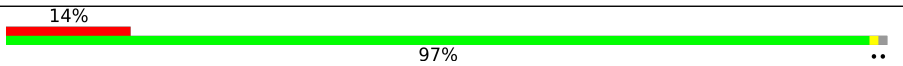
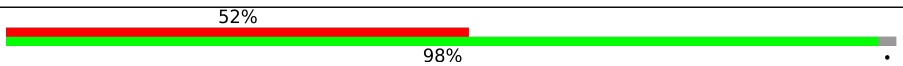
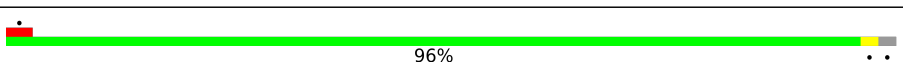
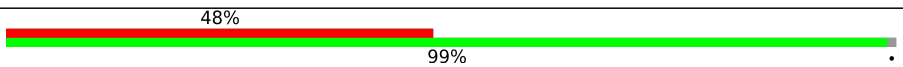
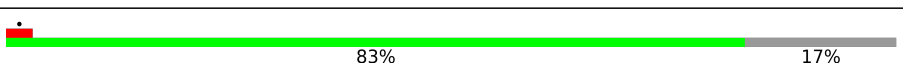
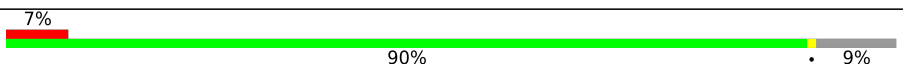
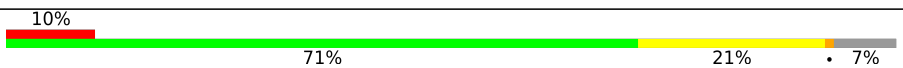
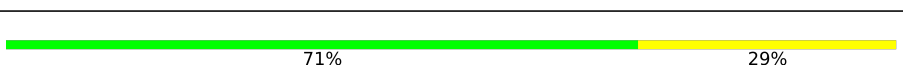
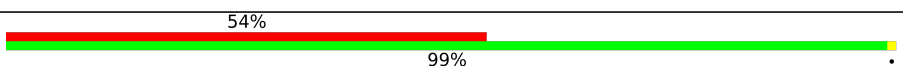
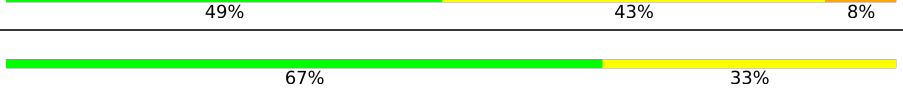
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 59 | AB | 112 |   |
| 60 | BB | 124 |   |
| 61 | CB | 244 |   |
| 62 | DB | 389 |   |
| 63 | EB | 404 |   |
| 64 | FB | 206 |   |
| 65 | GB | 92 |   |
| 66 | HB | 217 |   |
| 67 | IB | 25 |   |
| 68 | JB | 129 |   |
| 69 | KB | 208 |   |
| 70 | LB | 219 |   |
| 71 | MB | 112 |   |
| 72 | NB | 69 |   |
| 73 | OB | 60 |   |
| 74 | PB | 119 |   |
| 75 | RB | 3386 |   |
| 76 | SB | 160 |   |
| 77 | TB | 120 |   |
| 78 | al | 7 |   |
| 79 | bl | 437 |   |
| 80 | cl | 75 |   |
| 81 | dl | 3 |   |

# 2 Entry composition (i)

There are 83 unique types of molecules in this entry. The entry contains 201231 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | aa | 1695 | 36156 | 16155 | 6463 | 11845 | 1693 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| aa | ? | - | G | deletion | GB 2123606567 |
| aa | 1399 | G | C | conflict | GB 2123606567 |
| aa | 1411 | C | G | conflict | GB 2123606567 |
| aa | 1441 | C | G | conflict | GB 2123606567 |
| aa | 1762 | C | G | conflict | GB 2123606567 |

- Molecule 2 is a protein called 40S ribosomal protein eS24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | ba | 113 | 929 | 593 | 178 | 156 | 2 | 0 | 0 |

- Molecule 3 is a protein called 40S ribosomal protein eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | ca | 178 | 1443 | 891 | 291 | 257 | 4 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | da | 81 | 703 | 461 | 117 | 122 | 3 | 0 | 0 |

- Molecule 5 is a protein called 40S ribosomal protein uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | ga | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1070 | 679 | 207 | 181 | 3 | | |

- Molecule 6 is a protein called RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | ha | 322 | Total | C | N | O | S | 0 | 0 |
| | | | 2473 | 1555 | 429 | 478 | 11 | | |

- Molecule 7 is a protein called 40S ribosomal protein uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | ia | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1673 | 1061 | 303 | 300 | 9 | | |

- Molecule 8 is a protein called 40S ribosomal protein eS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | ja | 261 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1325 | 388 | 362 | 7 | | |

- Molecule 9 is a protein called 40S ribosomal protein uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | ka | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1516 | 947 | 285 | 277 | 7 | | |

- Molecule 10 is a protein called 40S ribosomal protein uS9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | la | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1119 | 712 | 215 | 187 | 5 | | |

- Molecule 11 is a protein called 40S ribosomal protein uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | ma | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 806 | 504 | 147 | 151 | 4 | | |

- Molecule 12 is a protein called 40S ribosomal protein uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | na | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 941 | 579 | 185 | 173 | 4 | | |

- Molecule 13 is a protein called 40S ribosomal protein uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | oa | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1114 | 695 | 220 | 193 | 6 | | |

- Molecule 14 is a protein called 40S ribosomal protein uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | pa | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1195 | 765 | 224 | 204 | 2 | | |

- Molecule 15 is a protein called 40S ribosomal protein eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | qa | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 975 | 607 | 185 | 177 | 6 | | |

- Molecule 16 is a protein called 40S ribosomal protein eS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | ra | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1065 | 672 | 200 | 189 | 4 | | |

- Molecule 17 is a protein called 40S ribosomal protein uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | sa | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 807 | 518 | 151 | 133 | 5 | | |

- Molecule 18 is a protein called 40S ribosomal protein eS25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | ta | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 618 | 387 | 116 | 113 | 2 | | |

- Molecule 19 is a protein called 40S ribosomal protein eS28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | ua | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 314 | 104 | 93 | 2 | | |

- Molecule 20 is a protein called 40S ribosomal protein uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | va | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1039 | 653 | 199 | 182 | 5 | | |

- Molecule 21 is a protein called 40S ribosomal protein uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | wa | 39 | Total | C | N | O | S | 0 | 0 |
| | | | 314 | 193 | 65 | 50 | 6 | | |

- Molecule 22 is a protein called 40S ribosomal protein eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | xa | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 546 | 342 | 101 | 96 | 7 | | |

- Molecule 23 is a protein called 40S ribosomal protein eS30.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 23 | ya | 39 | Total | C | N | O | 0 | 0 |
| | | | 322 | 199 | 74 | 49 | | |

- Molecule 24 is a protein called 40S ribosomal protein uS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | za | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1609 | 1018 | 291 | 289 | 11 | | |

- Molecule 25 is a protein called 40S ribosomal protein eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | bb | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1720 | 1096 | 311 | 304 | 9 | | |

- Molecule 26 is a protein called 40S ribosomal protein eS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | cb | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 596 | 368 | 111 | 114 | 3 | | |

- Molecule 27 is a protein called 40S ribosomal protein eS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | db | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 771 | 472 | 168 | 124 | 7 | | |

- Molecule 28 is a protein called 40S ribosomal protein uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | eb | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1493 | 945 | 298 | 246 | 4 | | |

- Molecule 29 is a protein called 40S ribosomal protein uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | fb | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1660 | 1070 | 294 | 287 | 9 | | |

- Molecule 30 is a protein called 40S ribosomal protein eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | gb | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1199 | 749 | 233 | 209 | 8 | | |

- Molecule 31 is a protein called 40S ribosomal protein eS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | hb | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1389 | 889 | 255 | 243 | 2 | | |

- Molecule 32 is a protein called 40S ribosomal protein uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | ib | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1166 | 745 | 223 | 192 | 6 | | |

- Molecule 33 is a protein called 40S ribosomal protein eL8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | AA | 229 | Total | C | N | O | S | 0 | 0 |
| | | | 1847 | 1191 | 341 | 309 | 6 | | |

- Molecule 34 is a protein called 60S ribosomal protein eL21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | BA | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1256 | 795 | 246 | 212 | 3 | | |

- Molecule 35 is a protein called 60S ribosomal protein eL27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | CA | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1090 | 704 | 205 | 177 | 4 | | |

- Molecule 36 is a protein called 60S ribosomal protein uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | DA | 251 | Total | C | N | O | S | 0 | 0 |
| | | | 1919 | 1193 | 395 | 324 | 7 | | |

- Molecule 37 is a protein called 60S ribosomal protein uL5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | EA | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1332 | 841 | 248 | 235 | 8 | | |

- Molecule 38 is a protein called 60S ribosomal protein uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | FA | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1459 | 925 | 265 | 263 | 6 | | |

- Molecule 39 is a protein called 60S ribosomal protein uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | GA | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 976 | 618 | 181 | 168 | 9 | | |

- Molecule 40 is a protein called 60S ribosomal protein eL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | HA | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1720 | 1078 | 370 | 269 | 3 | | |

- Molecule 41 is a protein called 60S ribosomal protein uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | IA | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 720 | 218 | 181 | 4 | | |

- Molecule 42 is a protein called 60S ribosomal protein eL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | JA | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1487 | 938 | 296 | 248 | 5 | | |

- Molecule 43 is a protein called 60S ribosomal protein uL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | KA | 273 | Total | C | N | O | S | 0 | 0 |
| | | | 2209 | 1390 | 406 | 408 | 5 | | |

- Molecule 44 is a protein called 60S ribosomal protein eL19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | LA | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1414 | 880 | 295 | 231 | 8 | | |

- Molecule 45 is a protein called 60S ribosomal protein uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | MA | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1253 | 780 | 247 | 221 | 5 | | |

- Molecule 46 is a protein called 60S ribosomal protein uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | NA | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 935 | 600 | 165 | 168 | 2 | | |

- Molecule 47 is a protein called 60S ribosomal protein eL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | OA | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 517 | 335 | 99 | 79 | 4 | | |

- Molecule 48 is a protein called 60S ribosomal protein uL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | PA | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1054 | 651 | 223 | 177 | 3 | | |

- Molecule 49 is a protein called 60S ribosomal protein eL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | QA | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1125 | 711 | 207 | 203 | 4 | | |

- Molecule 50 is a protein called 60S ribosomal protein eL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | RA | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 757 | 480 | 131 | 140 | 6 | | |

- Molecule 51 is a protein called 60S ribosomal protein eL31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | SA | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 863 | 540 | 167 | 154 | 2 | | |

- Molecule 52 is a protein called 60S ribosomal protein eL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | TA | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1042 | 662 | 207 | 168 | 5 | | |

- Molecule 53 is a protein called 60S ribosomal protein eL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | UA | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 656 | 402 | 144 | 104 | 6 | | |

- Molecule 54 is a protein called 60S ribosomal protein eL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | VA | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 452 | 286 | 99 | 66 | 1 | | |

- Molecule 55 is a protein called 60S ribosomal protein eL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | WA | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 794 | 498 | 157 | 134 | 5 | | |

- Molecule 56 is a protein called 60S ribosomal protein eL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | XA | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1066 | 684 | 196 | 181 | 5 | | |

- Molecule 57 is a protein called 60S ribosomal protein eL20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | YA | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1496 | 963 | 275 | 250 | 8 | | |

- Molecule 58 is a protein called 60S ribosomal protein eL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | ZA | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 520 | 144 | 148 | 2 | | |

- Molecule 59 is a protein called 60S ribosomal protein eL36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | AB | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 803 | 505 | 166 | 130 | 2 | | |

- Molecule 60 is a protein called 60S ribosomal protein uL29.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 60 | BB | 119 | Total | C | N | O | 0 | 0 |
| | | | 979 | 617 | 196 | 166 | | |

- Molecule 61 is a protein called 60S ribosomal protein uL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | CB | 234 | Total | C | N | O | S | 0 | 0 |
| | | | 1917 | 1230 | 357 | 325 | 5 | | |

- Molecule 62 is a protein called 60S ribosomal protein uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | DB | 384 | Total | C | N | O | S | 0 | 0 |
| | | | 3099 | 1972 | 575 | 535 | 17 | | |

- Molecule 63 is a protein called 60S ribosomal protein uL4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | EB | 399 | Total | C | N | O | S | 0 | 0 |
| | | | 3075 | 1934 | 590 | 540 | 11 | | |

- Molecule 64 is a protein called 60S ribosomal protein uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | FB | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1641 | 1040 | 319 | 272 | 10 | | |

- Molecule 65 is a protein called 60S ribosomal protein eL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | GB | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 707 | 442 | 136 | 123 | 6 | | |

- Molecule 66 is a protein called 60S ribosomal protein uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | HB | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1635 | 1034 | 321 | 271 | 9 | | |

- Molecule 67 is a protein called 60S ribosomal protein eL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | IB | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 237 | 145 | 62 | 27 | 3 | | |

- Molecule 68 is a protein called 60S ribosomal protein eL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | JB | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 420 | 262 | 88 | 65 | 5 | | |

- Molecule 69 is a protein called 60S ribosomal protein eL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | KB | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1670 | 1045 | 334 | 285 | 6 | | |

- Molecule 70 is a protein called 60S ribosomal protein eL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | LB | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1703 | 1088 | 310 | 302 | 3 | | |

- Molecule 71 is a protein called 60S ribosomal protein eL33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | MB | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 551 | 168 | 152 | 4 | | |

- Molecule 72 is a protein called 60S ribosomal protein eL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | NB | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 557 | 354 | 105 | 96 | 2 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| NB | 48 | PHE | HIS | conflict | UNP A0A1D5W6Q2 |
| NB | 50 | ALA | THR | conflict | UNP A0A1D5W6Q2 |
| NB | 65 | SER | ASN | conflict | UNP A0A1D5W6Q2 |

- Molecule 73 is a protein called 60S ribosomal protein eL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | OB | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 416 | 254 | 93 | 68 | 1 | | |

- Molecule 74 is a protein called 60S ribosomal protein eL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | PB | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 879 | 555 | 179 | 144 | 1 | | |

- Molecule 75 is a RNA chain called 60S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | RB | 3147 | Total | C | N | O | P | 0 | 0 |
| | | | 67383 | 30051 | 12300 | 21886 | 3146 | | |

- Molecule 76 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | SB | 160 | Total | C | N | O | P | 0 | 0 |
| | | | 3408 | 1522 | 614 | 1113 | 159 | | |

- Molecule 77 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | TB | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2561 | 1144 | 461 | 837 | 119 | | |

- Molecule 78 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | al | 7 | Total | C | N | O | P | 0 | 0 |
| | | | 147 | 68 | 29 | 44 | 6 | | |

- Molecule 79 is a protein called eukaryotic release factor 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 79 | bl | 437 | Total | C | N | O | S | 0 | 0 |
| | | | 3446 | 2168 | 589 | 675 | 14 | | |

- Molecule 80 is a RNA chain called tRNAi.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 80 | cl | 75 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1622 | 730 | 298 | 518 | 75 | 1 | | |

- Molecule 81 is a RNA chain called CCA end of E-tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 81 | dl | 3 | Total | C | N | O | P | 0 | 0 |
| | | | 62 | 28 | 11 | 20 | 3 | | |

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 82 | aa | 83 | Total | Mg | 0 |
| | | | 83 | 83 | |
| 82 | ja | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | ka | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | BA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | DA | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 82 | FA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | GA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | JA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | DB | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | OB | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | PB | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | RB | 209 | Total | Mg | 0 |
| | | | 209 | 209 | |
| 82 | TB | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 82 | cl | 3 | Total | Mg | 0 |
| | | | 3 | 3 | |

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 83 | wa | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 83 | db | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 83 | WA | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

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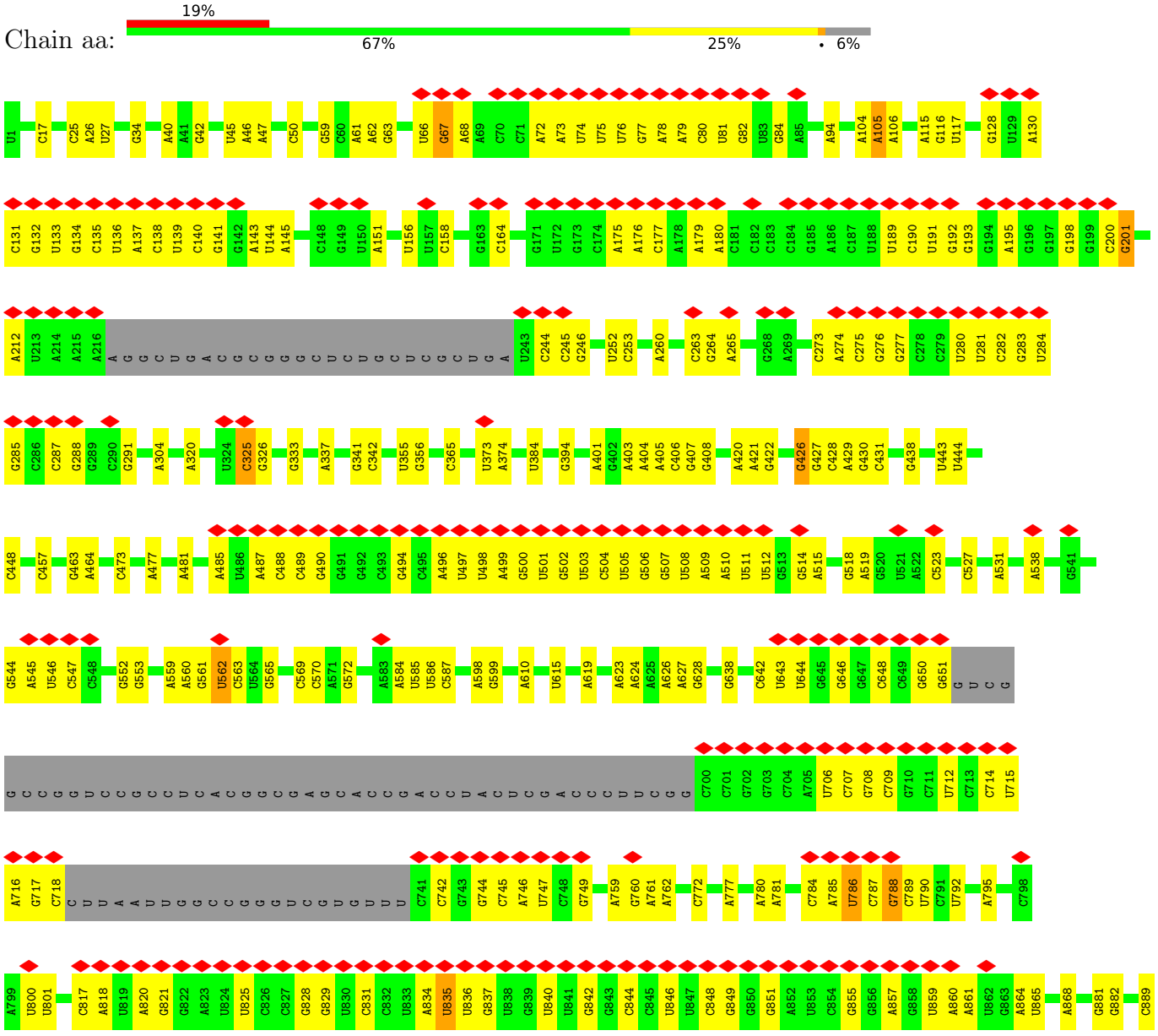
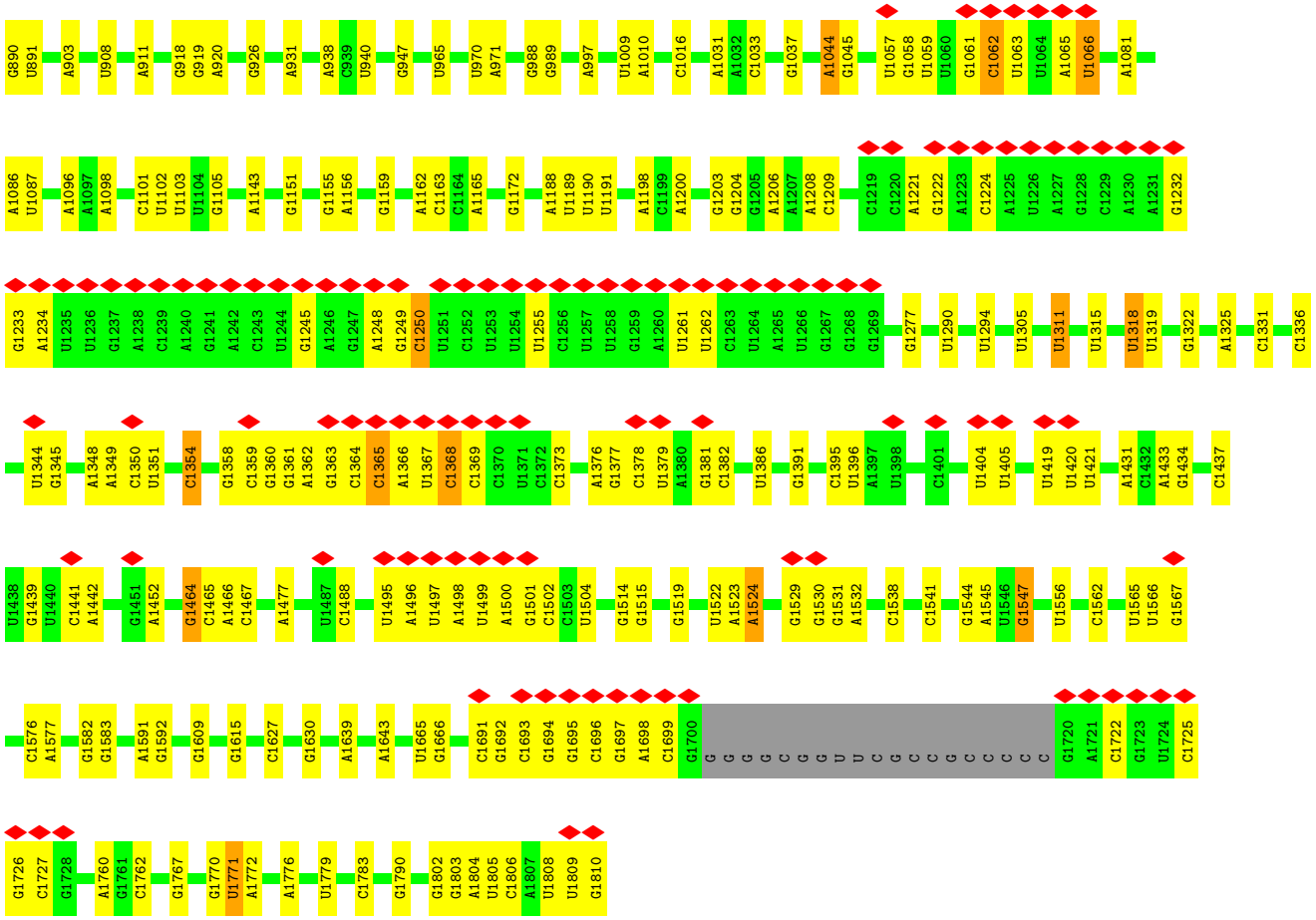
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 83 | GB | 1 | 1 | 1 | 0 |

# 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.

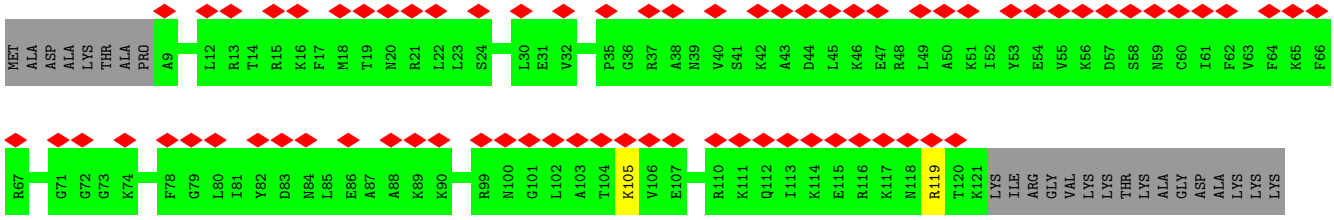
- Molecule 1: 18S ribosomal RNA





• Molecule 2: 40S ribosomal protein eS24

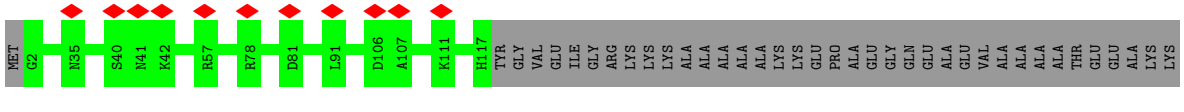
Chain ba:

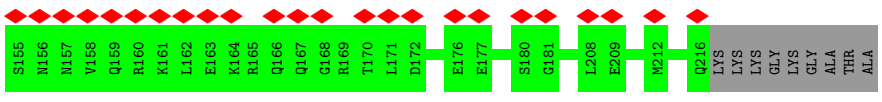





• Molecule 3: 40S ribosomal protein eS8

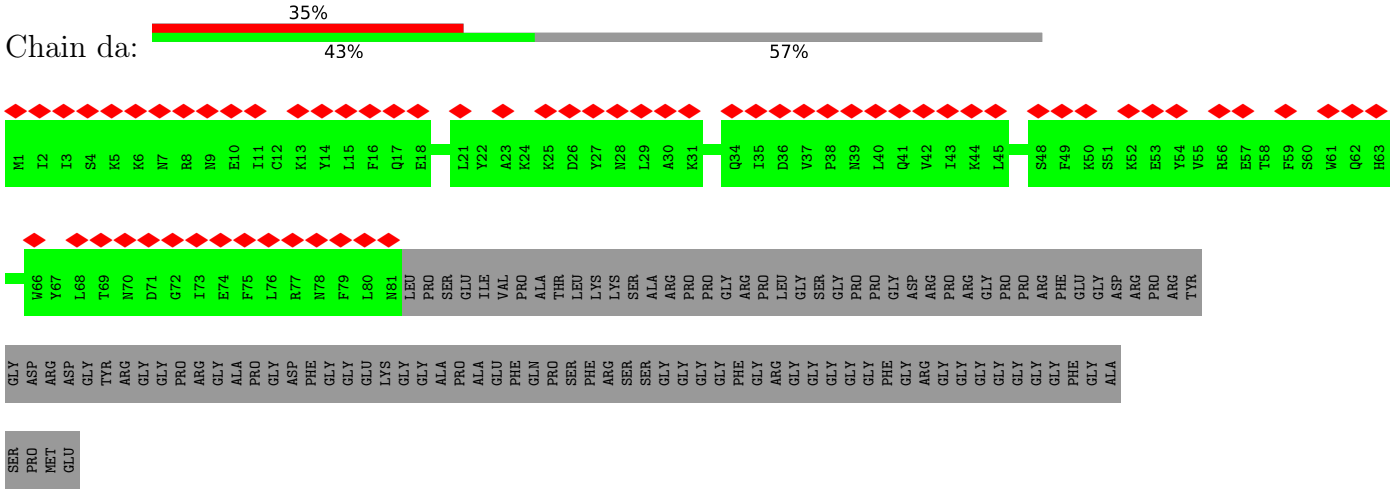
Chain ca:



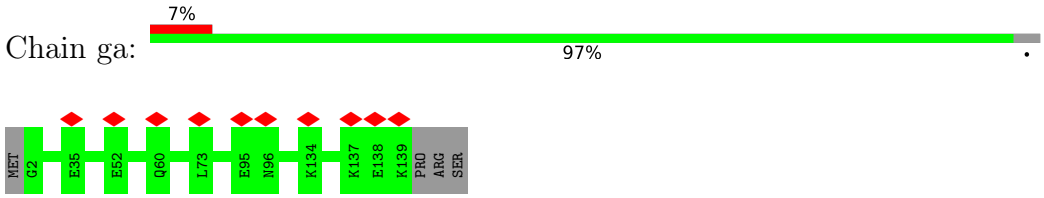
• Molecule 4: 40S ribosomal protein eS10

Chain da:



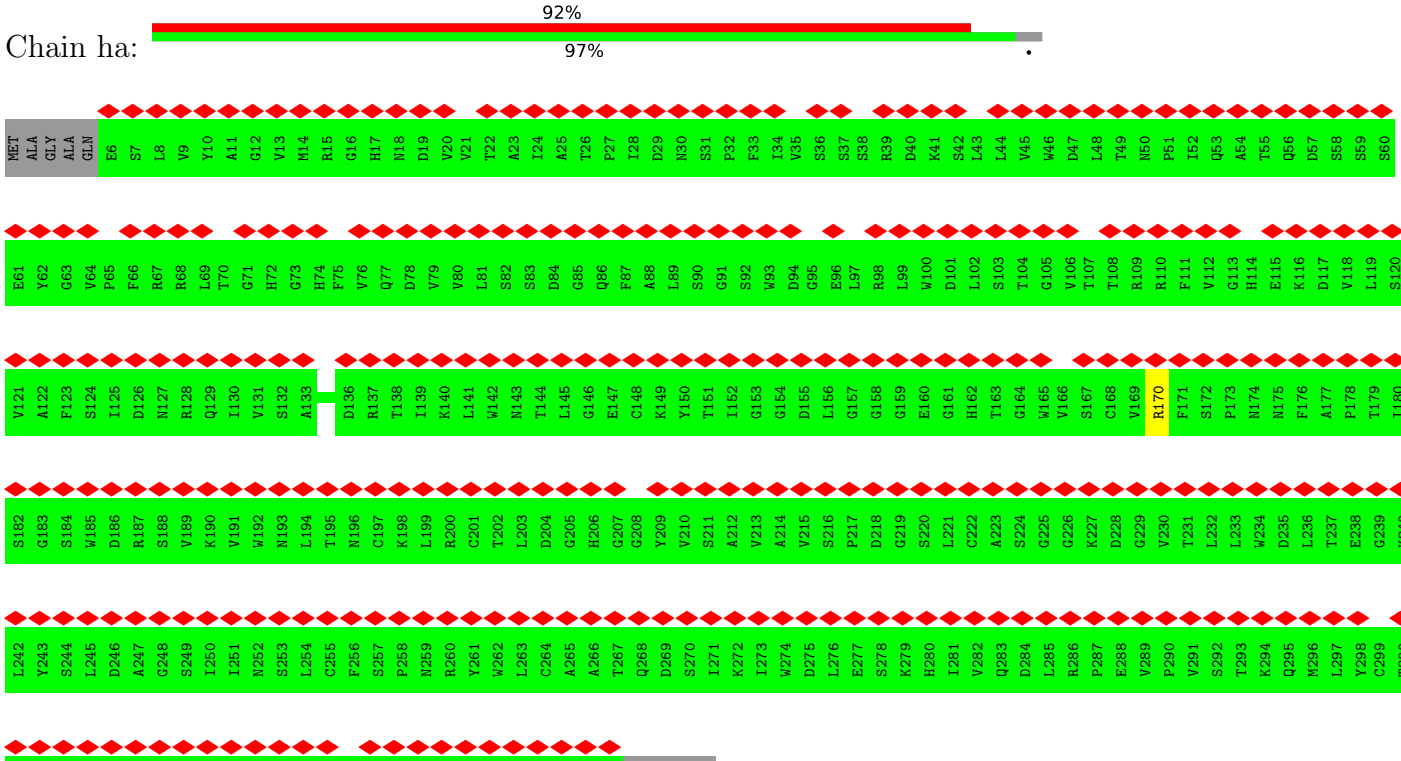

• Molecule 5: 40S ribosomal protein uS12

Chain ga:



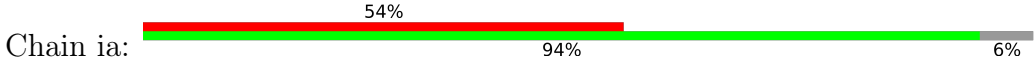

• Molecule 6: RACK1

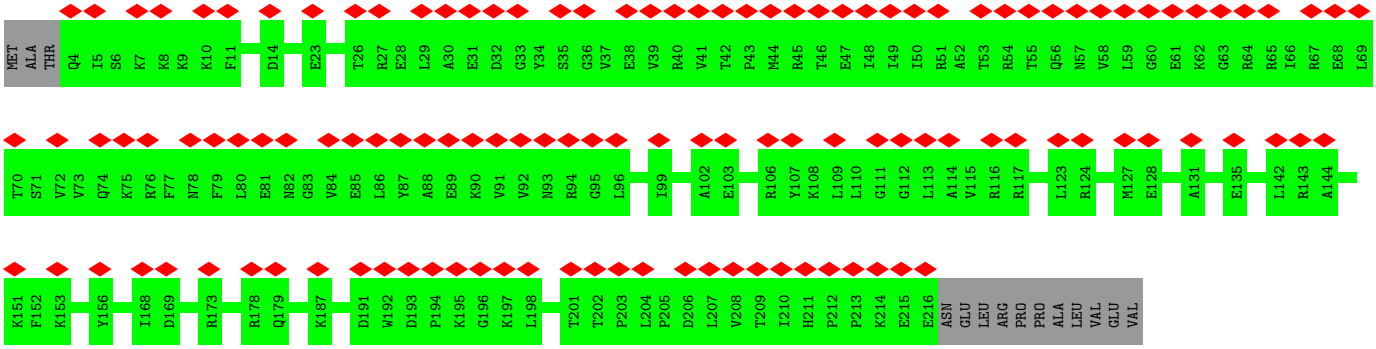
Chain ha:




• Molecule 7: 40S ribosomal protein uS3

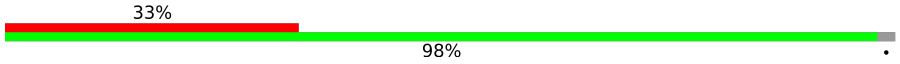
Chain ia:

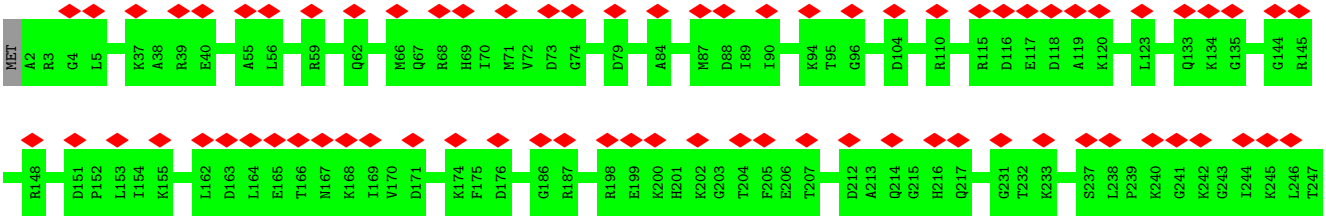





• Molecule 8: 40S ribosomal protein eS4

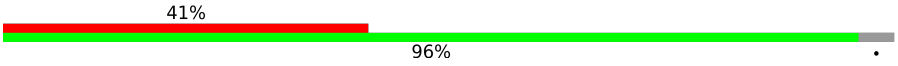
Chain ja:

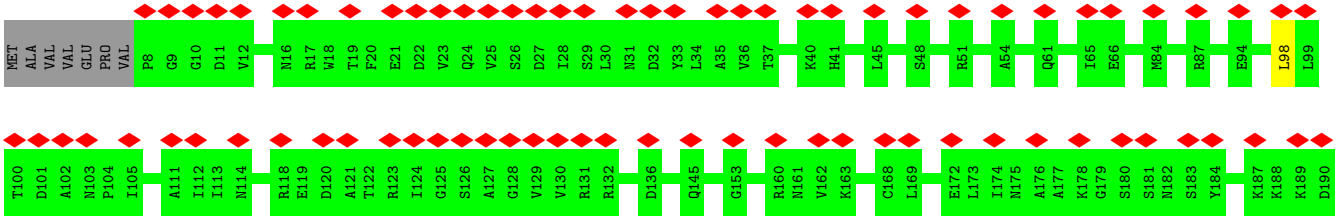



• Molecule 9: 40S ribosomal protein uS7

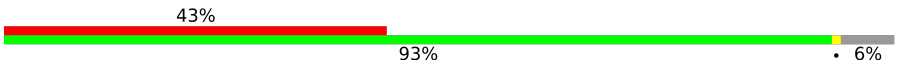
Chain ka:

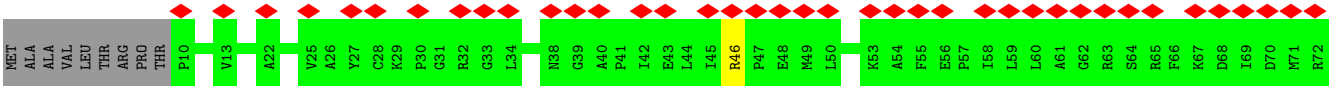


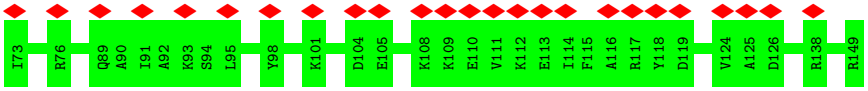




• Molecule 10: 40S ribosomal protein uS9

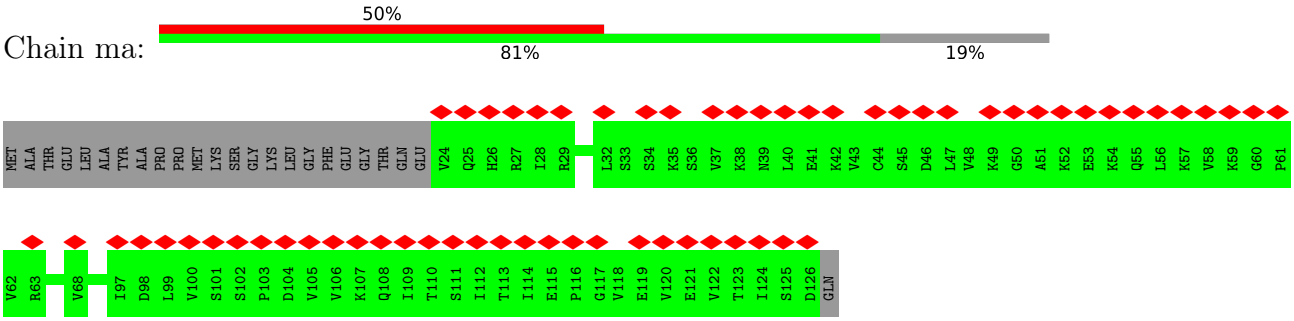
Chain la:



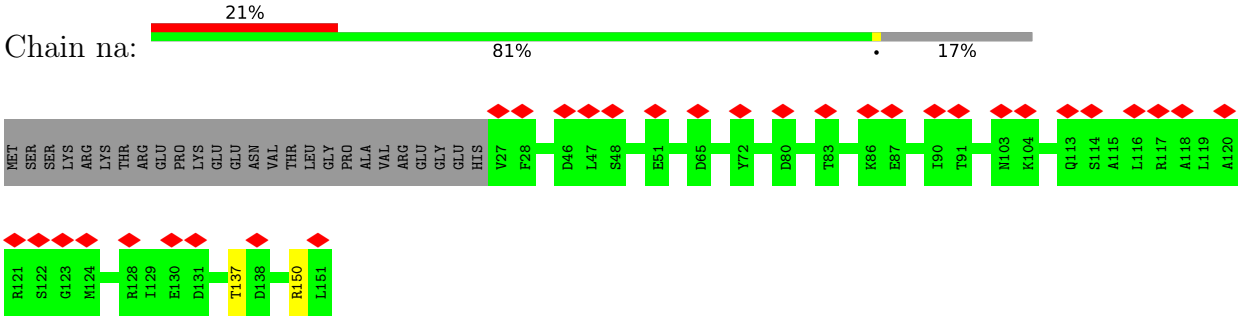





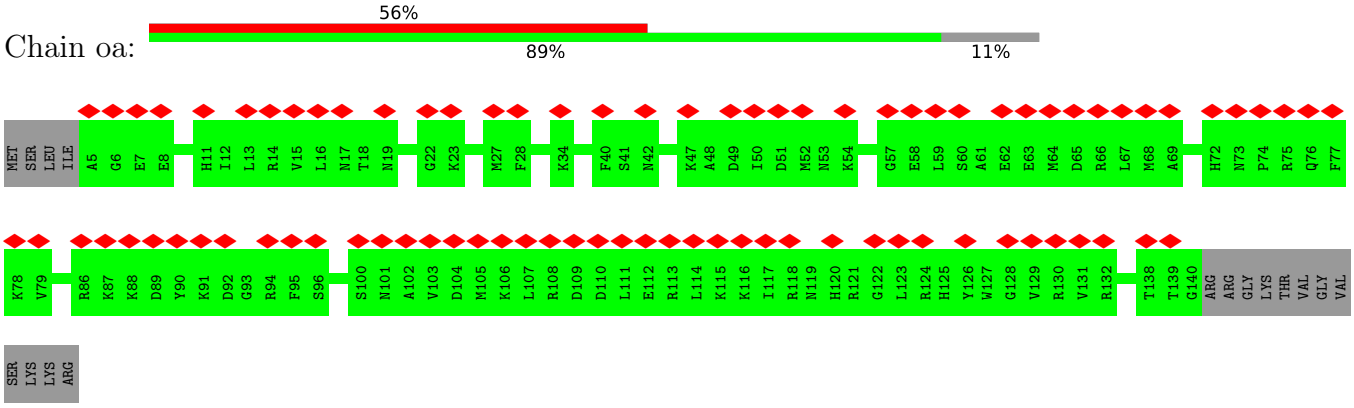

• Molecule 11: 40S ribosomal protein uS10



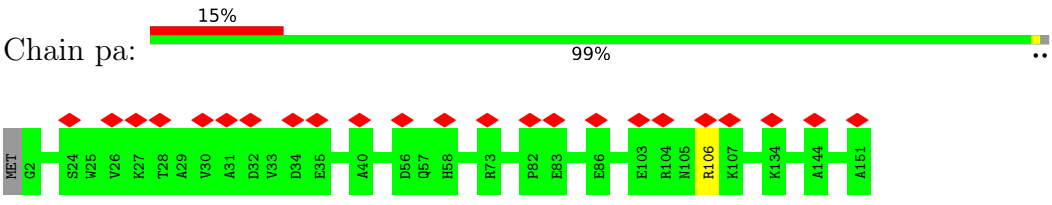

• Molecule 12: 40S ribosomal protein uS11




• Molecule 13: 40S ribosomal protein uS13

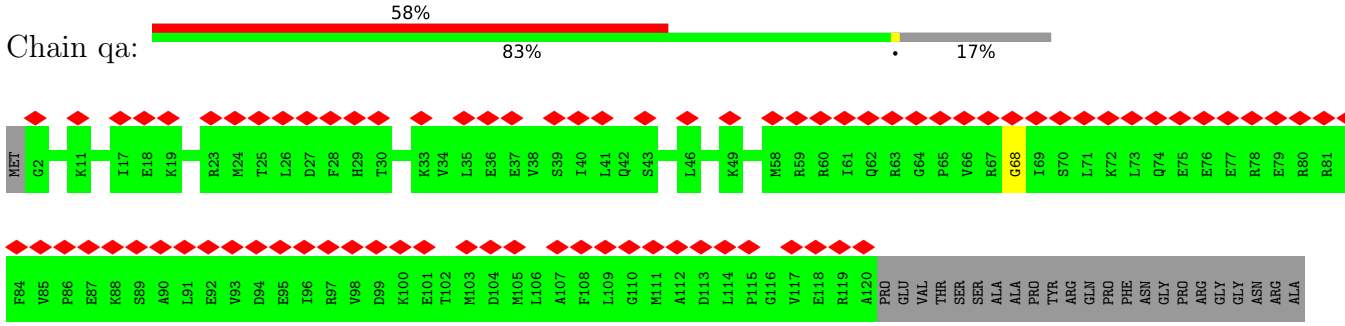



• Molecule 14: 40S ribosomal protein uS15



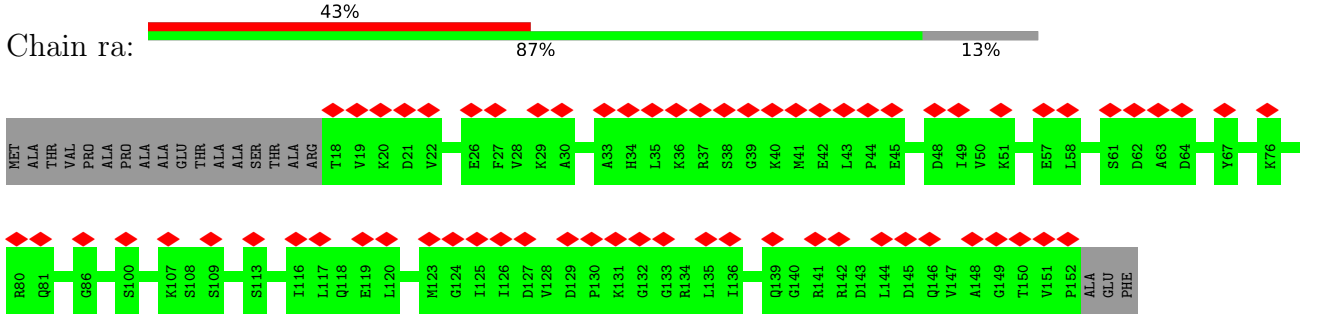

• Molecule 15: 40S ribosomal protein eS17

Chain qa:



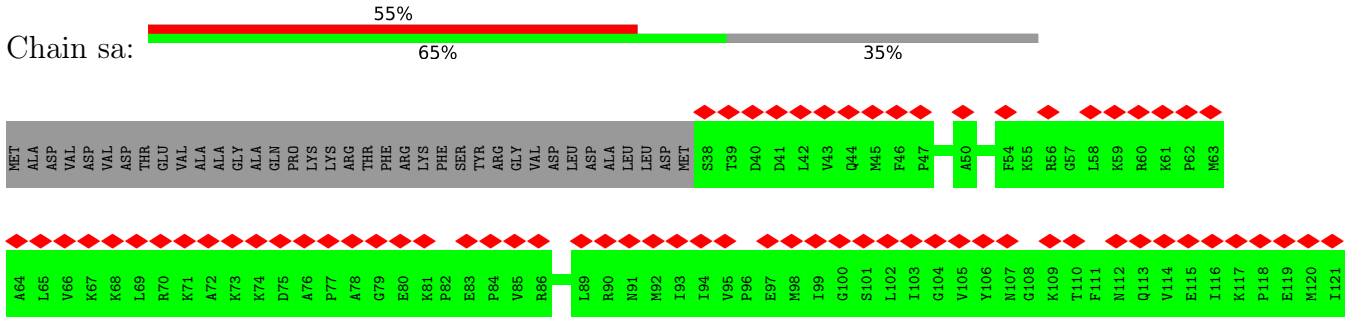

• Molecule 16: 40S ribosomal protein eS19

Chain ra:



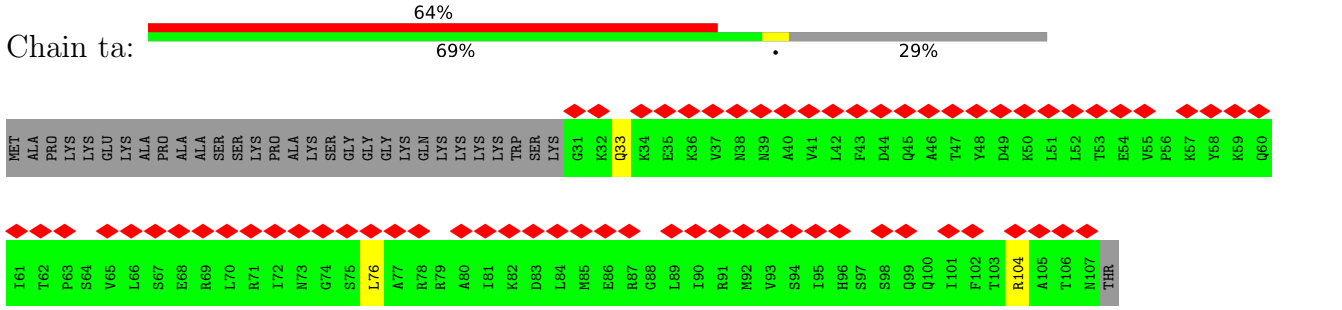

• Molecule 17: 40S ribosomal protein uS19

Chain sa:



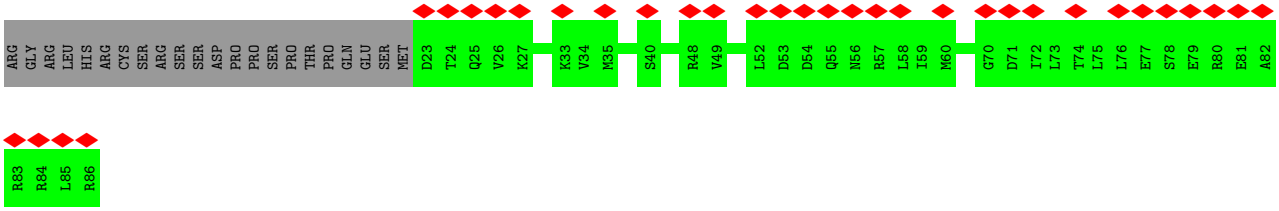

• Molecule 18: 40S ribosomal protein eS25

Chain ta:

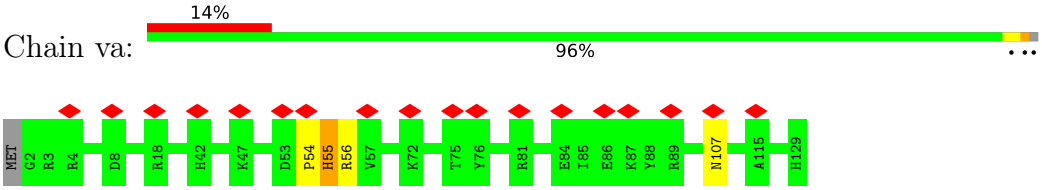



• Molecule 19: 40S ribosomal protein eS28

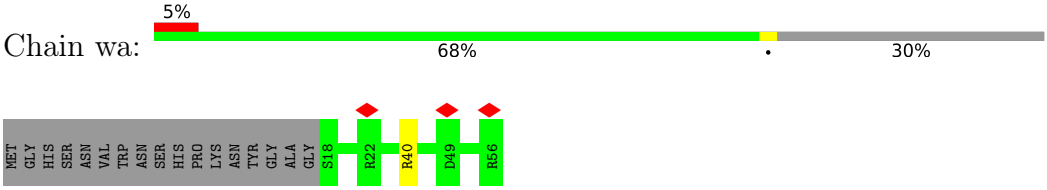
Chain ua:



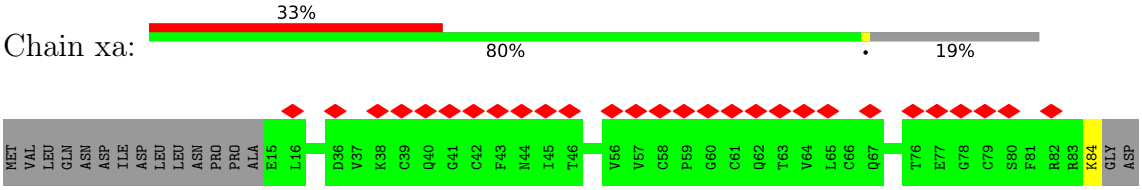

• Molecule 20: 40S ribosomal protein uS8



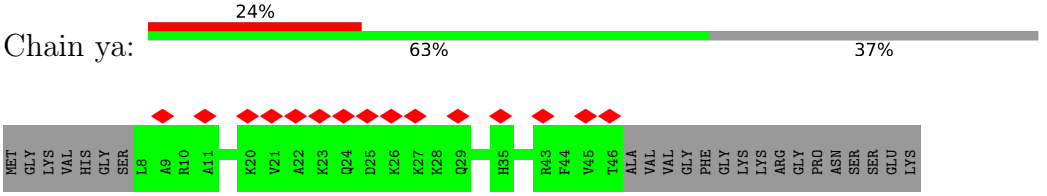

• Molecule 21: 40S ribosomal protein uS14



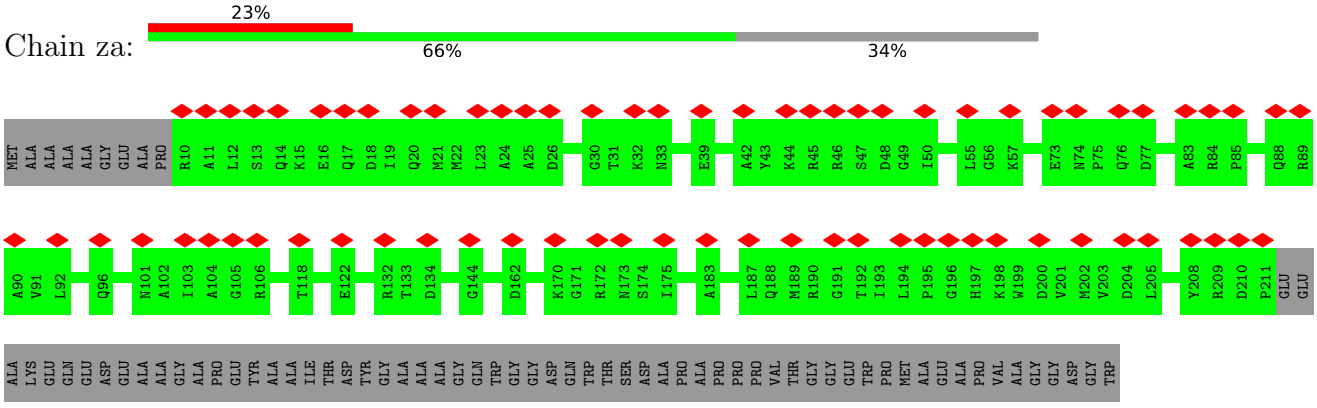

• Molecule 22: 40S ribosomal protein eS27

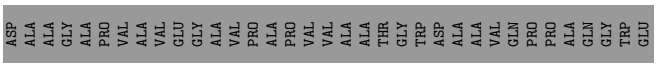



• Molecule 23: 40S ribosomal protein eS30

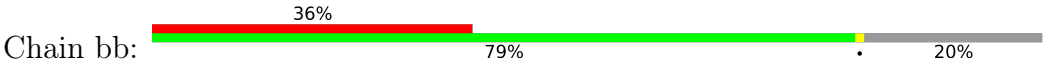


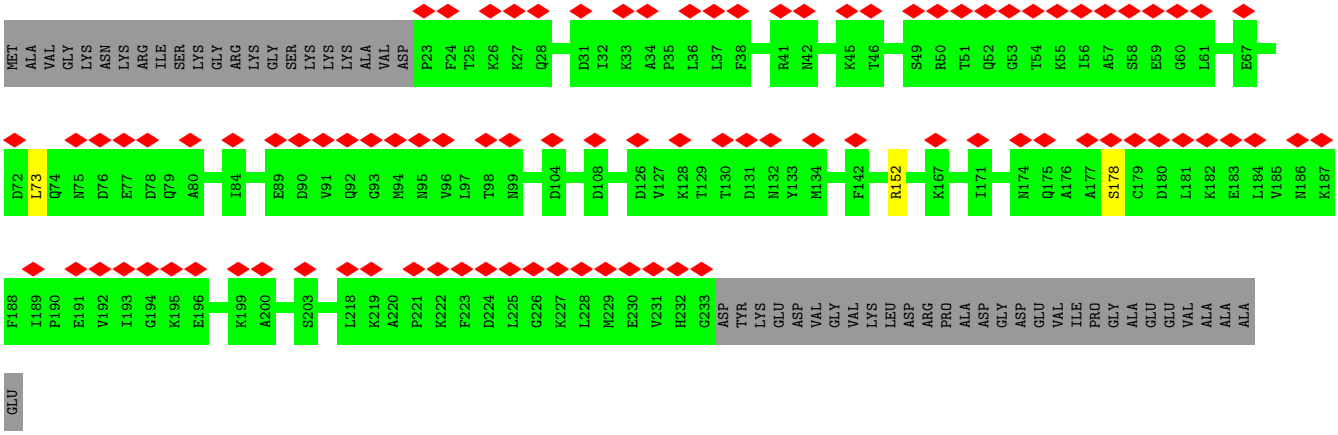

• Molecule 24: 40S ribosomal protein uS2



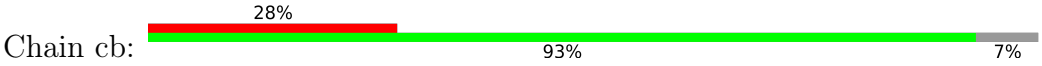


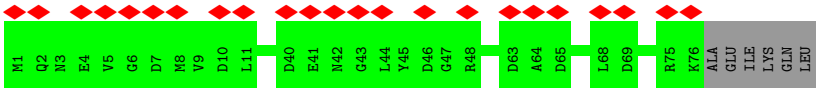

• Molecule 25: 40S ribosomal protein eS1



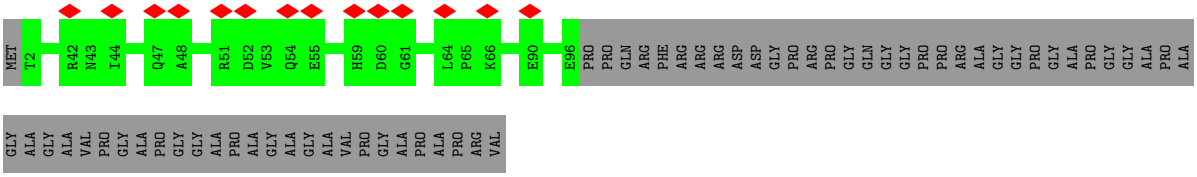




• Molecule 26: 40S ribosomal protein eS21

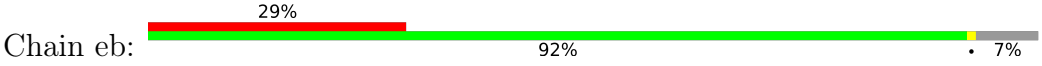


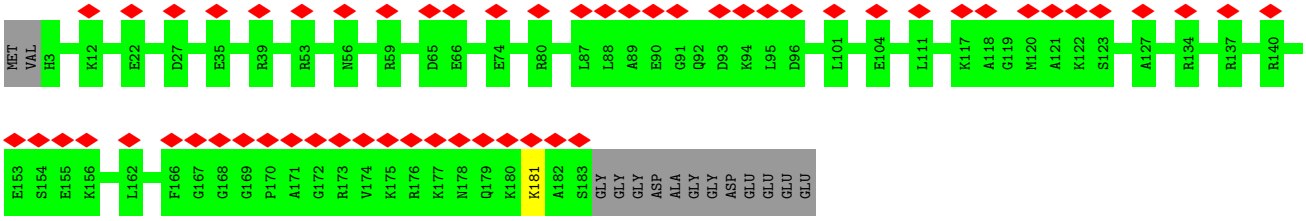




• Molecule 27: 40S ribosomal protein eS26

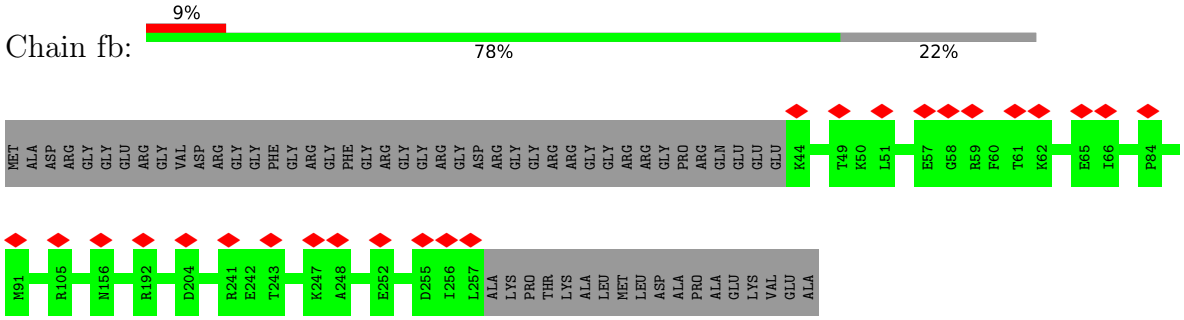

• Molecule 28: 40S ribosomal protein uS4



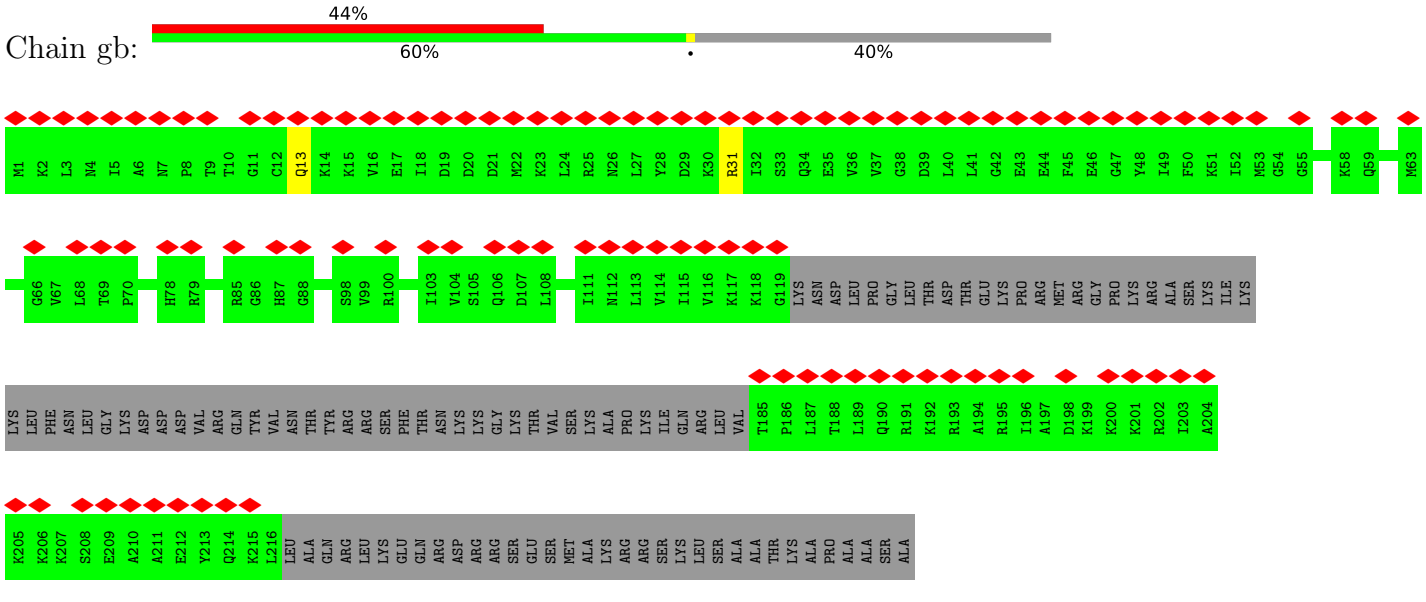

• Molecule 29: 40S ribosomal protein uS5

Chain fb:



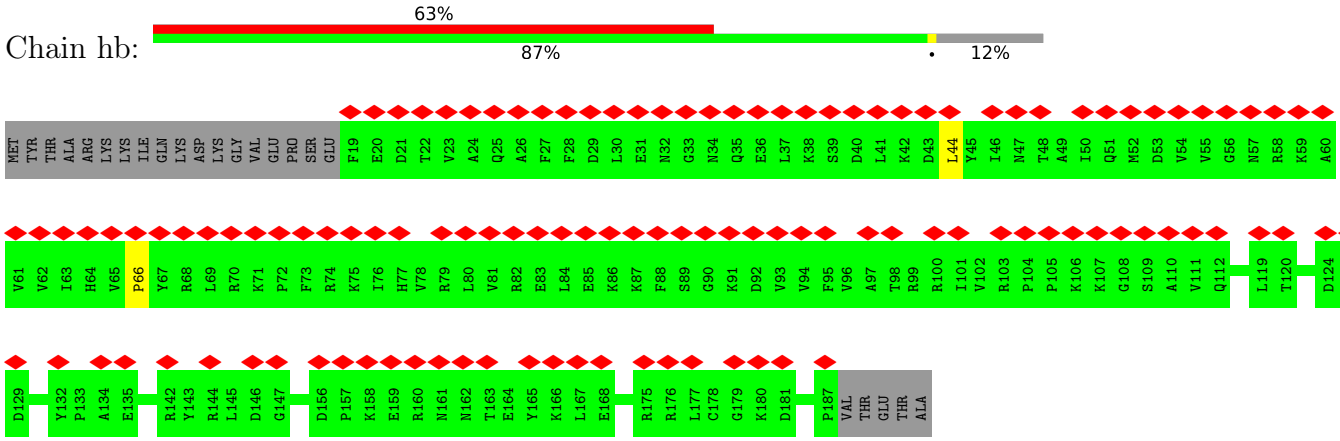

• Molecule 30: 40S ribosomal protein eS6

Chain gb:



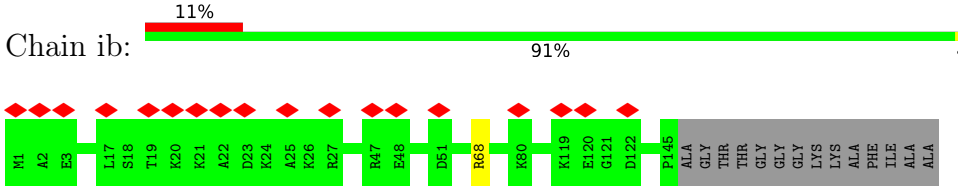

• Molecule 31: 40S ribosomal protein eS7

Chain hb:



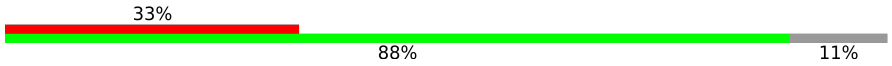

• Molecule 32: 40S ribosomal protein uS17

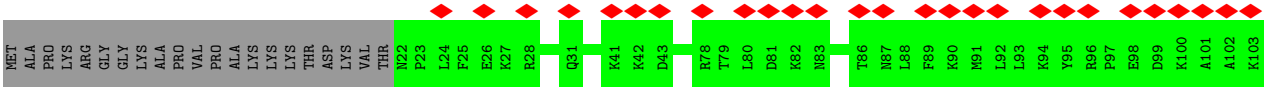
Chain ib:

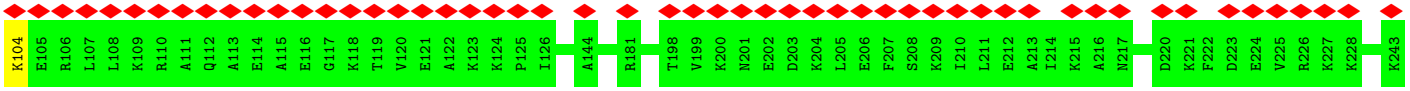


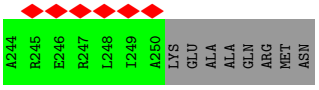
• Molecule 33: 40S ribosomal protein eL8

Chain AA:



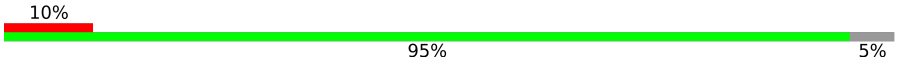



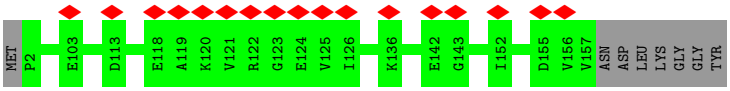




• Molecule 34: 60S ribosomal protein eL21

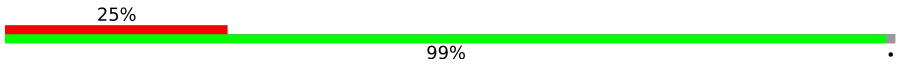
Chain BA:

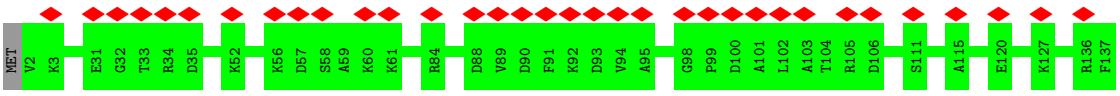



• Molecule 35: 60S ribosomal protein eL27

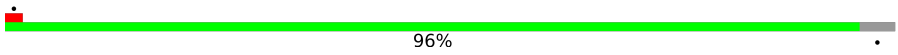
Chain CA:

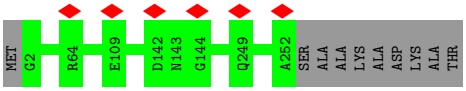



• Molecule 36: 60S ribosomal protein uL2

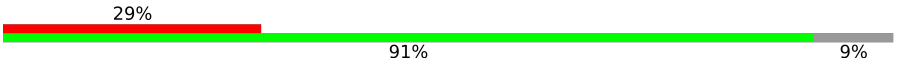
Chain DA:

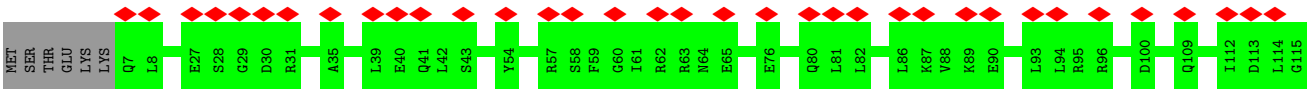


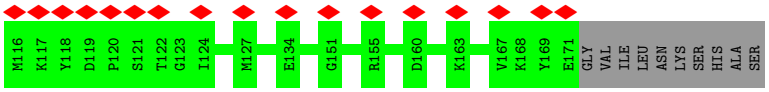




• Molecule 37: 60S ribosomal protein uL5

Chain EA:

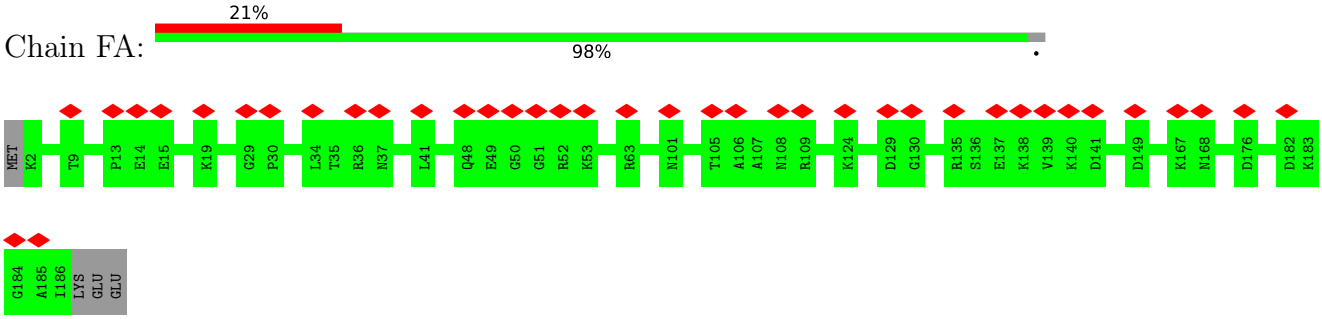


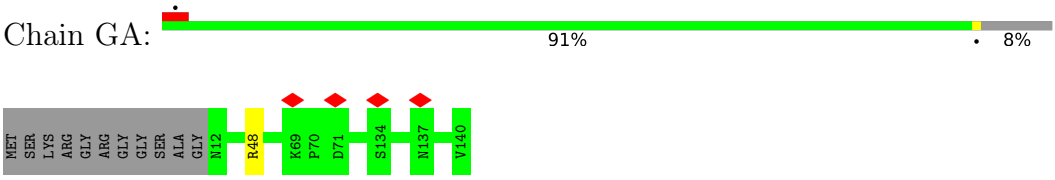

• Molecule 38: 60S ribosomal protein uL6

Chain FA:



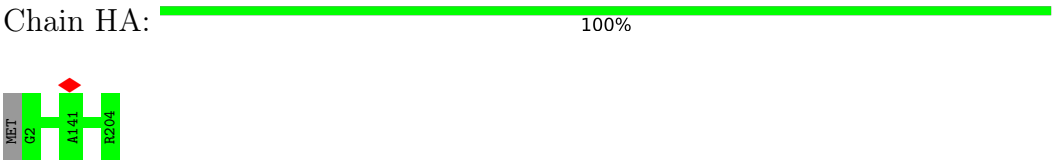

• Molecule 39: 60S ribosomal protein uL14

Chain GA:



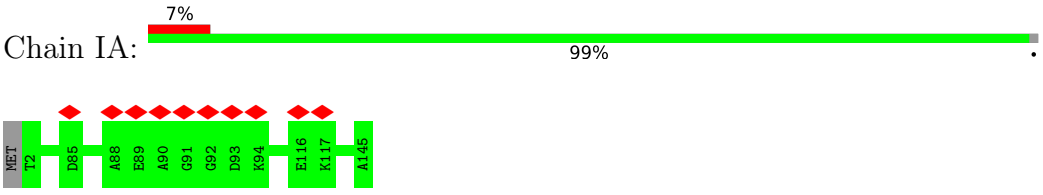

• Molecule 40: 60S ribosomal protein eL15

Chain HA:



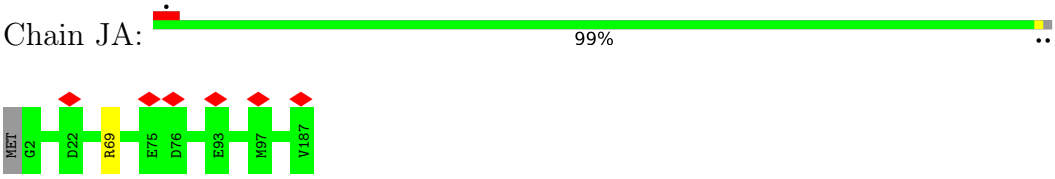

• Molecule 41: 60S ribosomal protein uL15

Chain IA:



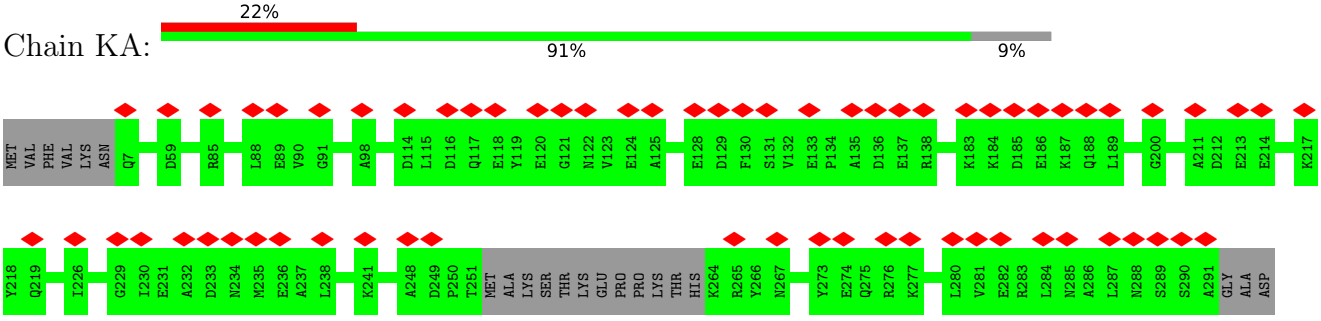

• Molecule 42: 60S ribosomal protein eL18

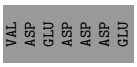
Chain JA:




• Molecule 43: 60S ribosomal protein uL18

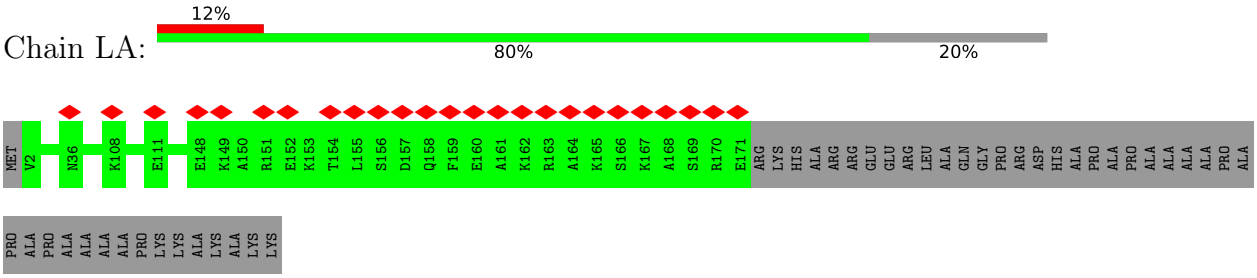
Chain KA:





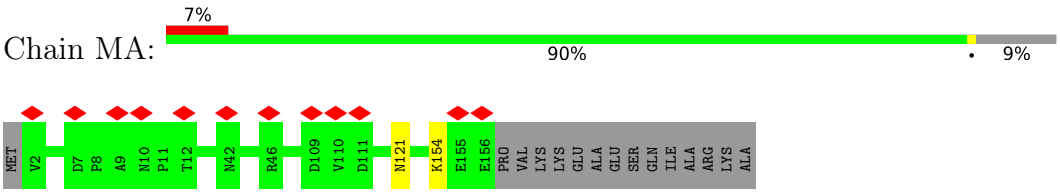

• Molecule 44: 60S ribosomal protein eL19

Chain LA:



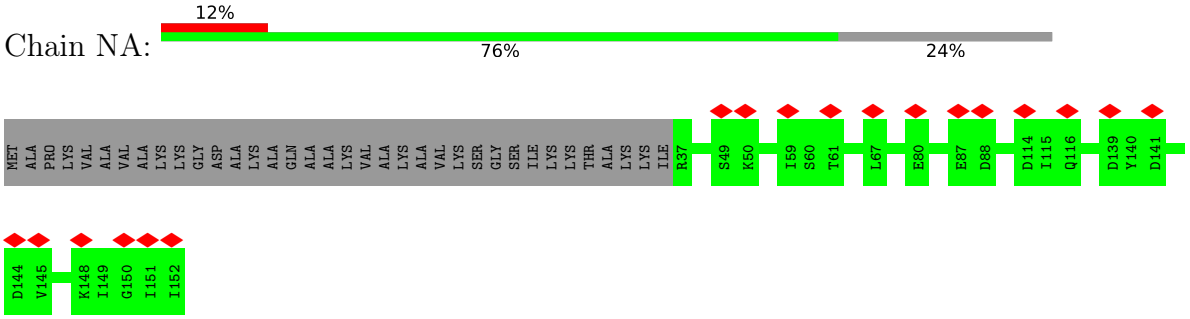

• Molecule 45: 60S ribosomal protein uL22

Chain MA:



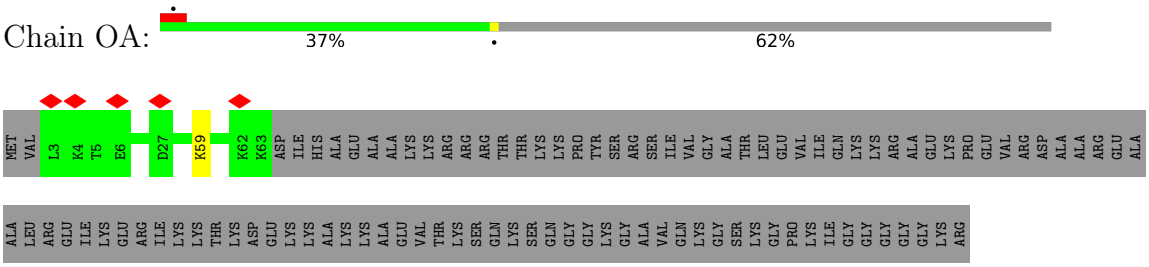

• Molecule 46: 60S ribosomal protein uL23

Chain NA:



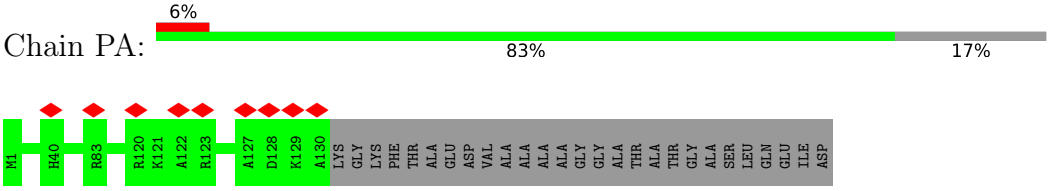

• Molecule 47: 60S ribosomal protein eL24

Chain OA:



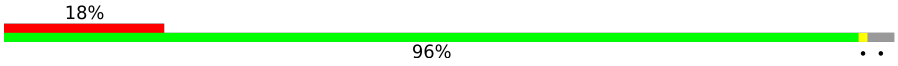

• Molecule 48: 60S ribosomal protein uL24

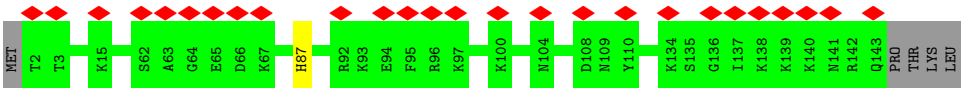
Chain PA:




• Molecule 49: 60S ribosomal protein eL28

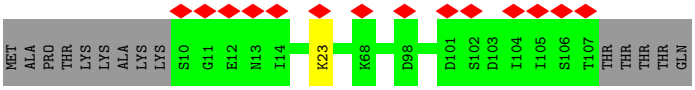
Chain QA:



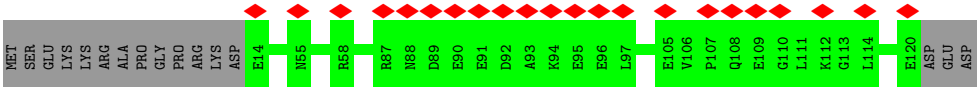

• Molecule 50: 60S ribosomal protein eL30

Chain RA:

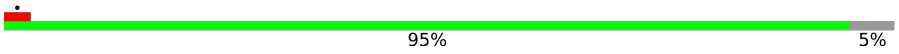

• Molecule 51: 60S ribosomal protein eL31

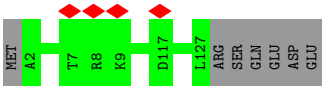
Chain SA:


• Molecule 52: 60S ribosomal protein eL32

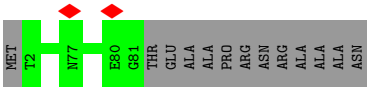
Chain TA:



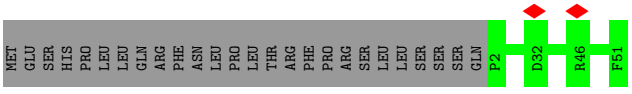

• Molecule 53: 60S ribosomal protein eL37

Chain UA:

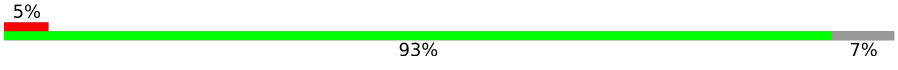

• Molecule 54: 60S ribosomal protein eL39

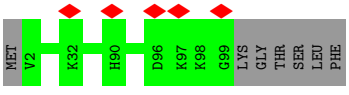
Chain VA:


• Molecule 55: 60S ribosomal protein eL42

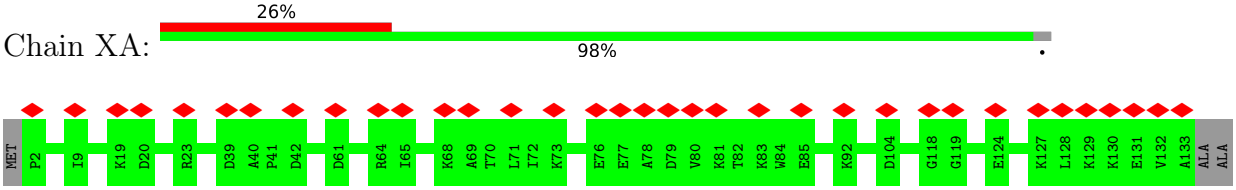
Chain WA:



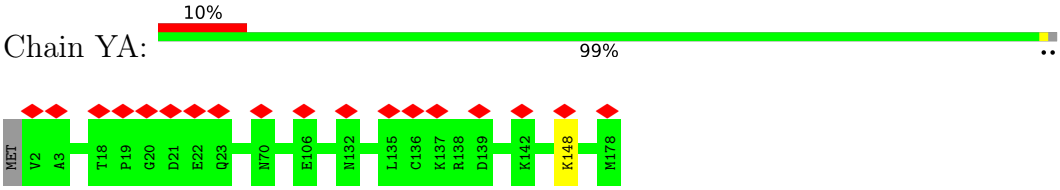
• Molecule 56: 60S ribosomal protein eL14

Chain XA:



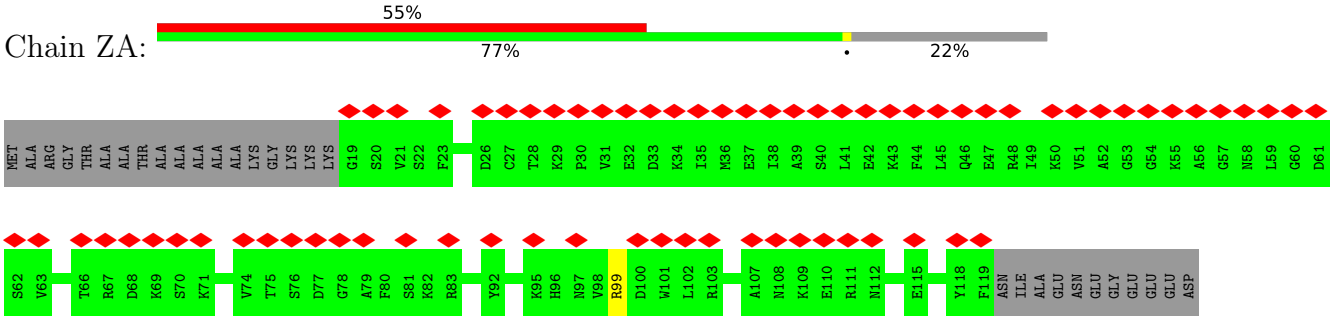

• Molecule 57: 60S ribosomal protein eL20

Chain YA:



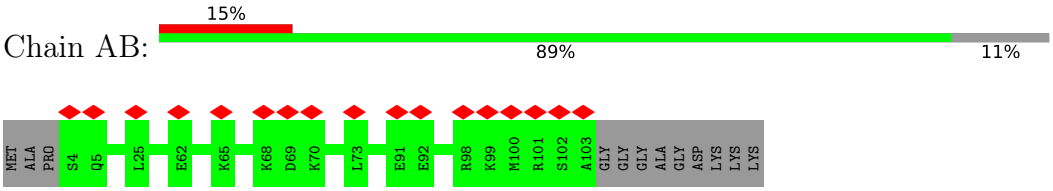

• Molecule 58: 60S ribosomal protein eL22

Chain ZA:



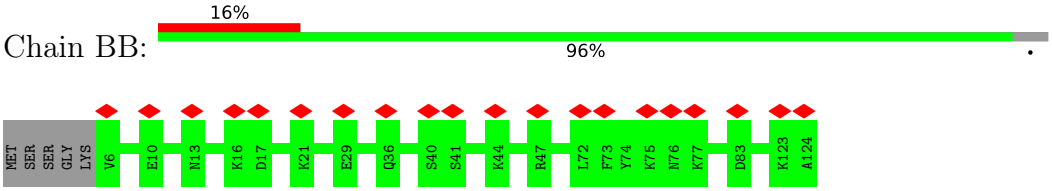

• Molecule 59: 60S ribosomal protein eL36

Chain AB:



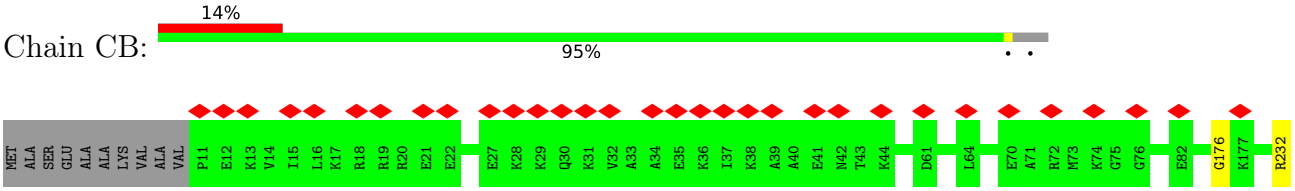

• Molecule 60: 60S ribosomal protein uL29

Chain BB:



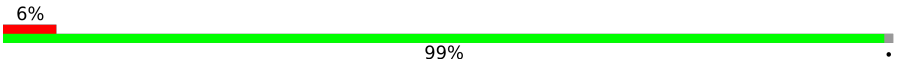

• Molecule 61: 60S ribosomal protein uL30

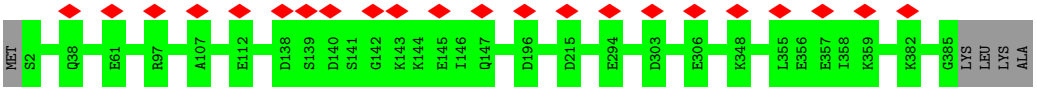
Chain CB:




• Molecule 62: 60S ribosomal protein uL3

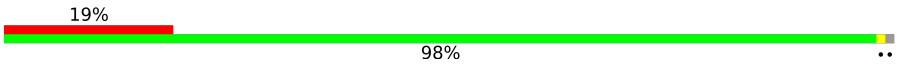
Chain DB:

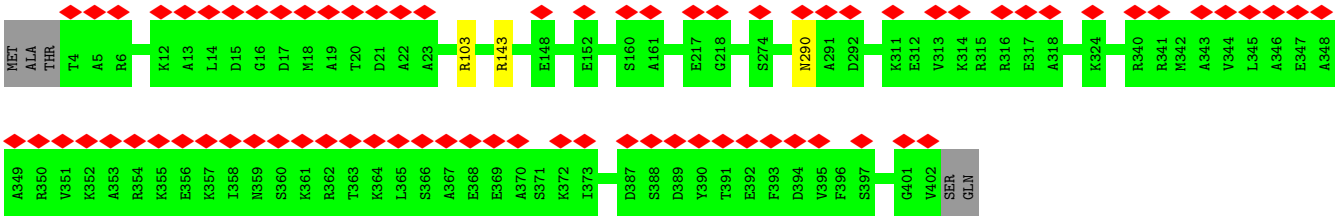



• Molecule 63: 60S ribosomal protein uL4

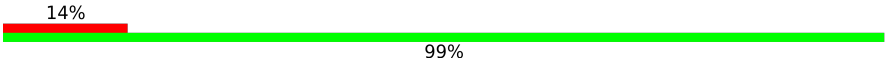
Chain EB:

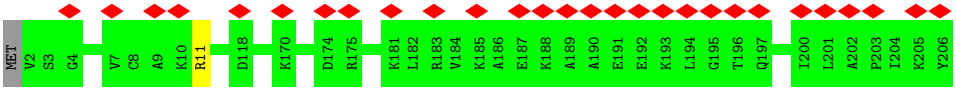



• Molecule 64: 60S ribosomal protein uL13

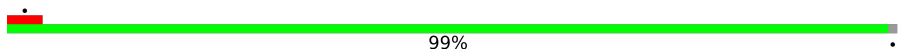
Chain FB:

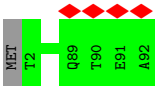



• Molecule 65: 60S ribosomal protein eL43

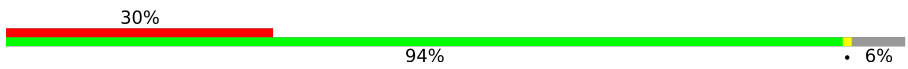
Chain GB:

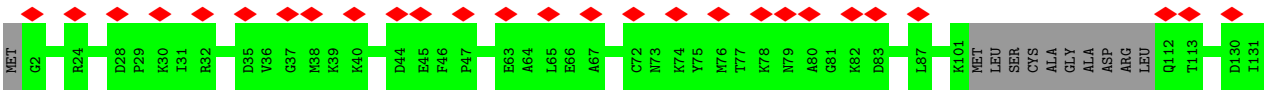



• Molecule 66: 60S ribosomal protein uL16

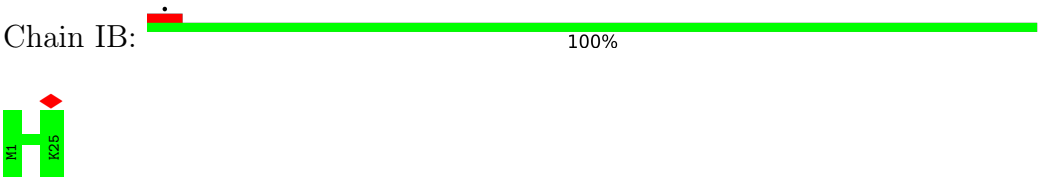
Chain HB:



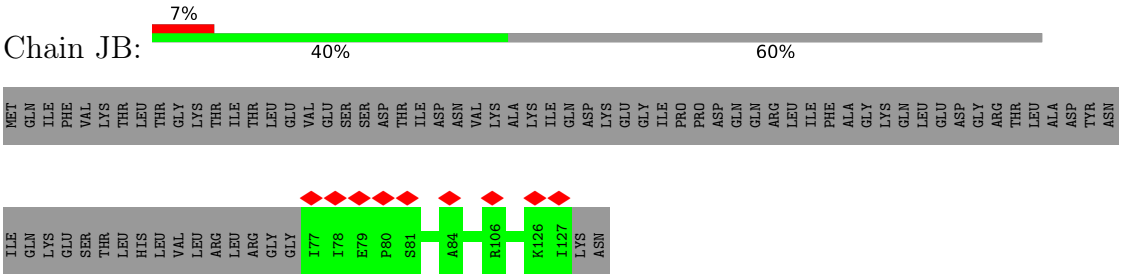

• Molecule 67: 60S ribosomal protein eL41

Chain IB:



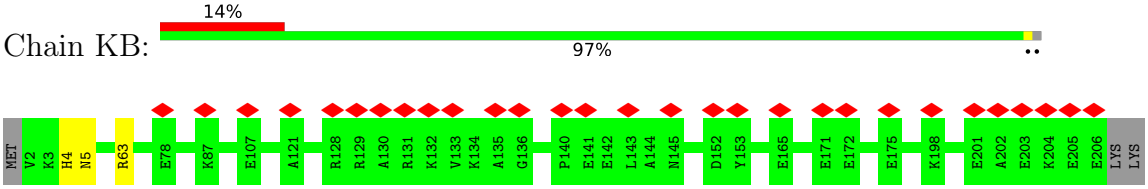

• Molecule 68: 60S ribosomal protein eL40

Chain JB:



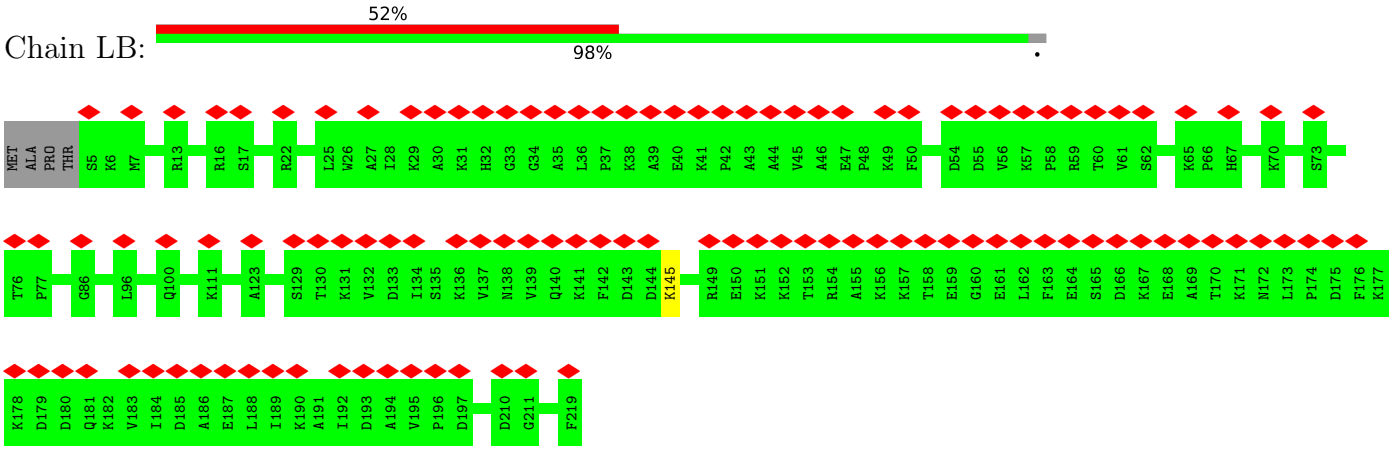

• Molecule 69: 60S ribosomal protein eL13

Chain KB:



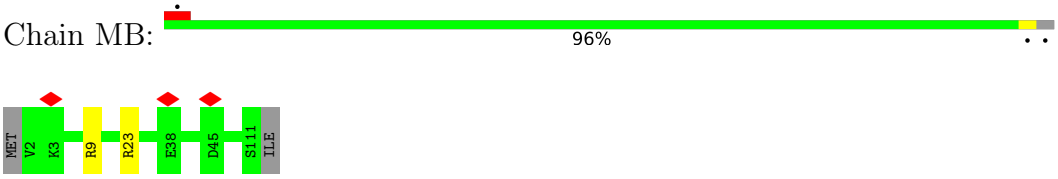

• Molecule 70: 60S ribosomal protein eL6

Chain LB:



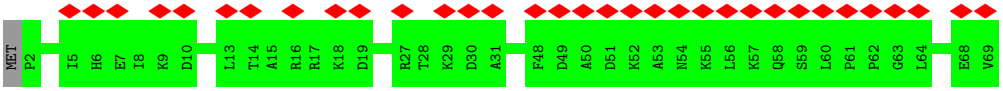

• Molecule 71: 60S ribosomal protein eL33

Chain MB:



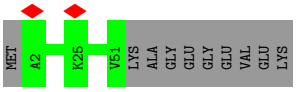

• Molecule 72: 60S ribosomal protein eL38

Chain NB:



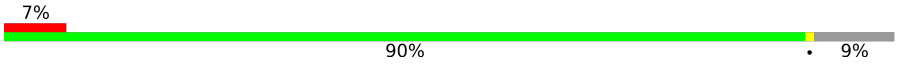

• Molecule 73: 60S ribosomal protein eL29

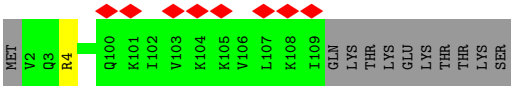
Chain OB:


• Molecule 74: 60S ribosomal protein eL34

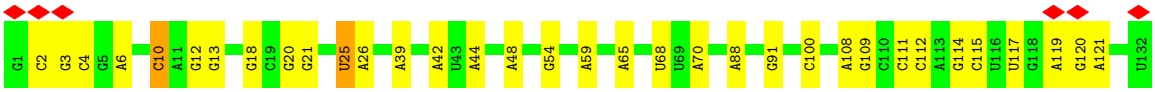
Chain PB:

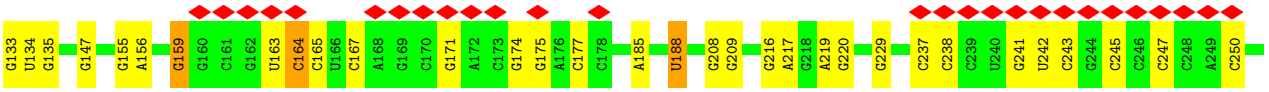


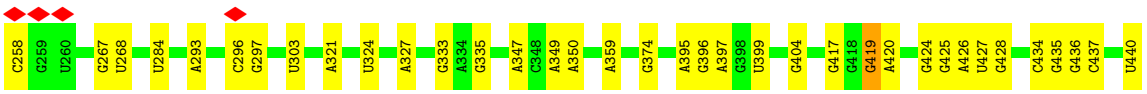




• Molecule 75: 60S ribosomal RNA

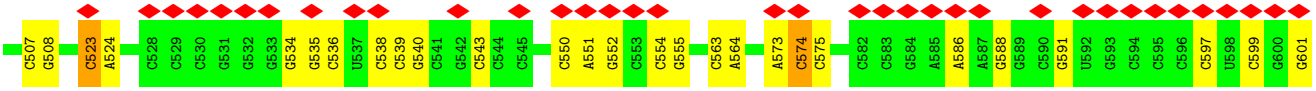
Chain RB:

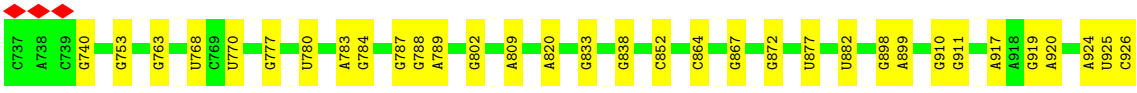



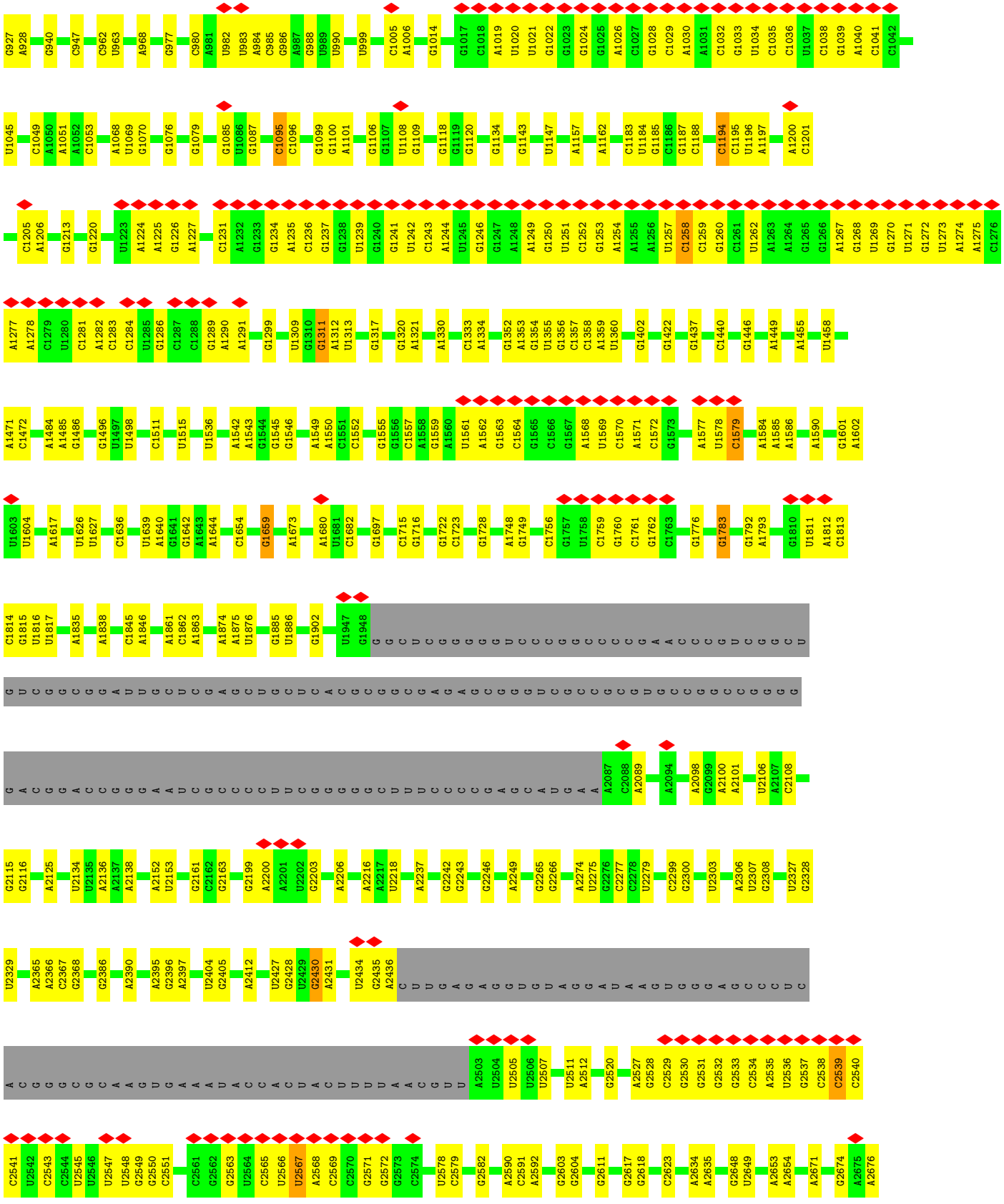



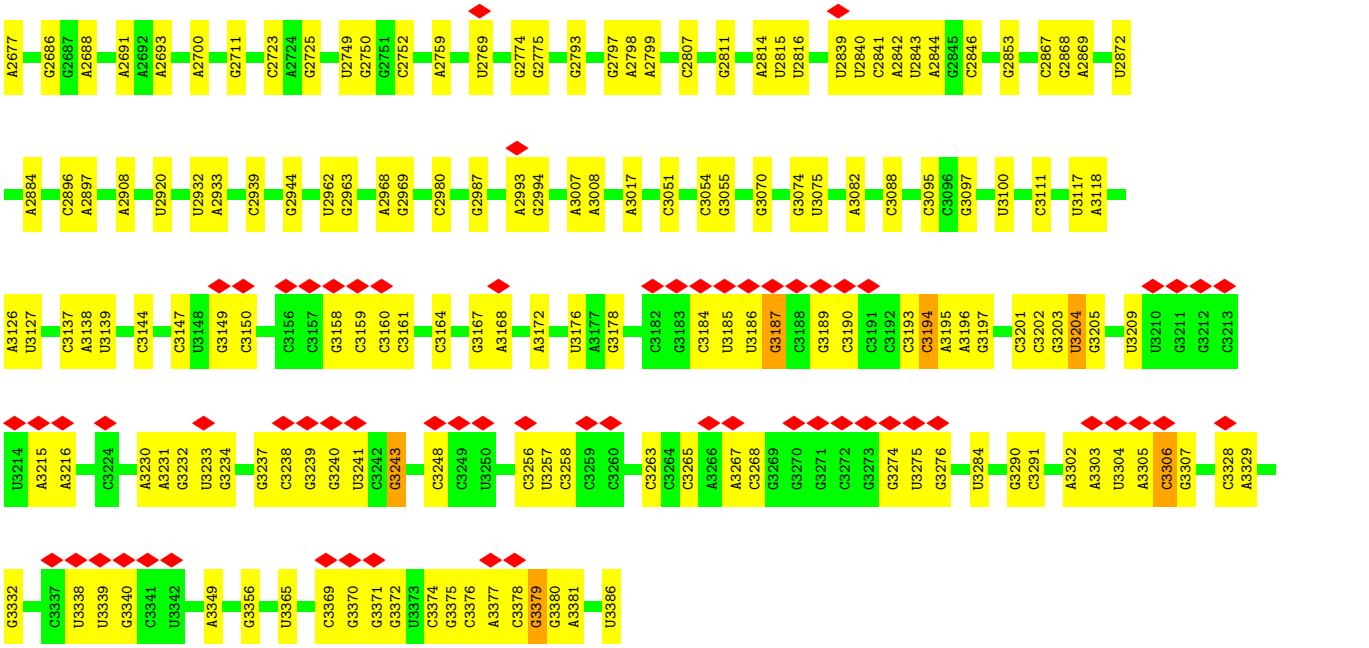






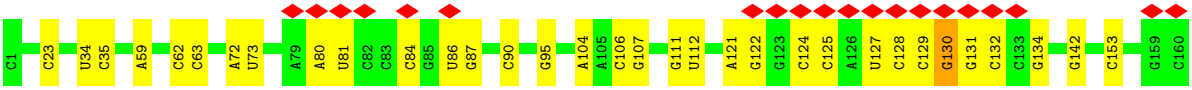






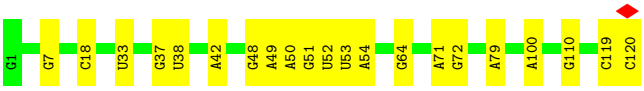

• Molecule 76: 5.8S ribosomal RNA

Chain SB:


• Molecule 77: 5S ribosomal RNA

Chain TB:

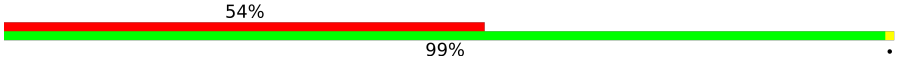

• Molecule 78: mRNA

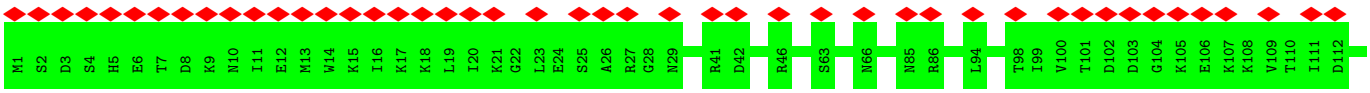
Chain al:

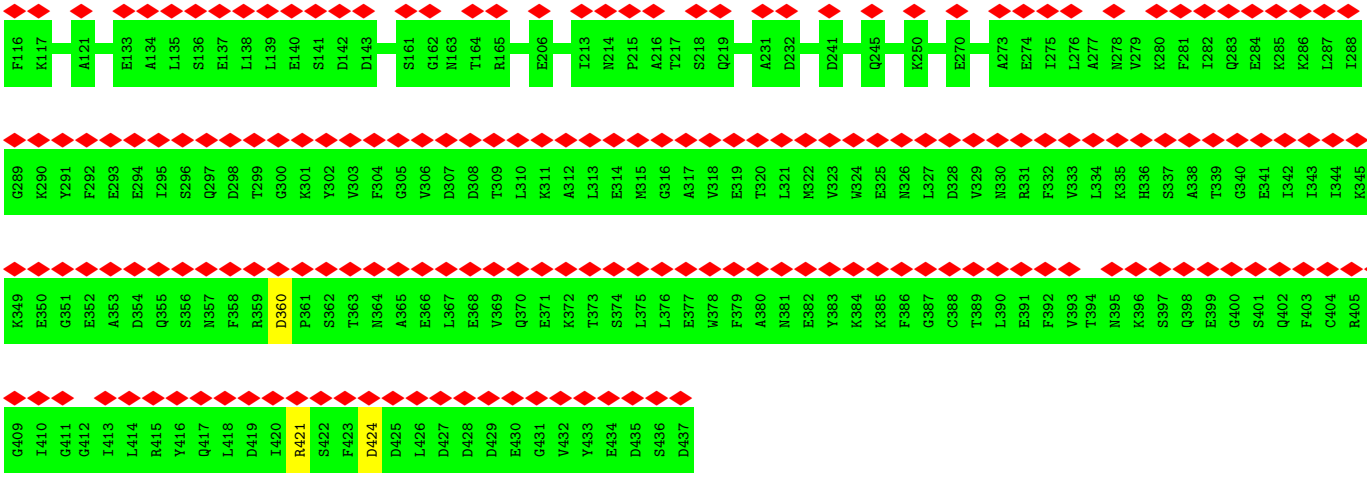


• Molecule 79: eukaryotic release factor 1

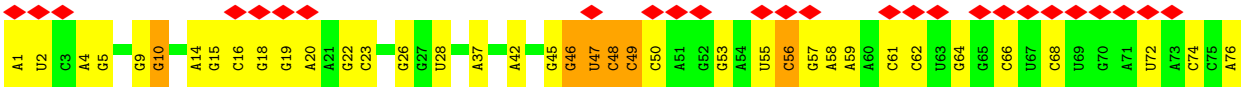
Chain bl:






- Molecule 80: tRNAi


- Molecule 81: CCA end of E-tRNA


# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 96104 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | JEOL CRYO ARM 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 40.0 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | 60000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.086 | Depositor |
| Minimum map value | -0.031 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.004 | Depositor |
| Recommended contour level | 0.016 | Depositor |
| Map size (Å) | 441.28, 441.28, 441.28 | wwPDB |
| Map dimensions | 560, 560, 560 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.788, 0.788, 0.788 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 1MA, 1MG, 2MG, G7M, ZN, 5MC, H2U, MG, PSU

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 | aa | 0.75 | 0/40441 | 0.94 | 69/63026 (0.1%) |
| 2 | ba | 0.35 | 0/943 | 0.56 | 0/1253 |
| 3 | ca | 0.41 | 0/1464 | 0.57 | 0/1957 |
| 4 | da | 0.39 | 0/722 | 0.62 | 0/972 |
| 5 | ga | 0.41 | 0/1088 | 0.57 | 0/1448 |
| 6 | ha | 0.33 | 0/2530 | 0.60 | 0/3443 |
| 7 | ia | 0.33 | 0/1697 | 0.53 | 0/2279 |
| 8 | ja | 0.38 | 0/2123 | 0.56 | 0/2853 |
| 9 | ka | 0.37 | 0/1538 | 0.58 | 1/2070 (0.0%) |
| 10 | la | 0.41 | 0/1138 | 0.61 | 0/1517 |
| 11 | ma | 0.37 | 0/815 | 0.60 | 0/1098 |
| 12 | na | 0.38 | 0/953 | 0.59 | 0/1278 |
| 13 | oa | 0.38 | 0/1132 | 0.63 | 0/1511 |
| 14 | pa | 0.40 | 0/1219 | 0.52 | 0/1638 |
| 15 | qa | 0.31 | 0/985 | 0.55 | 0/1313 |
| 16 | ra | 0.41 | 0/1088 | 0.57 | 0/1463 |
| 17 | sa | 0.37 | 0/824 | 0.58 | 0/1102 |
| 18 | ta | 0.36 | 0/624 | 0.70 | 0/836 |
| 19 | ua | 0.37 | 0/514 | 0.57 | 0/685 |
| 20 | va | 0.45 | 0/1057 | 0.70 | 2/1421 (0.1%) |
| 21 | wa | 0.43 | 0/318 | 0.60 | 0/418 |
| 22 | xa | 0.37 | 0/555 | 0.56 | 0/742 |
| 23 | ya | 0.36 | 0/326 | 0.57 | 0/430 |
| 24 | za | 0.37 | 0/1644 | 0.50 | 0/2226 |
| 25 | bb | 0.40 | 0/1749 | 0.65 | 1/2349 (0.0%) |
| 26 | cb | 0.42 | 0/605 | 0.61 | 0/814 |
| 27 | db | 0.43 | 0/784 | 0.49 | 0/1047 |
| 28 | eb | 0.38 | 0/1521 | 0.55 | 0/2035 |
| 29 | fb | 0.44 | 0/1696 | 0.54 | 0/2292 |
| 30 | gb | 0.33 | 0/1210 | 0.59 | 0/1606 |
| 31 | hb | 0.37 | 0/1415 | 0.61 | 1/1907 (0.1%) |
| 32 | ib | 0.43 | 0/1192 | 0.54 | 0/1597 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | AA | 0.38 | 0/1881 | 0.53 | 0/2523 |
| 34 | BA | 0.45 | 0/1284 | 0.52 | 0/1728 |
| 35 | CA | 0.40 | 0/1111 | 0.55 | 0/1481 |
| 36 | DA | 0.46 | 0/1965 | 0.56 | 0/2644 |
| 37 | EA | 0.40 | 0/1353 | 0.58 | 0/1807 |
| 38 | FA | 0.39 | 0/1478 | 0.55 | 0/1983 |
| 39 | GA | 0.45 | 0/992 | 0.55 | 0/1333 |
| 40 | HA | 0.50 | 0/1760 | 0.57 | 0/2354 |
| 41 | IA | 0.48 | 0/1152 | 0.54 | 0/1538 |
| 42 | JA | 0.44 | 0/1511 | 0.53 | 0/2021 |
| 43 | KA | 0.42 | 0/2249 | 0.53 | 0/3020 |
| 44 | LA | 0.40 | 0/1433 | 0.51 | 0/1892 |
| 45 | MA | 0.45 | 0/1276 | 0.54 | 0/1713 |
| 46 | NA | 0.42 | 0/950 | 0.54 | 0/1275 |
| 47 | OA | 0.44 | 0/530 | 0.49 | 0/703 |
| 48 | PA | 0.44 | 0/1067 | 0.57 | 0/1425 |
| 49 | QA | 0.41 | 0/1144 | 0.53 | 0/1536 |
| 50 | RA | 0.43 | 0/769 | 0.55 | 0/1035 |
| 51 | SA | 0.41 | 0/874 | 0.54 | 0/1171 |
| 52 | TA | 0.44 | 0/1061 | 0.55 | 0/1417 |
| 53 | UA | 0.47 | 0/669 | 0.58 | 0/886 |
| 54 | VA | 0.41 | 0/464 | 0.49 | 0/616 |
| 55 | WA | 0.44 | 0/807 | 0.51 | 0/1064 |
| 56 | XA | 0.40 | 0/1079 | 0.56 | 0/1440 |
| 57 | YA | 0.46 | 0/1534 | 0.55 | 0/2061 |
| 58 | ZA | 0.36 | 0/826 | 0.57 | 0/1106 |
| 59 | AB | 0.41 | 0/814 | 0.57 | 0/1077 |
| 60 | BB | 0.41 | 0/990 | 0.55 | 0/1317 |
| 61 | CB | 0.42 | 0/1952 | 0.53 | 0/2614 |
| 62 | DB | 0.48 | 0/3167 | 0.56 | 0/4238 |
| 63 | EB | 0.42 | 0/3133 | 0.53 | 0/4220 |
| 64 | FB | 0.43 | 0/1669 | 0.51 | 0/2236 |
| 65 | GB | 0.45 | 0/716 | 0.56 | 0/948 |
| 66 | HB | 0.42 | 0/1670 | 0.57 | 2/2237 (0.1%) |
| 67 | IB | 0.43 | 0/238 | 0.58 | 0/302 |
| 68 | JB | 0.42 | 0/426 | 0.51 | 0/564 |
| 69 | KB | 0.41 | 0/1699 | 0.53 | 0/2269 |
| 70 | LB | 0.37 | 0/1737 | 0.54 | 0/2334 |
| 71 | MB | 0.49 | 0/893 | 0.58 | 0/1198 |
| 72 | NB | 0.39 | 0/565 | 0.60 | 0/753 |
| 73 | OB | 0.40 | 0/424 | 0.49 | 0/561 |
| 74 | PB | 0.48 | 0/894 | 0.59 | 0/1197 |
| 75 | RB | 0.92 | 4/75401 (0.0%) | 0.94 | 90/117598 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | SB | 0.88 | 0/3809 | 0.94 | 5/5936 (0.1%) |
| 77 | TB | 0.88 | 0/2864 | 0.89 | 2/4464 (0.0%) |
| 78 | al | 0.98 | 0/165 | 1.02 | 0/256 |
| 79 | bl | 0.36 | 0/3503 | 0.59 | 0/4711 |
| 80 | cl | 0.71 | 1/1534 (0.1%) | 0.94 | 1/2386 (0.0%) |
| 81 | dl | 0.89 | 0/68 | 0.97 | 0/103 |
| All | All | 0.71 | 5/215460 (0.0%) | 0.81 | 174/315917 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 10 | la | 0 | 1 |
| 12 | na | 0 | 1 |
| 18 | ta | 0 | 2 |
| 25 | bb | 0 | 1 |
| 61 | CB | 0 | 1 |
| 71 | MB | 0 | 2 |
| 79 | bl | 0 | 2 |
| All | All | 0 | 10 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 80 | cl | 1 | A | OP3-P | -10.87 | 1.48 | 1.61 |
| 75 | RB | 26 | A | N9-C4 | -6.64 | 1.33 | 1.37 |
| 75 | RB | 702 | G | N9-C4 | -5.62 | 1.33 | 1.38 |
| 75 | RB | 1659 | G | N9-C4 | -5.13 | 1.33 | 1.38 |
| 75 | RB | 26 | A | N3-C4 | -5.02 | 1.31 | 1.34 |

The worst 5 of 174 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | aa | 1441 | C | C2-N1-C1' | 9.07 | 128.78 | 118.80 |
| 1 | aa | 457 | C | C2-N1-C1' | 8.71 | 128.38 | 118.80 |
| 75 | RB | 26 | A | C2-N3-C4 | -8.62 | 106.29 | 110.60 |
| 9 | ka | 98 | LEU | CA-CB-CG | 8.41 | 134.64 | 115.30 |
| 75 | RB | 1659 | G | N3-C4-N9 | -8.33 | 121.00 | 126.00 |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 25 | bb | 178 | SER | Peptide |
| 10 | la | 46 | ARG | Peptide |
| 12 | na | 137 | THR | Peptide |
| 18 | ta | 33 | GLN | Peptide |
| 18 | ta | 76 | LEU | Peptide |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | ba | 111/137 (81%) | 101 (91%) | 10 (9%) | 0 | 100 | 100 |
| 3 | ca | 174/225 (77%) | 162 (93%) | 12 (7%) | 0 | 100 | 100 |
| 4 | da | 79/188 (42%) | 68 (86%) | 11 (14%) | 0 | 100 | 100 |
| 5 | ga | 136/142 (96%) | 130 (96%) | 6 (4%) | 0 | 100 | 100 |
| 6 | ha | 320/332 (96%) | 257 (80%) | 63 (20%) | 0 | 100 | 100 |
| 7 | ia | 211/227 (93%) | 195 (92%) | 16 (8%) | 0 | 100 | 100 |
| 8 | ja | 259/265 (98%) | 240 (93%) | 19 (7%) | 0 | 100 | 100 |
| 9 | ka | 191/200 (96%) | 177 (93%) | 14 (7%) | 0 | 100 | 100 |
| 10 | la | 138/149 (93%) | 123 (89%) | 15 (11%) | 0 | 100 | 100 |
| 11 | ma | 101/127 (80%) | 94 (93%) | 7 (7%) | 0 | 100 | 100 |
| 12 | na | 123/151 (82%) | 114 (93%) | 9 (7%) | 0 | 100 | 100 |
| 13 | oa | 134/152 (88%) | 124 (92%) | 10 (8%) | 0 | 100 | 100 |
| 14 | pa | 148/151 (98%) | 145 (98%) | 3 (2%) | 0 | 100 | 100 |
| 15 | qa | 117/143 (82%) | 105 (90%) | 11 (9%) | 1 (1%) | 17 | 48 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 16 | ra | 133/155 (86%) | 124 (93%) | 9 (7%) | 0 | 100 | 100 |
| 17 | sa | 98/154 (64%) | 84 (86%) | 14 (14%) | 0 | 100 | 100 |
| 18 | ta | 75/108 (69%) | 60 (80%) | 15 (20%) | 0 | 100 | 100 |
| 19 | ua | 62/86 (72%) | 58 (94%) | 4 (6%) | 0 | 100 | 100 |
| 20 | va | 126/129 (98%) | 116 (92%) | 8 (6%) | 2 (2%) | 9 | 32 |
| 21 | wa | 37/56 (66%) | 37 (100%) | 0 | 0 | 100 | 100 |
| 22 | xa | 68/86 (79%) | 60 (88%) | 8 (12%) | 0 | 100 | 100 |
| 23 | ya | 37/62 (60%) | 32 (86%) | 5 (14%) | 0 | 100 | 100 |
| 24 | za | 200/308 (65%) | 193 (96%) | 7 (4%) | 0 | 100 | 100 |
| 25 | bb | 209/263 (80%) | 186 (89%) | 23 (11%) | 0 | 100 | 100 |
| 26 | cb | 74/82 (90%) | 67 (90%) | 7 (10%) | 0 | 100 | 100 |
| 27 | db | 93/156 (60%) | 91 (98%) | 2 (2%) | 0 | 100 | 100 |
| 28 | eb | 179/195 (92%) | 166 (93%) | 13 (7%) | 0 | 100 | 100 |
| 29 | fb | 212/274 (77%) | 201 (95%) | 11 (5%) | 0 | 100 | 100 |
| 30 | gb | 147/250 (59%) | 135 (92%) | 12 (8%) | 0 | 100 | 100 |
| 31 | hb | 167/192 (87%) | 144 (86%) | 22 (13%) | 1 (1%) | 25 | 58 |
| 32 | ib | 143/159 (90%) | 139 (97%) | 4 (3%) | 0 | 100 | 100 |
| 33 | AA | 227/258 (88%) | 210 (92%) | 17 (8%) | 0 | 100 | 100 |
| 34 | BA | 154/164 (94%) | 146 (95%) | 8 (5%) | 0 | 100 | 100 |
| 35 | CA | 134/137 (98%) | 123 (92%) | 11 (8%) | 0 | 100 | 100 |
| 36 | DA | 249/261 (95%) | 241 (97%) | 8 (3%) | 0 | 100 | 100 |
| 37 | EA | 162/180 (90%) | 144 (89%) | 18 (11%) | 0 | 100 | 100 |
| 38 | FA | 183/189 (97%) | 173 (94%) | 10 (6%) | 0 | 100 | 100 |
| 39 | GA | 127/140 (91%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |
| 40 | HA | 201/204 (98%) | 192 (96%) | 9 (4%) | 0 | 100 | 100 |
| 41 | IA | 142/145 (98%) | 136 (96%) | 6 (4%) | 0 | 100 | 100 |
| 42 | JA | 184/187 (98%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 43 | KA | 269/301 (89%) | 257 (96%) | 12 (4%) | 0 | 100 | 100 |
| 44 | LA | 168/213 (79%) | 163 (97%) | 5 (3%) | 0 | 100 | 100 |
| 45 | MA | 153/170 (90%) | 147 (96%) | 6 (4%) | 0 | 100 | 100 |
| 46 | NA | 114/152 (75%) | 109 (96%) | 5 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 47 | OA | 59/162 (36%) | 57 (97%) | 2 (3%) | 0 | 100 | 100 |
| 48 | PA | 128/157 (82%) | 126 (98%) | 2 (2%) | 0 | 100 | 100 |
| 49 | QA | 140/147 (95%) | 130 (93%) | 10 (7%) | 0 | 100 | 100 |
| 50 | RA | 96/112 (86%) | 96 (100%) | 0 | 0 | 100 | 100 |
| 51 | SA | 105/123 (85%) | 102 (97%) | 3 (3%) | 0 | 100 | 100 |
| 52 | TA | 124/133 (93%) | 122 (98%) | 2 (2%) | 0 | 100 | 100 |
| 53 | UA | 78/93 (84%) | 72 (92%) | 6 (8%) | 0 | 100 | 100 |
| 54 | VA | 48/76 (63%) | 48 (100%) | 0 | 0 | 100 | 100 |
| 55 | WA | 96/105 (91%) | 93 (97%) | 3 (3%) | 0 | 100 | 100 |
| 56 | XA | 130/135 (96%) | 124 (95%) | 6 (5%) | 0 | 100 | 100 |
| 57 | YA | 175/178 (98%) | 169 (97%) | 6 (3%) | 0 | 100 | 100 |
| 58 | ZA | 99/130 (76%) | 82 (83%) | 16 (16%) | 1 (1%) | 15 | 45 |
| 59 | AB | 98/112 (88%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 60 | BB | 117/124 (94%) | 105 (90%) | 12 (10%) | 0 | 100 | 100 |
| 61 | CB | 232/244 (95%) | 224 (97%) | 7 (3%) | 1 (0%) | 34 | 66 |
| 62 | DB | 382/389 (98%) | 372 (97%) | 10 (3%) | 0 | 100 | 100 |
| 63 | EB | 397/404 (98%) | 379 (96%) | 18 (4%) | 0 | 100 | 100 |
| 64 | FB | 203/206 (98%) | 196 (97%) | 7 (3%) | 0 | 100 | 100 |
| 65 | GB | 89/92 (97%) | 85 (96%) | 4 (4%) | 0 | 100 | 100 |
| 66 | HB | 201/217 (93%) | 191 (95%) | 10 (5%) | 0 | 100 | 100 |
| 67 | IB | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 68 | JB | 49/129 (38%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 69 | KB | 203/208 (98%) | 192 (95%) | 8 (4%) | 3 (2%) | 10 | 34 |
| 70 | LB | 213/219 (97%) | 189 (89%) | 24 (11%) | 0 | 100 | 100 |
| 71 | MB | 108/112 (96%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 72 | NB | 66/69 (96%) | 61 (92%) | 5 (8%) | 0 | 100 | 100 |
| 73 | OB | 48/60 (80%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 74 | PB | 106/119 (89%) | 102 (96%) | 4 (4%) | 0 | 100 | 100 |
| 79 | bl | 435/437 (100%) | 384 (88%) | 51 (12%) | 0 | 100 | 100 |
| All | All | 11017/12722 (87%) | 10288 (93%) | 720 (6%) | 9 (0%) | 54 | 82 |

5 of 9 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | va | 56 | ARG |
| 58 | ZA | 99 | ARG |
| 69 | KB | 4 | HIS |
| 69 | KB | 63 | ARG |
| 20 | va | 55 | HIS |

### 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 |
|---|---|---|---|---|---|
| 2 | ba | 99/116 (85%) | 97 (98%) | 2 (2%) | 55 82 |
| 3 | ca | 153/181 (84%) | 153 (100%) | 0 | 100 100 |
| 4 | da | 77/143 (54%) | 77 (100%) | 0 | 100 100 |
| 5 | ga | 109/113 (96%) | 109 (100%) | 0 | 100 100 |
| 6 | ha | 274/281 (98%) | 273 (100%) | 1 (0%) | 91 97 |
| 7 | ia | 180/192 (94%) | 180 (100%) | 0 | 100 100 |
| 8 | ja | 222/224 (99%) | 222 (100%) | 0 | 100 100 |
| 9 | ka | 163/169 (96%) | 163 (100%) | 0 | 100 100 |
| 10 | la | 113/120 (94%) | 113 (100%) | 0 | 100 100 |
| 11 | ma | 97/115 (84%) | 97 (100%) | 0 | 100 100 |
| 12 | na | 98/121 (81%) | 97 (99%) | 1 (1%) | 76 92 |
| 13 | oa | 119/133 (90%) | 119 (100%) | 0 | 100 100 |
| 14 | pa | 129/130 (99%) | 128 (99%) | 1 (1%) | 81 94 |
| 15 | qa | 108/126 (86%) | 108 (100%) | 0 | 100 100 |
| 16 | ra | 112/124 (90%) | 112 (100%) | 0 | 100 100 |
| 17 | sa | 87/130 (67%) | 87 (100%) | 0 | 100 100 |
| 18 | ta | 69/92 (75%) | 68 (99%) | 1 (1%) | 67 89 |
| 19 | ua | 57/78 (73%) | 57 (100%) | 0 | 100 100 |
| 20 | va | 110/111 (99%) | 109 (99%) | 1 (1%) | 78 93 |
| 21 | wa | 34/47 (72%) | 33 (97%) | 1 (3%) | 42 76 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 22 | xa | 64/78 (82%) | 63 (98%) | 1 (2%) | 62 86 |
| 23 | ya | 32/49 (65%) | 32 (100%) | 0 | 100 100 |
| 24 | za | 172/233 (74%) | 172 (100%) | 0 | 100 100 |
| 25 | bb | 189/228 (83%) | 188 (100%) | 1 (0%) | 88 96 |
| 26 | cb | 63/68 (93%) | 63 (100%) | 0 | 100 100 |
| 27 | db | 82/113 (73%) | 82 (100%) | 0 | 100 100 |
| 28 | eb | 154/162 (95%) | 153 (99%) | 1 (1%) | 86 96 |
| 29 | fb | 181/219 (83%) | 181 (100%) | 0 | 100 100 |
| 30 | gb | 130/215 (60%) | 128 (98%) | 2 (2%) | 65 87 |
| 31 | hb | 151/171 (88%) | 151 (100%) | 0 | 100 100 |
| 32 | ib | 126/132 (96%) | 125 (99%) | 1 (1%) | 81 94 |
| 33 | AA | 200/222 (90%) | 199 (100%) | 1 (0%) | 88 96 |
| 34 | BA | 135/141 (96%) | 135 (100%) | 0 | 100 100 |
| 35 | CA | 113/114 (99%) | 113 (100%) | 0 | 100 100 |
| 36 | DA | 193/199 (97%) | 193 (100%) | 0 | 100 100 |
| 37 | EA | 142/156 (91%) | 142 (100%) | 0 | 100 100 |
| 38 | FA | 159/163 (98%) | 159 (100%) | 0 | 100 100 |
| 39 | GA | 103/109 (94%) | 102 (99%) | 1 (1%) | 76 92 |
| 40 | HA | 177/178 (99%) | 177 (100%) | 0 | 100 100 |
| 41 | IA | 113/114 (99%) | 113 (100%) | 0 | 100 100 |
| 42 | JA | 156/157 (99%) | 155 (99%) | 1 (1%) | 86 96 |
| 43 | KA | 227/252 (90%) | 227 (100%) | 0 | 100 100 |
| 44 | LA | 150/176 (85%) | 150 (100%) | 0 | 100 100 |
| 45 | MA | 132/144 (92%) | 130 (98%) | 2 (2%) | 65 87 |
| 46 | NA | 104/128 (81%) | 104 (100%) | 0 | 100 100 |
| 47 | OA | 55/133 (41%) | 54 (98%) | 1 (2%) | 59 85 |
| 48 | PA | 115/130 (88%) | 115 (100%) | 0 | 100 100 |
| 49 | QA | 127/132 (96%) | 126 (99%) | 1 (1%) | 81 94 |
| 50 | RA | 86/98 (88%) | 85 (99%) | 1 (1%) | 71 91 |
| 51 | SA | 94/108 (87%) | 94 (100%) | 0 | 100 100 |
| 52 | TA | 114/121 (94%) | 114 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 53 | UA | 69/77 (90%) | 69 (100%) | 0 | 100 100 |
| 54 | VA | 47/73 (64%) | 47 (100%) | 0 | 100 100 |
| 55 | WA | 87/93 (94%) | 87 (100%) | 0 | 100 100 |
| 56 | XA | 114/115 (99%) | 114 (100%) | 0 | 100 100 |
| 57 | YA | 162/163 (99%) | 161 (99%) | 1 (1%) | 86 96 |
| 58 | ZA | 89/106 (84%) | 89 (100%) | 0 | 100 100 |
| 59 | AB | 86/92 (94%) | 86 (100%) | 0 | 100 100 |
| 60 | BB | 105/109 (96%) | 105 (100%) | 0 | 100 100 |
| 61 | CB | 199/205 (97%) | 199 (100%) | 0 | 100 100 |
| 62 | DB | 332/336 (99%) | 332 (100%) | 0 | 100 100 |
| 63 | EB | 317/321 (99%) | 314 (99%) | 3 (1%) | 78 93 |
| 64 | FB | 172/173 (99%) | 171 (99%) | 1 (1%) | 86 96 |
| 65 | GB | 72/73 (99%) | 72 (100%) | 0 | 100 100 |
| 66 | HB | 170/178 (96%) | 170 (100%) | 0 | 100 100 |
| 67 | IB | 24/24 (100%) | 24 (100%) | 0 | 100 100 |
| 68 | JB | 46/115 (40%) | 46 (100%) | 0 | 100 100 |
| 69 | KB | 175/178 (98%) | 175 (100%) | 0 | 100 100 |
| 70 | LB | 182/185 (98%) | 181 (100%) | 1 (0%) | 88 96 |
| 71 | MB | 91/93 (98%) | 91 (100%) | 0 | 100 100 |
| 72 | NB | 62/63 (98%) | 62 (100%) | 0 | 100 100 |
| 73 | OB | 44/51 (86%) | 44 (100%) | 0 | 100 100 |
| 74 | PB | 96/107 (90%) | 95 (99%) | 1 (1%) | 76 92 |
| 79 | bl | 378/378 (100%) | 377 (100%) | 1 (0%) | 92 98 |
| All | All | 9568/10697 (89%) | 9538 (100%) | 30 (0%) | 92 98 |

5 of 30 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | AA | 104 | LYS |
| 70 | LB | 145 | LYS |
| 45 | MA | 121 | ASN |
| 79 | bl | 421 | ARG |
| 63 | EB | 143 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 42 | JA | 89 | GLN |
| 66 | HB | 144 | ASN |
| 79 | bl | 198 | HIS |
| 69 | KB | 61 | GLN |
| 16 | ra | 25 | HIS |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | aa | 1690/1810 (93%) | 466 (27%) | 0 |
| 75 | RB | 3143/3386 (92%) | 684 (21%) | 49 (1%) |
| 76 | SB | 159/160 (99%) | 29 (18%) | 2 (1%) |
| 77 | TB | 119/120 (99%) | 18 (15%) | 2 (1%) |
| 78 | al | 6/7 (85%) | 2 (33%) | 0 |
| 80 | cl | 73/75 (97%) | 31 (42%) | 0 |
| 81 | dl | 2/3 (66%) | 1 (50%) | 0 |
| All | All | 5192/5561 (93%) | 1231 (23%) | 53 (1%) |

5 of 1231 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | aa | 17 | C |
| 1 | aa | 25 | C |
| 1 | aa | 26 | A |
| 1 | aa | 27 | U |
| 1 | aa | 34 | G |

5 of 53 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | RB | 1861 | A |
| 75 | RB | 2539 | C |
| 76 | SB | 72 | A |
| 75 | RB | 2100 | A |
| 75 | RB | 2535 | A |

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

11 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 | $\#\|Z\| > 2$ |
| 80 | 1MG | cl | 9 | 80 | 18,26,27 | 2.59 | 5 (27%) | 19,39,42 | 1.40 | 3 (15%) |
| 80 | PSU | cl | 28 | 80 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.86 | 5 (22%) |
| 80 | 2MG | cl | 10 | 80 | 18,26,27 | 2.53 | 7 (38%) | 16,38,41 | 1.56 | 4 (25%) |
| 80 | MIA | cl | 37 | 80,82 | 24,31,32 | 2.40 | 3 (12%) | 26,44,47 | 3.57 | 7 (26%) |
| 80 | PSU | cl | 55 | 80 | 18,21,22 | 1.10 | 1 (5%) | 22,30,33 | 1.77 | 5 (22%) |
| 80 | G7M | cl | 46 | 80 | 20,26,27 | 2.73 | 7 (35%) | 17,39,42 | 1.09 | 2 (11%) |
| 80 | 5MC | cl | 49 | 80 | 18,22,23 | 3.75 | 8 (44%) | 26,32,35 | 1.03 | 1 (3%) |
| 80 | 1MA | cl | 58 | 80 | 16,25,26 | 4.22 | 4 (25%) | 18,37,40 | 1.69 | 3 (16%) |
| 80 | 2MG | cl | 26 | 80 | 18,26,27 | 2.47 | 6 (33%) | 16,38,41 | 1.54 | 4 (25%) |
| 80 | H2U | cl | 47 | 80 | 18,21,22 | 3.10 | 5 (27%) | 21,30,33 | 2.02 | 5 (23%) |
| 80 | 5MC | cl | 48 | 80 | 18,22,23 | 3.69 | 8 (44%) | 26,32,35 | 1.20 | 2 (7%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 80 | 1MG | cl | 9 | 80 | - | 0/3/25/26 | 0/3/3/3 |
| 80 | PSU | cl | 28 | 80 | - | 0/7/25/26 | 0/2/2/2 |
| 80 | 2MG | cl | 10 | 80 | - | 2/5/27/28 | 0/3/3/3 |
| 80 | MIA | cl | 37 | 80,82 | - | 5/11/33/34 | 0/3/3/3 |
| 80 | PSU | cl | 55 | 80 | - | 1/7/25/26 | 0/2/2/2 |
| 80 | G7M | cl | 46 | 80 | - | 1/3/25/26 | 0/3/3/3 |
| 80 | 5MC | cl | 49 | 80 | - | 3/7/25/26 | 0/2/2/2 |
| 80 | 1MA | cl | 58 | 80 | - | 0/3/25/26 | 0/3/3/3 |
| 80 | 2MG | cl | 26 | 80 | - | 0/5/27/28 | 0/3/3/3 |
| 80 | H2U | cl | 47 | 80 | - | 5/7/38/39 | 0/2/2/2 |
| 80 | 5MC | cl | 48 | 80 | - | 2/7/25/26 | 0/2/2/2 |

The worst 5 of 55 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 80 | cl | 58 | 1MA | C2-N3 | 15.52 | 1.47 | 1.29 |
| 80 | cl | 47 | H2U | C2-N1 | 9.59 | 1.49 | 1.35 |
| 80 | cl | 49 | 5MC | C6-C5 | 9.48 | 1.50 | 1.34 |
| 80 | cl | 48 | 5MC | C6-C5 | 9.25 | 1.49 | 1.34 |
| 80 | cl | 37 | MIA | C2-S10 | 7.86 | 1.82 | 1.75 |

The worst 5 of 41 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | cl | 37 | MIA | C11-S10-C2 | 13.68 | 112.48 | 102.27 |
| 80 | cl | 37 | MIA | C1'-N9-C4 | 9.00 | 142.46 | 126.64 |
| 80 | cl | 47 | H2U | C4-N3-C2 | -7.05 | 119.95 | 125.79 |
| 80 | cl | 28 | PSU | N1-C2-N3 | 4.92 | 120.70 | 115.13 |
| 80 | cl | 58 | 1MA | N1-C2-N3 | -4.78 | 120.45 | 126.02 |

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | cl | 37 | MIA | O4'-C4'-C5'-O5' |
| 80 | cl | 37 | MIA | C13-C12-N6-C6 |
| 80 | cl | 37 | MIA | N1-C2-S10-C11 |
| 80 | cl | 37 | MIA | N3-C2-S10-C11 |
| 80 | cl | 47 | H2U | C4'-C5'-O5'-P |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 311 ligands modelled in this entry, 311 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)

There are no chain breaks in this entry.

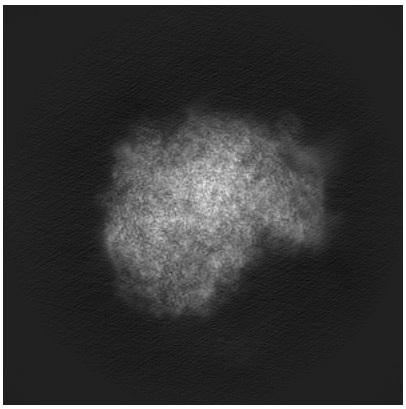
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35634. These allow visual inspection of the internal detail of the map and identification of artifacts.

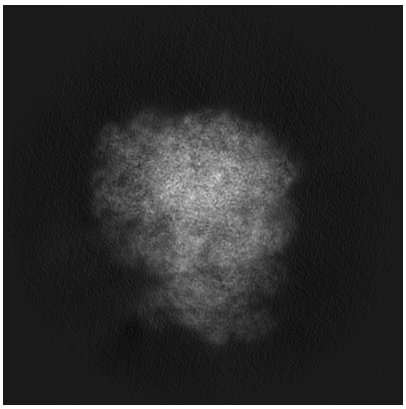
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

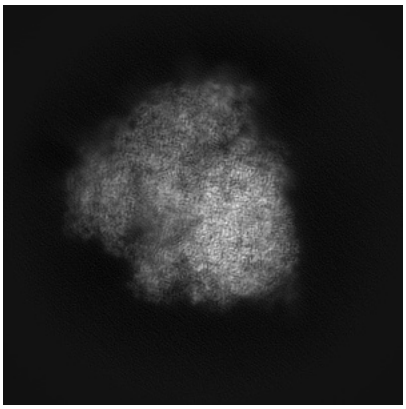
### 6.1.1 Primary map



X

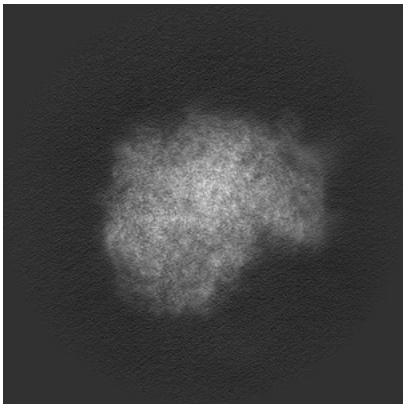


Y

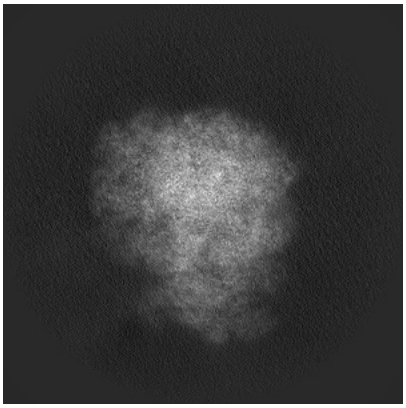


Z

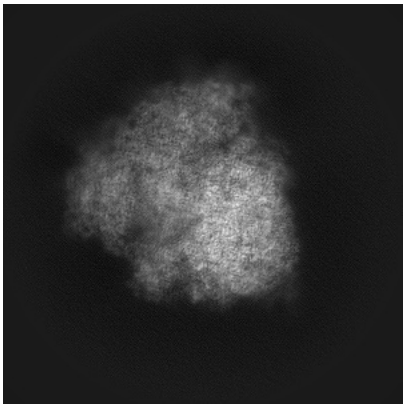
### 6.1.2 Raw map



X



Y

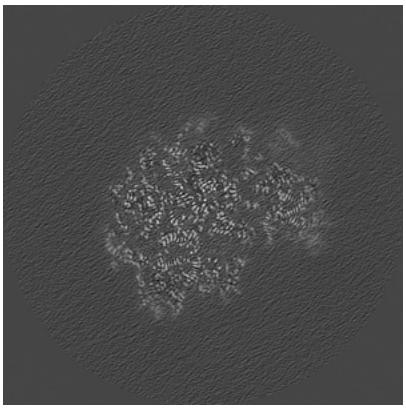


Z

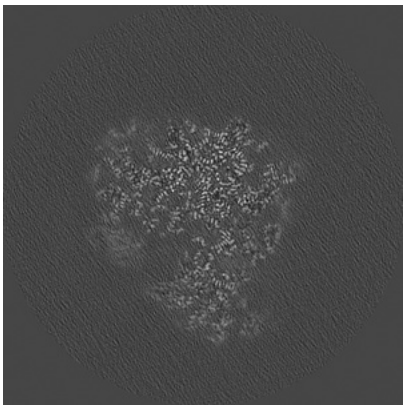
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

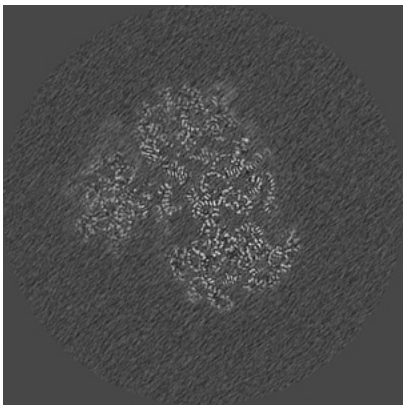
### 6.2.1 Primary map



X Index: 280

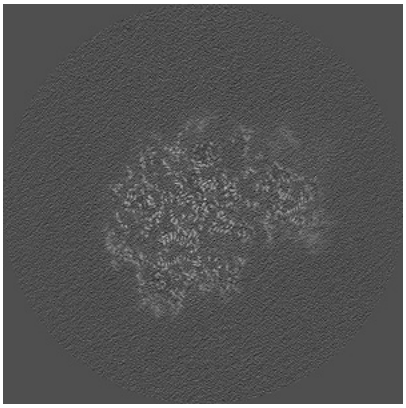


Y Index: 280

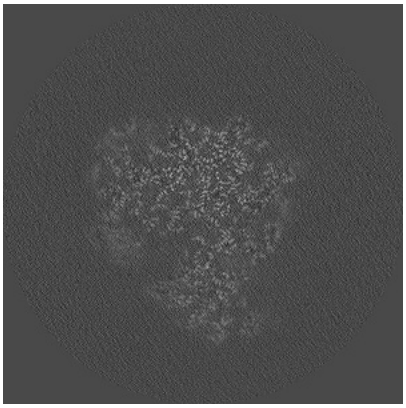


Z Index: 280

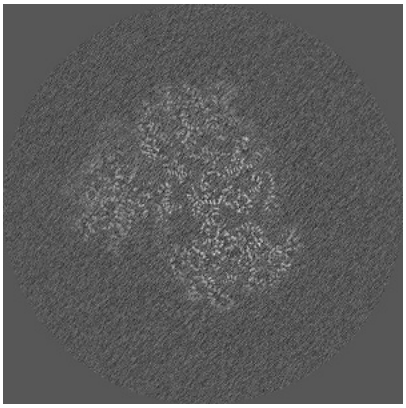
### 6.2.2 Raw map



X Index: 280



Y Index: 280

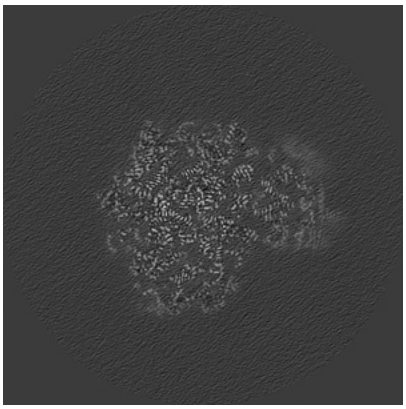


Z Index: 280

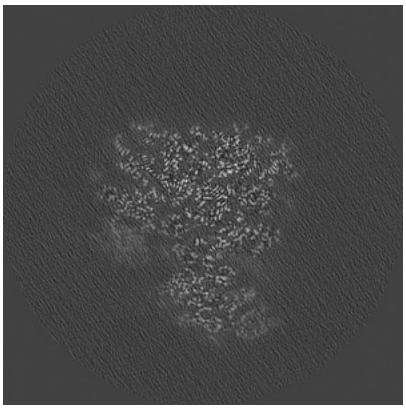
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

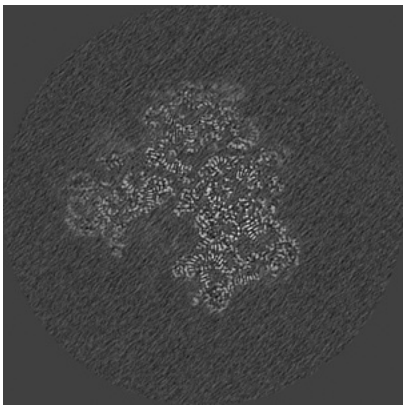
### 6.3.1 Primary map



X Index: 297

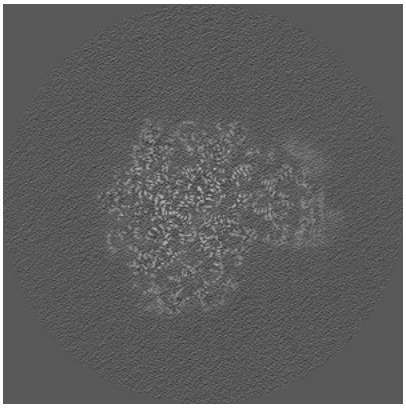


Y Index: 291

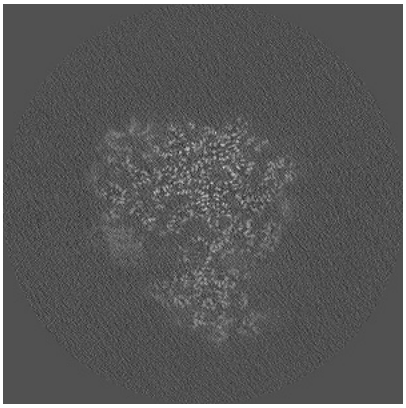


Z Index: 291

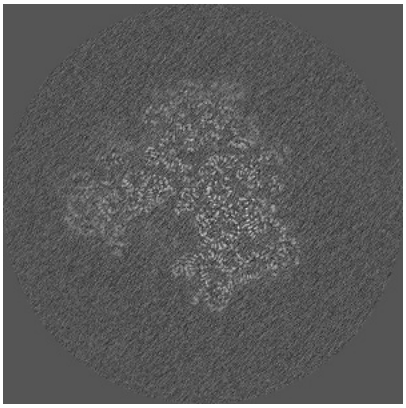
### 6.3.2 Raw map



X Index: 298



Y Index: 282

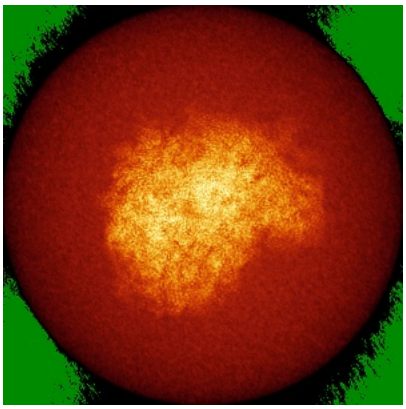


Z Index: 291

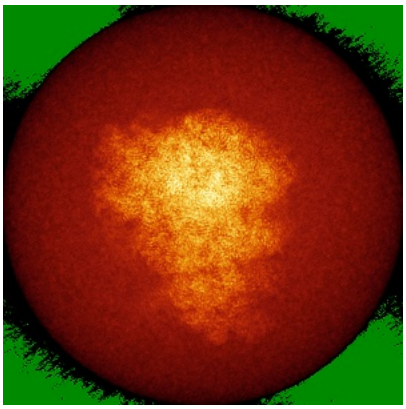
The images above show the largest variance slices of the map in three orthogonal directions.

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

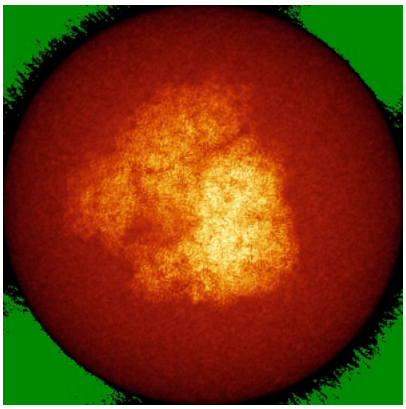
### 6.4.1 Primary map



X

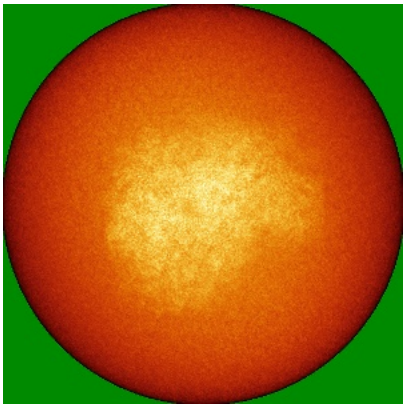


Y

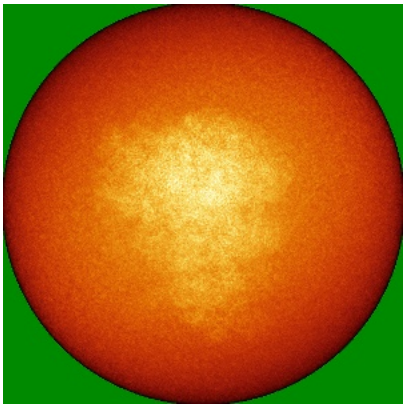


Z

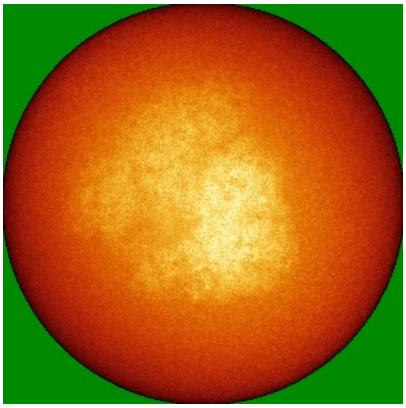
### 6.4.2 Raw map



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 0.016. 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.

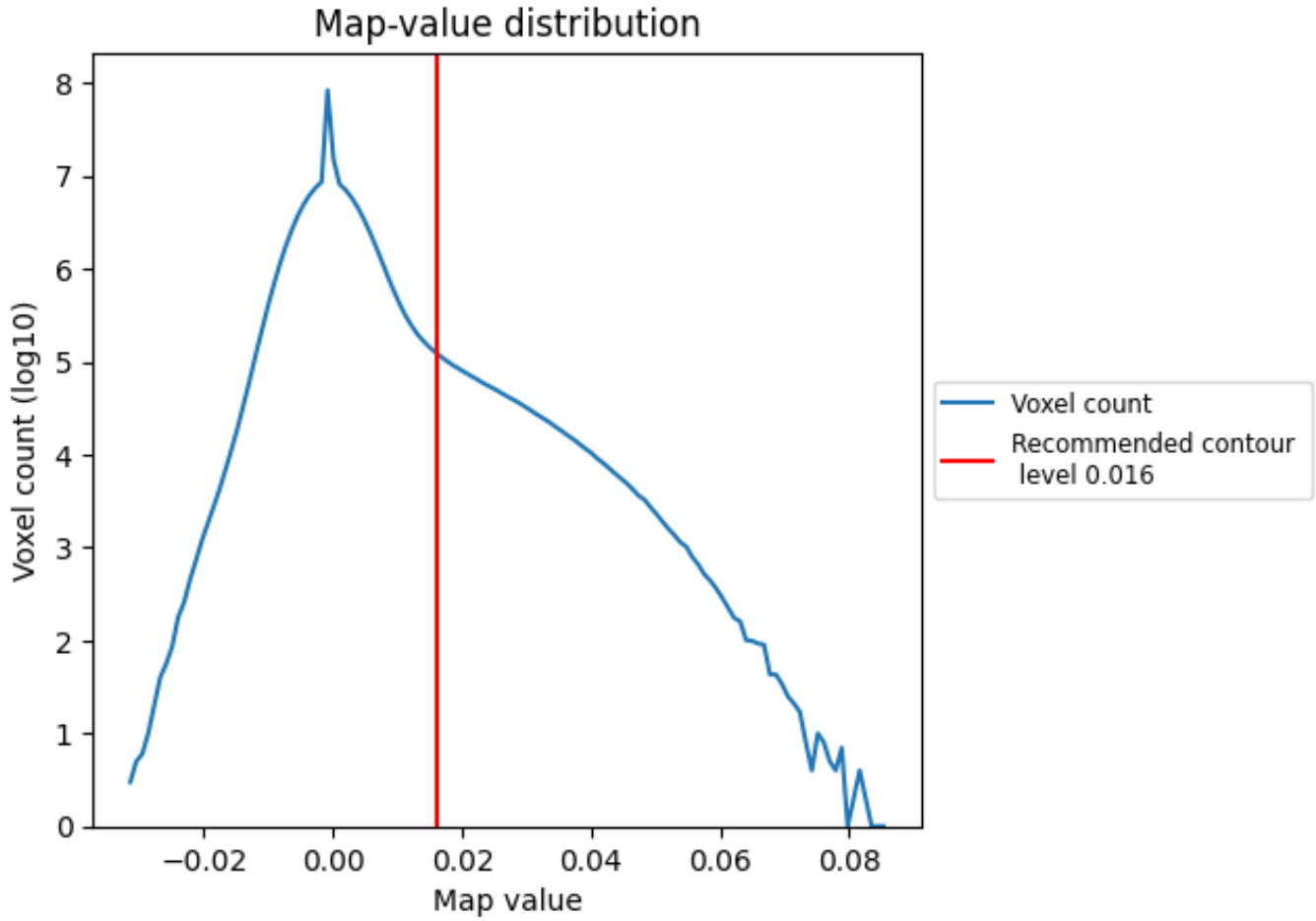
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

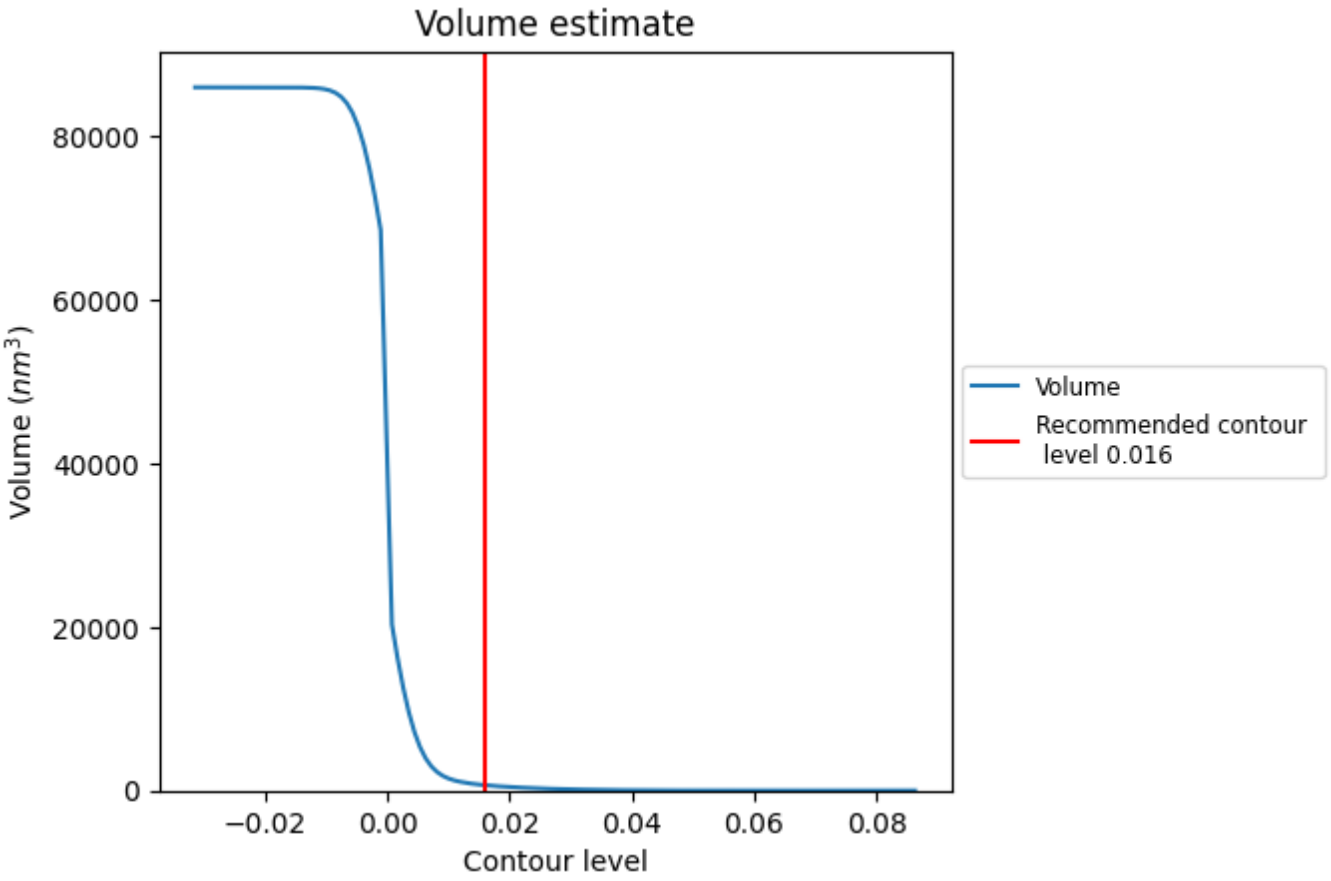
This section contains the results of statistical analysis of the map.

## 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.

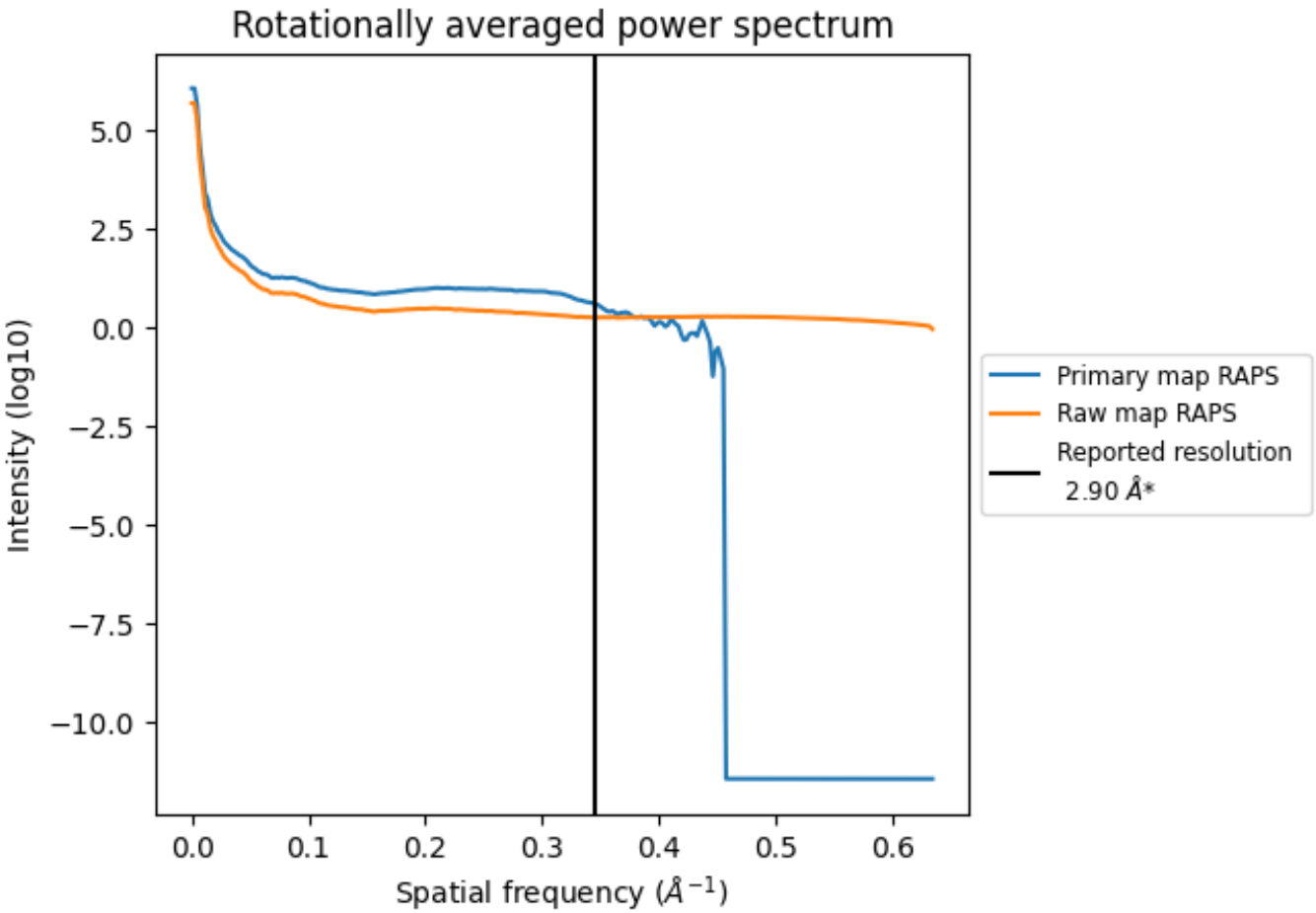
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 659 $nm^3$; this corresponds to an approximate mass of 596 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)

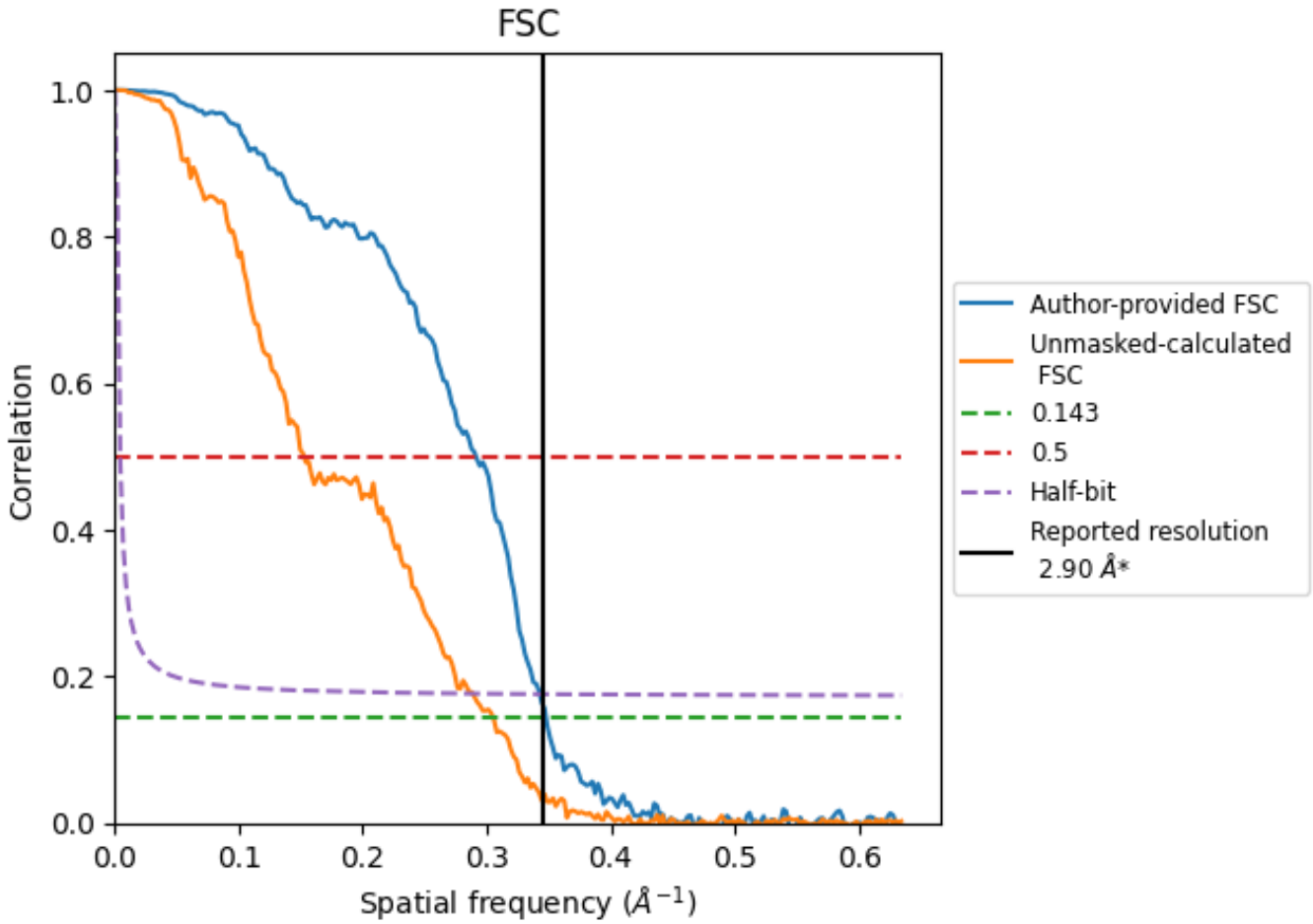



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

# 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 0.345 Å$^{-1}$

## 8.2 Resolution estimates (i)

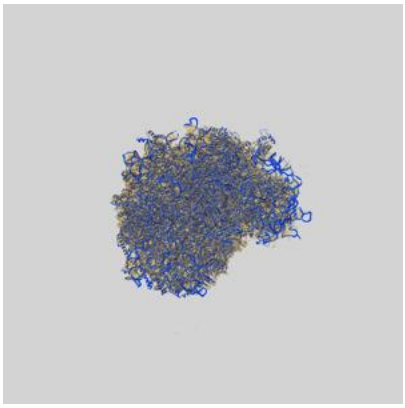
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.90 | - | - |
| Author-provided FSC curve | 2.87 | 3.43 | 2.92 |
| Unmasked-calculated* | 3.28 | 6.55 | 3.47 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.9 by more than 10 %

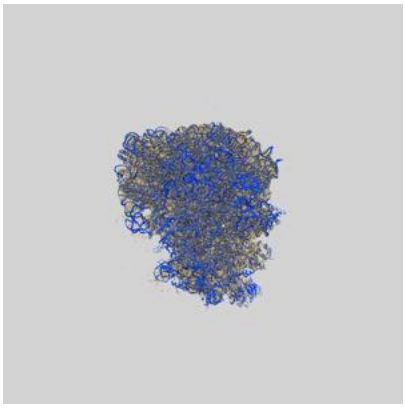
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35634 and PDB model 8IP8. Per-residue inclusion information can be found in section 3 on page 20.

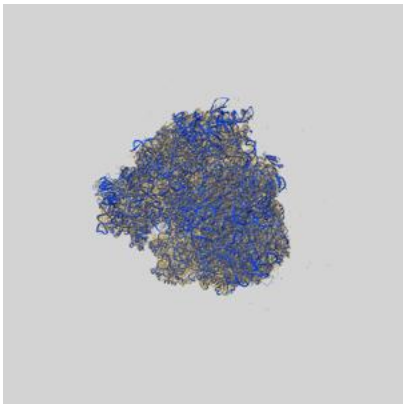
## 9.1 Map-model overlay



X



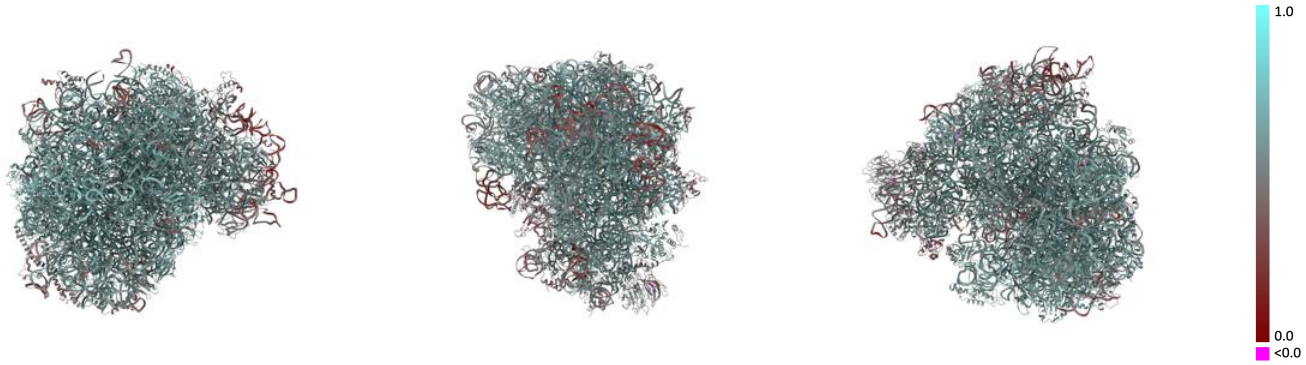
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

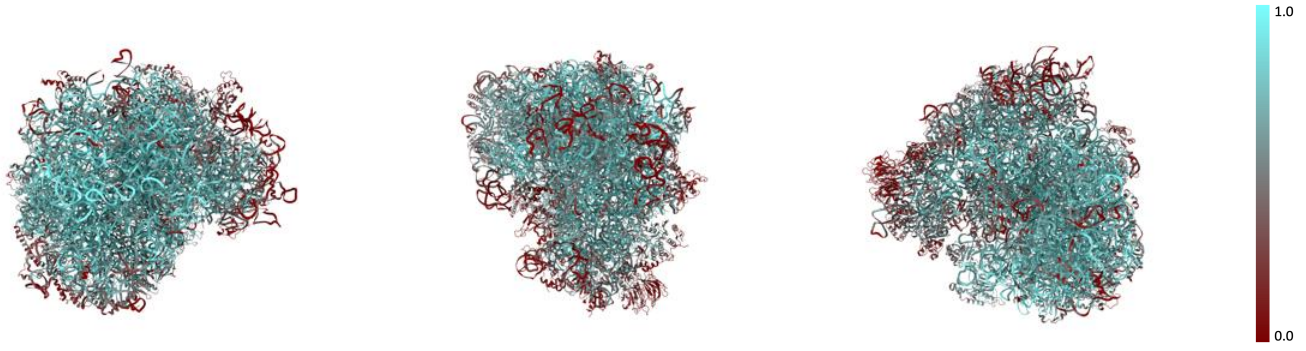
## 9.2 Q-score mapped to coordinate model




X Y Z

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

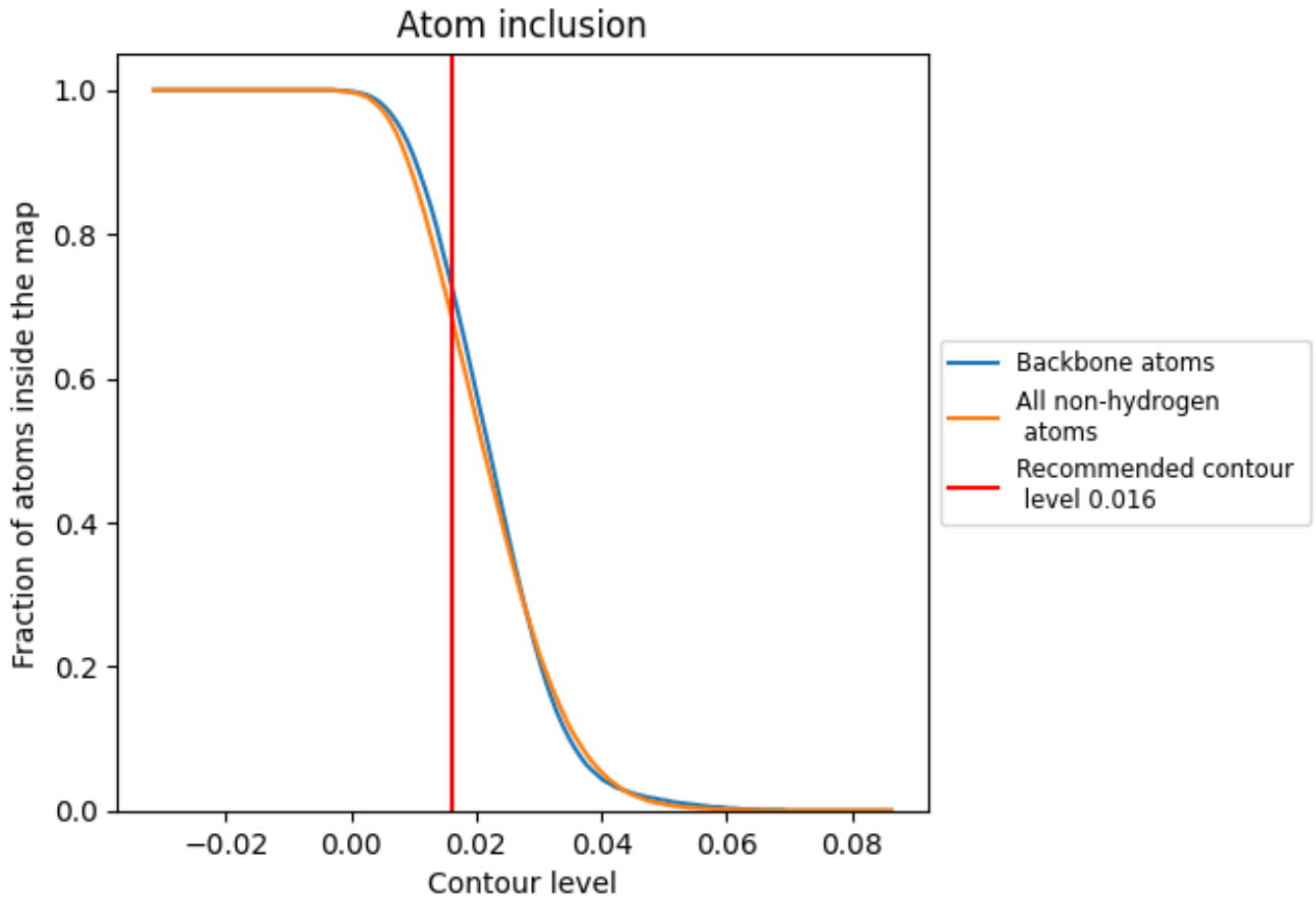
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

## 9.4 Atom inclusion (i)




At the recommended contour level, 73% of all backbone atoms, 69% 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 (0.016) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6880 | 0.5790 |
| AA | 0.4970 | 0.5480 |
| AB | 0.6150 | 0.5750 |
| BA | 0.7200 | 0.6160 |
| BB | 0.6070 | 0.5620 |
| CA | 0.5690 | 0.5620 |
| CB | 0.6990 | 0.6060 |
| DA | 0.8340 | 0.6480 |
| DB | 0.7490 | 0.6250 |
| EA | 0.5150 | 0.5480 |
| EB | 0.6570 | 0.5960 |
| FA | 0.5690 | 0.5820 |
| FB | 0.7050 | 0.6140 |
| GA | 0.7790 | 0.6380 |
| GB | 0.7510 | 0.6160 |
| HA | 0.8720 | 0.6480 |
| HB | 0.5580 | 0.5680 |
| IA | 0.8210 | 0.6430 |
| IB | 0.7390 | 0.5990 |
| JA | 0.7820 | 0.6360 |
| JB | 0.6920 | 0.6070 |
| KA | 0.6090 | 0.5850 |
| KB | 0.6930 | 0.6040 |
| LA | 0.6980 | 0.6000 |
| LB | 0.3890 | 0.5180 |
| MA | 0.7670 | 0.6320 |
| MB | 0.7820 | 0.6330 |
| NA | 0.6470 | 0.5930 |
| NB | 0.4690 | 0.5460 |
| OA | 0.7330 | 0.6170 |
| OB | 0.8060 | 0.6350 |
| PA | 0.7100 | 0.6060 |
| PB | 0.7800 | 0.6170 |
| QA | 0.6190 | 0.5970 |
| RA | 0.6220 | 0.5910 |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*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| RB | 0.8260 | 0.6060 |
| SA | 0.6430 | 0.5970 |
| SB | 0.8110 | 0.5950 |
| TA | 0.8030 | 0.6370 |
| TB | 0.8580 | 0.6160 |
| UA | 0.8970 | 0.6530 |
| VA | 0.8270 | 0.6420 |
| WA | 0.7550 | 0.6360 |
| XA | 0.5650 | 0.5710 |
| YA | 0.7220 | 0.6110 |
| ZA | 0.2980 | 0.5010 |
| aa | 0.6890 | 0.5500 |
| al | 0.8780 | 0.6260 |
| ba | 0.3160 | 0.5060 |
| bb | 0.4530 | 0.5250 |
| bl | 0.3470 | 0.4640 |
| ca | 0.6100 | 0.5750 |
| cb | 0.5440 | 0.5630 |
| cl | 0.5490 | 0.5220 |
| da | 0.2210 | 0.4170 |
| db | 0.6790 | 0.6050 |
| dl | 0.7420 | 0.6120 |
| eb | 0.5270 | 0.5570 |
| fb | 0.6480 | 0.6020 |
| ga | 0.7020 | 0.6130 |
| gb | 0.2790 | 0.4800 |
| ha | 0.1240 | 0.4430 |
| hb | 0.2680 | 0.4780 |
| ia | 0.3600 | 0.5320 |
| ib | 0.7000 | 0.6170 |
| ja | 0.5240 | 0.5610 |
| ka | 0.4540 | 0.5440 |
| la | 0.4430 | 0.5360 |
| ma | 0.3200 | 0.4960 |
| na | 0.5600 | 0.5670 |
| oa | 0.3440 | 0.5040 |
| pa | 0.6350 | 0.5930 |
| qa | 0.2790 | 0.4920 |
| ra | 0.4460 | 0.5220 |
| sa | 0.2240 | 0.4990 |
| ta | 0.1740 | 0.3080 |
| ua | 0.3690 | 0.5320 |

*Continued on next page...*

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| va | 0.6620 | 0.5650 |
| wa | 0.7040 | 0.5760 |
| xa | 0.4680 | 0.5390 |
| ya | 0.5110 | 0.5580 |
| za | 0.4860 | 0.5740 |