# wwPDB EM Validation Summary Report

Nov 19, 2022 – 10:51 PM EST

| | | |
|---|---|---|
| PDB ID | : | 3J9M |
| EMDB ID | : | EMD-2876 |
| Title | : | Structure of the human mitochondrial ribosome (class 1) |
| Authors | : | Amunts, A.; Brown, A.; Toots, J.; Scheres, S.H.; Ramakrishnan, V. |
| Deposited on | : | 2015-02-08 |
| Resolution | : | 3.50 Å(reported) |

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

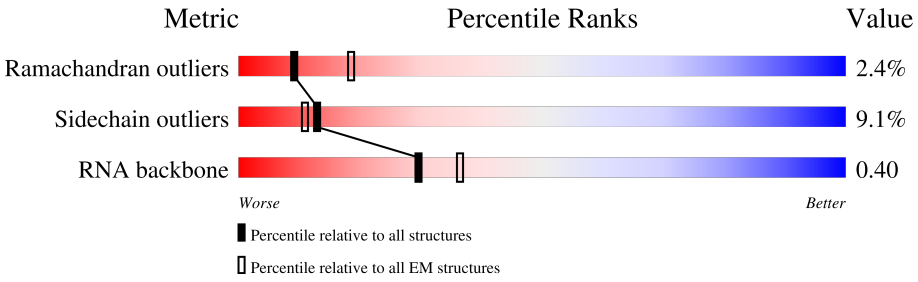
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 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 3.50 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%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1559 | 63% 31% · 6% |
| 2 | B | 73 | 49% 26% · 23% |
| 3 | D | 305 | 71% 7% 23% |
| 4 | E | 348 | 77% 9% 14% |
| 5 | F | 311 | 72% 8% 20% |
| 6 | H | 267 | 34% · 64% |
| 7 | I | 261 | 54% 6% 39% |
| 8 | J | 192 | 67% 6% 27% |
| 9 | K | 178 | 89% 10% ·· |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | L | 145 | 71% 8% 21% |
| 11 | M | 296 | 86% 11% |
| 12 | N | 251 | 73% 8% 18% |
| 13 | O | 175 | 74% 12% 13% |
| 14 | P | 179 | 65% 8% 26% |
| 15 | Q | 292 | 67% 7% 25% |
| 16 | R | 149 | 83% 10% 6% |
| 17 | S | 205 | 70% 6% 24% |
| 18 | T | 212 | 75% 22% |
| 19 | U | 153 | 63% 9% 27% |
| 20 | V | 216 | 80% 7% 12% |
| 21 | W | 148 | 69% 6% 25% |
| 22 | X | 256 | 85% 9% 5% |
| 23 | Y | 250 | 65% 6% 30% |
| 24 | Z | 161 | 68% 6% 25% |
| 25 | 0 | 188 | 47% 9% 43% |
| 26 | 1 | 65 | 69% 11% 20% |
| 27 | 2 | 92 | 46% 50% |
| 28 | 3 | 188 | 47% 49% |
| 29 | 4 | 103 | 31% 65% |
| 30 | 5 | 423 | 79% 10% 11% |
| 31 | 6 | 380 | 78% 8% 14% |
| 32 | 7 | 338 | 74% 5% 21% |
| 33 | 8 | 206 | 46% 52% |
| 34 | 9 | 137 | 73% 7% 20% |

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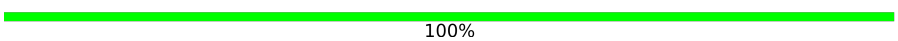
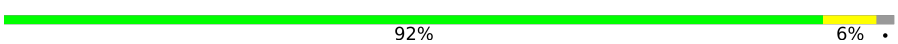
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 35 | a | 142 |   |
| 36 | b | 155 |   |
| 37 | c | 332 |   |
| 38 | d | 306 |   |
| 39 | e | 279 |   |
| 40 | f | 194 |   |
| 41 | g | 166 |   |
| 42 | h | 158 |   |
| 43 | i | 128 |   |
| 44 | j | 123 |   |
| 45 | k | 112 |   |
| 46 | l | 138 |   |
| 47 | m | 128 |   |
| 48 | o | 102 |   |
| 49 | p | 206 |   |
| 50 | q | 222 |   |
| 51 | r | 196 |   |
| 52 | s | 439 |   |
| 53 | t | 28 |   |
| 54 | u | 2 |   |
| 55 | AA | 954 |   |
| 56 | AB | 296 |   |
| 57 | AC | 167 |   |
| 58 | AD | 430 |   |
| 59 | AE | 125 |   |

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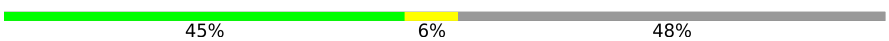
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 60 | AF | 242 |   |
| 61 | AG | 396 |   |
| 62 | AH | 201 |   |
| 63 | AI | 194 |   |
| 64 | AJ | 138 |   |
| 65 | AK | 128 |   |
| 66 | AL | 257 |   |
| 67 | AM | 137 |   |
| 68 | AN | 130 |   |
| 69 | AO | 258 |   |
| 70 | AP | 142 |   |
| 71 | AQ | 87 |   |
| 72 | AR | 360 |   |
| 73 | AS | 190 |   |
| 74 | AT | 173 |   |
| 75 | AU | 205 |   |
| 76 | AV | 414 |   |
| 77 | AW | 187 |   |
| 78 | AX | 398 |   |
| 79 | AY | 395 |   |
| 80 | AZ | 106 |   |
| 81 | A0 | 218 |   |
| 82 | A1 | 323 |   |
| 83 | A2 | 118 |   |
| 84 | A3 | 199 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 85 | A4 | 579 |   |

# 2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 158384 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 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | A | 1472 | 31261 | 14025 | 5642 | 10122 | 1472 | 0 | 0 |

- Molecule 2 is a RNA chain called mt-tRNAVal.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | B | 56 | 1191 | 534 | 214 | 387 | 56 | 0 | 0 |

- Molecule 3 is a protein called uL2m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | D | 236 | 1842 | 1145 | 373 | 315 | 9 | 0 | 0 |

- Molecule 4 is a protein called uL3m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | E | 300 | 2365 | 1523 | 410 | 422 | 10 | 0 | 0 |

- Molecule 5 is a protein called uL4m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | F | 250 | 2013 | 1294 | 365 | 348 | 6 | 0 | 0 |

- Molecule 6 is a protein called bL9m.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 6 | H | 95 | 784 | 498 | 152 | 134 | 0 | 0 |

- Molecule 7 is a protein called uL10m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | I | 158 | Total | C | N | O | S | 0 | 0 |
| | | | 1283 | 828 | 235 | 210 | 10 | | |

- Molecule 8 is a protein called uL11m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | J | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1061 | 680 | 192 | 187 | 2 | | |

- Molecule 9 is a protein called uL13m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | K | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1451 | 934 | 259 | 251 | 7 | | |

- Molecule 10 is a protein called uL14m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | L | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 889 | 559 | 171 | 154 | 5 | | |

- Molecule 11 is a protein called uL15m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | M | 287 | Total | C | N | O | S | 0 | 0 |
| | | | 2305 | 1472 | 425 | 402 | 6 | | |

- Molecule 12 is a protein called uL16m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | N | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1654 | 1056 | 308 | 280 | 10 | | |

- Molecule 13 is a protein called bL17m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | O | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1245 | 784 | 239 | 215 | 7 | | |

- Molecule 14 is a protein called uL18m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | P | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1080 | 677 | 209 | 189 | 5 | | |

- Molecule 15 is a protein called bL19m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | Q | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1822 | 1168 | 322 | 323 | 9 | | |

- Molecule 16 is a protein called bL20m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | R | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1153 | 732 | 231 | 186 | 4 | | |

- Molecule 17 is a protein called bL21m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | S | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1251 | 806 | 222 | 219 | 4 | | |

- Molecule 18 is a protein called uL22m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | T | 166 | Total | C | N | O | S | 0 | 0 |
| | | | 1368 | 875 | 254 | 232 | 7 | | |

- Molecule 19 is a protein called uL23m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | U | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 922 | 591 | 176 | 153 | 2 | | |

- Molecule 20 is a protein called uL24m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | V | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1551 | 987 | 278 | 278 | 8 | | |

- Molecule 21 is a protein called bL27m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | W | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 558 | 164 | 146 | 3 | | |

- Molecule 22 is a protein called bL28m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | X | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 2027 | 1310 | 350 | 362 | 5 | | |

- Molecule 23 is a protein called uL29m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | Y | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1517 | 970 | 291 | 252 | 4 | | |

- Molecule 24 is a protein called uL30m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | Z | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 978 | 626 | 183 | 166 | 3 | | |

- Molecule 25 is a protein called bL32m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | 0 | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 880 | 545 | 172 | 157 | 6 | | |

- Molecule 26 is a protein called bL33m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 1 | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 433 | 278 | 83 | 70 | 2 | | |

- Molecule 27 is a protein called bL34m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 376 | 233 | 83 | 59 | 1 | | |

- Molecule 28 is a protein called bL35m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | 3 | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 831 | 539 | 162 | 127 | 3 | | |

- Molecule 29 is a protein called bL36m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | 4 | 36 | Total | C | N | O | S | 0 | 0 |
| | | | 322 | 203 | 70 | 46 | 3 | | |

- Molecule 30 is a protein called mL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 5 | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 3064 | 1987 | 529 | 538 | 10 | | |

- Molecule 31 is a protein called mL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | 6 | 325 | Total | C | N | O | S | 0 | 0 |
| | | | 2636 | 1692 | 465 | 470 | 9 | | |

- Molecule 32 is a protein called mL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 7 | 266 | Total | C | N | O | S | 0 | 0 |
| | | | 2158 | 1383 | 371 | 388 | 16 | | |

- Molecule 33 is a protein called mL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | 8 | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 836 | 535 | 144 | 155 | 2 | | |

- Molecule 34 is a protein called mL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | 9 | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 873 | 565 | 152 | 154 | 2 | | |

- Molecule 35 is a protein called mL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | a | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 686 | 434 | 124 | 123 | 5 | | |

- Molecule 36 is a protein called mL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | b | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1178 | 733 | 229 | 213 | 3 | | |

- Molecule 37 is a protein called mL44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | c | 275 | Total | C | N | O | S | 0 | 0 |
| | | | 2217 | 1415 | 383 | 410 | 9 | | |

- Molecule 38 is a protein called mL45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | d | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1347 | 870 | 234 | 235 | 8 | | |

- Molecule 39 is a protein called mL46.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | e | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1762 | 1124 | 310 | 323 | 5 | | |

- Molecule 40 is a protein called mL48.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | f | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1039 | 663 | 169 | 203 | 4 | | |

- Molecule 41 is a protein called mL49.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | g | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1067 | 690 | 185 | 190 | 2 | | |

- Molecule 42 is a protein called mL50.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | h | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 827 | 524 | 146 | 155 | 2 | | |

- Molecule 43 is a protein called mL51.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | i | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 827 | 532 | 165 | 126 | 4 | | |

- Molecule 44 is a protein called mL52.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | j | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 684 | 423 | 133 | 126 | 2 | | |

- Molecule 45 is a protein called mL53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | k | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 655 | 407 | 122 | 121 | 5 | | |

- Molecule 46 is a protein called mL54.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 46 | l | 23 | Total | C | N | O | 0 | 0 |
| | | | 221 | 137 | 52 | 32 | | |

- Molecule 47 is a protein called bL31m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | m | 45 | Total | C | N | O | S | 0 | 0 |
| | | | 372 | 232 | 76 | 62 | 2 | | |

- Molecule 48 is a protein called mL63.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | o | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 797 | 501 | 165 | 128 | 3 | | |

- Molecule 49 is a protein called mL62 (ICT1).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | p | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1058 | 661 | 201 | 192 | 4 | | |

- Molecule 50 is a protein called mL64 (CRIF1).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | q | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1076 | 671 | 208 | 192 | 5 | | |

- Molecule 51 is a protein called mL66 (bS18a).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | r | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1203 | 764 | 232 | 199 | 8 | | |

- Molecule 52 is a protein called mL65 (mS30).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | s | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 3036 | 1946 | 542 | 534 | 14 | | |

- Molecule 53 is a protein called Unknown protein/protein extension.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 53 | t | 28 | Total | C | N | O | 0 | 0 |
| | | | 140 | 84 | 28 | 28 | | |

- Molecule 54 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | u | 2 | Total | C | N | O | P | 0 | 0 |
| | | | 42 | 19 | 8 | 13 | 2 | | |

- Molecule 55 is a RNA chain called 12S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | AA | 923 | Total | C | N | O | P | 0 | 0 |
| | | | 19606 | 8790 | 3535 | 6358 | 923 | | |

- Molecule 56 is a protein called uS2m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | AB | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1768 | 1131 | 321 | 306 | 10 | | |

- Molecule 57 is a protein called uS3m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | AC | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1082 | 699 | 195 | 184 | 4 | | |

- Molecule 58 is a protein called uS5m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | AD | 322 | Total | C | N | O | S | 0 | 0 |
| | | | 2557 | 1611 | 476 | 457 | 13 | | |

- Molecule 59 is a protein called bS6m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | AE | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 972 | 614 | 177 | 177 | 4 | | |

- Molecule 60 is a protein called uS7m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | AF | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1668 | 1069 | 305 | 283 | 11 | | |

- Molecule 61 is a protein called uS9m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | AG | 305 | Total | C | N | O | S | 0 | 0 |
| | | | 2516 | 1599 | 448 | 455 | 14 | | |

- Molecule 62 is a protein called uS10m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | AH | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 999 | 643 | 168 | 185 | 3 | | |

- Molecule 63 is a protein called uS11m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | AI | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 637 | 192 | 178 | 4 | | |

- Molecule 64 is a protein called uS12m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | AJ | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 838 | 521 | 169 | 142 | 6 | | |

- Molecule 65 is a protein called uS14m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | AK | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 861 | 537 | 179 | 140 | 5 | | |

- Molecule 66 is a protein called uS15m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | AL | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1382 | 883 | 257 | 235 | 7 | | |

- Molecule 67 is a protein called bS16m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | AM | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 920 | 582 | 182 | 150 | 6 | | |

- Molecule 68 is a protein called uS17m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | AN | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 846 | 549 | 153 | 141 | 3 | | |

- Molecule 69 is a protein called mS40 (bS18b).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | AO | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1528 | 970 | 285 | 267 | 6 | | |

- Molecule 70 is a protein called bS18m (bS18c).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | AP | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 774 | 498 | 133 | 135 | 8 | | |

- Molecule 71 is a protein called bS21m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | AQ | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 458 | 150 | 124 | 8 | | |

- Molecule 72 is a protein called mS22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | AR | 242 | Total | C | N | O | S | 0 | 0 |
| | | | 2008 | 1285 | 343 | 372 | 8 | | |

- Molecule 73 is a protein called mS23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | AS | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1042 | 673 | 183 | 185 | 1 | | |

- Molecule 74 is a protein called mS25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | AT | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1330 | 850 | 231 | 238 | 11 | | |

- Molecule 75 is a protein called mS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | AU | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1461 | 900 | 294 | 263 | 4 | | |

- Molecule 76 is a protein called mS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | AV | 328 | Total | C | N | O | S | 0 | 0 |
| | | | 2702 | 1737 | 452 | 502 | 11 | | |

- Molecule 77 is a protein called bS1m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | AW | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 766 | 486 | 137 | 139 | 4 | | |

- Molecule 78 is a protein called mS29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | AX | 316 | Total | C | N | O | S | 0 | 0 |
| | | | 2531 | 1625 | 440 | 455 | 11 | | |

- Molecule 79 is a protein called mS31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 79 | AY | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 914 | 593 | 150 | 169 | 2 | | |

- Molecule 80 is a protein called mS33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 80 | AZ | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 473 | 133 | 130 | 4 | | |

- Molecule 81 is a protein called mS34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 81 | A0 | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1684 | 1065 | 322 | 292 | 5 | | |

- Molecule 82 is a protein called mS35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 82 | A1 | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 2076 | 1321 | 350 | 395 | 10 | | |

- Molecule 83 is a protein called mS37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 83 | A2 | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 925 | 574 | 181 | 162 | 8 | | |

- Molecule 84 is a protein called mS38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 84 | A3 | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 610 | 393 | 130 | 86 | 1 | | |

- Molecule 85 is a protein called mS39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 85 | A4 | 414 | Total | C | N | O | S | 0 | 0 |
| | | | 2838 | 1805 | 490 | 529 | 14 | | |

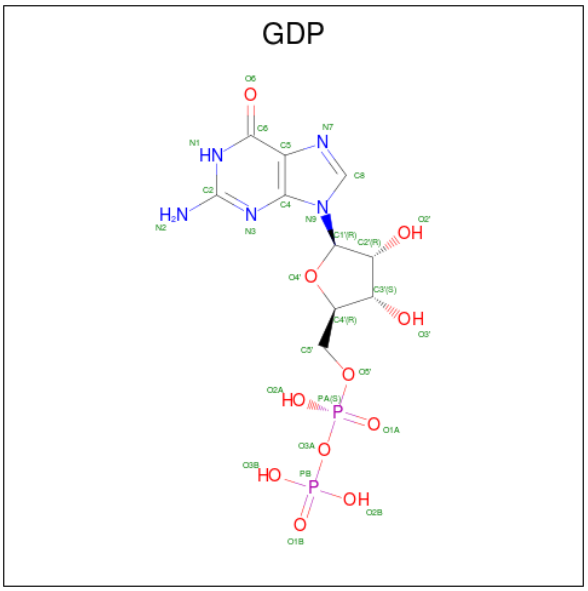
- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 86 | A | 97 | Total | Mg | 0 |
| | | | 97 | 97 | |
| 86 | M | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 86 | g | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 86 | AA | 28 | Total | Mg | 0 |
| | | | 28 | 28 | |

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 87 | 0 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | r | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | AB | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | AO | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | AP | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | AT | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



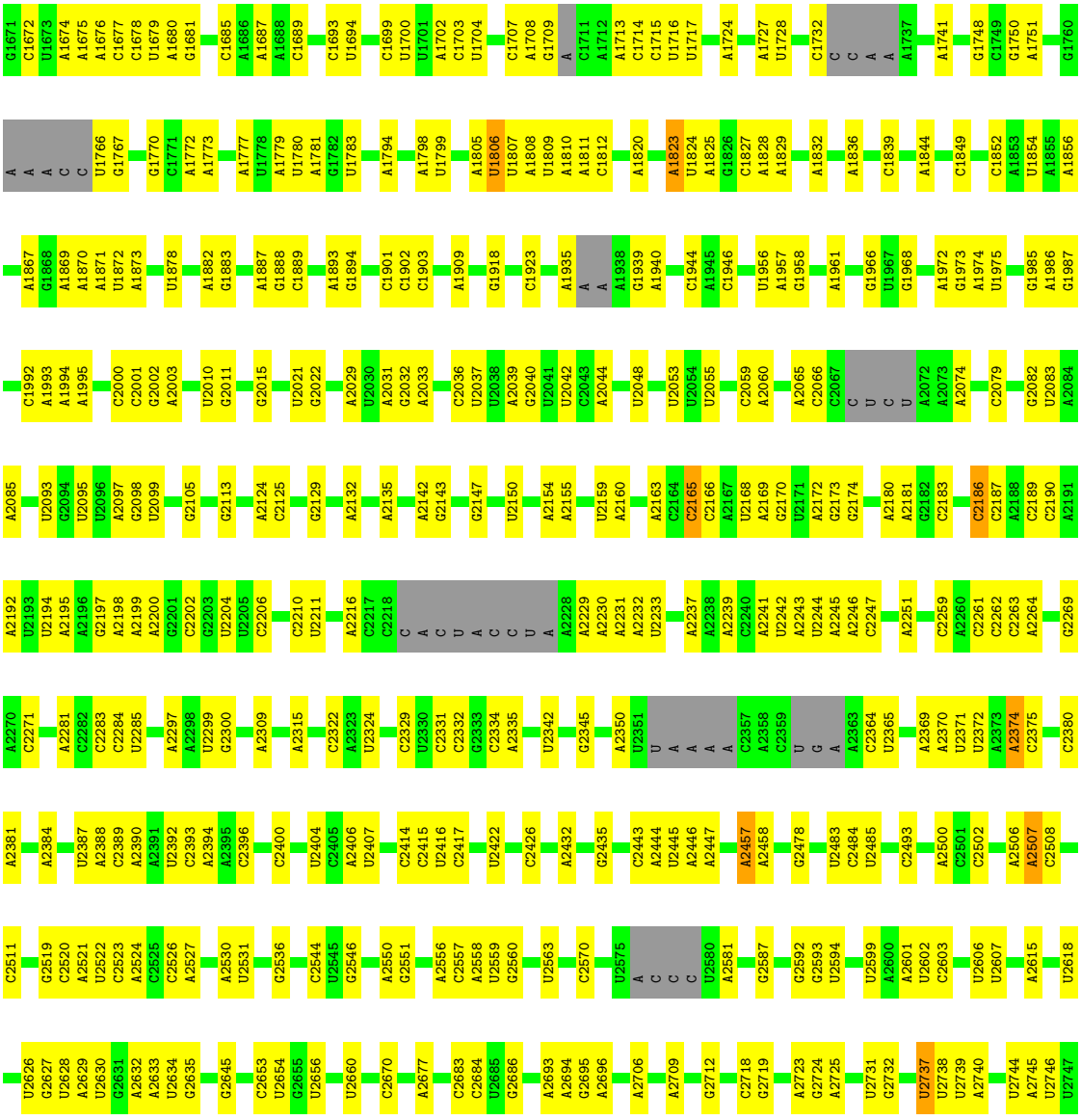

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 88 | AX | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

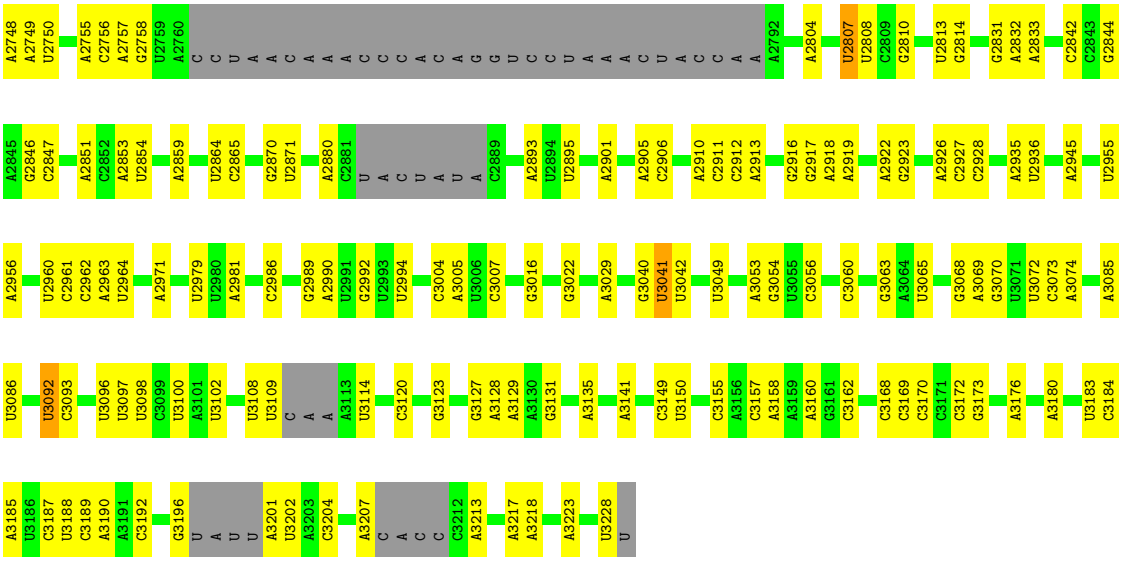
# 3 Residue-property plots (i)

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. 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. 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: 16S rRNA

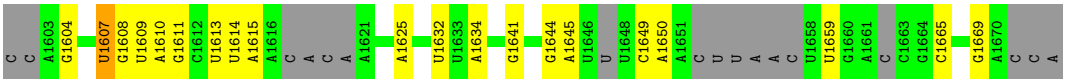
Chain A:



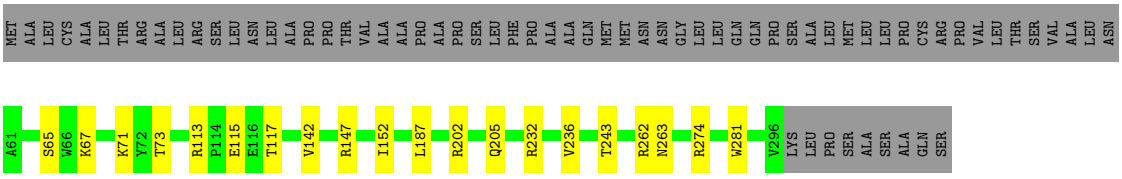
• Molecule 2: mt-tRNAVal

Chain B:

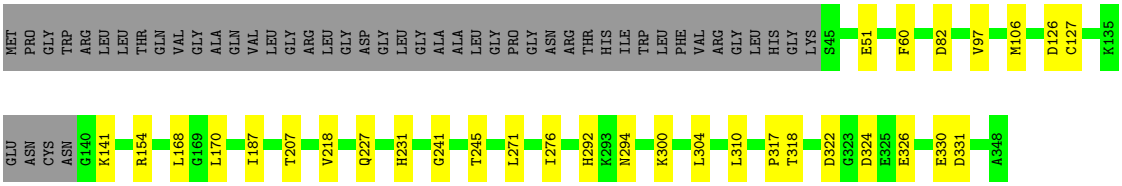
• Molecule 3: uL2m

Chain D:

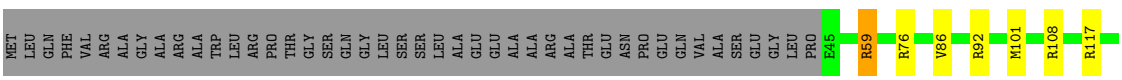
• Molecule 4: uL3m

Chain E:

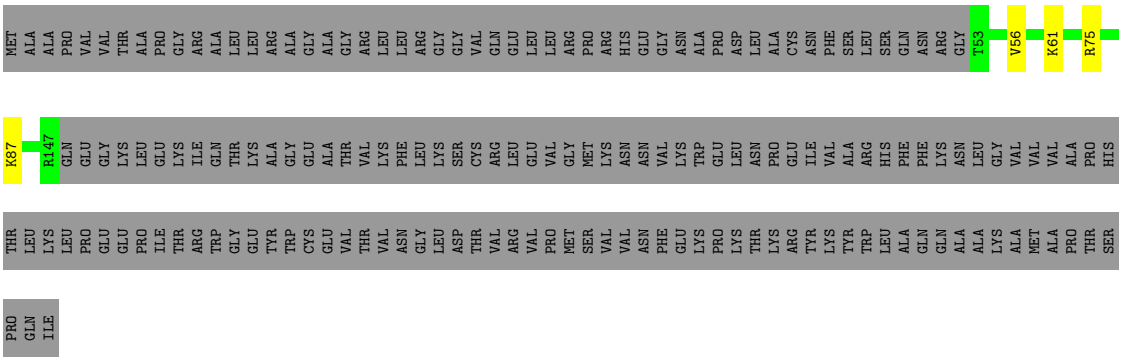
• Molecule 5: uL4m

Chain F:

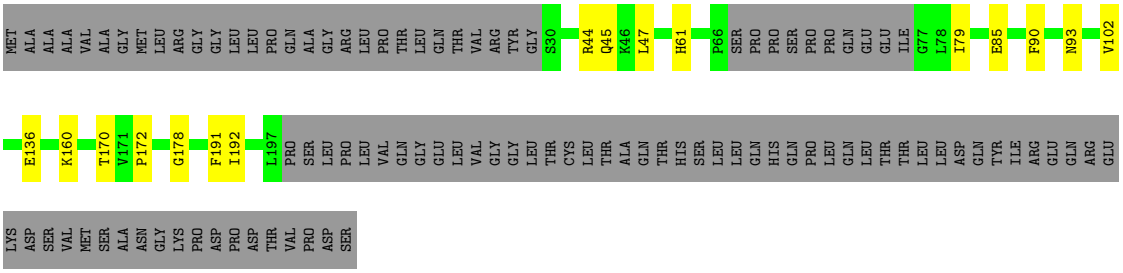

• Molecule 6: bL9m

Chain H:

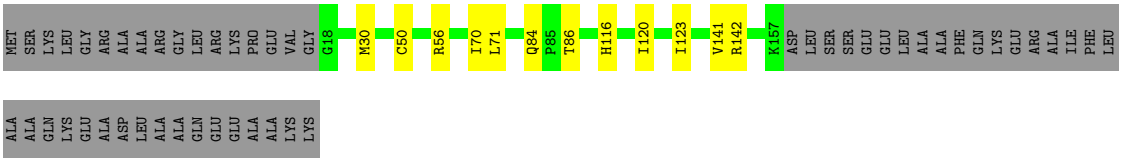

• Molecule 7: uL10m

Chain I:


• Molecule 8: uL11m

Chain J:


• Molecule 9: uL13m

Chain K:



• Molecule 10: uL14m

Chain L:


• Molecule 11: uL15m

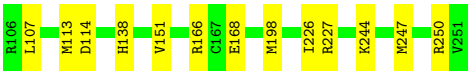
Chain M:




• Molecule 12: uL16m

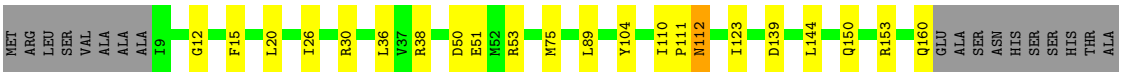
Chain N:






• Molecule 13: bL17m

Chain O:

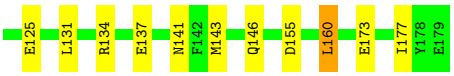





• Molecule 14: uL18m

Chain P:






• Molecule 15: bL19m

Chain Q:



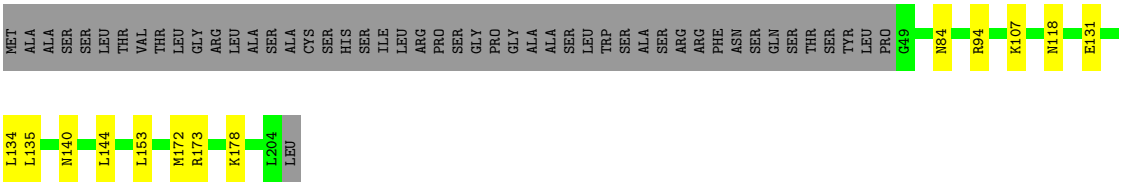
• Molecule 16: bL20m

Chain R:



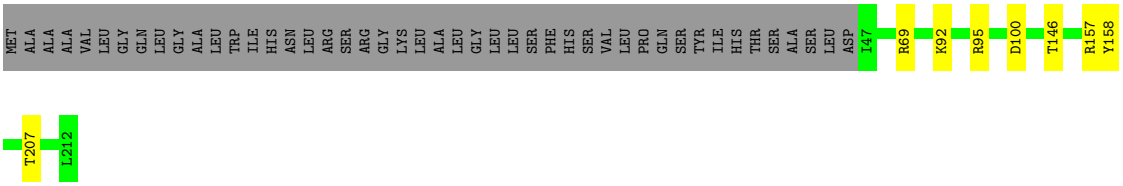
• Molecule 17: bL21m

Chain S:

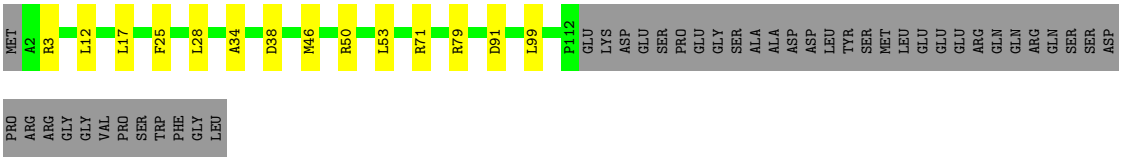

• Molecule 18: uL22m

Chain T:

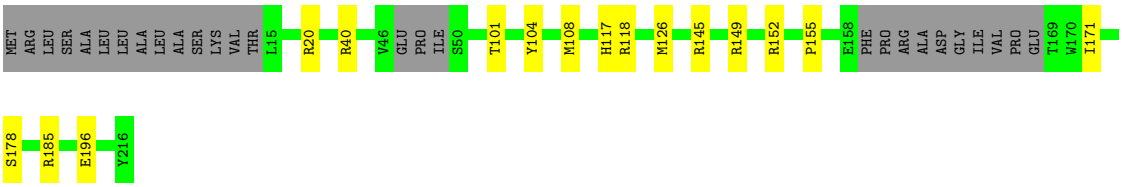

• Molecule 19: uL23m

Chain U:

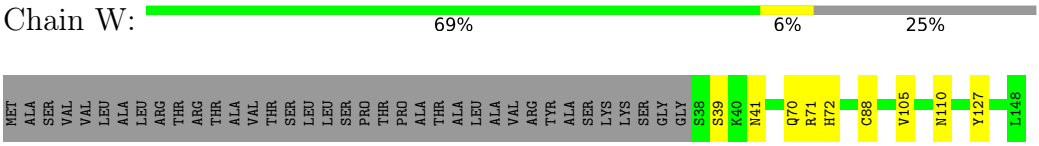

• Molecule 20: uL24m

Chain V:

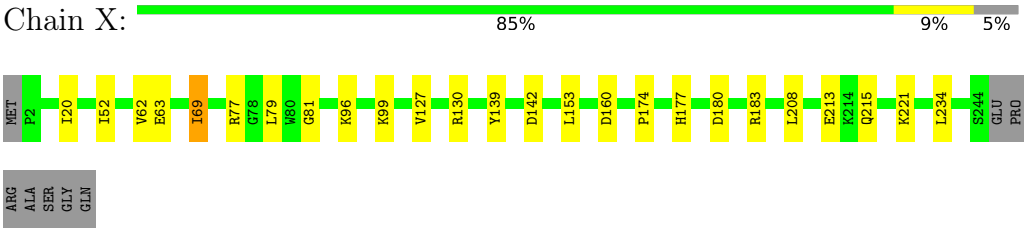

• Molecule 21: bL27m

Chain W:



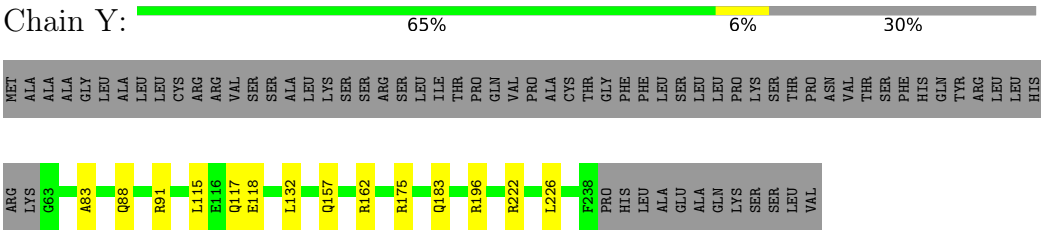

• Molecule 22: bL28m

Chain X:



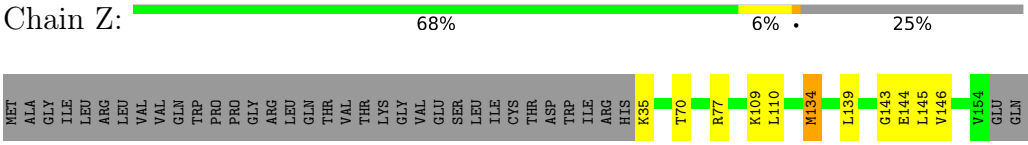

• Molecule 23: uL29m

Chain Y:



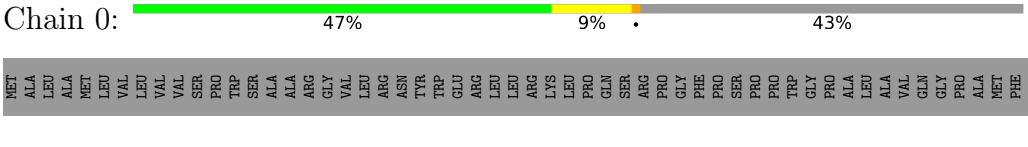

• Molecule 24: uL30m

Chain Z:



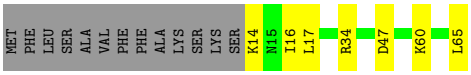

• Molecule 25: bL32m

Chain 0:



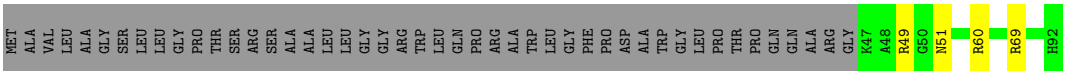

• Molecule 26: bL33m

Chain 1:


• Molecule 27: bL34m

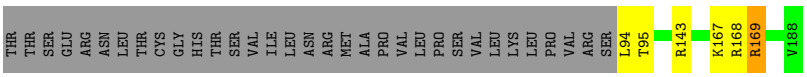
Chain 2:




• Molecule 28: bL35m

Chain 3:





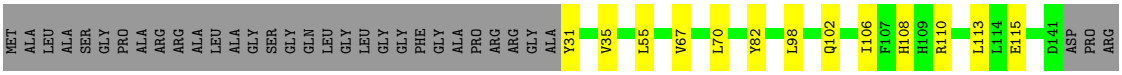

• Molecule 29: bL36m

Chain 4:




• Molecule 30: mL37

Chain 5:

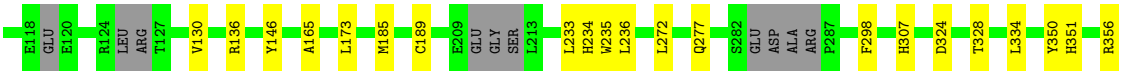



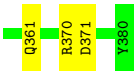



• Molecule 31: mL38

Chain 6:






• Molecule 32: mL39

Chain 7:



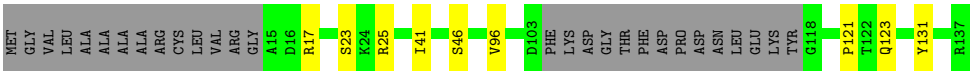

• Molecule 33: mL40

Chain 8:



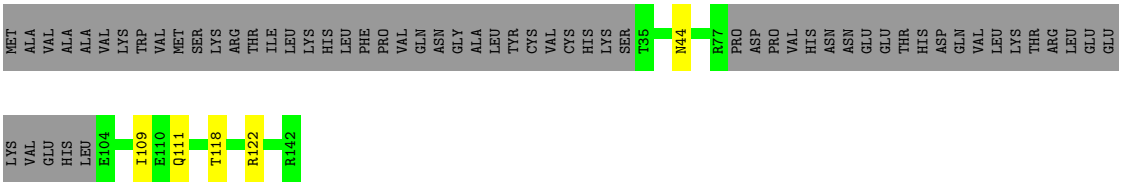

• Molecule 34: mL41

Chain 9:

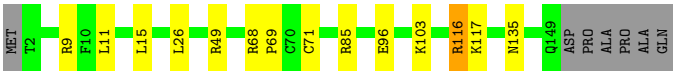

• Molecule 35: mL42

Chain a:

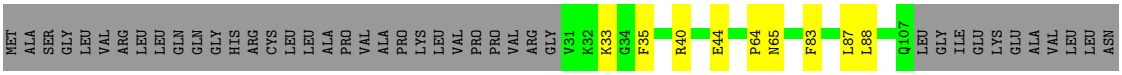

• Molecule 36: mL43

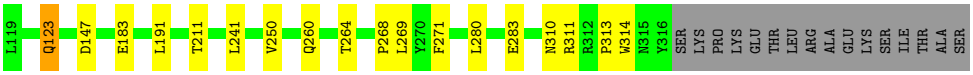
Chain b:


• Molecule 37: mL44

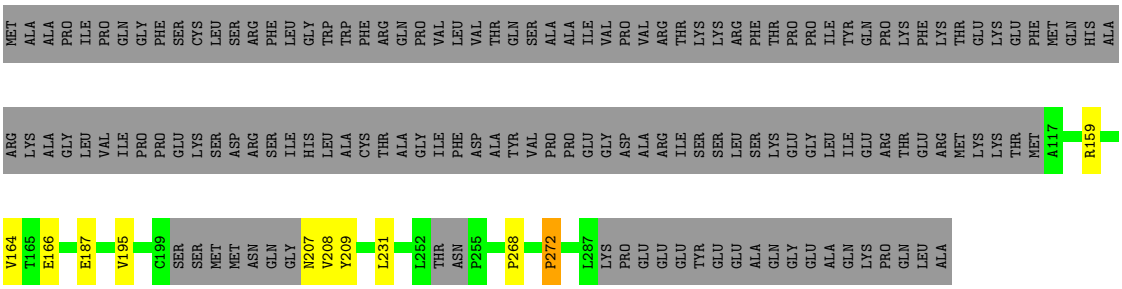
Chain c:



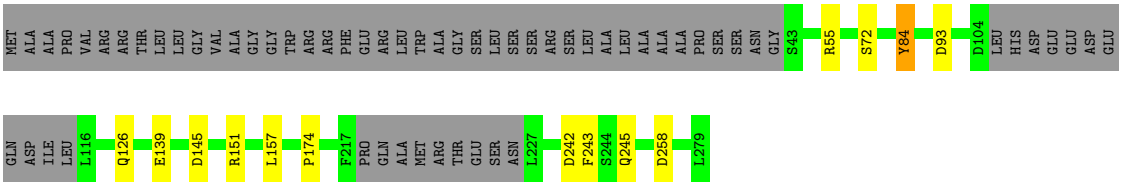

• Molecule 38: mL45

Chain d:

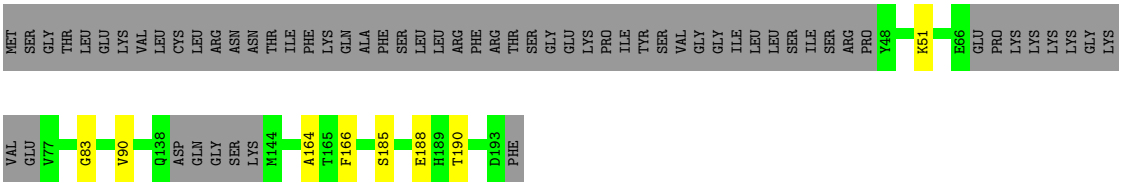

• Molecule 39: mL46

Chain e:

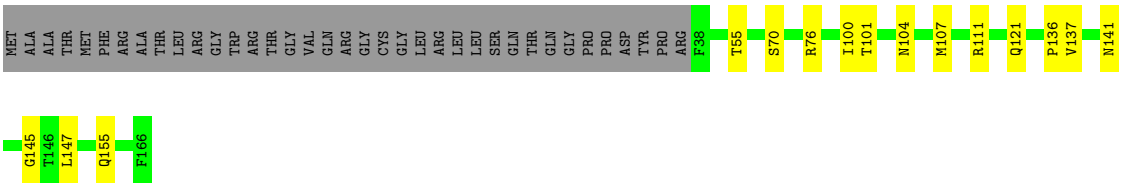

• Molecule 40: mL48

Chain f:

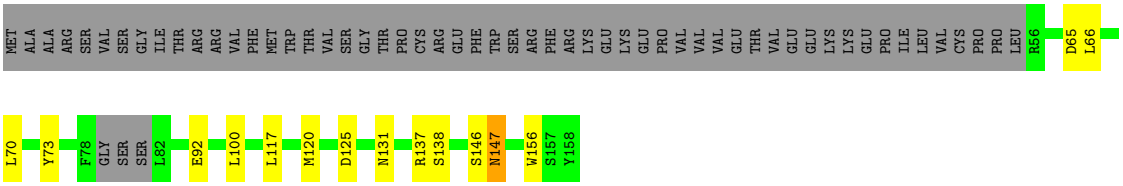

• Molecule 41: mL49

Chain g:


• Molecule 42: mL50

Chain h:



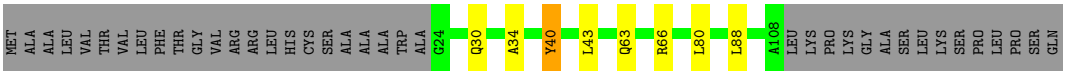

• Molecule 43: mL51

Chain i:



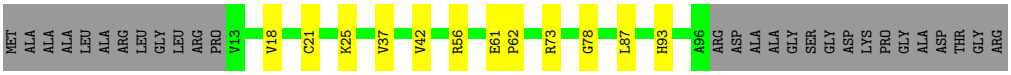
• Molecule 44: mL52

Chain j:

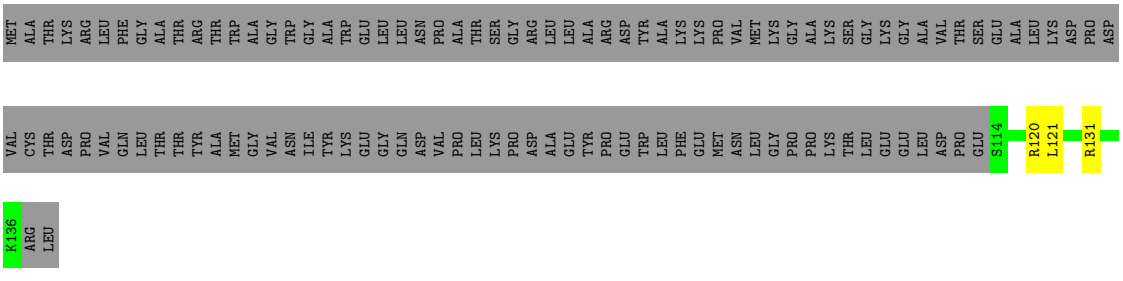

• Molecule 45: mL53

Chain k:

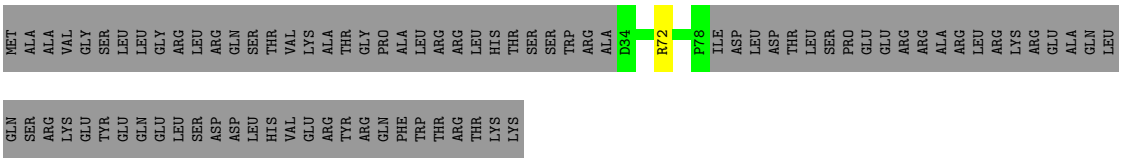

• Molecule 46: mL54

Chain l:

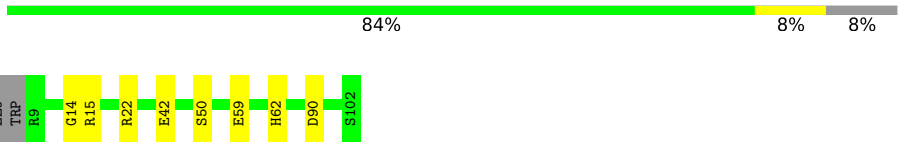

• Molecule 47: bL31m

Chain m:

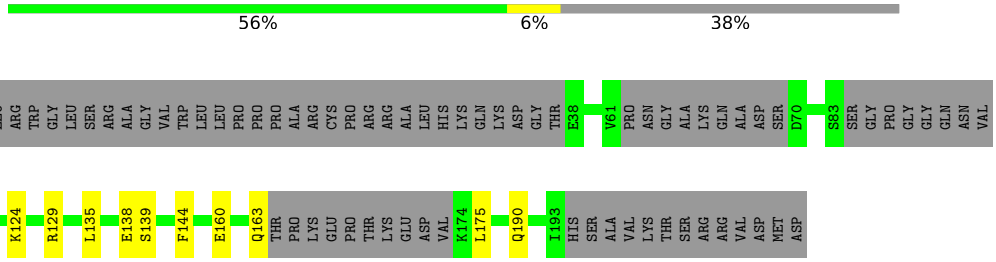

• Molecule 48: mL63

Chain o:



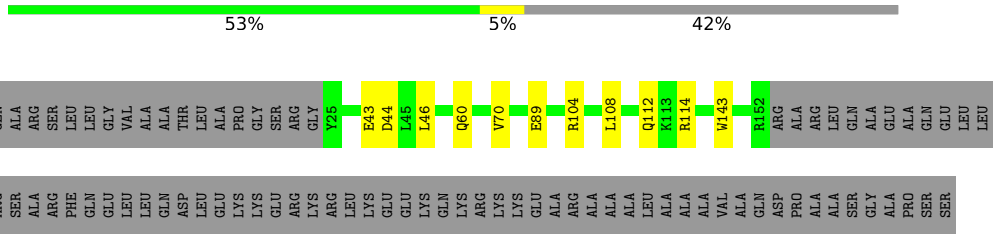

• Molecule 49: mL62 (ICT1)

Chain p:



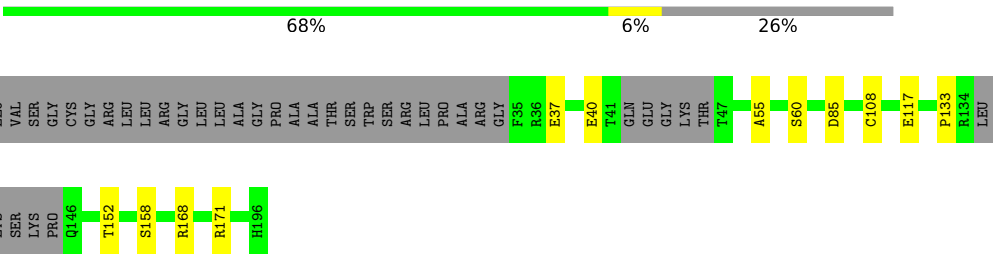

• Molecule 50: mL64 (CRIF1)

Chain q:



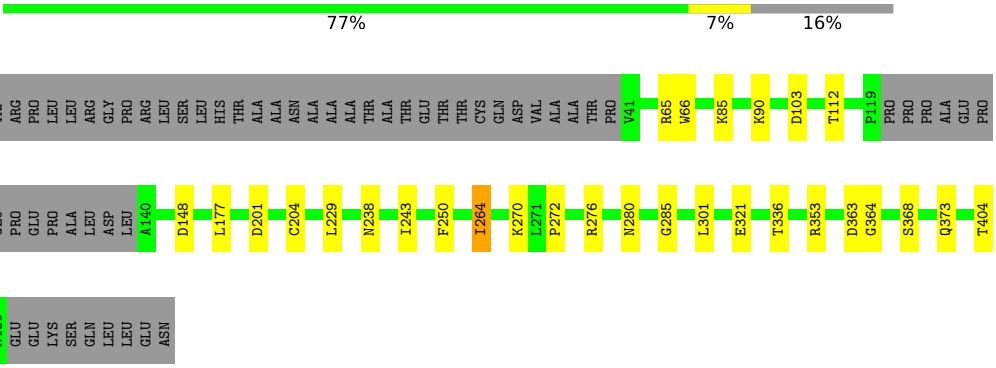

• Molecule 51: mL66 (bS18a)

Chain r:



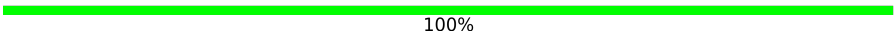

• Molecule 52: mL65 (mS30)

Chain s:




• Molecule 53: Unknown protein/protein extension

Chain t:



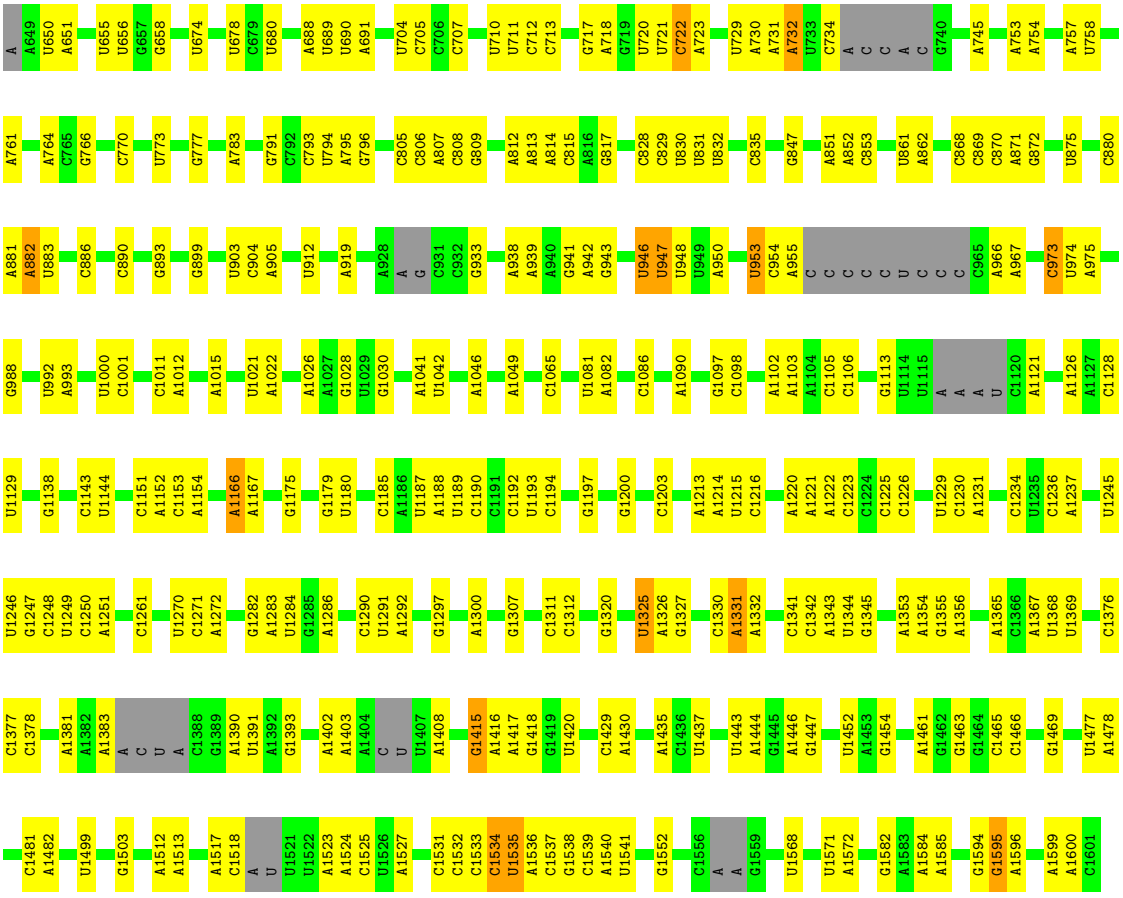

There are no outlier residues recorded for this chain.

• Molecule 54: E-site tRNA

Chain u:

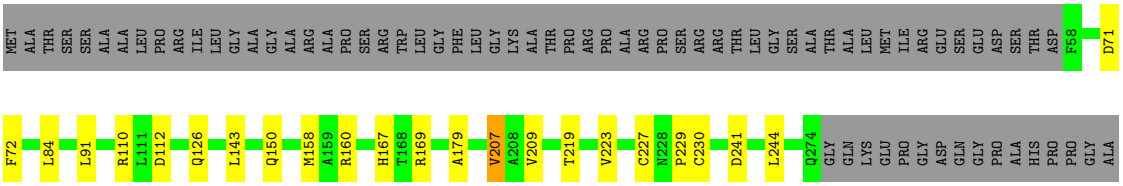

• Molecule 55: 12S rRNA

Chain AA:

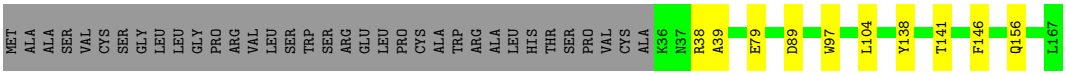
• Molecule 56: uS2m

Chain AB:

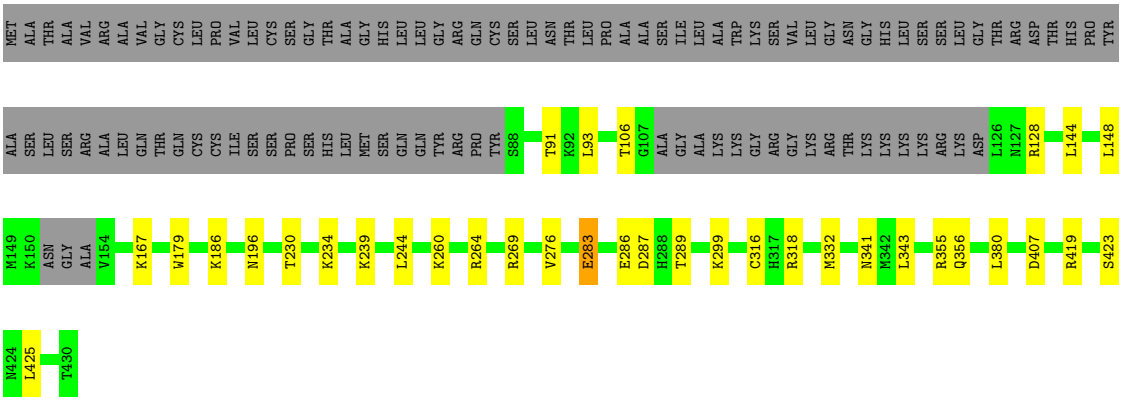

• Molecule 57: uS3m

Chain AC:

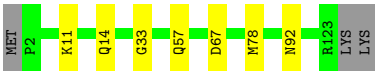

• Molecule 58: uS5m

Chain AD:

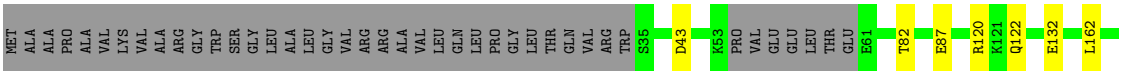

• Molecule 59: bS6m

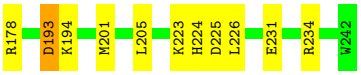
Chain AE:


• Molecule 60: uS7m

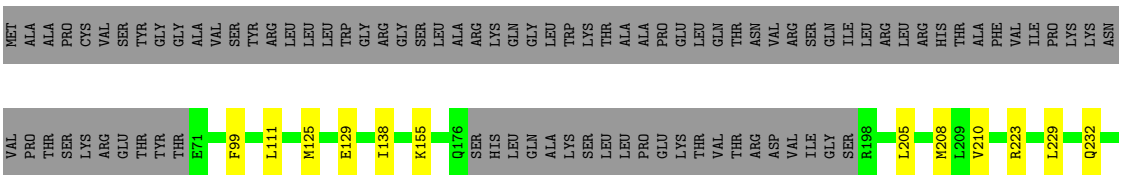
Chain AF:

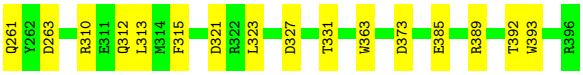




• Molecule 61: uS9m

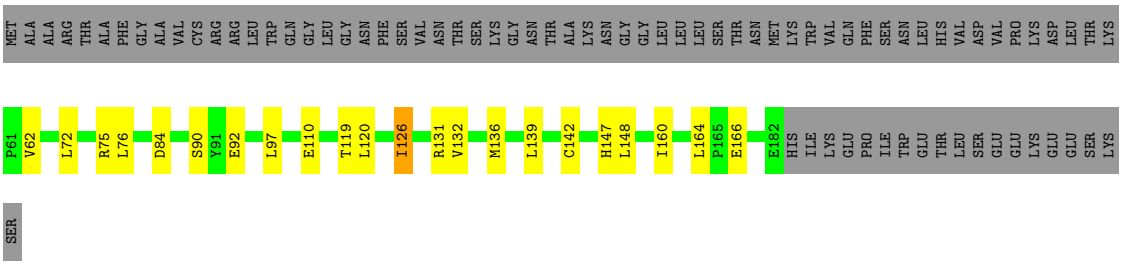
Chain AG:



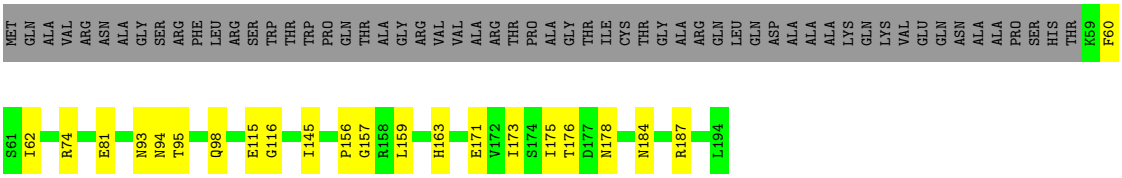

• Molecule 62: uS10m

Chain AH:

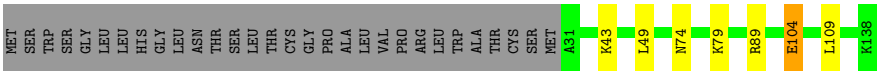

• Molecule 63: uS11m

Chain AI:


• Molecule 64: uS12m

Chain AJ:

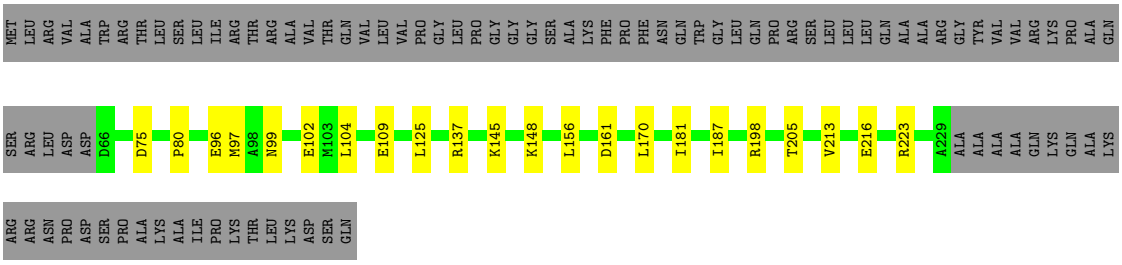

• Molecule 65: uS14m

Chain AK:



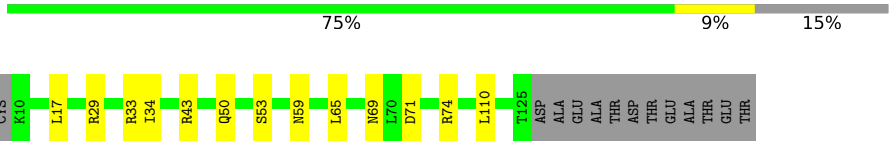
• Molecule 66: uS15m

Chain AL:

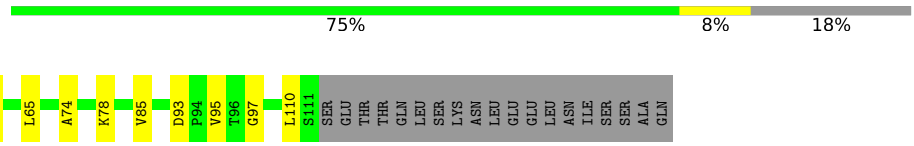
• Molecule 67: bS16m

Chain AM:



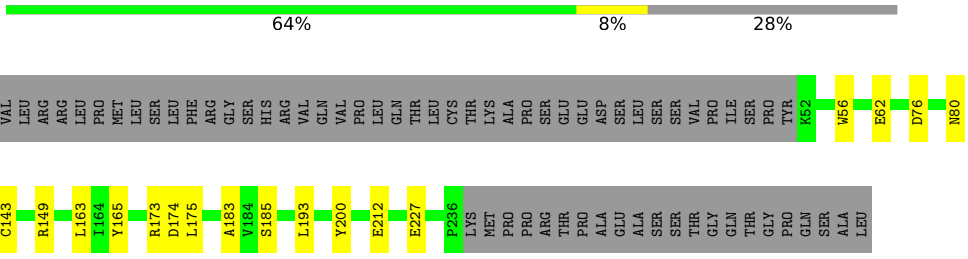

• Molecule 68: uS17m

Chain AN:



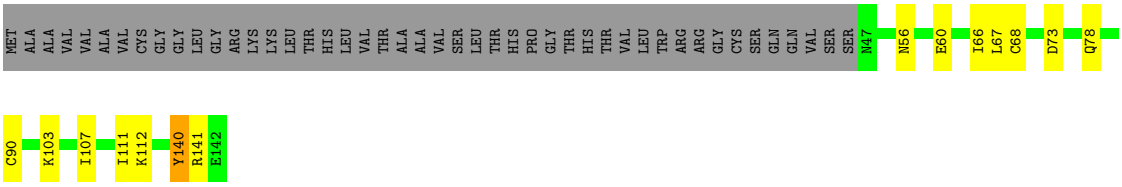

• Molecule 69: mS40 (bS18b)

Chain AO:



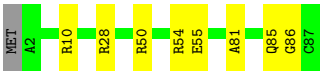

• Molecule 70: bS18m (bS18c)

Chain AP:

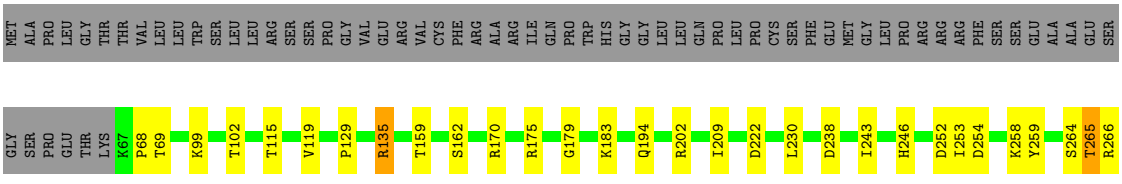

• Molecule 71: bS21m

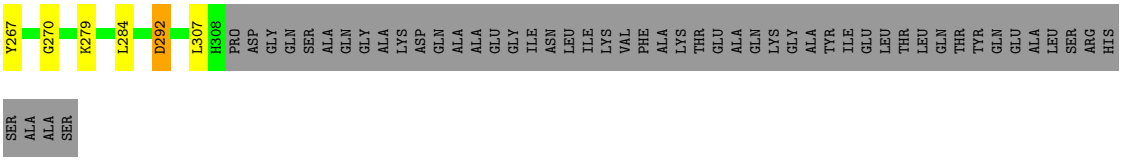
Chain AQ:


• Molecule 72: mS22

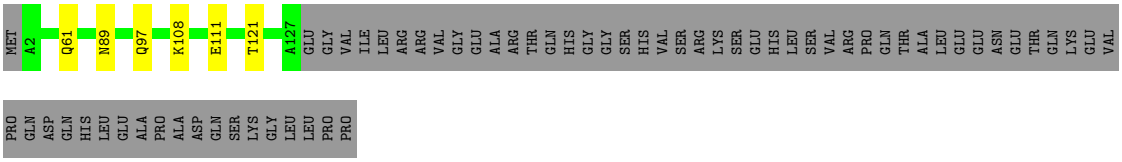
Chain AR:




• Molecule 73: mS23

Chain AS:

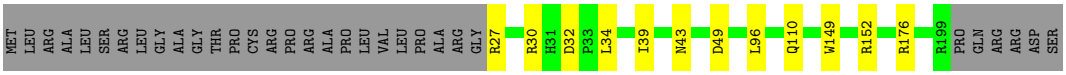

• Molecule 74: mS25

Chain AT:



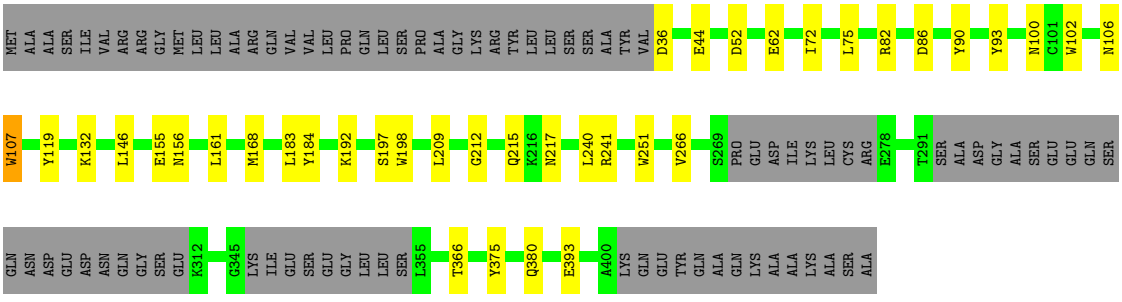
• Molecule 75: mS26

Chain AU:

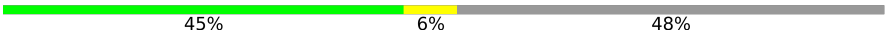

• Molecule 76: mS27

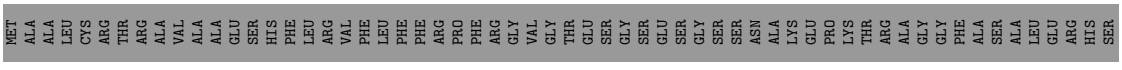
Chain AV:

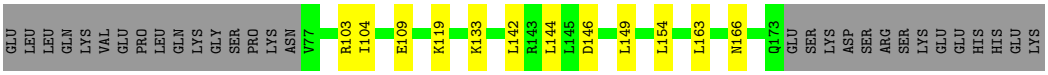




• Molecule 77: bS1m

Chain AW:



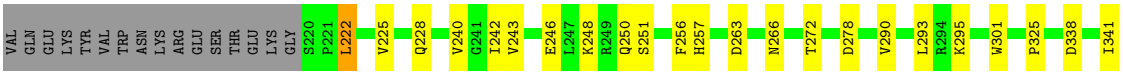






• Molecule 78: mS29

Chain AX:



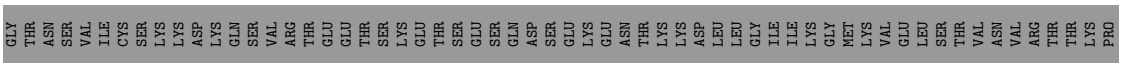





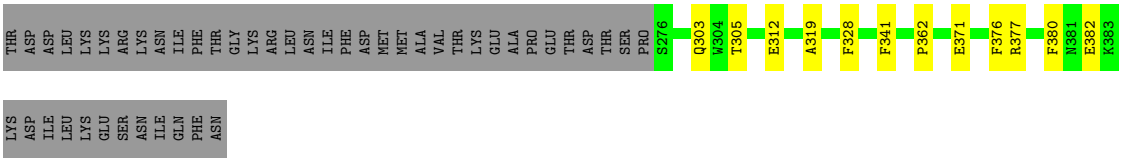
• Molecule 79: mS31

Chain AY:



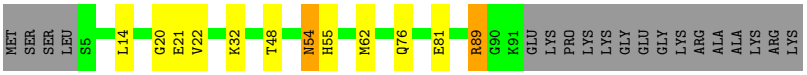




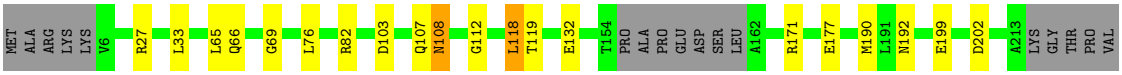

• Molecule 80: mS33

Chain AZ:

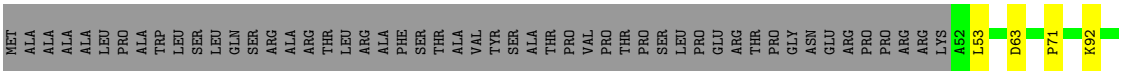

• Molecule 81: mS34

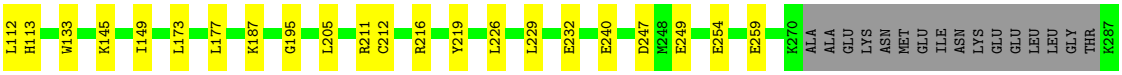
Chain A0:




- Molecule 82: mS35

Chain A1:



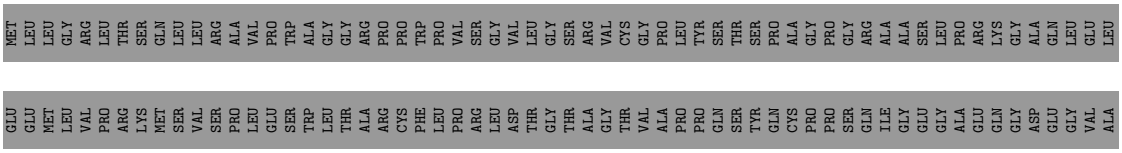
- Molecule 83: mS37

Chain A2:



- Molecule 84: mS38

Chain A3:

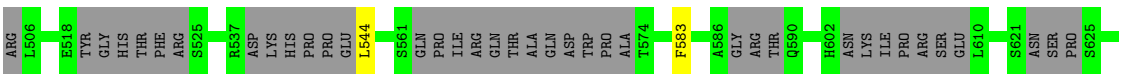



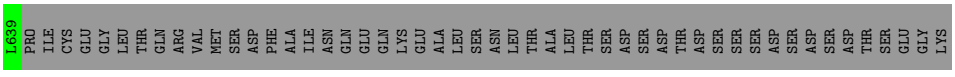


- Molecule 85: mS39

Chain A4:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 884122 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | |
| Microscope | FEI TITAN KRIOS, FEI TITAN KRIOS, FEI TITAN KRIOS, FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300, 300, 300, 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 25 | Depositor |
| Minimum defocus (nm) | 1500, 1500, 1500, 1500 | Depositor |
| Maximum defocus (nm) | 3500, 3500, 3500, 3500 | Depositor |
| Magnification | 104478, 104478, 104478, 104478 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GDP, MG

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 | A | 0.27 | 0/34967 | 0.75 | 14/54407 (0.0%) |
| 2 | B | 0.22 | 0/1328 | 0.67 | 1/2056 (0.0%) |
| 3 | D | 0.39 | 1/1879 (0.1%) | 0.73 | 0/2527 |
| 4 | E | 0.37 | 0/2433 | 0.69 | 0/3299 |
| 5 | F | 0.39 | 0/2071 | 0.73 | 0/2817 |
| 6 | H | 0.41 | 0/798 | 0.72 | 0/1073 |
| 7 | I | 0.42 | 0/1308 | 0.79 | 0/1761 |
| 8 | J | 0.42 | 0/1077 | 0.73 | 0/1452 |
| 9 | K | 0.45 | 0/1495 | 0.78 | 1/2029 (0.0%) |
| 10 | L | 0.35 | 0/904 | 0.70 | 0/1218 |
| 11 | M | 0.44 | 0/2359 | 0.78 | 0/3185 |
| 12 | N | 0.38 | 0/1697 | 0.72 | 0/2281 |
| 13 | O | 0.42 | 0/1269 | 0.84 | 0/1708 |
| 14 | P | 0.42 | 0/1103 | 0.77 | 1/1491 (0.1%) |
| 15 | Q | 0.43 | 0/1863 | 0.73 | 1/2509 (0.0%) |
| 16 | R | 0.43 | 0/1174 | 0.86 | 0/1572 |
| 17 | S | 0.37 | 0/1276 | 0.71 | 0/1729 |
| 18 | T | 0.37 | 0/1402 | 0.73 | 0/1886 |
| 19 | U | 0.39 | 0/946 | 0.77 | 0/1283 |
| 20 | V | 0.39 | 0/1590 | 0.67 | 0/2151 |
| 21 | W | 0.35 | 0/893 | 0.70 | 0/1204 |
| 22 | X | 0.42 | 0/2081 | 0.73 | 0/2812 |
| 23 | Y | 0.43 | 0/1552 | 0.80 | 0/2079 |
| 24 | Z | 0.36 | 0/1003 | 0.68 | 0/1354 |
| 25 | 0 | 0.44 | 0/895 | 0.80 | 0/1201 |
| 26 | 1 | 0.37 | 0/438 | 0.70 | 0/583 |
| 27 | 2 | 0.40 | 0/382 | 0.97 | 1/507 (0.2%) |
| 28 | 3 | 0.39 | 0/852 | 0.74 | 1/1136 (0.1%) |
| 29 | 4 | 0.36 | 0/329 | 0.71 | 0/435 |
| 30 | 5 | 0.41 | 0/3154 | 0.75 | 1/4295 (0.0%) |
| 31 | 6 | 0.41 | 0/2722 | 0.71 | 0/3709 |
| 32 | 7 | 0.39 | 0/2207 | 0.69 | 0/2978 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 33 | 8 | 0.42 | 0/855 | 0.73 | 0/1152 |
| 34 | 9 | 0.40 | 0/896 | 0.73 | 0/1205 |
| 35 | a | 0.40 | 0/709 | 0.61 | 0/963 |
| 36 | b | 0.39 | 0/1202 | 0.74 | 0/1626 |
| 37 | c | 0.42 | 0/2264 | 0.76 | 0/3059 |
| 38 | d | 0.40 | 0/1385 | 0.65 | 0/1877 |
| 39 | e | 0.40 | 0/1797 | 0.66 | 1/2422 (0.0%) |
| 40 | f | 0.38 | 0/1055 | 0.61 | 0/1427 |
| 41 | g | 0.39 | 0/1102 | 0.69 | 0/1503 |
| 42 | h | 0.43 | 0/847 | 0.74 | 0/1150 |
| 43 | i | 0.42 | 0/849 | 0.86 | 0/1135 |
| 44 | j | 0.43 | 0/698 | 0.79 | 0/940 |
| 45 | k | 0.46 | 0/665 | 0.73 | 0/897 |
| 46 | l | 0.45 | 0/226 | 0.87 | 0/299 |
| 47 | m | 0.38 | 0/379 | 0.70 | 0/510 |
| 48 | o | 0.44 | 0/818 | 0.88 | 0/1097 |
| 49 | p | 0.38 | 0/1071 | 0.68 | 0/1433 |
| 50 | q | 0.46 | 0/1107 | 0.76 | 0/1498 |
| 51 | r | 0.39 | 0/1238 | 0.67 | 0/1676 |
| 52 | s | 0.40 | 0/3114 | 0.73 | 0/4225 |
| 54 | u | 0.29 | 0/46 | 1.12 | 0/69 |
| 55 | AA | 0.25 | 0/21926 | 0.76 | 17/34121 (0.0%) |
| 56 | AB | 0.42 | 0/1811 | 0.79 | 0/2451 |
| 57 | AC | 0.41 | 0/1112 | 0.67 | 0/1505 |
| 58 | AD | 0.46 | 2/2607 (0.1%) | 0.73 | 0/3498 |
| 59 | AE | 0.38 | 0/989 | 0.78 | 0/1335 |
| 60 | AF | 0.42 | 0/1708 | 0.80 | 0/2291 |
| 61 | AG | 0.41 | 0/2570 | 0.75 | 0/3443 |
| 62 | AH | 0.39 | 0/1019 | 0.73 | 0/1379 |
| 63 | AI | 0.36 | 0/1031 | 0.69 | 0/1390 |
| 64 | AJ | 0.36 | 0/854 | 0.67 | 0/1148 |
| 65 | AK | 0.40 | 0/879 | 0.85 | 1/1182 (0.1%) |
| 66 | AL | 0.43 | 0/1406 | 0.79 | 0/1878 |
| 67 | AM | 0.41 | 0/941 | 0.82 | 0/1265 |
| 68 | AN | 0.35 | 0/864 | 0.66 | 0/1169 |
| 69 | AO | 0.41 | 0/1580 | 0.73 | 0/2150 |
| 70 | AP | 0.42 | 0/791 | 0.71 | 0/1062 |
| 71 | AQ | 0.42 | 0/752 | 0.91 | 0/1001 |
| 72 | AR | 0.44 | 0/2050 | 0.82 | 4/2770 (0.1%) |
| 73 | AS | 0.43 | 0/1069 | 0.75 | 0/1441 |
| 74 | AT | 0.40 | 0/1361 | 0.73 | 0/1829 |
| 75 | AU | 0.43 | 0/1482 | 0.84 | 0/1987 |
| 76 | AV | 0.45 | 0/2758 | 0.83 | 2/3724 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 77 | AW | 0.41 | 0/778 | 0.74 | 0/1048 |
| 78 | AX | 0.44 | 0/2596 | 0.76 | 3/3519 (0.1%) |
| 79 | AY | 0.57 | 2/943 (0.2%) | 0.71 | 0/1274 |
| 80 | AZ | 0.45 | 0/757 | 0.82 | 0/1011 |
| 81 | A0 | 0.40 | 0/1727 | 0.78 | 1/2338 (0.0%) |
| 82 | A1 | 0.41 | 0/2121 | 0.70 | 1/2873 (0.0%) |
| 83 | A2 | 0.42 | 0/939 | 0.79 | 0/1256 |
| 84 | A3 | 0.43 | 0/621 | 0.92 | 0/820 |
| 85 | A4 | 0.42 | 0/2137 | 0.75 | 0/2872 |
| All | All | 0.37 | 5/165949 (0.0%) | 0.75 | 51/235920 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 8 | J | 0 | 1 |
| 15 | Q | 0 | 1 |
| 58 | AD | 0 | 1 |
| 72 | AR | 0 | 1 |
| 74 | AT | 0 | 1 |
| 78 | AX | 0 | 2 |
| 80 | AZ | 0 | 1 |
| All | All | 0 | 8 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 79 | AY | 371 | GLU | CD-OE1 | 8.47 | 1.34 | 1.25 |
| 79 | AY | 371 | GLU | CD-OE2 | 7.81 | 1.34 | 1.25 |
| 58 | AD | 283 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 58 | AD | 283 | GLU | CD-OE1 | 6.94 | 1.33 | 1.25 |
| 3 | D | 115 | GLU | CD-OE1 | 5.13 | 1.31 | 1.25 |

The worst 5 of 51 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 55 | AA | 947 | U | N1-C1'-C2' | -12.05 | 98.33 | 114.00 |
| 55 | AA | 946 | U | N1-C1'-C2' | -9.06 | 102.04 | 112.00 |
| 55 | AA | 1596 | A | N9-C1'-C2' | -8.73 | 102.40 | 112.00 |
| 72 | AR | 135 | ARG | NE-CZ-NH2 | 7.44 | 124.02 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 2507 | A | C2'-C3'-O3' | 7.32 | 125.61 | 109.50 |

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 58 | AD | 287 | ASP | Peptide |
| 72 | AR | 265 | THR | Peptide |
| 74 | AT | 147 | VAL | Peptide |
| 8 | J | 30 | MET | Peptide |
| 15 | Q | 215 | VAL | 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 |
|---|---|---|---|---|---|---|
| 3 | D | 234/305 (77%) | 214 (92%) | 18 (8%) | 2 (1%) | 17 56 |
| 4 | E | 296/348 (85%) | 266 (90%) | 20 (7%) | 10 (3%) | 3 28 |
| 5 | F | 248/311 (80%) | 228 (92%) | 13 (5%) | 7 (3%) | 5 32 |
| 6 | H | 93/267 (35%) | 84 (90%) | 8 (9%) | 1 (1%) | 14 52 |
| 7 | I | 154/261 (59%) | 139 (90%) | 11 (7%) | 4 (3%) | 5 33 |
| 8 | J | 138/192 (72%) | 126 (91%) | 11 (8%) | 1 (1%) | 22 61 |
| 9 | K | 175/178 (98%) | 156 (89%) | 11 (6%) | 8 (5%) | 2 21 |
| 10 | L | 113/145 (78%) | 100 (88%) | 11 (10%) | 2 (2%) | 8 41 |
| 11 | M | 285/296 (96%) | 247 (87%) | 34 (12%) | 4 (1%) | 11 46 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 12 | N | 203/251 (81%) | 186 (92%) | 16 (8%) | 1 (0%) | 29 68 |
| 13 | O | 150/175 (86%) | 130 (87%) | 16 (11%) | 4 (3%) | 5 33 |
| 14 | P | 129/179 (72%) | 117 (91%) | 9 (7%) | 3 (2%) | 6 36 |
| 15 | Q | 217/292 (74%) | 186 (86%) | 22 (10%) | 9 (4%) | 3 23 |
| 16 | R | 138/149 (93%) | 126 (91%) | 9 (6%) | 3 (2%) | 6 37 |
| 17 | S | 154/205 (75%) | 141 (92%) | 11 (7%) | 2 (1%) | 12 48 |
| 18 | T | 164/212 (77%) | 154 (94%) | 7 (4%) | 3 (2%) | 8 41 |
| 19 | U | 109/153 (71%) | 95 (87%) | 10 (9%) | 4 (4%) | 3 26 |
| 20 | V | 183/216 (85%) | 159 (87%) | 20 (11%) | 4 (2%) | 6 37 |
| 21 | W | 109/148 (74%) | 100 (92%) | 6 (6%) | 3 (3%) | 5 32 |
| 22 | X | 241/256 (94%) | 211 (88%) | 22 (9%) | 8 (3%) | 4 28 |
| 23 | Y | 174/250 (70%) | 162 (93%) | 9 (5%) | 3 (2%) | 9 42 |
| 24 | Z | 118/161 (73%) | 110 (93%) | 5 (4%) | 3 (2%) | 5 34 |
| 25 | 0 | 106/188 (56%) | 93 (88%) | 8 (8%) | 5 (5%) | 2 20 |
| 26 | 1 | 50/65 (77%) | 44 (88%) | 5 (10%) | 1 (2%) | 7 39 |
| 27 | 2 | 44/92 (48%) | 43 (98%) | 1 (2%) | 0 | 100 100 |
| 28 | 3 | 93/188 (50%) | 88 (95%) | 4 (4%) | 1 (1%) | 14 52 |
| 29 | 4 | 34/103 (33%) | 34 (100%) | 0 | 0 | 100 100 |
| 30 | 5 | 368/423 (87%) | 326 (89%) | 32 (9%) | 10 (3%) | 5 33 |
| 31 | 6 | 313/380 (82%) | 281 (90%) | 25 (8%) | 7 (2%) | 6 37 |
| 32 | 7 | 258/338 (76%) | 226 (88%) | 28 (11%) | 4 (2%) | 9 43 |
| 33 | 8 | 97/206 (47%) | 90 (93%) | 6 (6%) | 1 (1%) | 15 54 |
| 34 | 9 | 105/137 (77%) | 92 (88%) | 10 (10%) | 3 (3%) | 4 31 |
| 35 | a | 78/142 (55%) | 74 (95%) | 3 (4%) | 1 (1%) | 12 48 |
| 36 | b | 146/155 (94%) | 127 (87%) | 16 (11%) | 3 (2%) | 7 38 |
| 37 | c | 271/332 (82%) | 236 (87%) | 28 (10%) | 7 (3%) | 5 33 |
| 38 | d | 156/306 (51%) | 137 (88%) | 12 (8%) | 7 (4%) | 2 21 |
| 39 | e | 211/279 (76%) | 193 (92%) | 14 (7%) | 4 (2%) | 8 40 |
| 40 | f | 125/194 (64%) | 115 (92%) | 6 (5%) | 4 (3%) | 4 29 |
| 41 | g | 127/166 (76%) | 114 (90%) | 8 (6%) | 5 (4%) | 3 25 |
| 42 | h | 96/158 (61%) | 82 (85%) | 9 (9%) | 5 (5%) | 2 18 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 43 | i | 95/128 (74%) | 76 (80%) | 16 (17%) | 3 (3%) | 4 29 |
| 44 | j | 83/123 (68%) | 77 (93%) | 4 (5%) | 2 (2%) | 6 35 |
| 45 | k | 82/112 (73%) | 64 (78%) | 12 (15%) | 6 (7%) | 1 11 |
| 46 | l | 21/138 (15%) | 20 (95%) | 1 (5%) | 0 | 100 100 |
| 47 | m | 43/128 (34%) | 39 (91%) | 4 (9%) | 0 | 100 100 |
| 48 | o | 92/102 (90%) | 77 (84%) | 12 (13%) | 3 (3%) | 4 28 |
| 49 | p | 119/206 (58%) | 113 (95%) | 4 (3%) | 2 (2%) | 9 42 |
| 50 | q | 126/222 (57%) | 118 (94%) | 8 (6%) | 0 | 100 100 |
| 51 | r | 140/196 (71%) | 124 (89%) | 13 (9%) | 3 (2%) | 7 38 |
| 52 | s | 366/439 (83%) | 332 (91%) | 28 (8%) | 6 (2%) | 9 43 |
| 56 | AB | 215/296 (73%) | 193 (90%) | 18 (8%) | 4 (2%) | 8 40 |
| 57 | AC | 130/167 (78%) | 117 (90%) | 12 (9%) | 1 (1%) | 19 58 |
| 58 | AD | 316/430 (74%) | 284 (90%) | 28 (9%) | 4 (1%) | 12 48 |
| 59 | AE | 120/125 (96%) | 114 (95%) | 5 (4%) | 1 (1%) | 19 58 |
| 60 | AF | 197/242 (81%) | 183 (93%) | 12 (6%) | 2 (1%) | 15 54 |
| 61 | AG | 301/396 (76%) | 265 (88%) | 30 (10%) | 6 (2%) | 7 39 |
| 62 | AH | 120/201 (60%) | 105 (88%) | 11 (9%) | 4 (3%) | 4 28 |
| 63 | AI | 134/194 (69%) | 116 (87%) | 11 (8%) | 7 (5%) | 2 18 |
| 64 | AJ | 106/138 (77%) | 91 (86%) | 14 (13%) | 1 (1%) | 17 56 |
| 65 | AK | 99/128 (77%) | 96 (97%) | 2 (2%) | 1 (1%) | 15 54 |
| 66 | AL | 162/257 (63%) | 148 (91%) | 13 (8%) | 1 (1%) | 25 64 |
| 67 | AM | 114/137 (83%) | 105 (92%) | 9 (8%) | 0 | 100 100 |
| 68 | AN | 105/130 (81%) | 94 (90%) | 8 (8%) | 3 (3%) | 4 31 |
| 69 | AO | 183/258 (71%) | 157 (86%) | 21 (12%) | 5 (3%) | 5 33 |
| 70 | AP | 94/142 (66%) | 85 (90%) | 6 (6%) | 3 (3%) | 4 29 |
| 71 | AQ | 84/87 (97%) | 75 (89%) | 6 (7%) | 3 (4%) | 3 26 |
| 72 | AR | 240/360 (67%) | 202 (84%) | 28 (12%) | 10 (4%) | 3 23 |
| 73 | AS | 124/190 (65%) | 110 (89%) | 14 (11%) | 0 | 100 100 |
| 74 | AT | 160/173 (92%) | 144 (90%) | 8 (5%) | 8 (5%) | 2 19 |
| 75 | AU | 171/205 (83%) | 163 (95%) | 8 (5%) | 0 | 100 100 |
| 76 | AV | 320/414 (77%) | 283 (88%) | 29 (9%) | 8 (2%) | 5 34 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 77 | AW | 95/187 (51%) | 82 (86%) | 9 (10%) | 4 (4%) | 3 23 |
| 78 | AX | 310/398 (78%) | 263 (85%) | 30 (10%) | 17 (6%) | 2 17 |
| 79 | AY | 106/395 (27%) | 95 (90%) | 8 (8%) | 3 (3%) | 5 32 |
| 80 | AZ | 85/106 (80%) | 72 (85%) | 8 (9%) | 5 (6%) | 1 15 |
| 81 | A0 | 197/218 (90%) | 175 (89%) | 19 (10%) | 3 (2%) | 10 45 |
| 82 | A1 | 252/323 (78%) | 212 (84%) | 34 (14%) | 6 (2%) | 6 35 |
| 83 | A2 | 114/118 (97%) | 97 (85%) | 13 (11%) | 4 (4%) | 3 27 |
| 84 | A3 | 67/199 (34%) | 62 (92%) | 4 (6%) | 1 (2%) | 10 45 |
| 85 | A4 | 237/579 (41%) | 230 (97%) | 5 (2%) | 2 (1%) | 19 58 |
| All | All | 12628/17789 (71%) | 11290 (89%) | 1039 (8%) | 299 (2%) | 9 35 |

5 of 299 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | E | 170 | LEU |
| 4 | E | 245 | THR |
| 5 | F | 223 | HIS |
| 7 | I | 102 | VAL |
| 8 | J | 70 | ILE |

### 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 |
|---|---|---|---|---|---|
| 3 | D | 190/245 (78%) | 173 (91%) | 17 (9%) | 9 37 |
| 4 | E | 255/290 (88%) | 233 (91%) | 22 (9%) | 10 38 |
| 5 | F | 217/262 (83%) | 198 (91%) | 19 (9%) | 10 38 |
| 6 | H | 86/228 (38%) | 83 (96%) | 3 (4%) | 36 67 |
| 7 | I | 145/232 (62%) | 133 (92%) | 12 (8%) | 11 40 |
| 8 | J | 113/150 (75%) | 103 (91%) | 10 (9%) | 10 38 |
| 9 | K | 155/156 (99%) | 145 (94%) | 10 (6%) | 17 50 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 10 | L | 98/124 (79%) | 88 (90%) | 10 (10%) | 7 | 32 |
| 11 | M | 245/249 (98%) | 217 (89%) | 28 (11%) | 5 | 26 |
| 12 | N | 172/211 (82%) | 152 (88%) | 20 (12%) | 5 | 26 |
| 13 | O | 133/150 (89%) | 114 (86%) | 19 (14%) | 3 | 19 |
| 14 | P | 115/154 (75%) | 102 (89%) | 13 (11%) | 6 | 27 |
| 15 | Q | 201/256 (78%) | 187 (93%) | 14 (7%) | 15 | 46 |
| 16 | R | 118/126 (94%) | 104 (88%) | 14 (12%) | 5 | 25 |
| 17 | S | 141/180 (78%) | 130 (92%) | 11 (8%) | 12 | 42 |
| 18 | T | 146/182 (80%) | 141 (97%) | 5 (3%) | 37 | 68 |
| 19 | U | 99/135 (73%) | 89 (90%) | 10 (10%) | 7 | 32 |
| 20 | V | 169/191 (88%) | 157 (93%) | 12 (7%) | 14 | 46 |
| 21 | W | 91/119 (76%) | 85 (93%) | 6 (7%) | 16 | 49 |
| 22 | X | 217/227 (96%) | 199 (92%) | 18 (8%) | 11 | 40 |
| 23 | Y | 159/223 (71%) | 148 (93%) | 11 (7%) | 15 | 47 |
| 24 | Z | 111/147 (76%) | 102 (92%) | 9 (8%) | 11 | 41 |
| 25 | 0 | 97/164 (59%) | 81 (84%) | 16 (16%) | 2 | 13 |
| 26 | 1 | 49/60 (82%) | 43 (88%) | 6 (12%) | 5 | 23 |
| 27 | 2 | 40/72 (56%) | 37 (92%) | 3 (8%) | 13 | 43 |
| 28 | 3 | 88/166 (53%) | 83 (94%) | 5 (6%) | 20 | 53 |
| 29 | 4 | 35/89 (39%) | 31 (89%) | 4 (11%) | 5 | 26 |
| 30 | 5 | 337/368 (92%) | 305 (90%) | 32 (10%) | 8 | 34 |
| 31 | 6 | 266/332 (80%) | 242 (91%) | 24 (9%) | 9 | 37 |
| 32 | 7 | 242/303 (80%) | 230 (95%) | 12 (5%) | 24 | 58 |
| 33 | 8 | 91/190 (48%) | 88 (97%) | 3 (3%) | 38 | 68 |
| 34 | 9 | 91/112 (81%) | 85 (93%) | 6 (7%) | 16 | 49 |
| 35 | a | 78/133 (59%) | 74 (95%) | 4 (5%) | 24 | 57 |
| 36 | b | 130/135 (96%) | 118 (91%) | 12 (9%) | 9 | 36 |
| 37 | c | 241/288 (84%) | 220 (91%) | 21 (9%) | 10 | 38 |
| 38 | d | 151/274 (55%) | 146 (97%) | 5 (3%) | 38 | 68 |
| 39 | e | 188/236 (80%) | 178 (95%) | 10 (5%) | 22 | 55 |
| 40 | f | 117/173 (68%) | 113 (97%) | 4 (3%) | 37 | 68 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 41 | g | 119/148 (80%) | 109 (92%) | 10 (8%) | 11 40 |
| 42 | h | 95/148 (64%) | 84 (88%) | 11 (12%) | 5 26 |
| 43 | i | 86/110 (78%) | 76 (88%) | 10 (12%) | 5 26 |
| 44 | j | 68/97 (70%) | 61 (90%) | 7 (10%) | 7 32 |
| 45 | k | 74/90 (82%) | 68 (92%) | 6 (8%) | 11 41 |
| 46 | l | 23/116 (20%) | 20 (87%) | 3 (13%) | 4 21 |
| 47 | m | 40/113 (35%) | 39 (98%) | 1 (2%) | 47 75 |
| 48 | o | 80/87 (92%) | 75 (94%) | 5 (6%) | 18 51 |
| 49 | p | 117/181 (65%) | 107 (92%) | 10 (8%) | 10 39 |
| 50 | q | 110/178 (62%) | 99 (90%) | 11 (10%) | 7 32 |
| 51 | r | 133/169 (79%) | 124 (93%) | 9 (7%) | 16 48 |
| 52 | s | 326/381 (86%) | 299 (92%) | 27 (8%) | 11 40 |
| 56 | AB | 191/249 (77%) | 171 (90%) | 20 (10%) | 7 31 |
| 57 | AC | 115/143 (80%) | 106 (92%) | 9 (8%) | 12 42 |
| 58 | AD | 269/357 (75%) | 239 (89%) | 30 (11%) | 6 27 |
| 59 | AE | 104/107 (97%) | 98 (94%) | 6 (6%) | 20 53 |
| 60 | AF | 178/209 (85%) | 161 (90%) | 17 (10%) | 8 34 |
| 61 | AG | 265/342 (78%) | 243 (92%) | 22 (8%) | 11 40 |
| 62 | AH | 112/180 (62%) | 93 (83%) | 19 (17%) | 2 12 |
| 63 | AI | 104/147 (71%) | 89 (86%) | 15 (14%) | 3 18 |
| 64 | AJ | 93/118 (79%) | 86 (92%) | 7 (8%) | 13 43 |
| 65 | AK | 91/113 (80%) | 82 (90%) | 9 (10%) | 8 33 |
| 66 | AL | 152/226 (67%) | 131 (86%) | 21 (14%) | 3 20 |
| 67 | AM | 95/113 (84%) | 82 (86%) | 13 (14%) | 3 20 |
| 68 | AN | 93/115 (81%) | 86 (92%) | 7 (8%) | 13 43 |
| 69 | AO | 166/230 (72%) | 150 (90%) | 16 (10%) | 8 34 |
| 70 | AP | 87/123 (71%) | 75 (86%) | 12 (14%) | 3 20 |
| 71 | AQ | 78/79 (99%) | 73 (94%) | 5 (6%) | 17 50 |
| 72 | AR | 224/318 (70%) | 198 (88%) | 26 (12%) | 5 26 |
| 73 | AS | 109/164 (66%) | 103 (94%) | 6 (6%) | 21 54 |
| 74 | AT | 150/157 (96%) | 128 (85%) | 22 (15%) | 3 18 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 75 | AU | 149/174 (86%) | 137 (92%) | 12 (8%) | 11 41 |
| 76 | AV | 295/364 (81%) | 266 (90%) | 29 (10%) | 8 33 |
| 77 | AW | 84/158 (53%) | 76 (90%) | 8 (10%) | 8 34 |
| 78 | AX | 275/351 (78%) | 231 (84%) | 44 (16%) | 2 14 |
| 79 | AY | 99/357 (28%) | 91 (92%) | 8 (8%) | 11 41 |
| 80 | AZ | 80/95 (84%) | 72 (90%) | 8 (10%) | 7 32 |
| 81 | A0 | 176/190 (93%) | 158 (90%) | 18 (10%) | 7 32 |
| 82 | A1 | 237/291 (81%) | 218 (92%) | 19 (8%) | 12 41 |
| 83 | A2 | 99/101 (98%) | 84 (85%) | 15 (15%) | 3 17 |
| 84 | A3 | 63/166 (38%) | 58 (92%) | 5 (8%) | 12 41 |
| 85 | A4 | 226/379 (60%) | 211 (93%) | 15 (7%) | 16 49 |
| All | All | 11347/15266 (74%) | 10314 (91%) | 1033 (9%) | 13 36 |

5 of 1033 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | AX | 243 | VAL |
| 80 | AZ | 14 | LEU |
| 78 | AX | 242 | ILE |
| 32 | 7 | 137 | GLU |
| 31 | 6 | 334 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | e | 198 | ASN |
| 51 | r | 65 | ASN |
| 78 | AX | 266 | ASN |
| 41 | g | 104 | ASN |
| 45 | k | 26 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 1459/1559 (93%) | 470 (32%) | 99 (6%) |
| 2 | B | 51/73 (69%) | 19 (37%) | 3 (5%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 54 | u | 1/2 (50%) | 1 (100%) | 0 |
| 55 | AA | 914/954 (95%) | 273 (29%) | 57 (6%) |
| All | All | 2425/2588 (93%) | 763 (31%) | 159 (6%) |

5 of 763 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1672 | C |
| 1 | A | 1674 | A |
| 1 | A | 1675 | A |
| 1 | A | 1676 | A |
| 1 | A | 1678 | C |

5 of 159 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | AA | 882 | A |
| 55 | AA | 1353 | A |
| 55 | AA | 953 | U |
| 55 | AA | 1189 | U |
| 55 | AA | 1465 | C |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 135 ligands modelled in this entry, 134 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 88 | GDP | AX | 500 | - | 24,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.35 | 4 (13%) |

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 |
|---|---|---|---|---|---|---|---|
| 88 | GDP | AX | 500 | - | - | 4/12/32/32 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 88 | AX | 500 | GDP | C6-N1 | -2.03 | 1.34 | 1.37 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 88 | AX | 500 | GDP | C3'-C2'-C1' | 3.83 | 106.74 | 100.98 |
| 88 | AX | 500 | GDP | PA-O3A-PB | -2.91 | 122.85 | 132.83 |
| 88 | AX | 500 | GDP | C5-C6-N1 | 2.47 | 118.31 | 113.95 |
| 88 | AX | 500 | GDP | C8-N7-C5 | 2.36 | 107.49 | 102.99 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 88 | AX | 500 | GDP | C5'-O5'-PA-O3A |
| 88 | AX | 500 | GDP | C3'-C4'-C5'-O5' |
| 88 | AX | 500 | GDP | O4'-C4'-C5'-O5' |
| 88 | AX | 500 | GDP | C5'-O5'-PA-O1A |

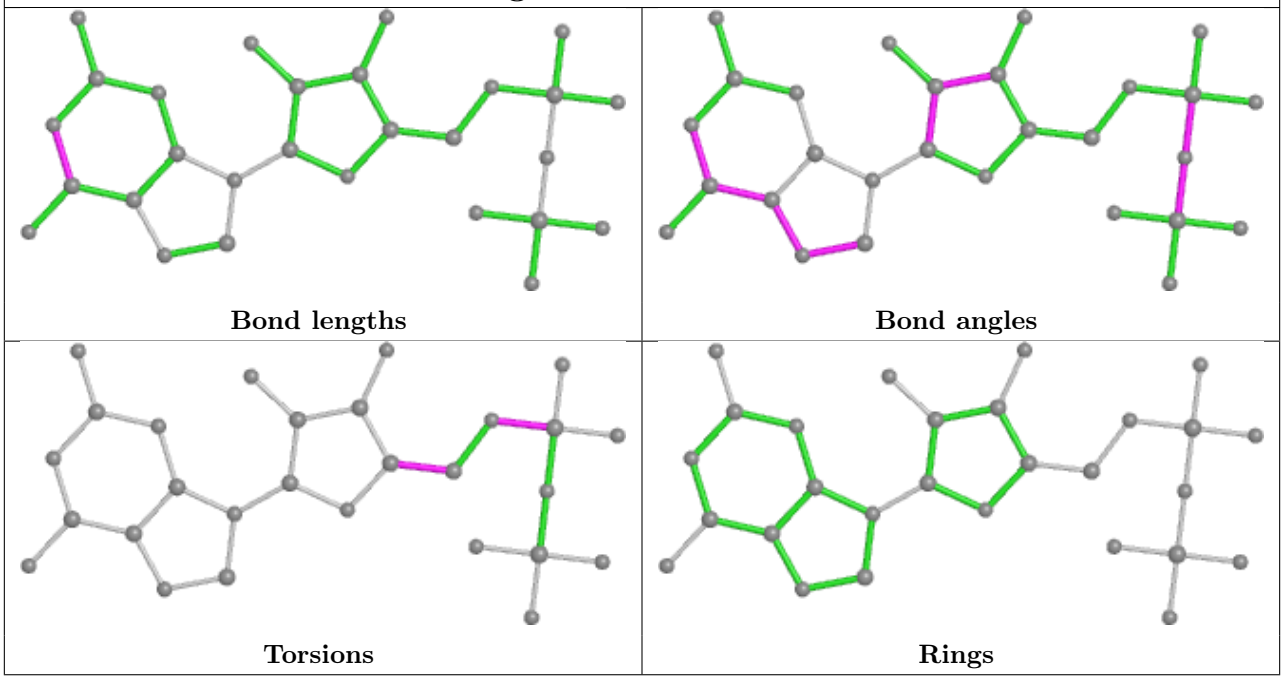
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

**Ligand GDP AX 500**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 85 | A4 | 13 |

The worst 5 of 13 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A4 | 380:ASP | C | 386:UNK | N | 26.68 |
| 1 | A4 | 143:GLU | C | 145:UNK | N | 21.71 |
| 1 | A4 | 399:UNK | C | 414:LYS | N | 20.81 |
| 1 | A4 | 173:UNK | C | 220:UNK | N | 13.65 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A4 | 300:UNK | C | 311:UNK | N | 13.15 |

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2876. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

This section was not generated.

## 6.2 Central slices

This section was not generated.

## 6.3 Largest variance slices

This section was not generated.

## 6.4 Orthogonal surface views

This section was not generated.

## 6.5 Mask visualisation

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

This section was not generated.

## 7.2 Volume estimate versus contour level

This section was not generated.

## 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit

This section was not generated.