# wwPDB EM Validation Summary Report

Dec 17, 2022 – 10:45 am GMT

| | | |
|---|---|---|
| PDB ID | : | 7AM2 |
| EMDB ID | : | EMD-11821 |
| Title | : | Intermediate assembly of the Large subunit from Leishmania major mitochondrial ribosome |
| Authors | : | Soufari, H.; Waltz, F.; Parrot, C.; Bochler, A.; Hashem, Y. |
| Deposited on | : | 2020-10-07 |
| Resolution | : | 3.40 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.

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

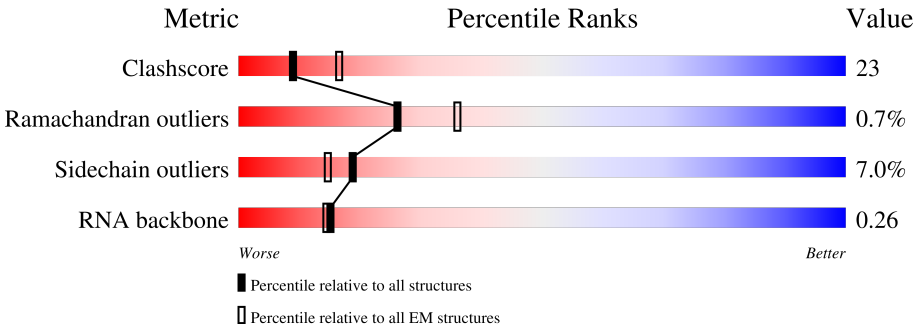
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| 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

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

The reported resolution of this entry is 3.40 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| 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 | 467 | 49% 25% • 24% |
| 2 | B | 436 | 70% 28% • |
| 3 | C | 262 | 48% 30% • 19% |
| 4 | E | 346 | 30% 33% • 35% |
| 5 | F | 171 | 53% 32% • 14% |
| 6 | G | 374 | 53% 31% 5% • 11% |
| 7 | I | 305 | 49% 33% • 16% |

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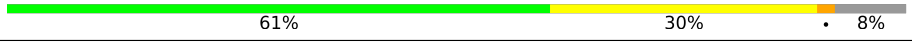
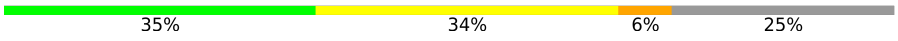
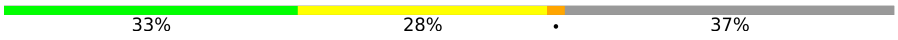
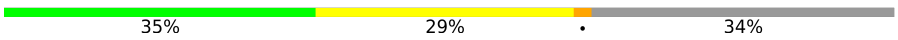
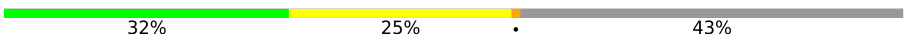
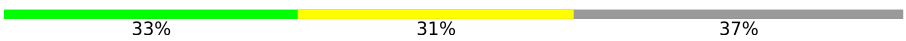
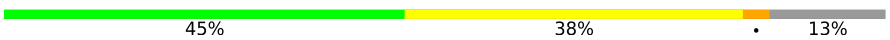
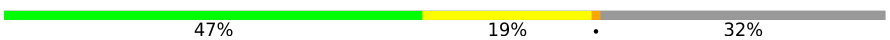
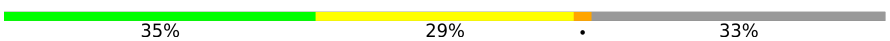
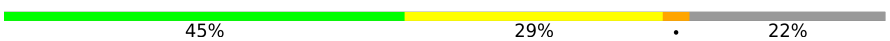
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | J | 144 |   |
| 9 | K | 194 |   |
| 10 | L | 186 |   |
| 11 | M | 279 |   |
| 12 | N | 252 |   |
| 13 | O | 476 |   |
| 14 | Q | 234 |   |
| 15 | R | 480 |   |
| 16 | S | 409 |   |
| 17 | T | 83 |   |
| 18 | V | 151 |   |
| 19 | Z | 197 |   |
| 20 | BA | 167 |   |
| 21 | CA | 618 |   |
| 22 | UA | 203 |   |
| 23 | BB | 156 |   |
| 24 | CB | 202 |   |
| 25 | BK | 893 |   |
| 26 | BQ | 445 |   |
| 27 | BN | 344 |   |
| 28 | BE | 118 |   |
| 29 | BO | 190 |   |
| 30 | At | 183 |   |
| 31 | Au | 186 |   |
| 32 | Ae | 311 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | Af | 155 | 88% 5% 6% |
| 34 | Ah | 570 | 66% 30% |
| 35 | Ap | 240 | 82% 7% 11% |
| 36 | Al | 346 | 61% 5% 34% |
| 37 | Ab | 262 | 61% 36% |
| 38 | Aa | 195 | 63% 7% 31% |
| 39 | BP | 254 | 33% 16% 48% |
| 40 | Az | 152 | 81% 5% 14% |
| 41 | Am | 340 | 83% 13% |
| 42 | As | 249 | 55% 42% |
| 43 | BG | 1347 | 94% |
| 44 | Ad | 237 | 76% 20% |
| 45 | Aw | 187 | 97% |
| 46 | BH | 229 | 47% 31% 21% |
| 47 | Aj | 503 | 65% 32% |
| 48 | Ar | 205 | 90% 5% 5% |
| 49 | An | 331 | 68% 28% |
| 50 | BF | 109 | 42% 28% 28% |
| 51 | Av | 192 | 48% 48% |
| 52 | BM | 457 | 40% 40% 5% 15% |
| 53 | Ag | 244 | 48% 49% |
| 54 | Bl | 266 | 67% 30% |
| 55 | Ax | 216 | 71% 6% 23% |
| 56 | BS | 416 | 18% 12% 70% |
| 57 | BX | 569 | 21% 23% 52% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 57 | BY | 569 | 20% 26% 52% |
| 58 | BZ | 413 | 38% 39% 7% 15% |
| 59 | CC | 150 | 29% 25% 44% |
| 60 | CD | 126 | 29% 40% 29% |
| 61 | BT | 464 | 38% 24% 35% |
| 62 | BU | 497 | 45% 43% 5% 7% |
| 63 | BW | 776 | 30% 24% 42% |
| 64 | BV | 787 | 14% 11% 75% |
| 65 | U7 | 40 | 85% 15% |
| 66 | U6 | 187 | 84% 14% |
| 67 | U1 | 46 | 76% 20% |
| 68 | U3 | 75 | 69% 31% |
| 69 | U4 | 136 | 88% 12% |
| 70 | U5 | 94 | 74% 23% |
| 71 | BR | 301 | 38% 33% 29% |
| 72 | U2 | 37 | 76% 24% |
| 73 | 1 | 19000 | 96% |
| 74 | R1 | 3 | 33% 67% |
| 75 | R2 | 35 | 14% 20% 60% |
| 76 | R5 | 5 | 40% 60% |
| 77 | U8 | 59 | 49% 29% 22% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 78 | GTP | BU | 501 | - | - | X | - |

# 2 Entry composition (i)

There are 79 unique types of molecules in this entry. The entry contains 139535 atoms, of which 12 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein L3-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 356 | 2909 | 1877 | 482 | 535 | 15 | 0 | 0 |

- Molecule 2 is a protein called uL4m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 435 | 3513 | 2237 | 615 | 642 | 19 | 0 | 0 |

- Molecule 3 is a protein called RIBOSOMAL_L9 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 212 | 1772 | 1144 | 303 | 321 | 4 | 0 | 0 |

- Molecule 4 is a protein called Putative ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | E | 225 | 1818 | 1176 | 319 | 314 | 9 | 0 | 0 |

- Molecule 5 is a protein called 50S ribosomal protein L13-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | F | 147 | 1231 | 788 | 223 | 210 | 10 | 0 | 0 |

- Molecule 6 is a protein called Ribosomal_L18e/L15P domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | G | 334 | 2767 | 1765 | 505 | 489 | 8 | 0 | 0 |

- Molecule 7 is a protein called Putative 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | I | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2153 | 1362 | 406 | 372 | 13 | | |

- Molecule 8 is a protein called bL19m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | J | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1146 | 727 | 211 | 202 | 6 | | |

- Molecule 9 is a protein called bL20m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | K | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1467 | 910 | 289 | 258 | 10 | | |

- Molecule 10 is a protein called bL21m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | L | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1419 | 907 | 257 | 250 | 5 | | |

- Molecule 11 is a protein called uL22m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | M | 259 | Total | C | N | O | S | 0 | 0 |
| | | | 2116 | 1345 | 385 | 371 | 15 | | |

- Molecule 12 is a protein called uL23m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | N | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1599 | 1031 | 296 | 269 | 3 | | |

- Molecule 13 is a protein called uL24m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | O | 300 | Total | C | N | O | S | 0 | 0 |
| | | | 2477 | 1561 | 446 | 463 | 7 | | |

- Molecule 14 is a protein called bL28m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | Q | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1785 | 1127 | 331 | 316 | 11 | | |

- Molecule 15 is a protein called uL29m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | R | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3755 | 2377 | 662 | 704 | 12 | | |

- Molecule 16 is a protein called uL30m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | S | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1244 | 782 | 247 | 207 | 8 | | |

- Molecule 17 is a protein called bL32m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | T | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 487 | 311 | 93 | 78 | 5 | | |

- Molecule 18 is a protein called bL35m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | V | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1202 | 755 | 242 | 197 | 8 | | |

- Molecule 19 is a protein called mL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | Z | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 907 | 582 | 167 | 154 | 4 | | |

- Molecule 20 is a protein called mL94.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | BA | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 489 | 144 | 149 | 4 | | |

- Molecule 21 is a protein called TRUD domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | CA | 537 | Total | C | N | O | S | 0 | 0 |
| | | | 4230 | 2664 | 783 | 765 | 18 | | |

- Molecule 22 is a protein called UA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 22 | UA | 203 | Total | C | N | O | 0 | 0 |
| | | | 1015 | 609 | 203 | 203 | | |

- Molecule 23 is a protein called mL95.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 23 | BB | 106 | Total | C | N | O | 0 | 0 |
| | | | 894 | 574 | 168 | 152 | | |

- Molecule 24 is a protein called RNA uridylyltransferase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | CB | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 673 | 192 | 201 | 8 | | |

- Molecule 25 is a protein called mL67.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | BK | 694 | Total | C | N | O | S | 0 | 0 |
| | | | 5419 | 3421 | 975 | 1002 | 21 | | |

- Molecule 26 is a protein called mL71.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | BQ | 413 | Total | C | N | O | S | 0 | 0 |
| | | | 3230 | 2031 | 571 | 615 | 13 | | |

- Molecule 27 is a protein called mL81.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | BN | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1507 | 939 | 275 | 286 | 7 | | |

- Molecule 28 is a protein called mL98.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 28 | BE | 37 | Total<br>325 | C<br>210 | N<br>55 | O<br>60 | 0 | 0 |

- Molecule 29 is a protein called Putative ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | BO | 158 | Total<br>1281 | C<br>805 | N<br>258 | O<br>209 | S<br>9 | 0 | 0 |

- Molecule 30 is a protein called mL86.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | At | 165 | Total<br>1346 | C<br>824 | N<br>260 | O<br>254 | S<br>8 | 0 | 0 |

- Molecule 31 is a protein called mL87.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | Au | 80 | Total<br>681 | C<br>432 | N<br>135 | O<br>109 | S<br>5 | 0 | 0 |

- Molecule 32 is a protein called mL53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | Ae | 290 | Total<br>2354 | C<br>1523 | N<br>417 | O<br>403 | S<br>11 | 0 | 0 |

- Molecule 33 is a protein called mL63.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | Af | 145 | Total<br>1192 | C<br>748 | N<br>228 | O<br>215 | S<br>1 | 0 | 0 |

- Molecule 34 is a protein called mL68.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | Ah | 399 | Total<br>3242 | C<br>2062 | N<br>567 | O<br>596 | S<br>17 | 0 | 0 |

- Molecule 35 is a protein called mL80.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | Ap | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1775 | 1111 | 327 | 328 | 9 | | |

- Molecule 36 is a protein called mL74.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | Al | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1857 | 1188 | 321 | 342 | 6 | | |

- Molecule 37 is a protein called L51_S25_CI-B8 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | Ab | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1413 | 886 | 268 | 254 | 5 | | |

- Molecule 38 is a protein called mL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | Aa | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1076 | 670 | 202 | 199 | 5 | | |

- Molecule 39 is a protein called mL52,mL52.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | BP | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1070 | 682 | 194 | 193 | 1 | | |

- Molecule 40 is a protein called mL93.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | Az | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1150 | 739 | 205 | 201 | 5 | | |

- Molecule 41 is a protein called mL75.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | Am | 296 | Total | C | N | O | S | 0 | 0 |
| | | | 2435 | 1553 | 435 | 431 | 16 | | |

- Molecule 42 is a protein called mL85.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | As | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1187 | 734 | 225 | 223 | 5 | | |

- Molecule 43 is a protein called mL100.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | BG | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 423 | 126 | 119 | 7 | | |

- Molecule 44 is a protein called mL49.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | Ad | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1502 | 969 | 264 | 262 | 7 | | |

- Molecule 45 is a protein called mL89.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | Aw | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 949 | 289 | 268 | 3 | | |

- Molecule 46 is a protein called Peptidyl-prolyl cis-trans isomerase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | BH | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1394 | 885 | 244 | 257 | 8 | | |

- Molecule 47 is a protein called mL72.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | Aj | 342 | Total | C | N | O | S | 0 | 0 |
| | | | 2777 | 1762 | 512 | 492 | 11 | | |

- Molecule 48 is a protein called mL84.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | Ar | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1644 | 1054 | 295 | 288 | 7 | | |

- Molecule 49 is a protein called mL76.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | An | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1946 | 1222 | 357 | 363 | 4 | | |

- Molecule 50 is a protein called mL99.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | BF | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 661 | 413 | 128 | 118 | 2 | | |

- Molecule 51 is a protein called mL88.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | Av | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 828 | 530 | 142 | 151 | 5 | | |

- Molecule 52 is a protein called mL70.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | BM | 389 | Total | C | N | O | S | 0 | 0 |
| | | | 3069 | 1954 | 548 | 551 | 16 | | |

- Molecule 53 is a protein called mL59/64.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | Ag | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1031 | 656 | 189 | 181 | 5 | | |

- Molecule 54 is a protein called Peptidyl-prolyl cis-trans isomerase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | Bl | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1409 | 895 | 242 | 264 | 8 | | |

- Molecule 55 is a protein called LIM zinc-binding domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | Ax | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 876 | 268 | 233 | 11 | | |

- Molecule 56 is a protein called DNAj-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | BS | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 978 | 624 | 177 | 173 | 4 | | |

- Molecule 57 is a protein called SpoU_methylase domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | BY | 275 | Total | C | N | O | S | 0 | 0 |
| | | | 2111 | 1317 | 384 | 401 | 9 | | |
| 57 | BX | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2086 | 1301 | 381 | 396 | 8 | | |

- Molecule 58 is a protein called Pseudouridylate synthase-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | BZ | 351 | Total | C | N | O | S | 0 | 0 |
| | | | 2829 | 1810 | 514 | 493 | 12 | | |

- Molecule 59 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | CC | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 668 | 429 | 104 | 134 | 1 | | |

- Molecule 60 is a protein called L0R8F8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | CD | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 761 | 475 | 146 | 136 | 4 | | |

- Molecule 61 is a protein called G domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | BT | 300 | Total | C | N | O | S | 0 | 0 |
| | | | 2346 | 1487 | 419 | 425 | 15 | | |

- Molecule 62 is a protein called GTPase Der.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | BU | 463 | Total | C | N | O | S | 0 | 0 |
| | | | 3680 | 2315 | 654 | 691 | 20 | | |

- Molecule 63 is a protein called DEAD/DEAH box helicase-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | BW | 447 | Total | C | N | O | S | 0 | 0 |
| | | | 3589 | 2282 | 661 | 622 | 24 | | |

- Molecule 64 is a protein called G domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | BV | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1596 | 1016 | 292 | 282 | 6 | | |

- Molecule 65 is a protein called mL78.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 65 | U7 | 40 | Total | C | N | O | 0 | 0 |
| | | | 200 | 120 | 40 | 40 | | |

- Molecule 66 is a protein called U6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 66 | U6 | 187 | Total | C | N | O | 0 | 0 |
| | | | 935 | 561 | 187 | 187 | | |

- Molecule 67 is a protein called U1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 67 | U1 | 46 | Total | C | N | O | 0 | 0 |
| | | | 230 | 138 | 46 | 46 | | |

- Molecule 68 is a protein called U3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 68 | U3 | 75 | Total | C | N | O | 0 | 0 |
| | | | 375 | 225 | 75 | 75 | | |

- Molecule 69 is a protein called U4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 69 | U4 | 136 | Total | C | N | O | 0 | 0 |
| | | | 680 | 408 | 136 | 136 | | |

- Molecule 70 is a protein called U5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 70 | U5 | 94 | Total | C | N | O | 0 | 0 |
| | | | 470 | 282 | 94 | 94 | | |

- Molecule 71 is a protein called mL78.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | BR | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1703 | 1071 | 329 | 300 | 3 | | |

- Molecule 72 is a protein called U2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 72 | U2 | 37 | Total | C | N | O | 0 | 0 |
| | | | 185 | 111 | 37 | 37 | | |

- Molecule 73 is a RNA chain called Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | 1 | 797 | Total | C | N | O | P | 0 | 0 |
| | | | 16777 | 7564 | 2796 | 5622 | 795 | | |

- Molecule 74 is a RNA chain called R1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | R1 | 3 | Total | C | N | O | P | 0 | 0 |
| | | | 62 | 28 | 9 | 22 | 3 | | |

- Molecule 75 is a RNA chain called R2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | R2 | 34 | Total | C | N | O | P | 0 | 0 |
| | | | 665 | 306 | 68 | 258 | 33 | | |

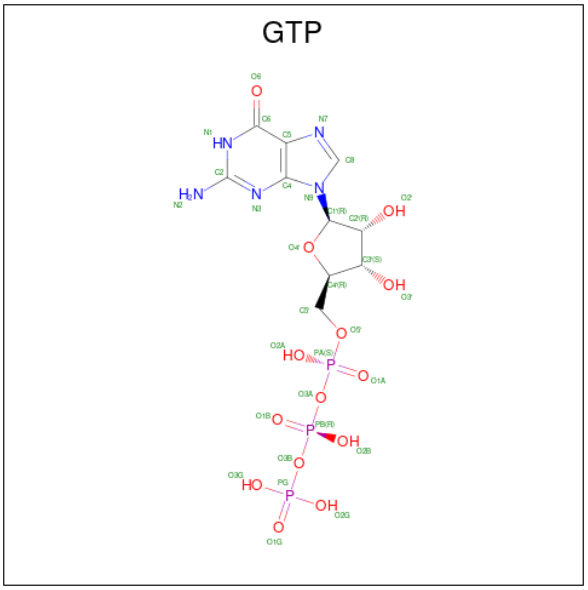
- Molecule 76 is a RNA chain called R5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | R5 | 5 | Total | C | N | O | P | 0 | 0 |
| | | | 100 | 45 | 10 | 40 | 5 | | |

- Molecule 77 is a protein called U8.

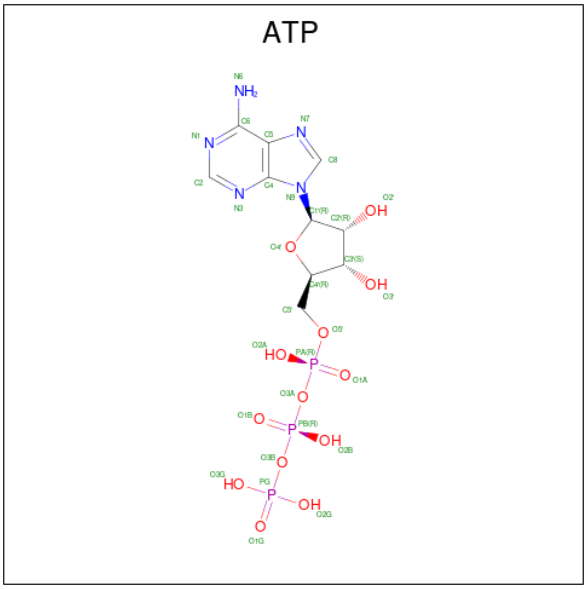
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 77 | U8 | 59 | Total | C | N | O | 0 | 0 |
| | | | 295 | 177 | 59 | 59 | | |

- Molecule 78 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 78 | BU | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

- Molecule 79 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



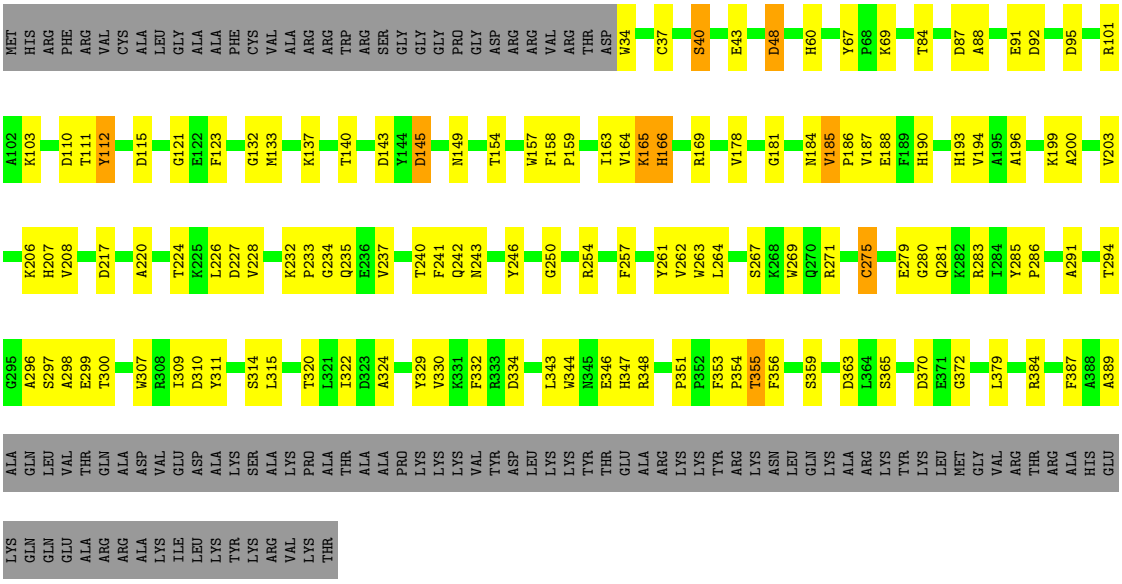
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 79 | BW | 1 | Total | C | H | N | O | P | 0 |
| | | | 43 | 10 | 12 | 5 | 13 | 3 | |

# 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.

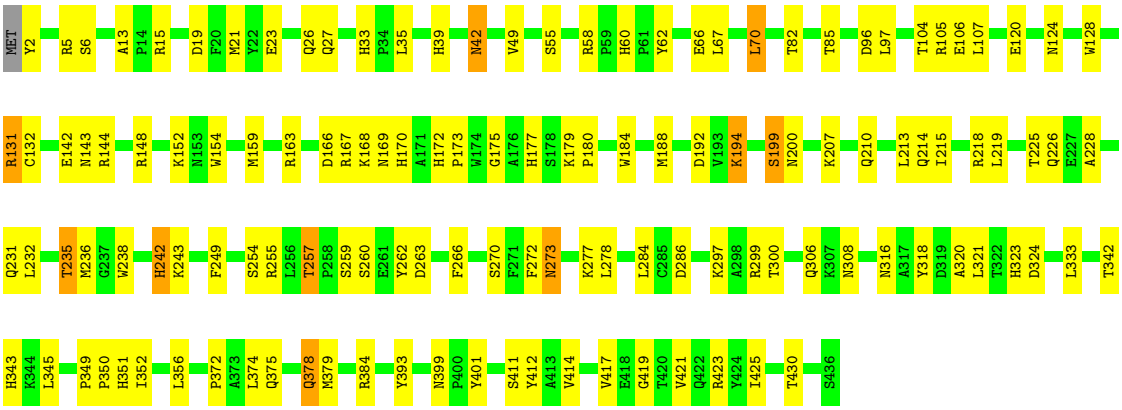
• Molecule 1: Ribosomal protein L3-like protein

Chain A:


• Molecule 2: uL4m

Chain B:

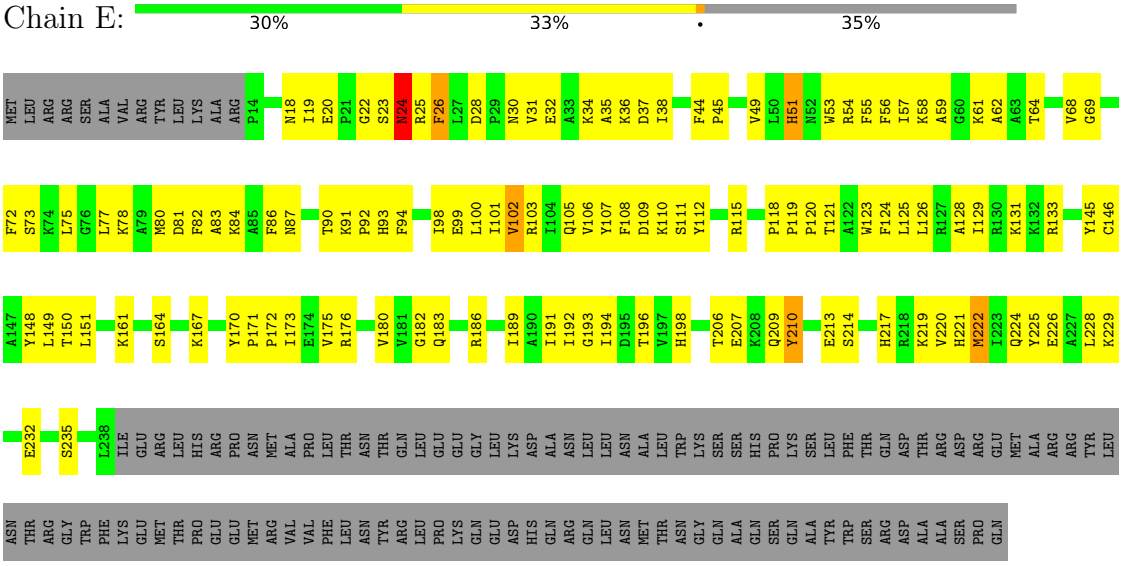




• Molecule 3: RIBOSOMAL_L9 domain-containing protein

Chain C:

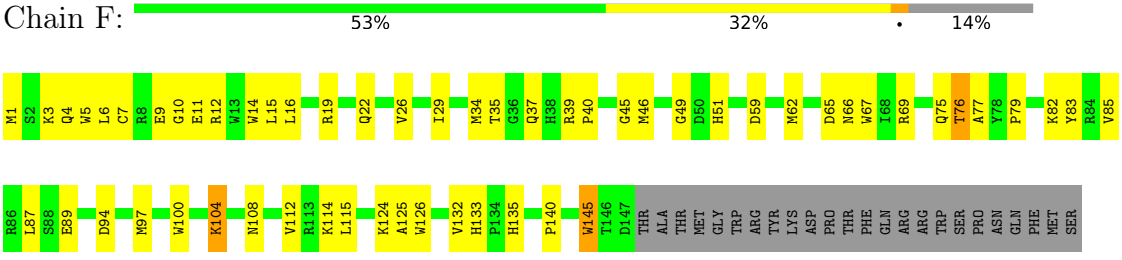

• Molecule 4: Putative ribosomal protein L11

Chain E:



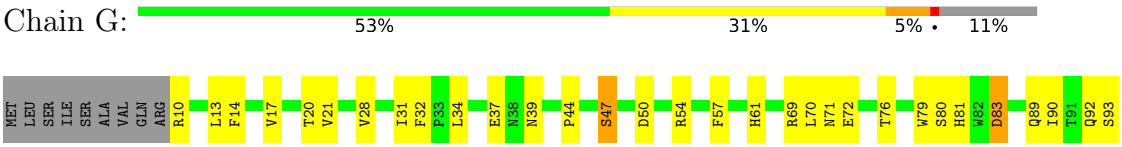

• Molecule 5: 50S ribosomal protein L13-like protein

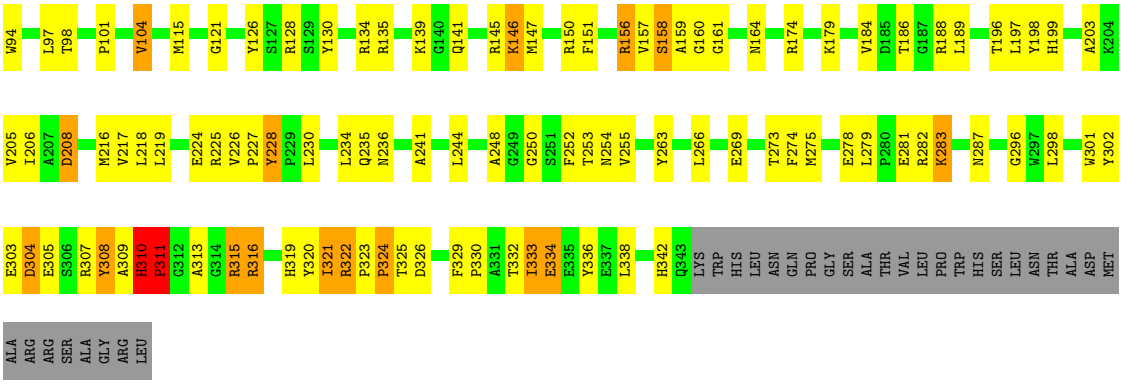
Chain F:




• Molecule 6: Ribosomal_L18e/L15P domain-containing protein

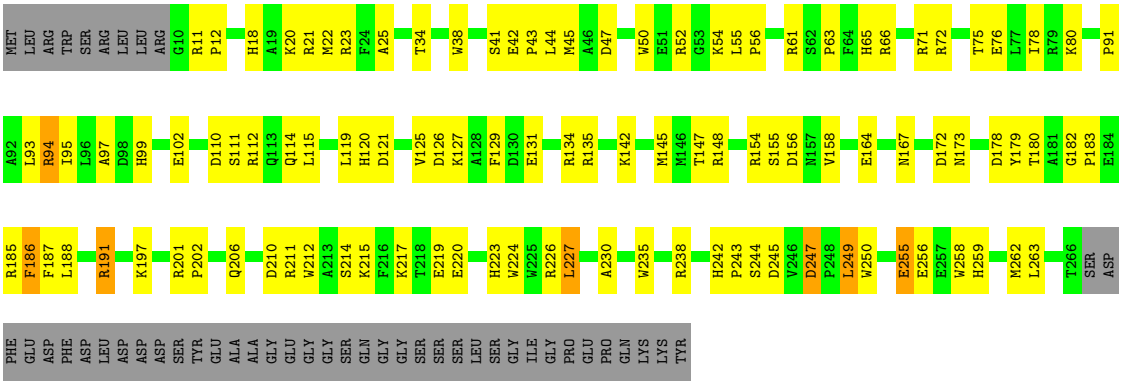
Chain G:





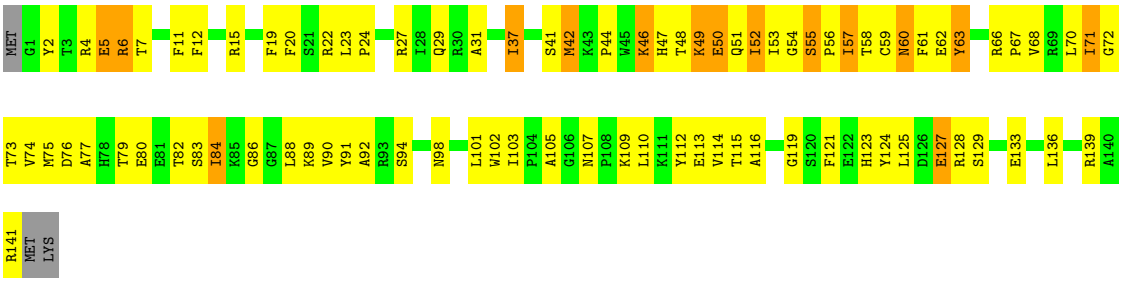
• Molecule 7: Putative 50S ribosomal protein L17

Chain I:

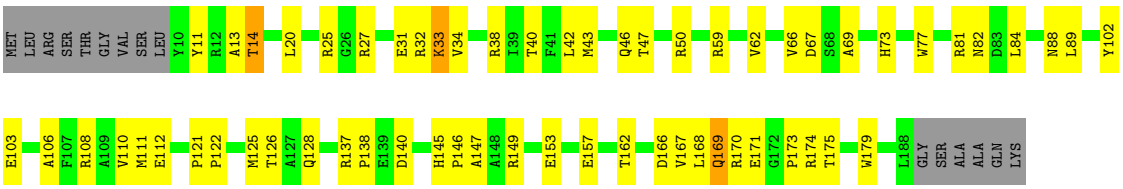
• Molecule 8: bL19m

Chain J:

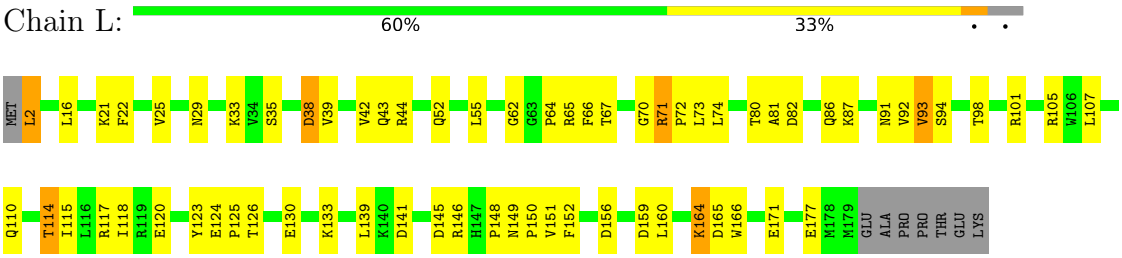
• Molecule 9: bL20m

Chain K:

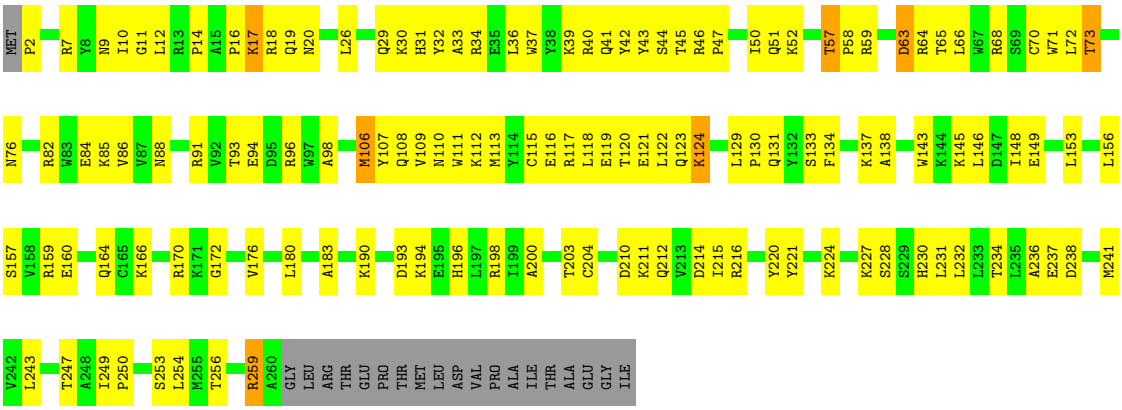
- Molecule 10: bL21m

Chain L:



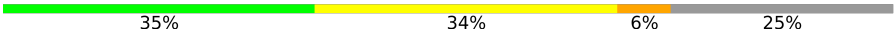

- Molecule 11: uL22m

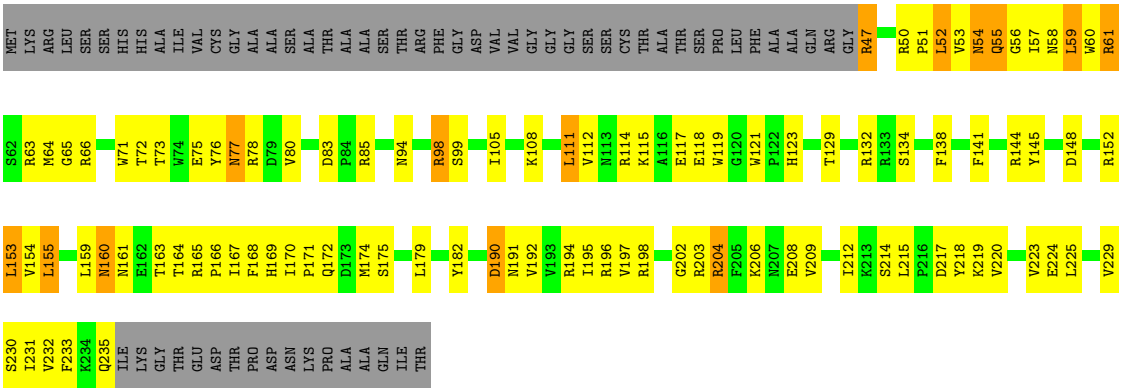
Chain M:

- Molecule 12: uL23m

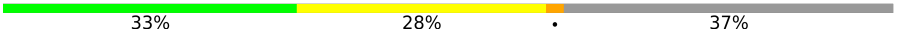
Chain N:

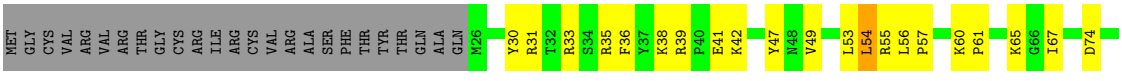


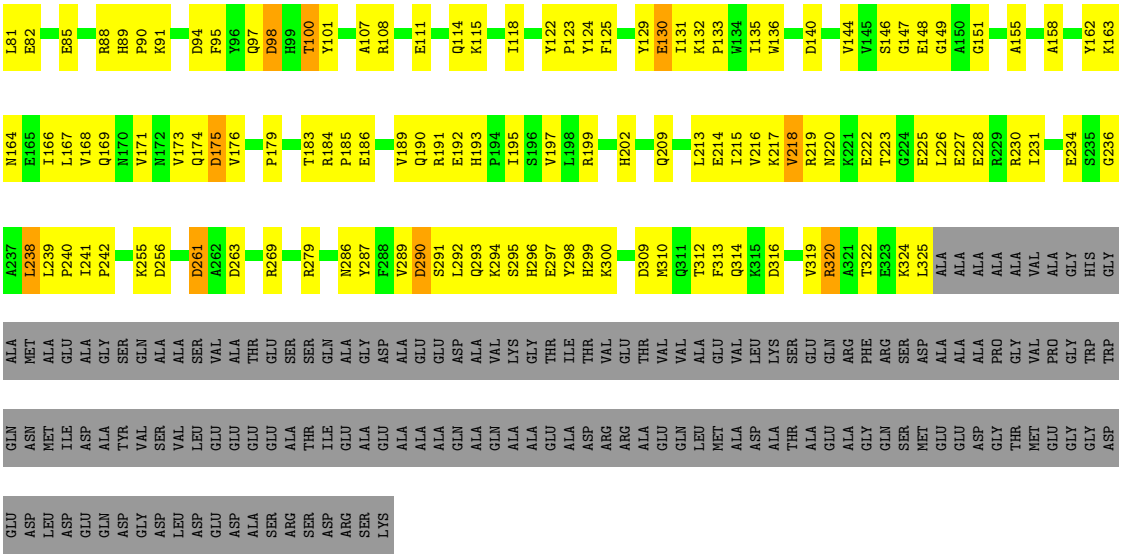



- Molecule 13: uL24m

Chain O:

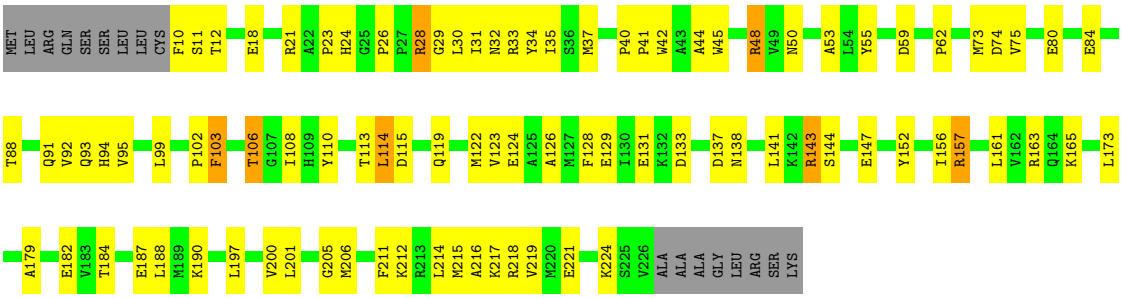




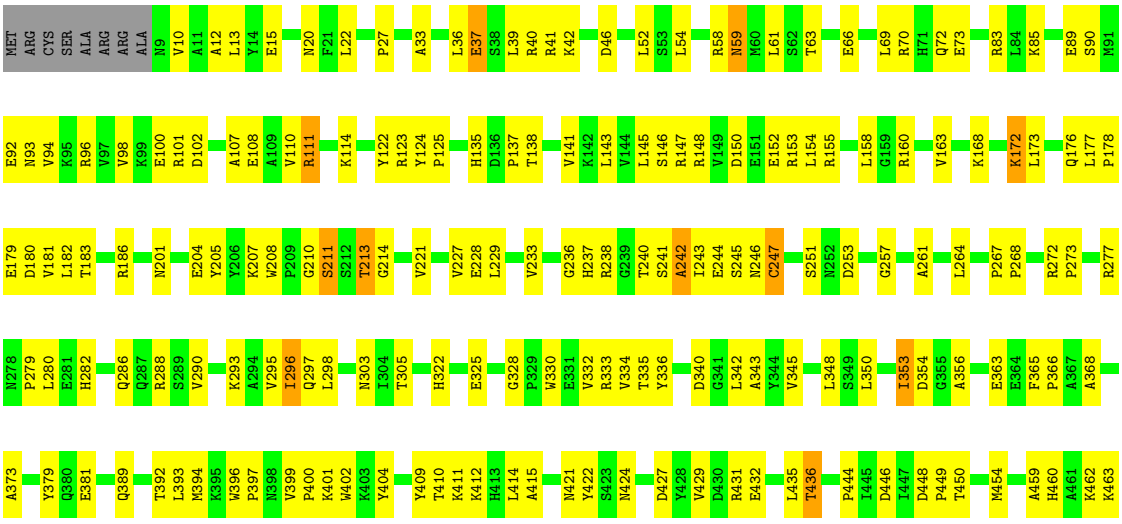
• Molecule 14: bL28m

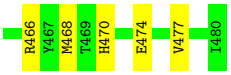
Chain Q:

• Molecule 15: uL29m

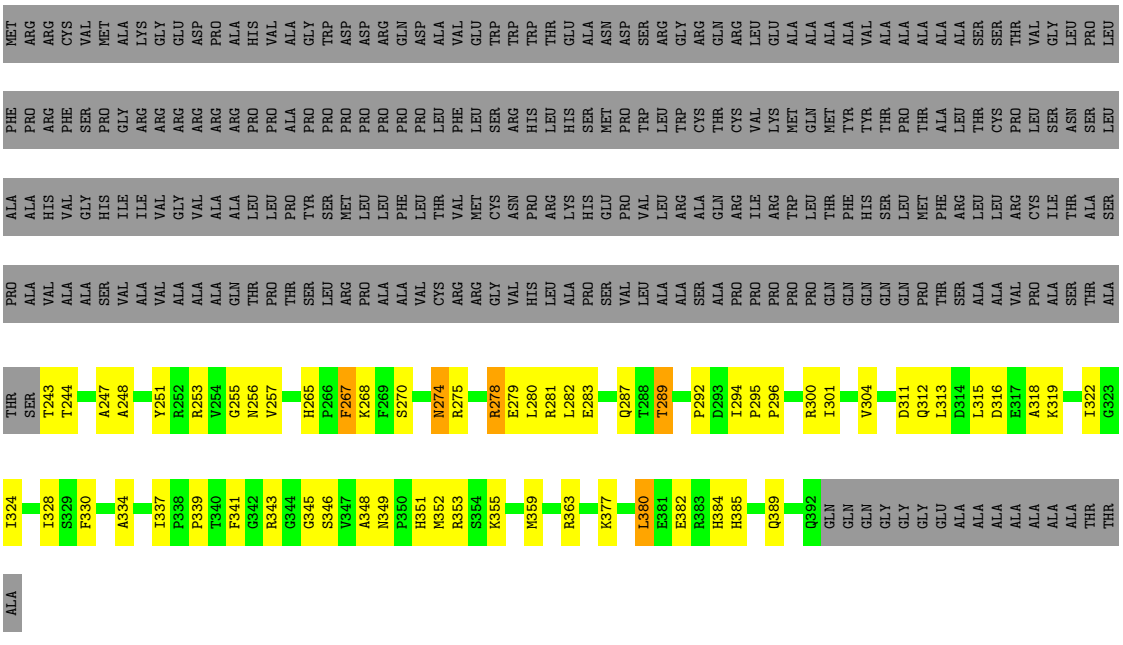
Chain R:



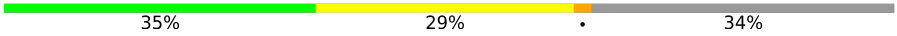

• Molecule 16: uL30m

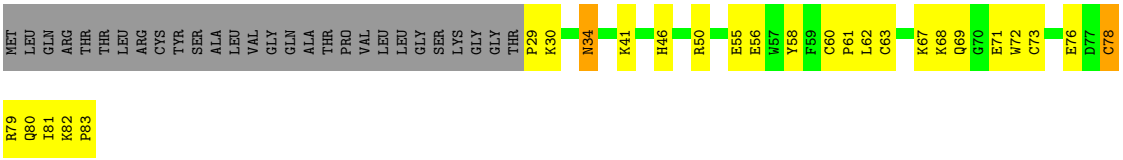
Chain S:


• Molecule 17: bL32m

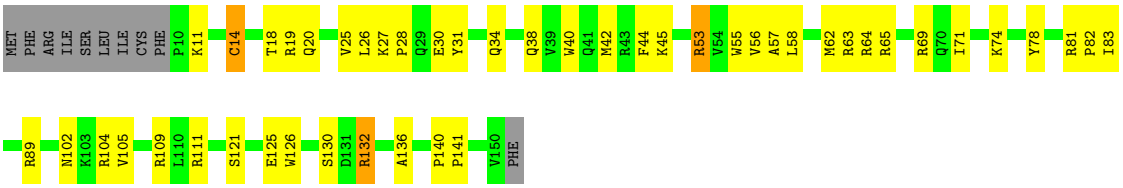
Chain T:



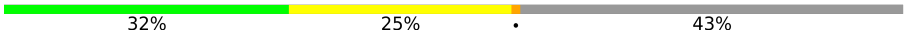

• Molecule 18: bL35m

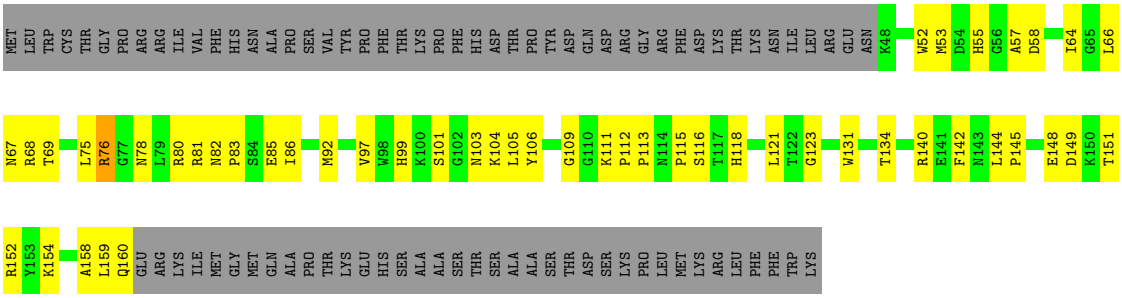
Chain V:


• Molecule 19: mL41

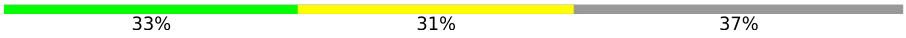
Chain Z:

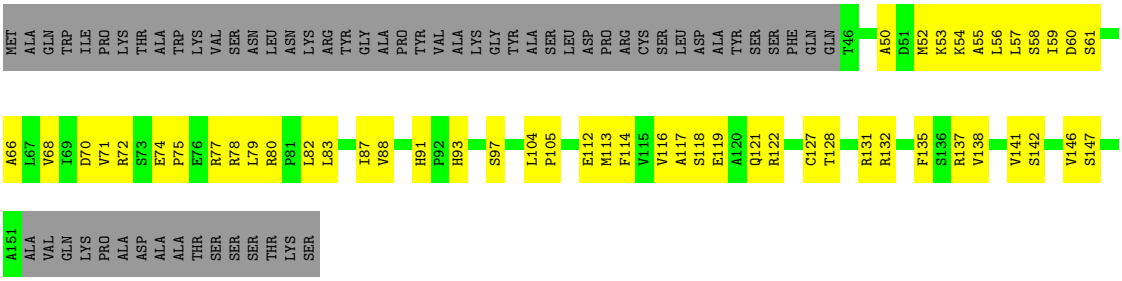




• Molecule 20: mL94

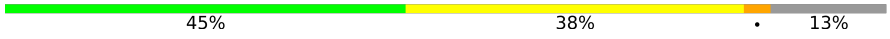
Chain BA:

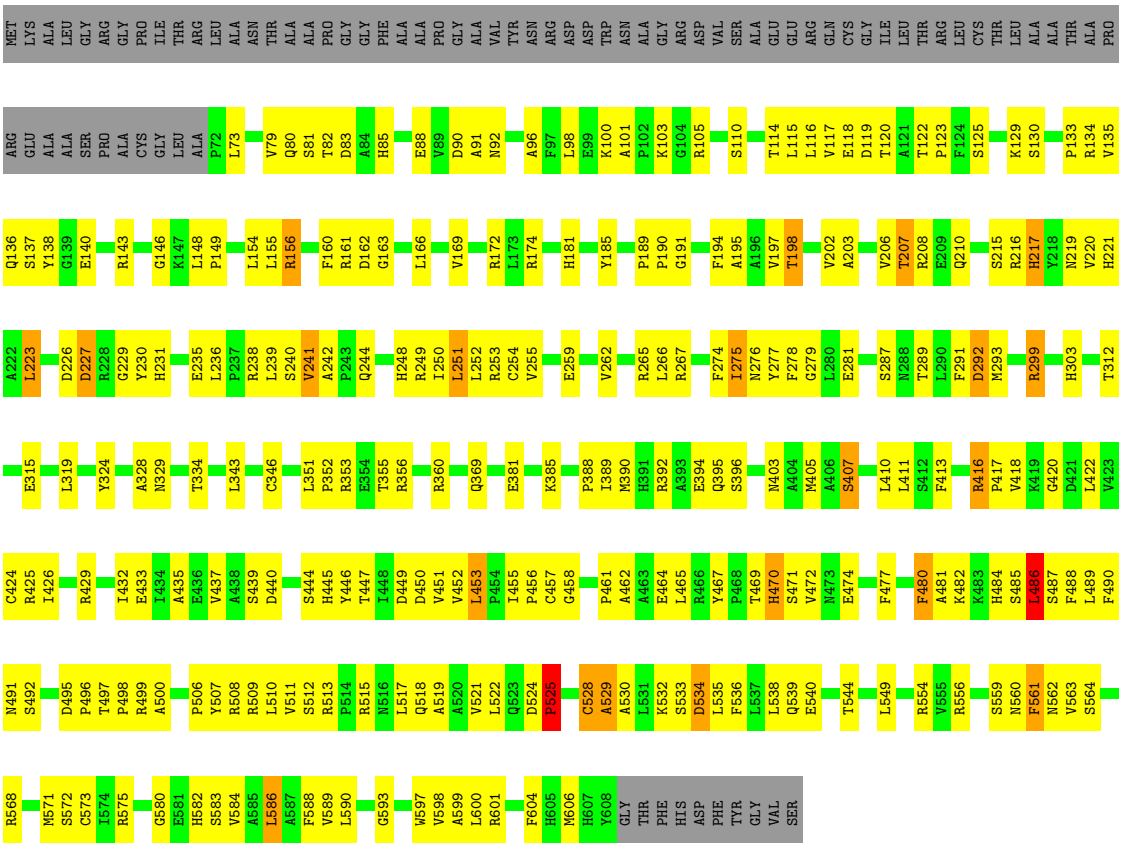


• Molecule 21: TRUD domain-containing protein

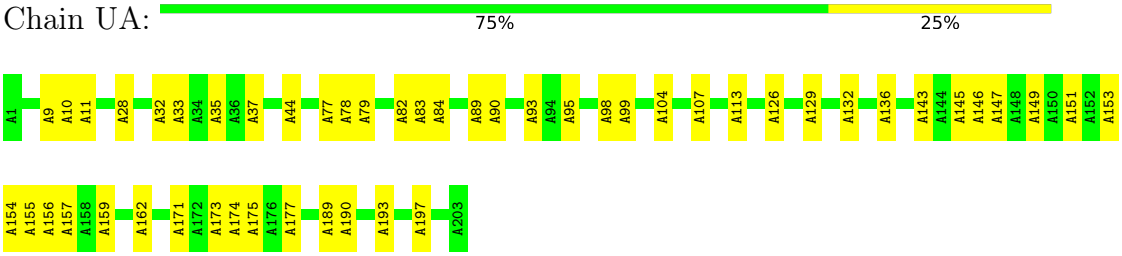
Chain CA:



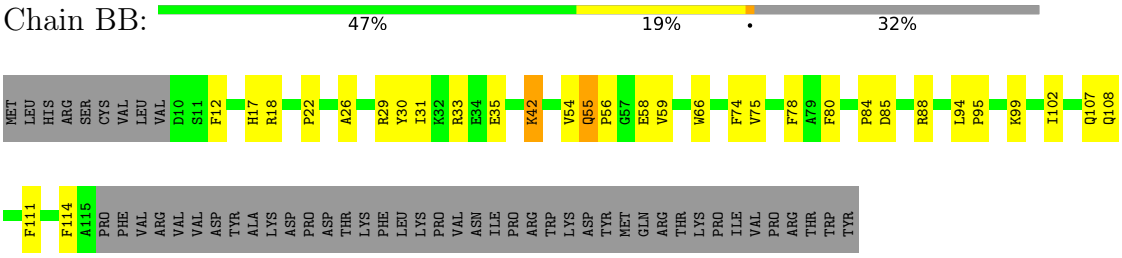
• Molecule 22: UA

Chain UA:



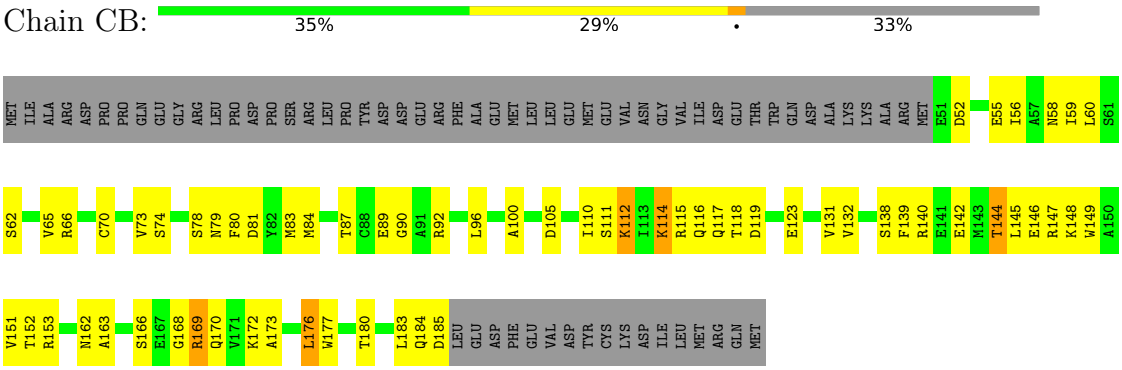

• Molecule 23: mL95

Chain BB:



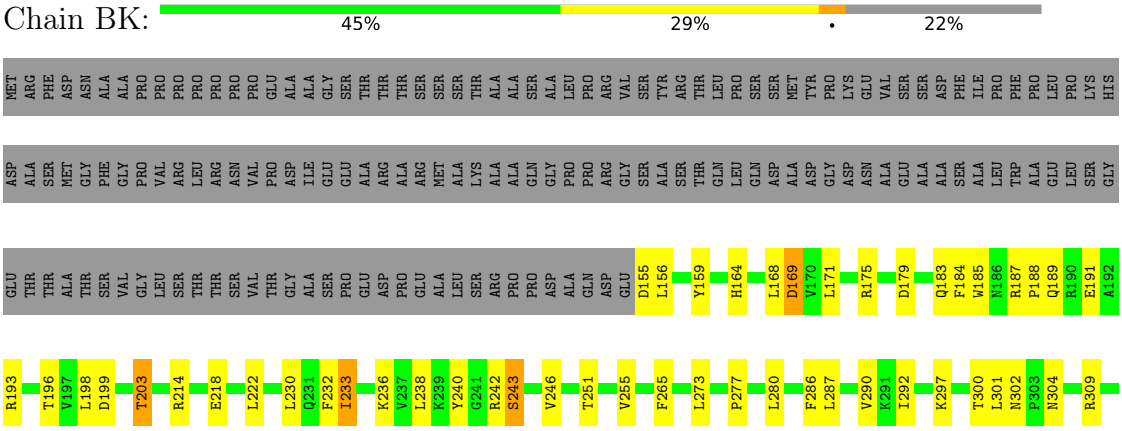

• Molecule 24: RNA uridylyltransferase

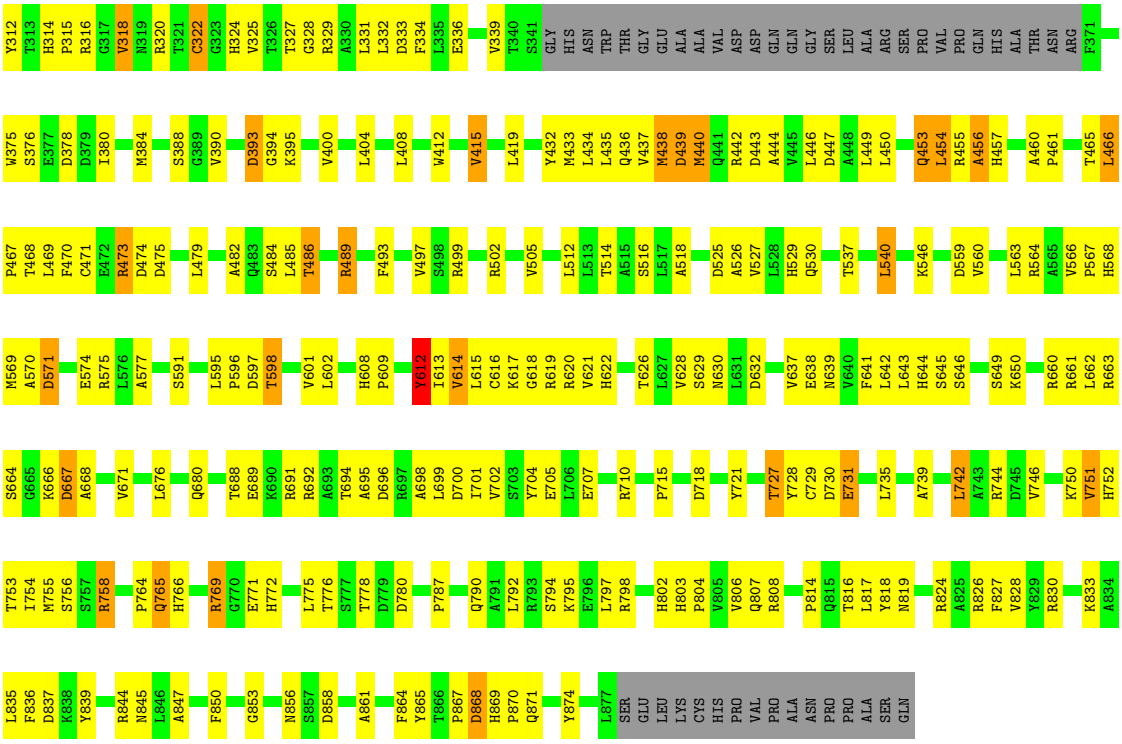
Chain CB:




• Molecule 25: mL67

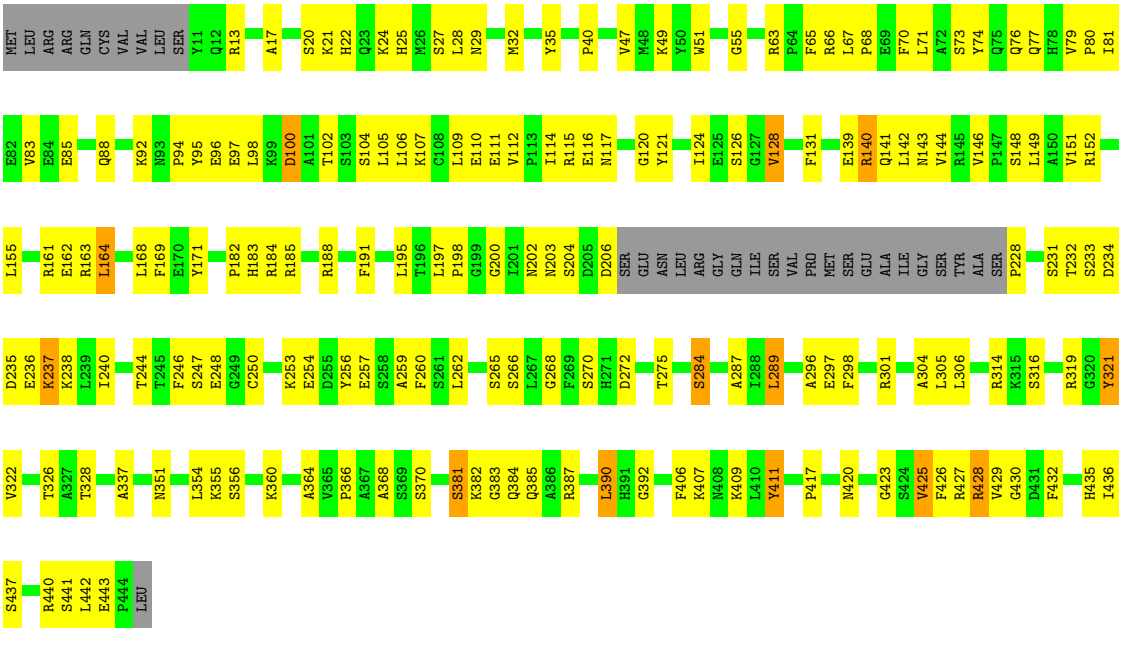
Chain BK:





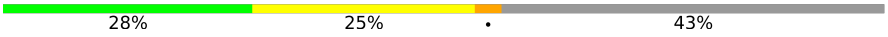
• Molecule 26: mL71

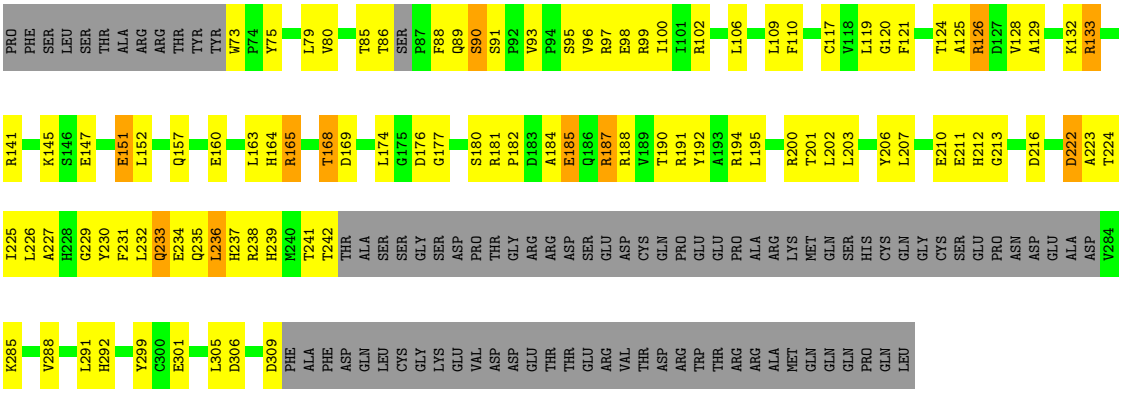
Chain BQ:

• Molecule 27: mL81

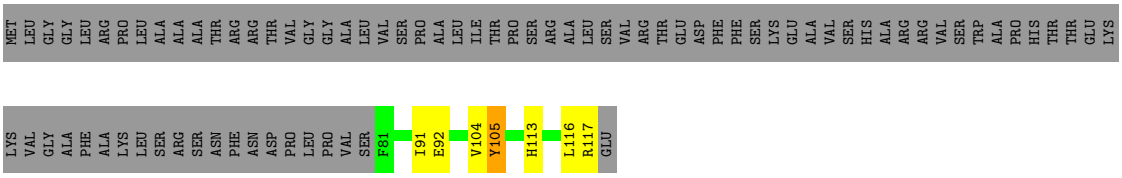
Chain BN:



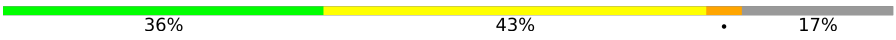
• Molecule 28: mL98

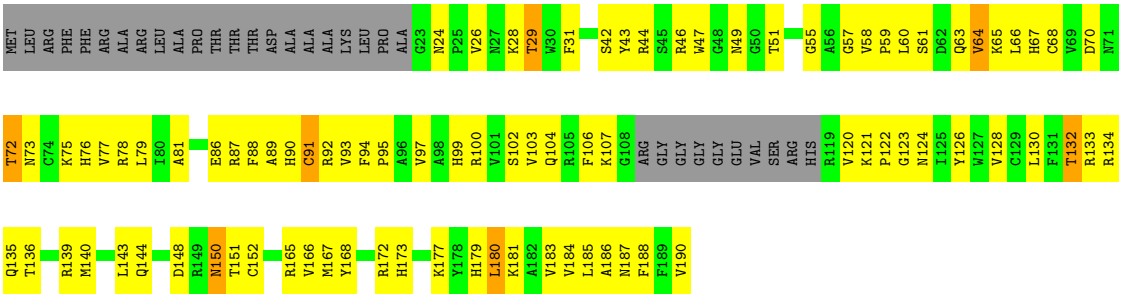
Chain BE:

• Molecule 29: Putative ribosomal protein L14

Chain BO:



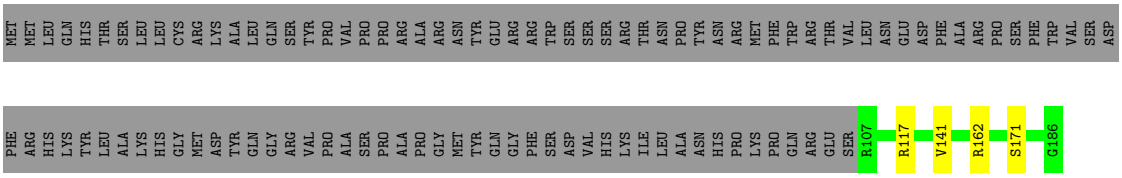



• Molecule 30: mL86

Chain At:

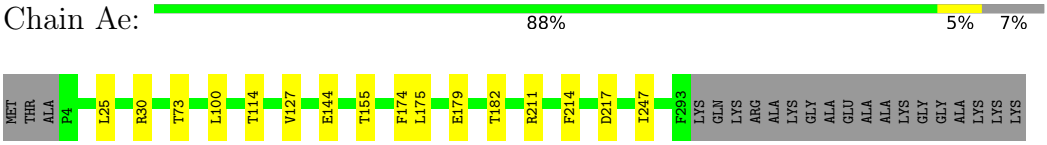

• Molecule 31: mL87

Chain Au:

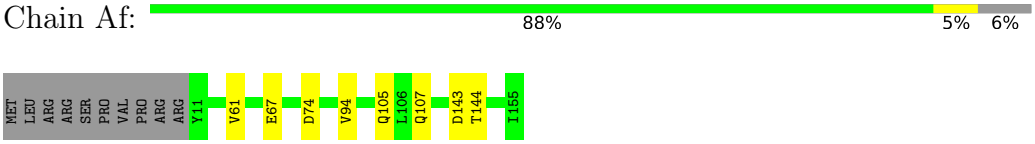
- Molecule 32: mL53

Chain Ae:



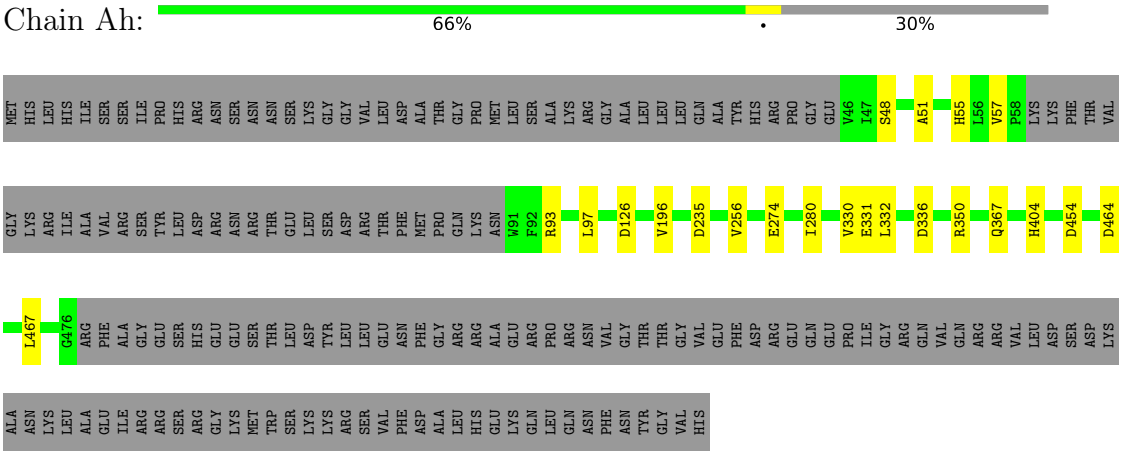

- Molecule 33: mL63

Chain Af:



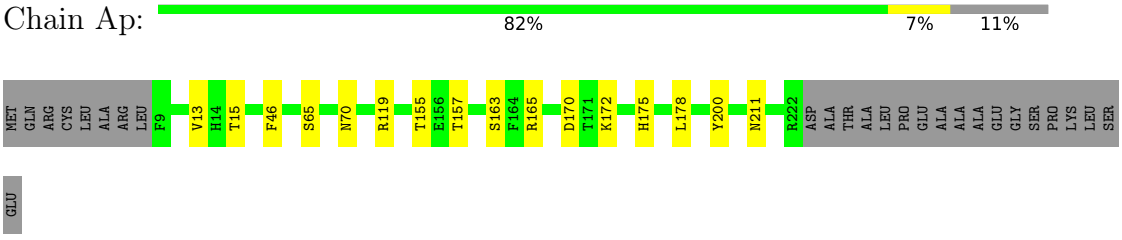

- Molecule 34: mL68

Chain Ah:



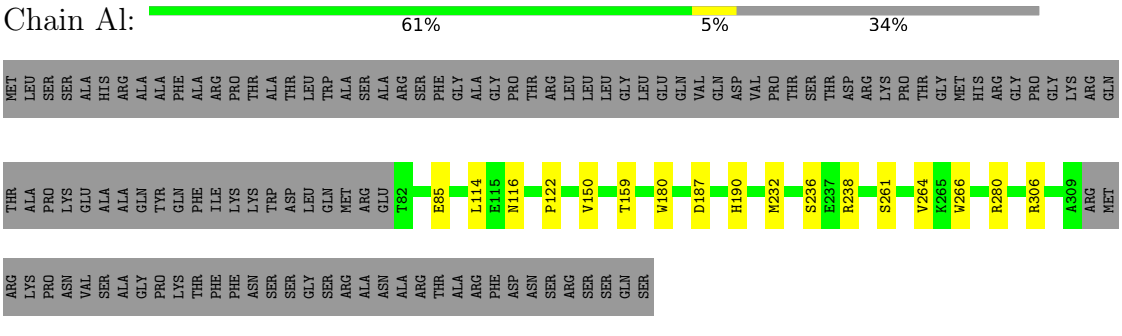

- Molecule 35: mL80

Chain Ap:



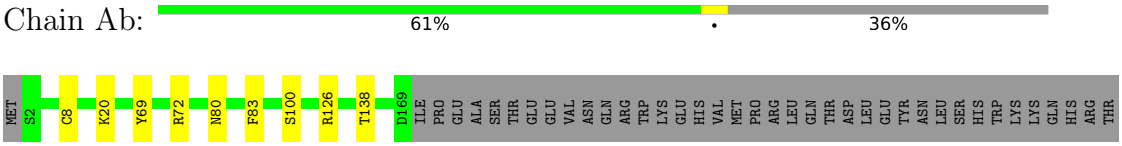

- Molecule 36: mL74

Chain Al:



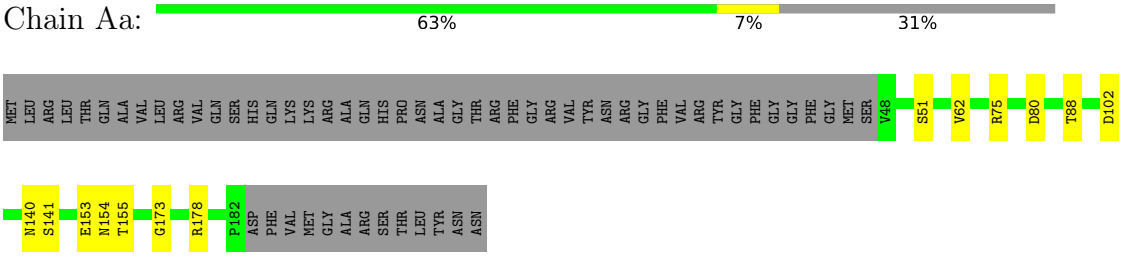
• Molecule 37: L51_S25_CI-B8 domain-containing protein

Chain Ab:



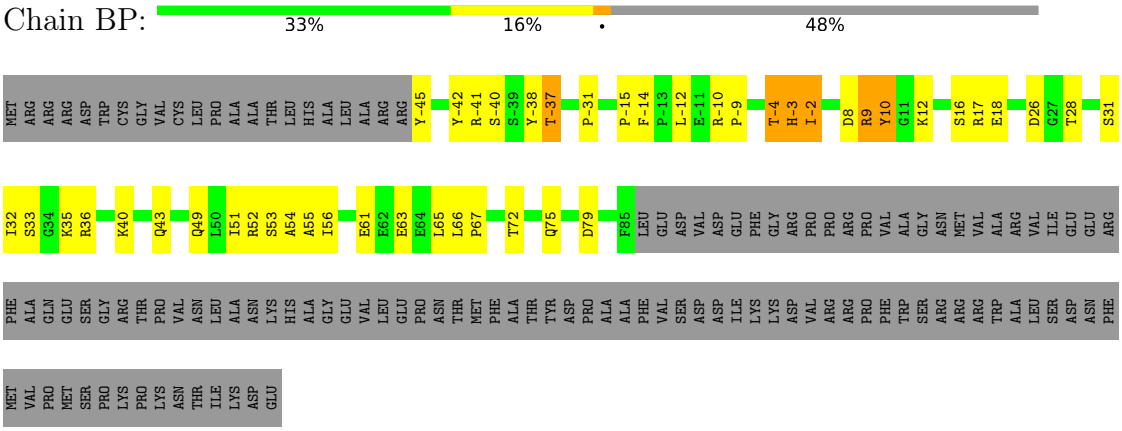

• Molecule 38: mL42

Chain Aa:



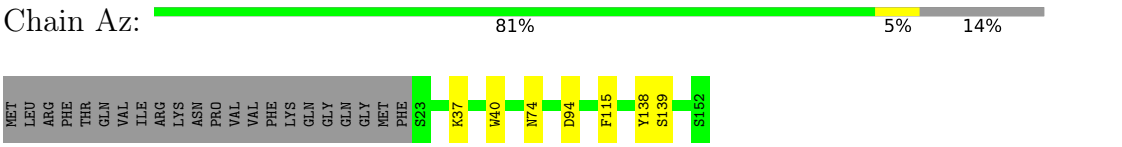

• Molecule 39: mL52,mL52

Chain BP:



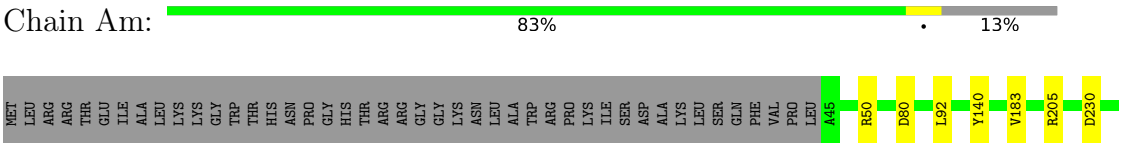

• Molecule 40: mL93

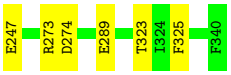
Chain Az:




• Molecule 41: mL75

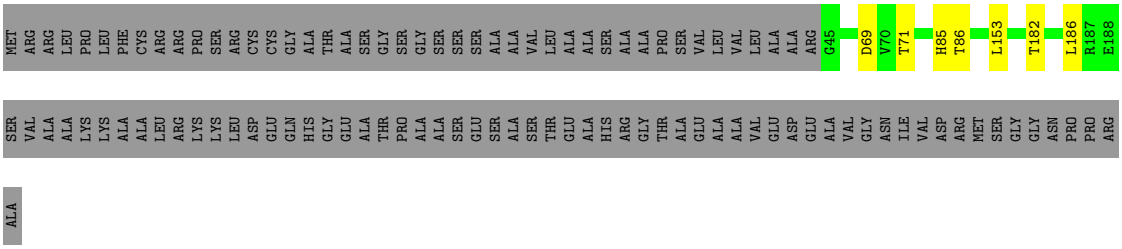
Chain Am:





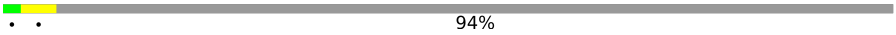

• Molecule 42: mL85

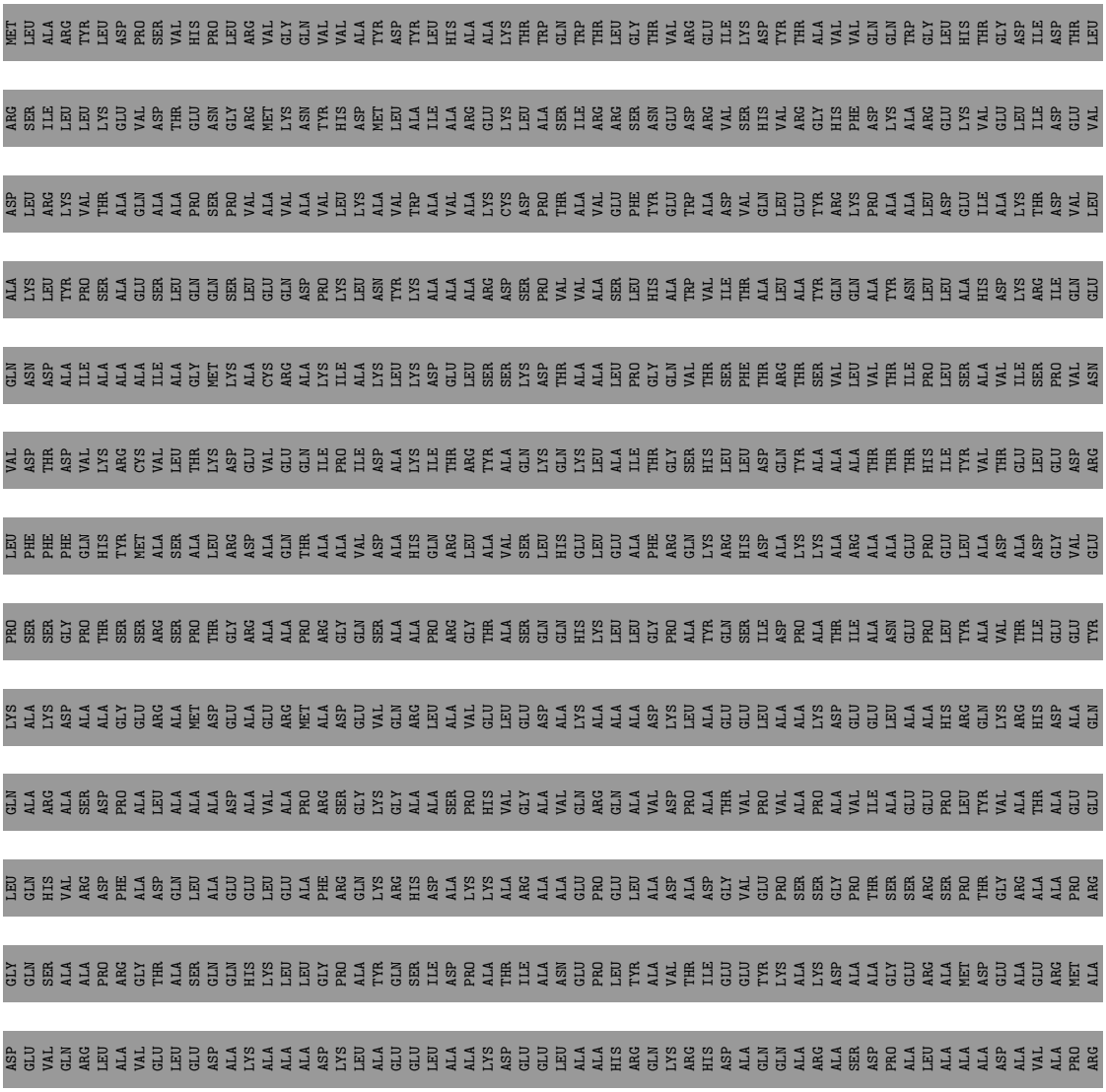
Chain As:

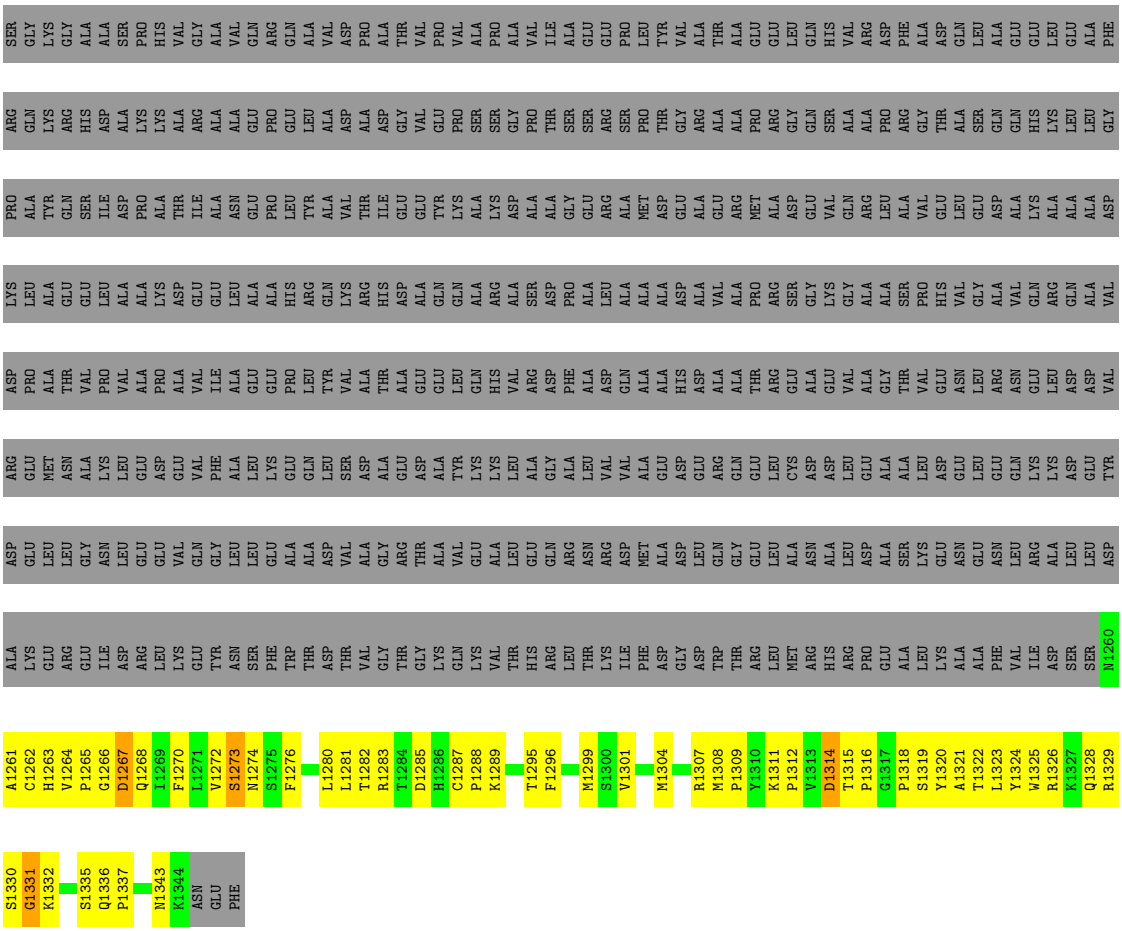




• Molecule 43: mL100

Chain BG:

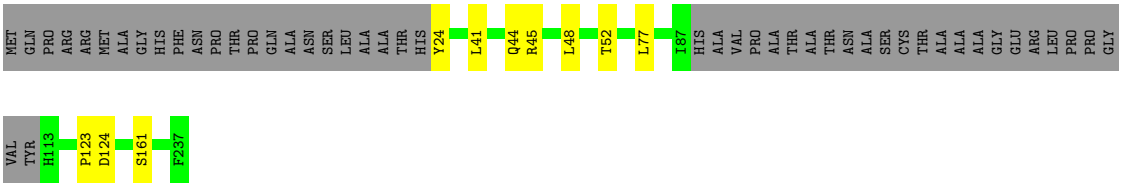




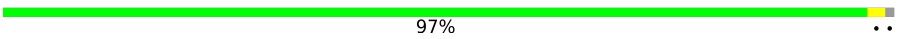
• Molecule 44: mL49

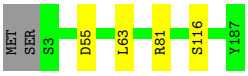
Chain Ad:

• Molecule 45: mL89

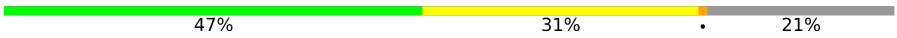
Chain Aw:

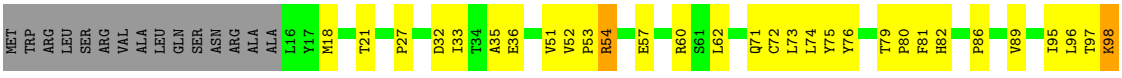


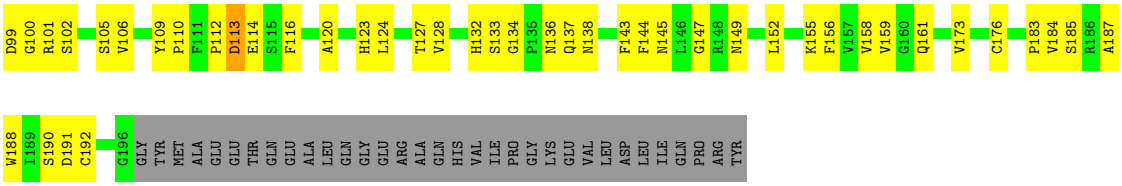



• Molecule 46: Peptidyl-prolyl cis-trans isomerase

Chain BH:

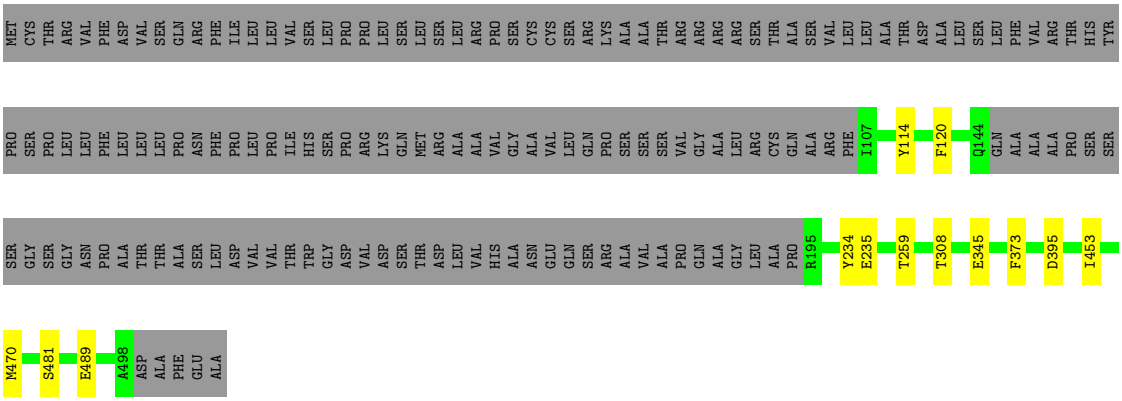





- Molecule 47: mL72

Chain Aj:

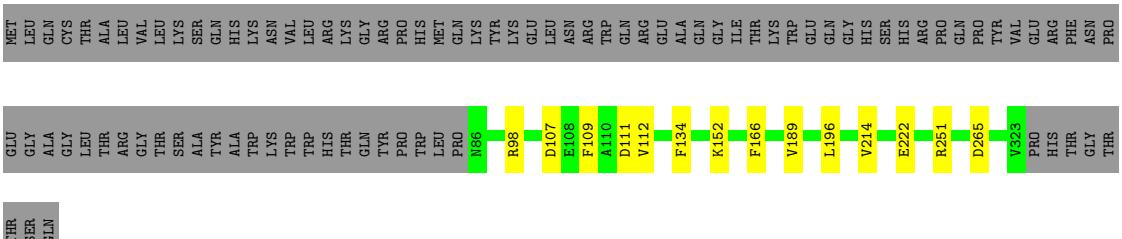

- Molecule 48: mL84

Chain Ar:



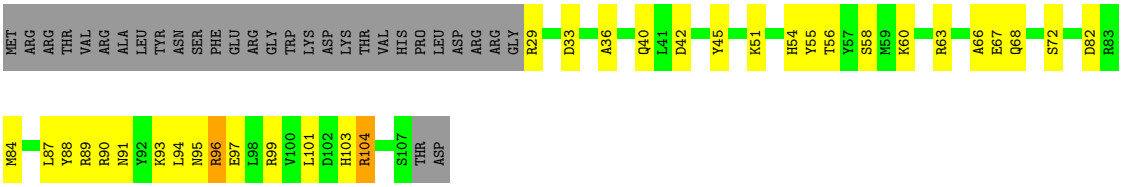
- Molecule 49: mL76

Chain An:

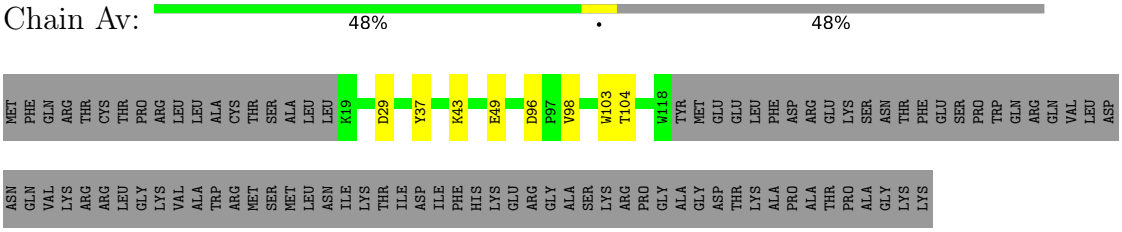

- Molecule 50: mL99

Chain BF:

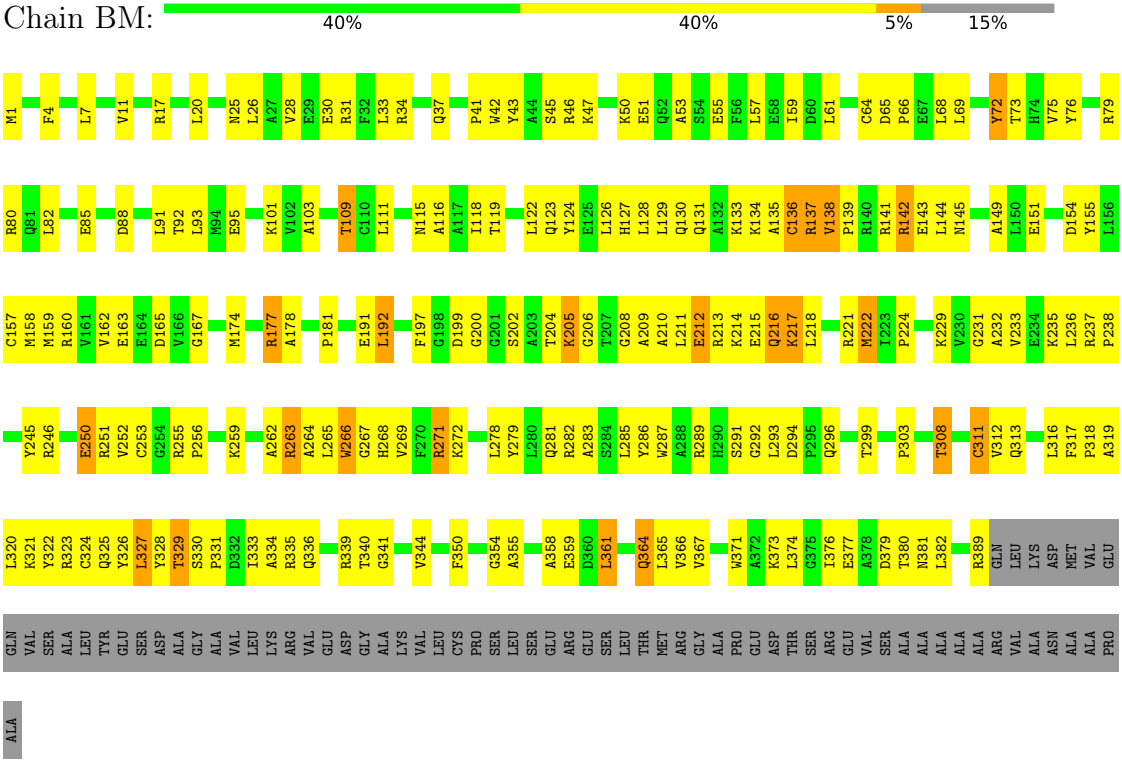
• Molecule 51: mL88

Chain Av:



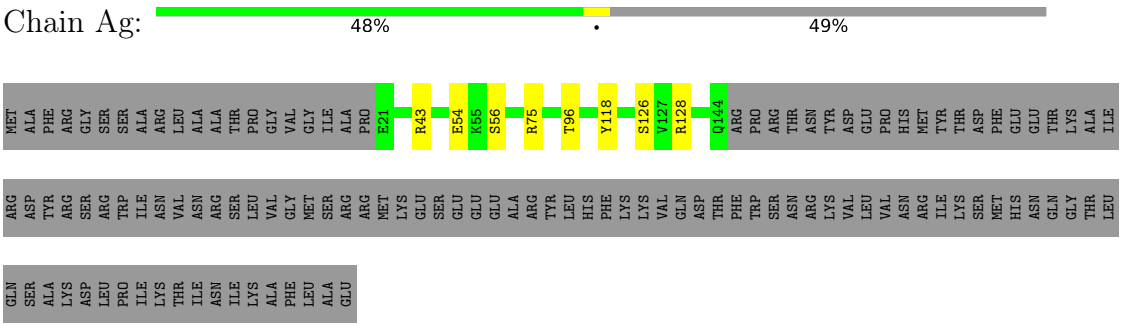

• Molecule 52: mL70

Chain BM:



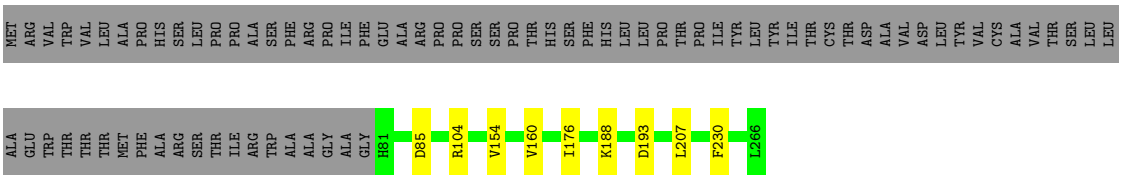

• Molecule 53: mL59/64

Chain Ag:




• Molecule 54: Peptidyl-prolyl cis-trans isomerase

Chain Bl:



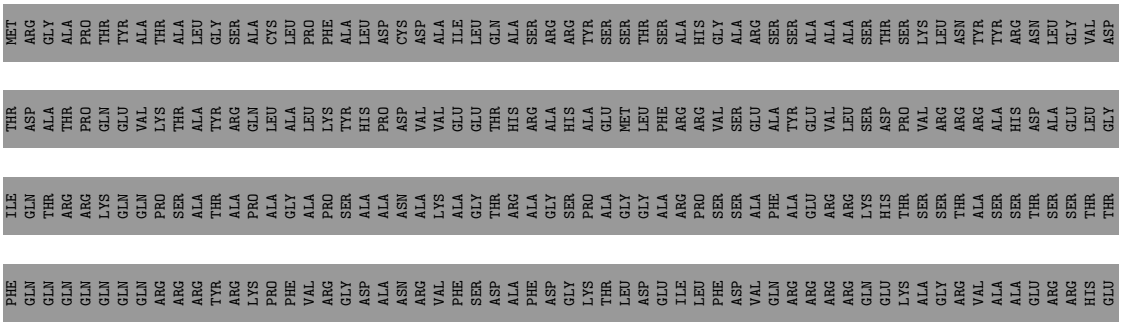

• Molecule 55: LIM zinc-binding domain-containing protein

Chain Ax:



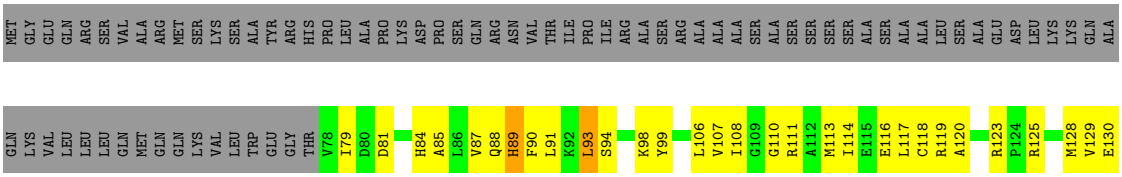

• Molecule 56: DNAj-like protein

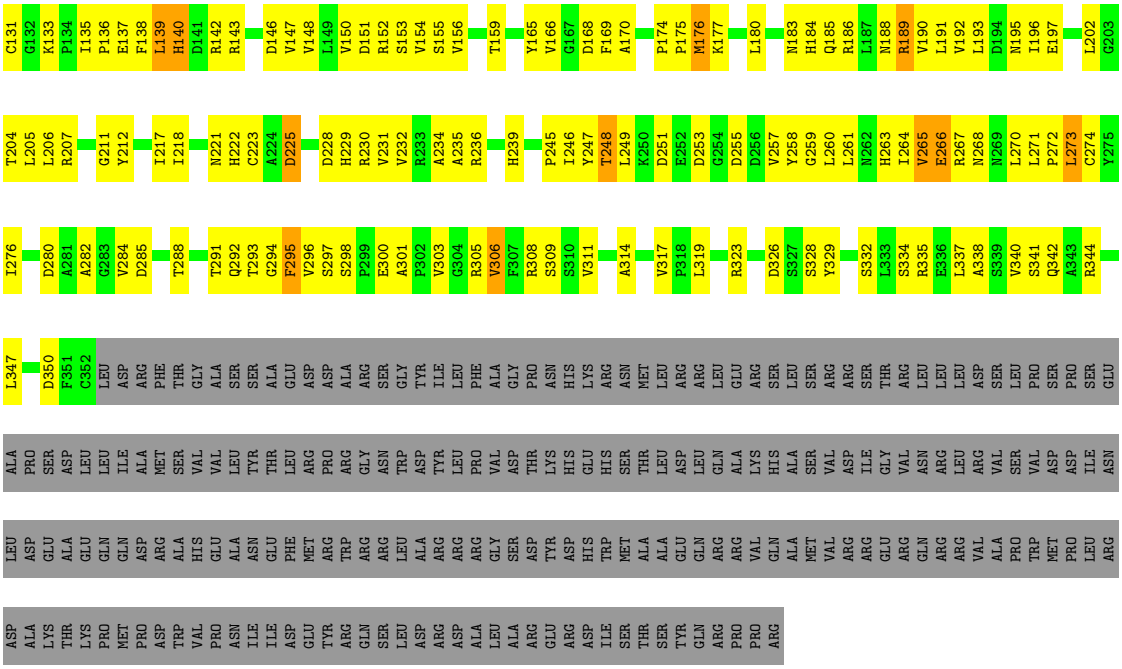
Chain BS:


• Molecule 57: SpoU_methylase domain-containing protein

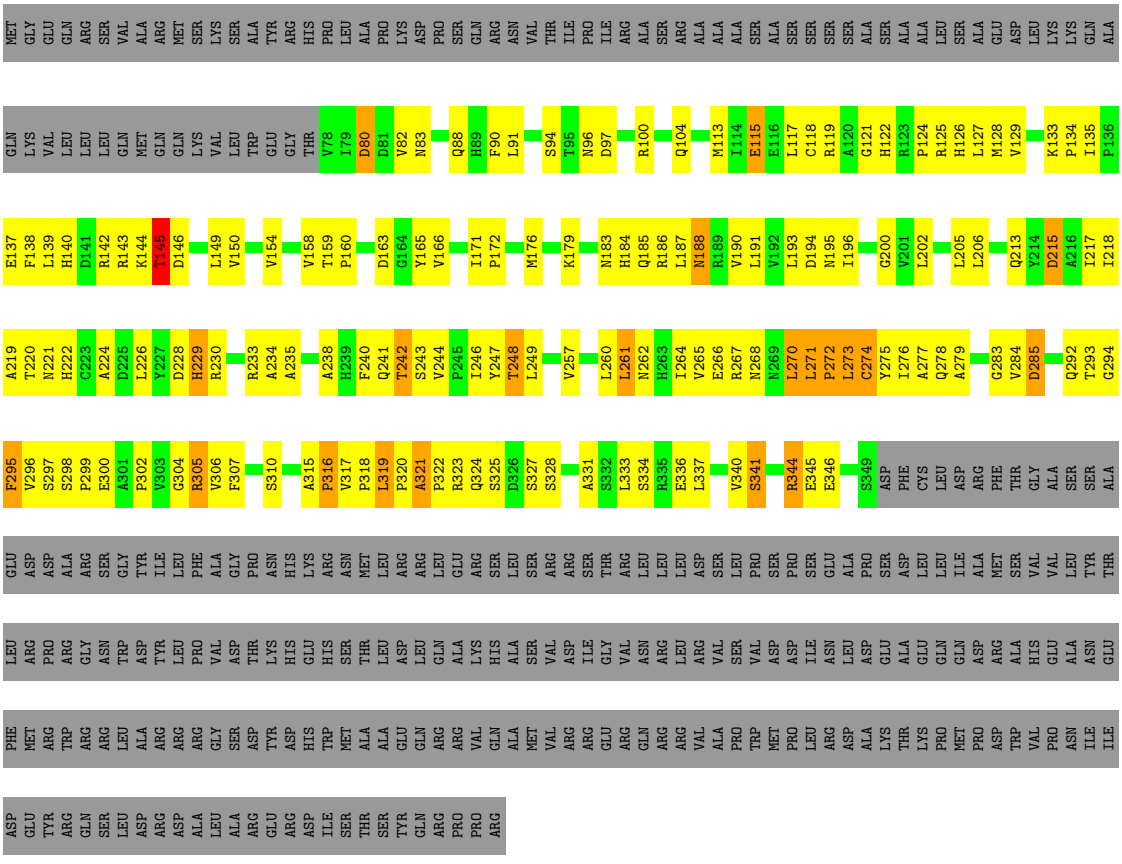
Chain BY:



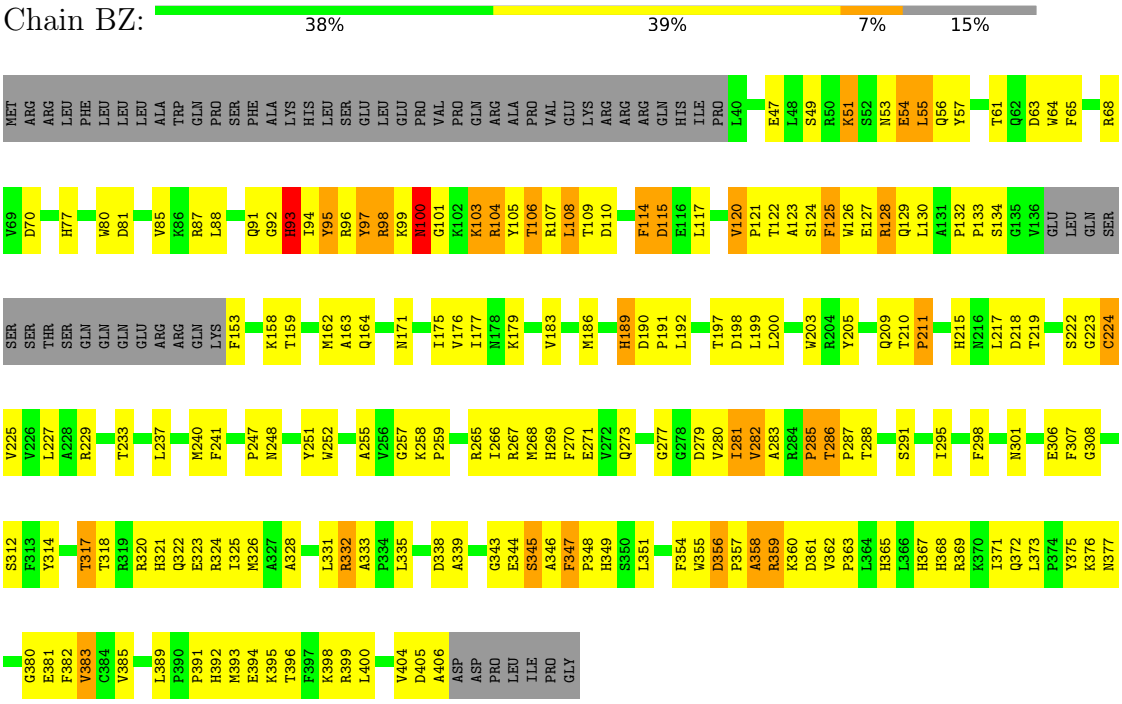
• Molecule 57: SpoU_methylase domain-containing protein

Chain BX:

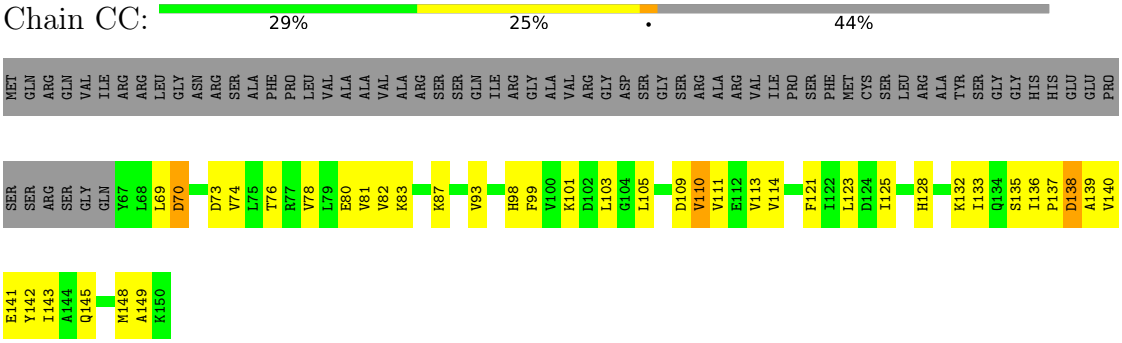
• Molecule 58: Pseudouridylate synthase-like protein

Chain BZ:



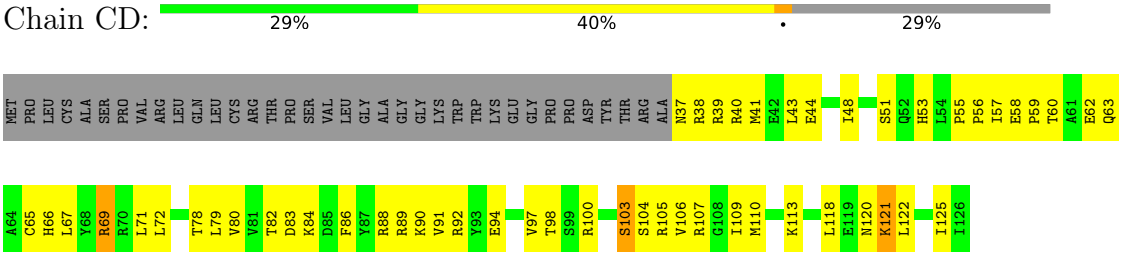

• Molecule 59: Acyl carrier protein

Chain CC:



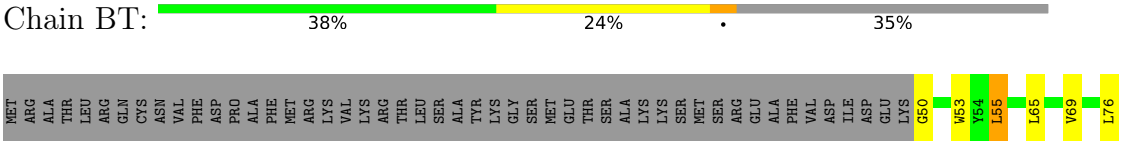

• Molecule 60: L0R8F8

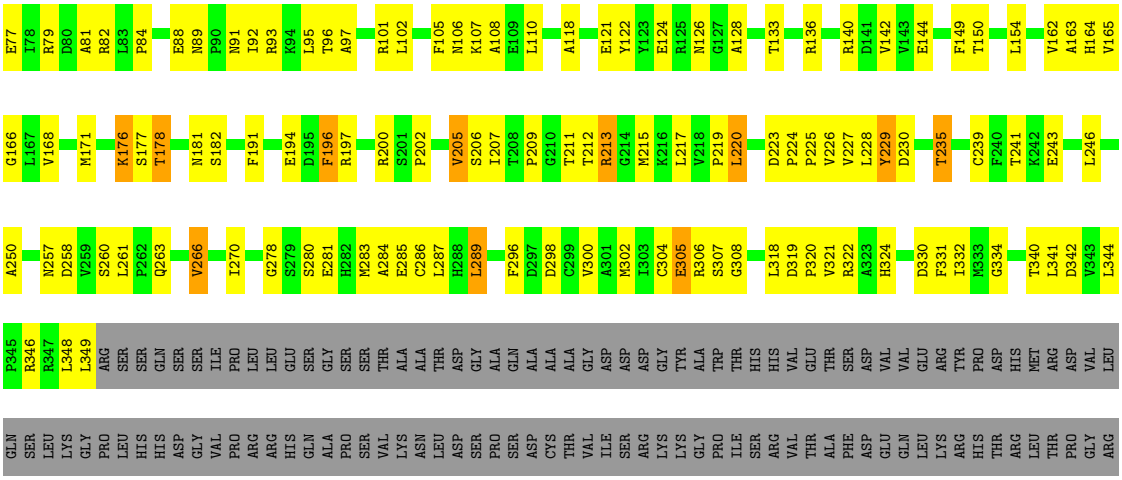
Chain CD:




• Molecule 61: G domain-containing protein

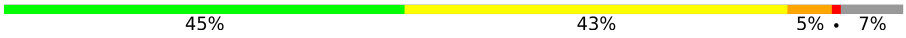
Chain BT:

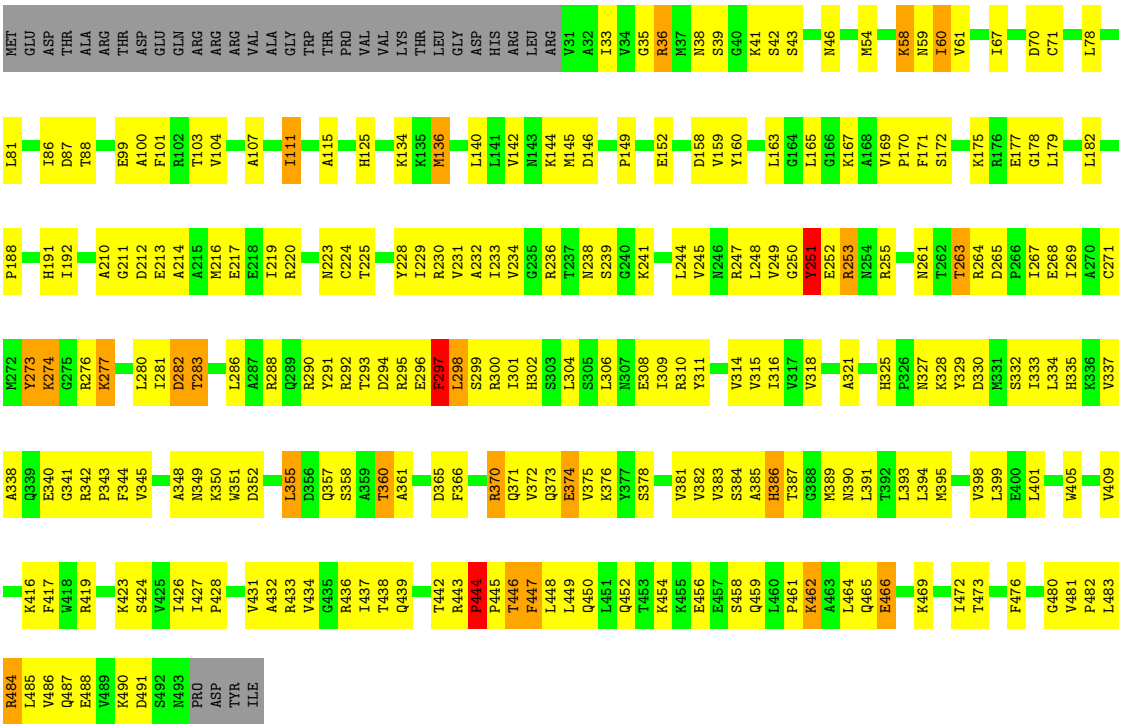




• Molecule 62: GTPase Der

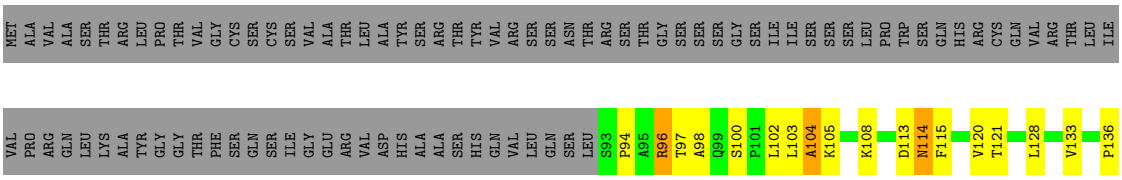
Chain BU:

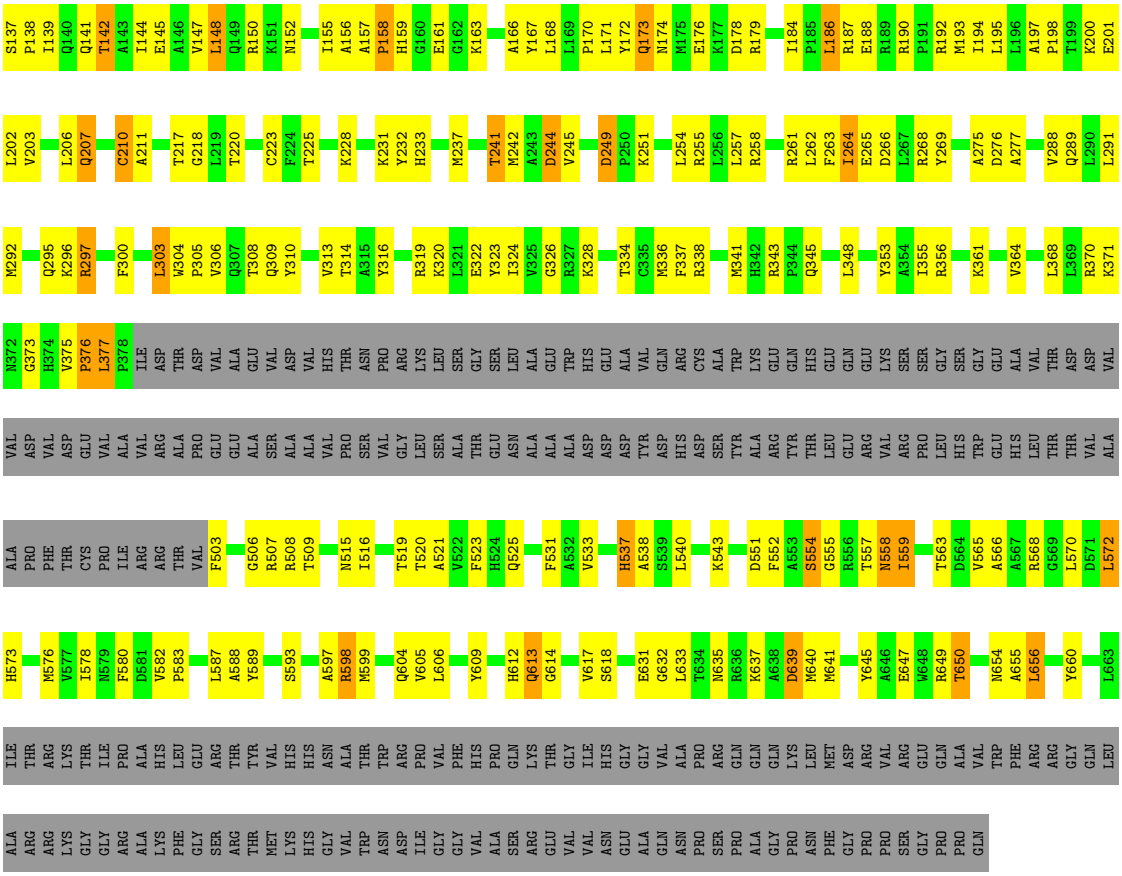


• Molecule 63: DEAD/DEAH box helicase-like protein

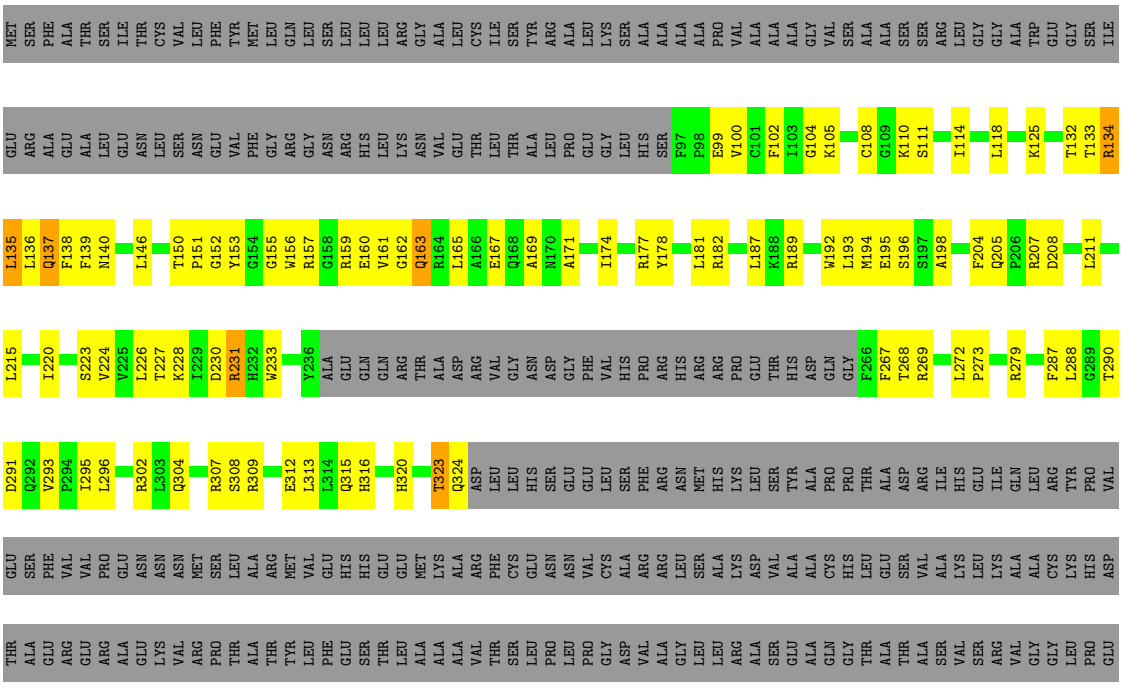
Chain BW:

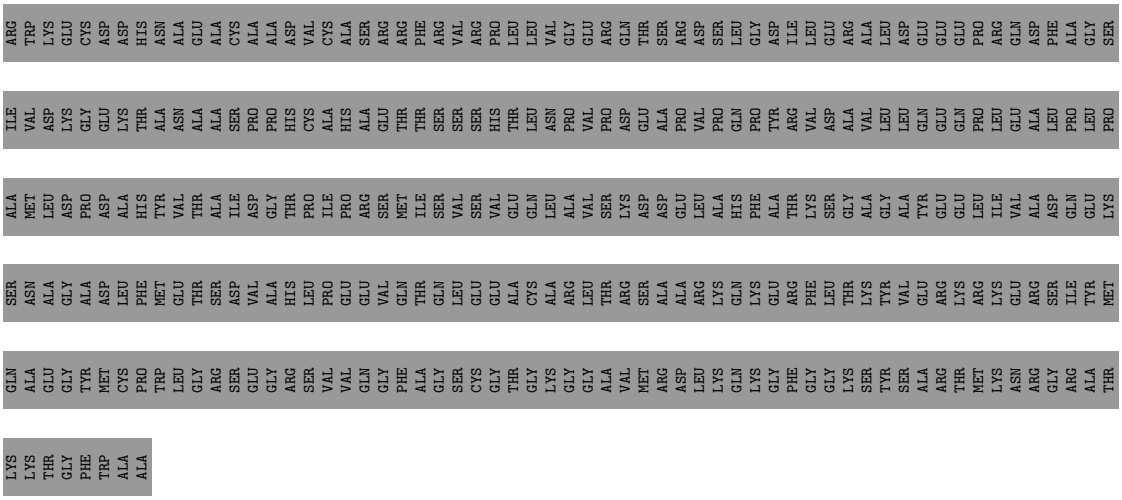





• Molecule 64: G domain-containing protein

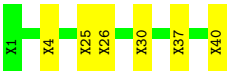
Chain BV: 14% 11% • 75%





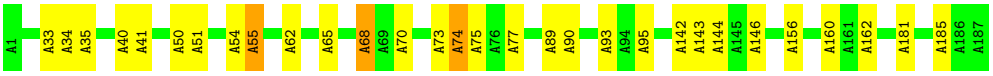

- Molecule 65: mL78

Chain U7:

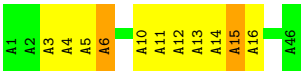

- Molecule 66: U6

Chain U6:

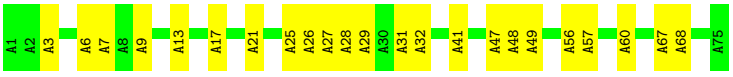

- Molecule 67: U1

Chain U1:

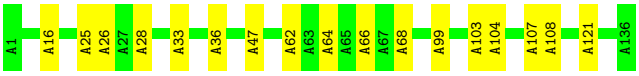

- Molecule 68: U3

Chain U3:

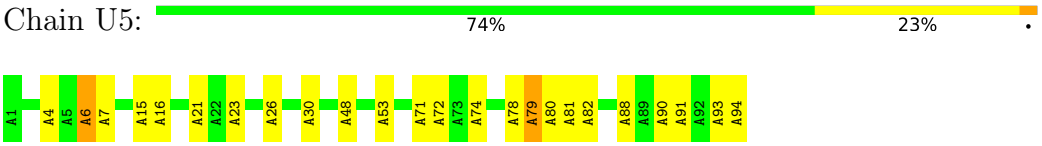

- Molecule 69: U4

Chain U4:

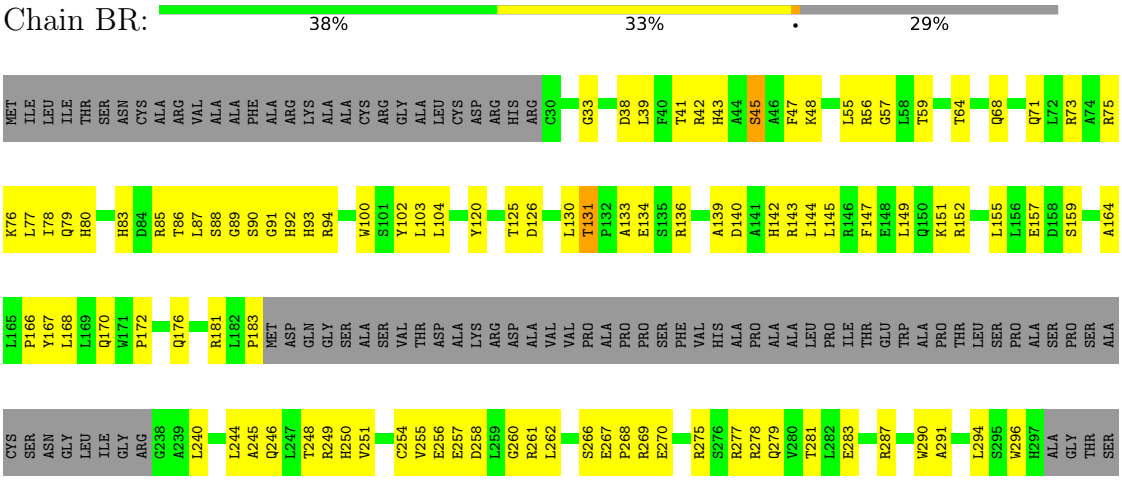

- Molecule 70: U5

Chain U5:



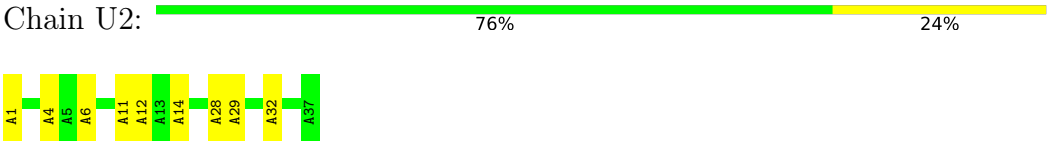

• Molecule 71: mL78

Chain BR:



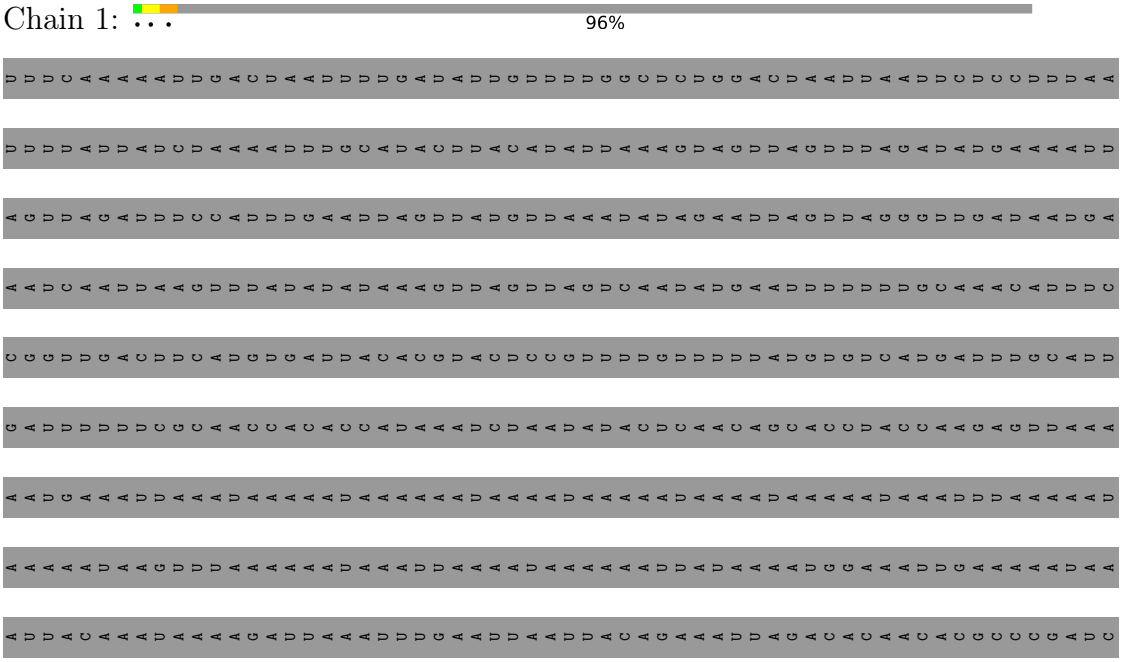

• Molecule 72: U2

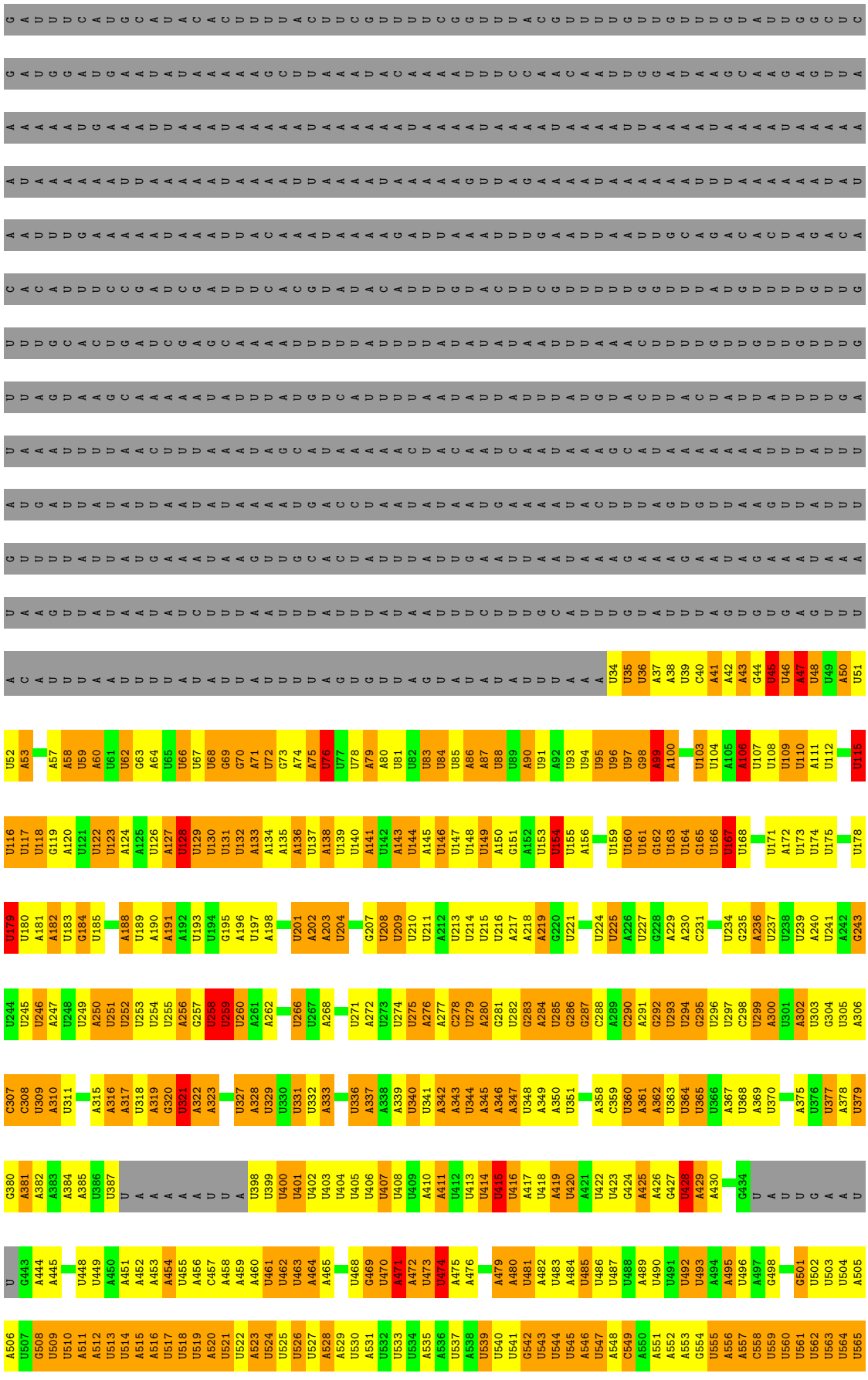
Chain U2:

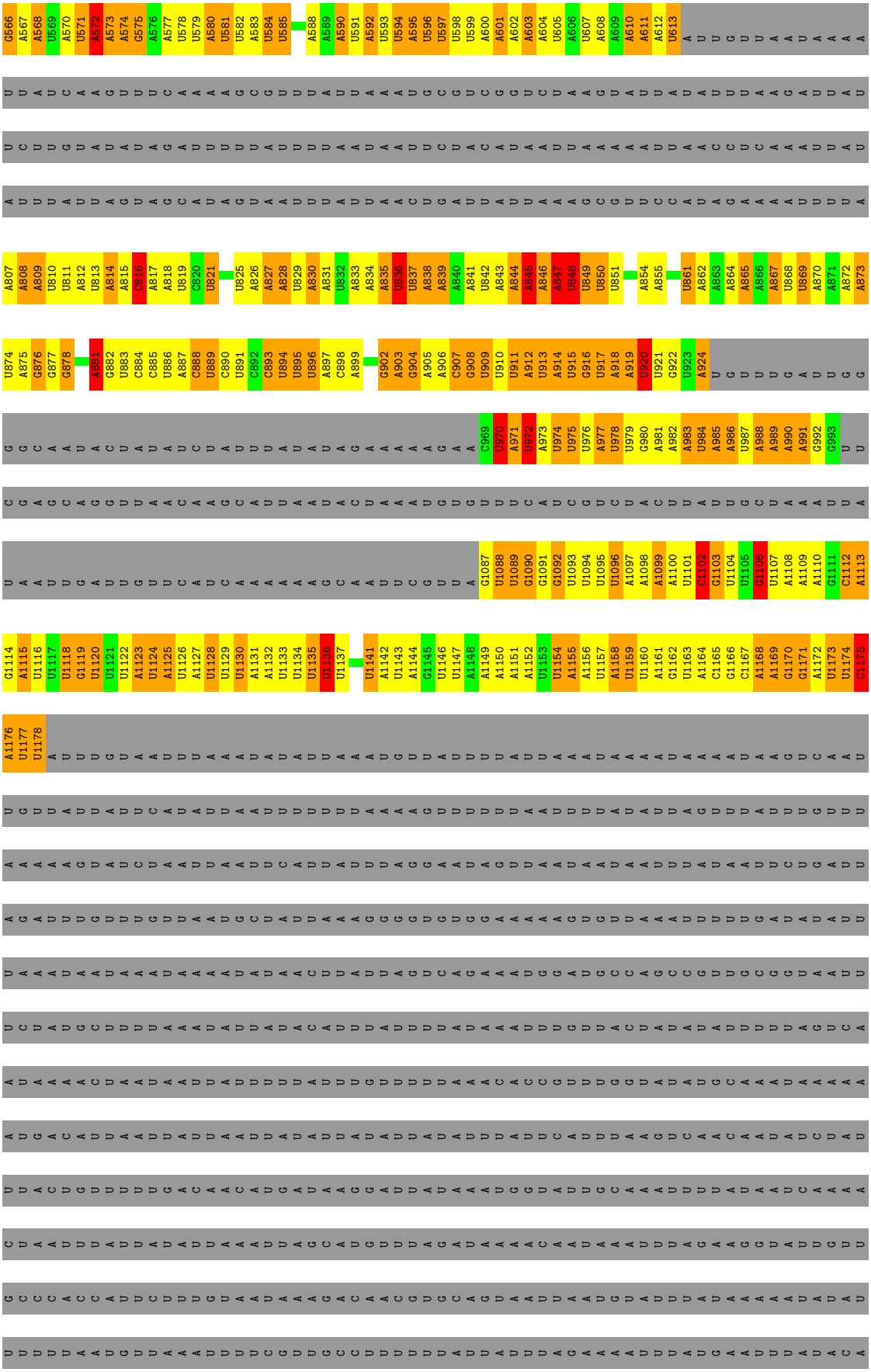


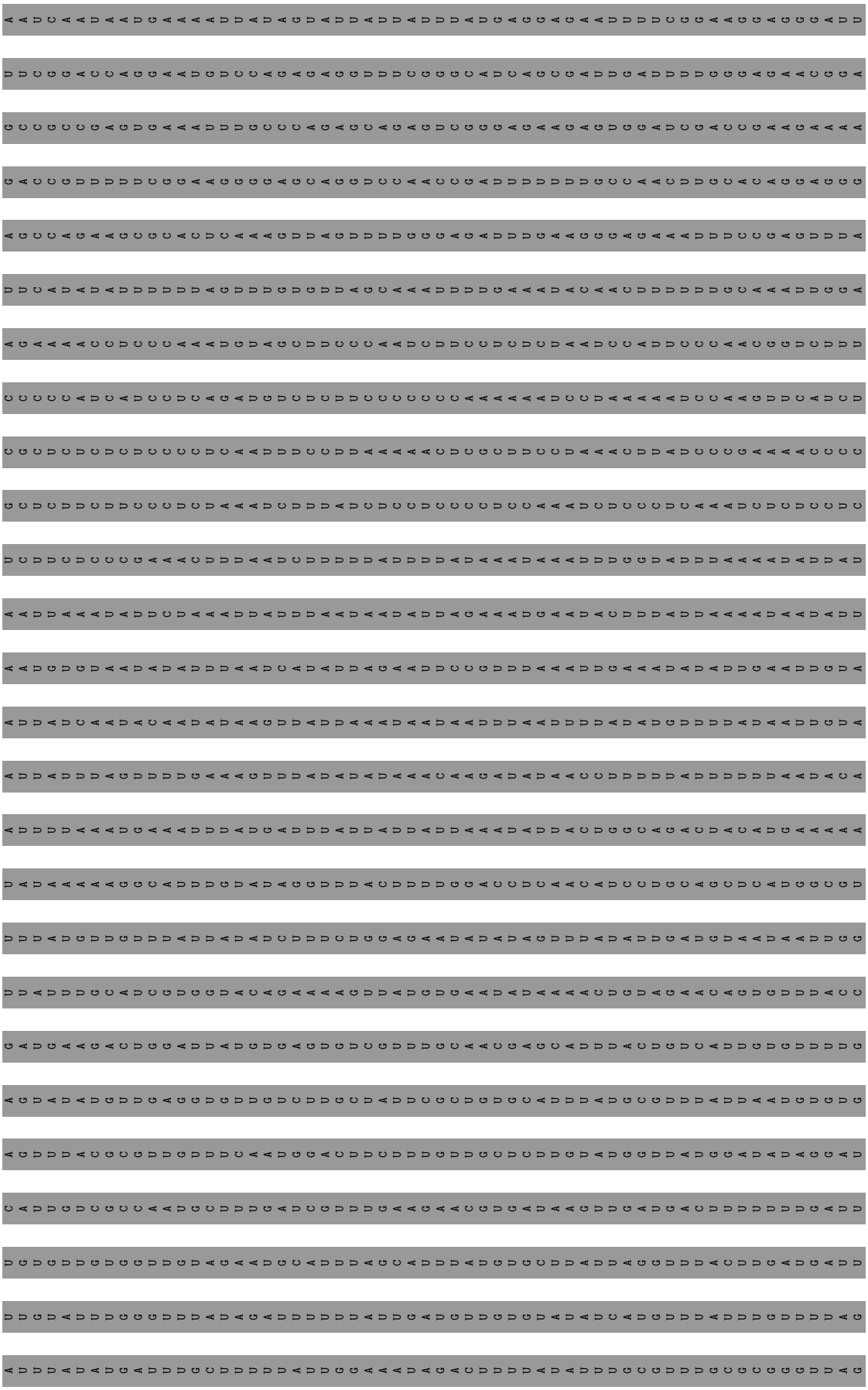

• Molecule 73: Ribosomal RNA

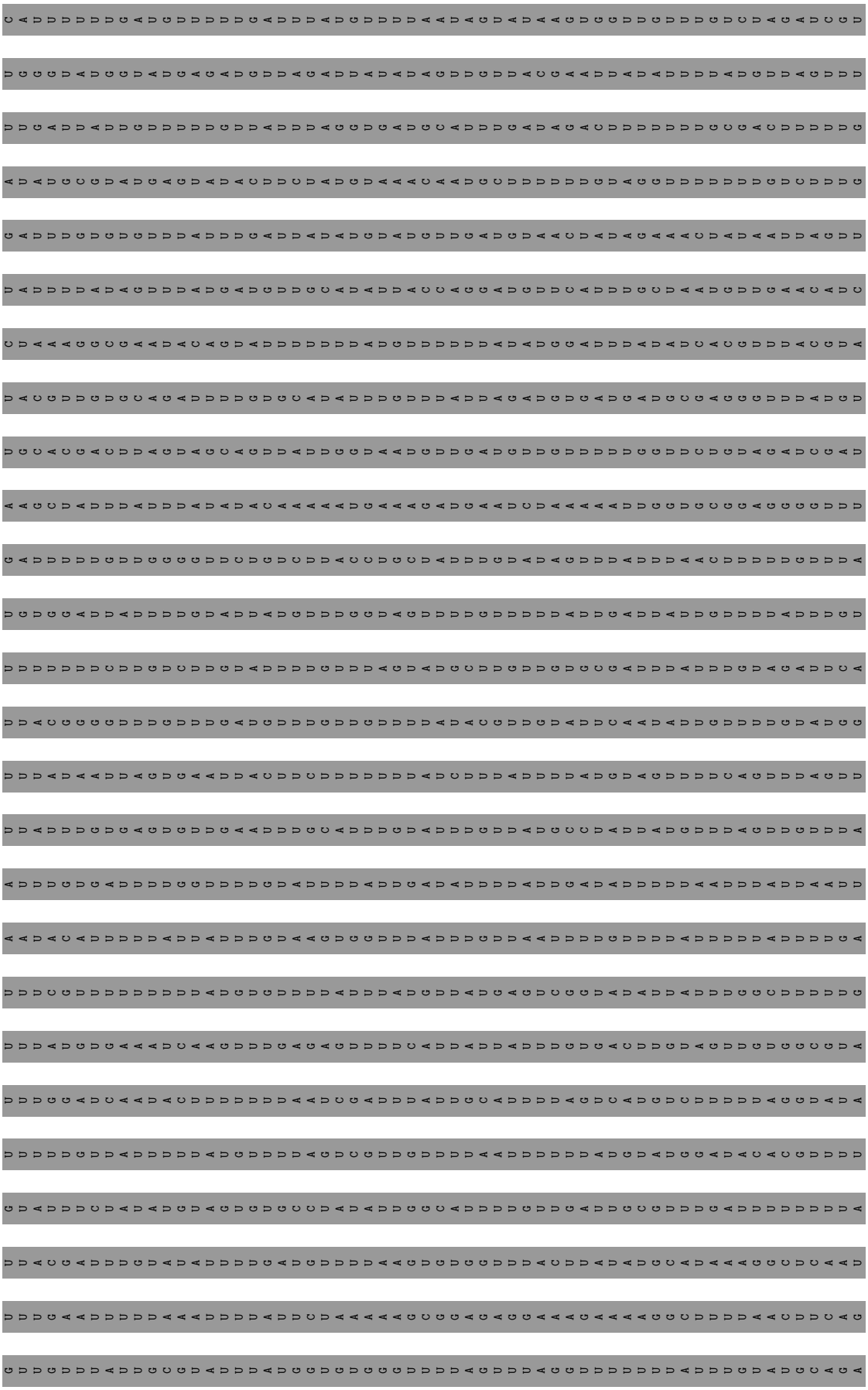
Chain 1:

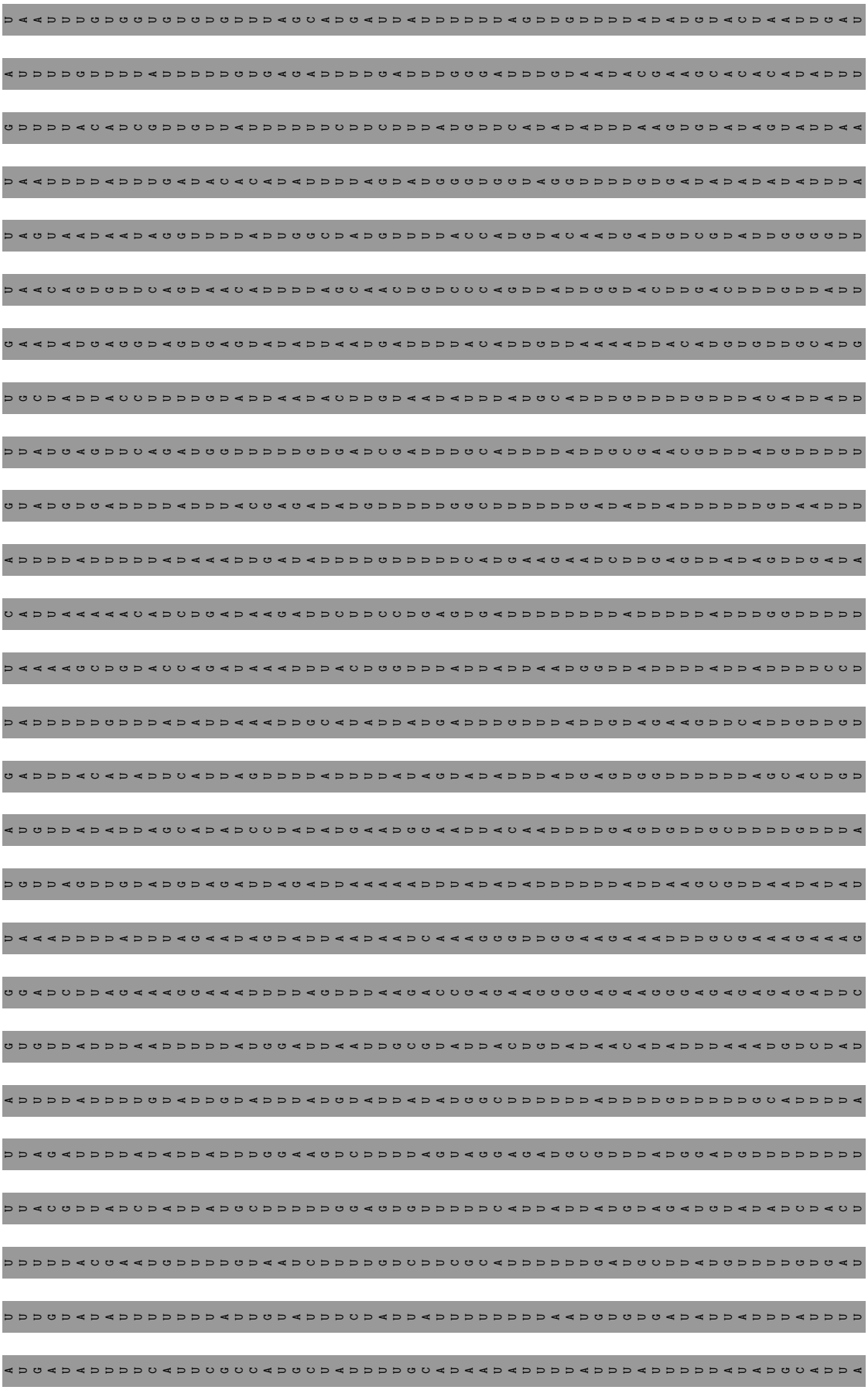


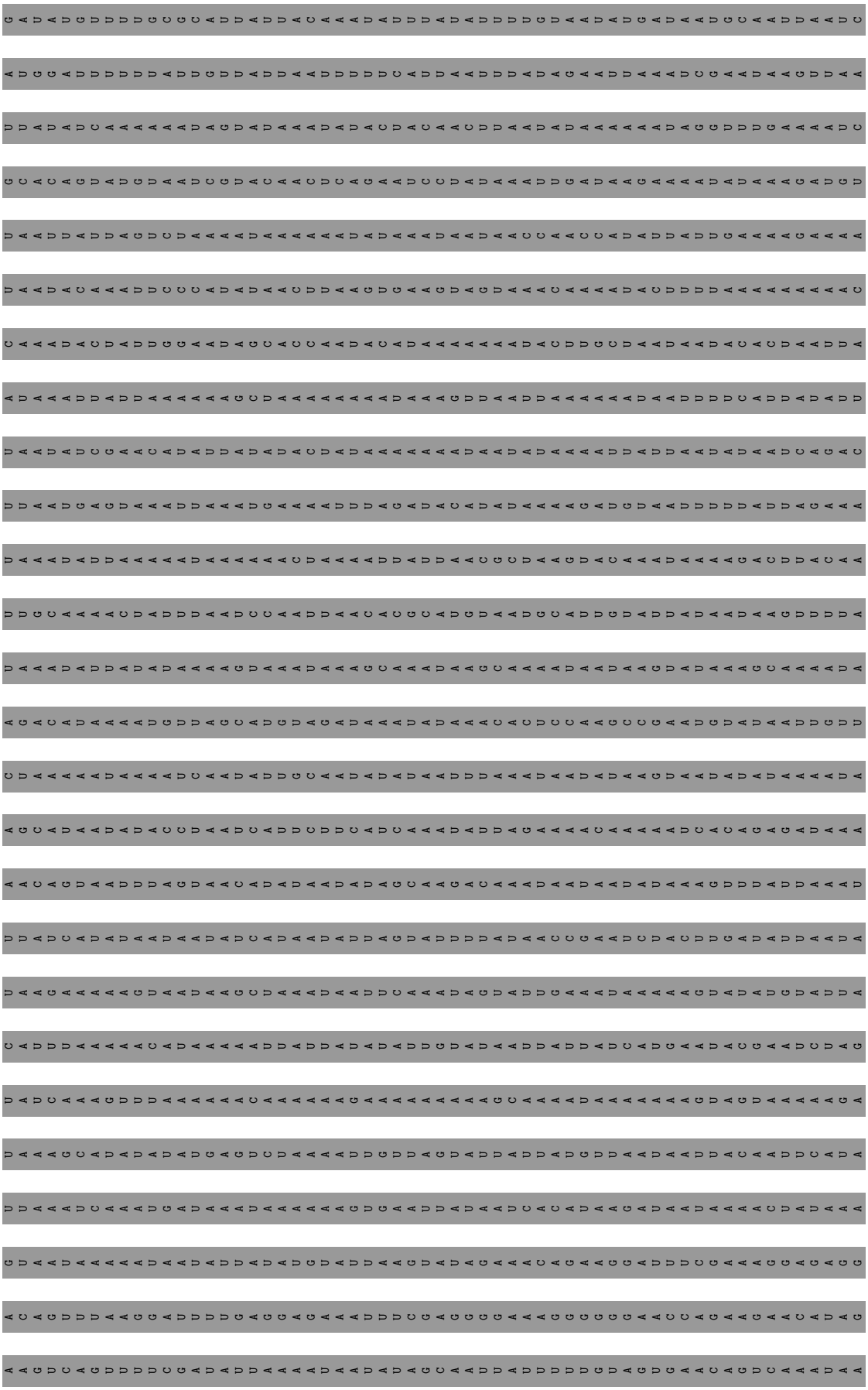


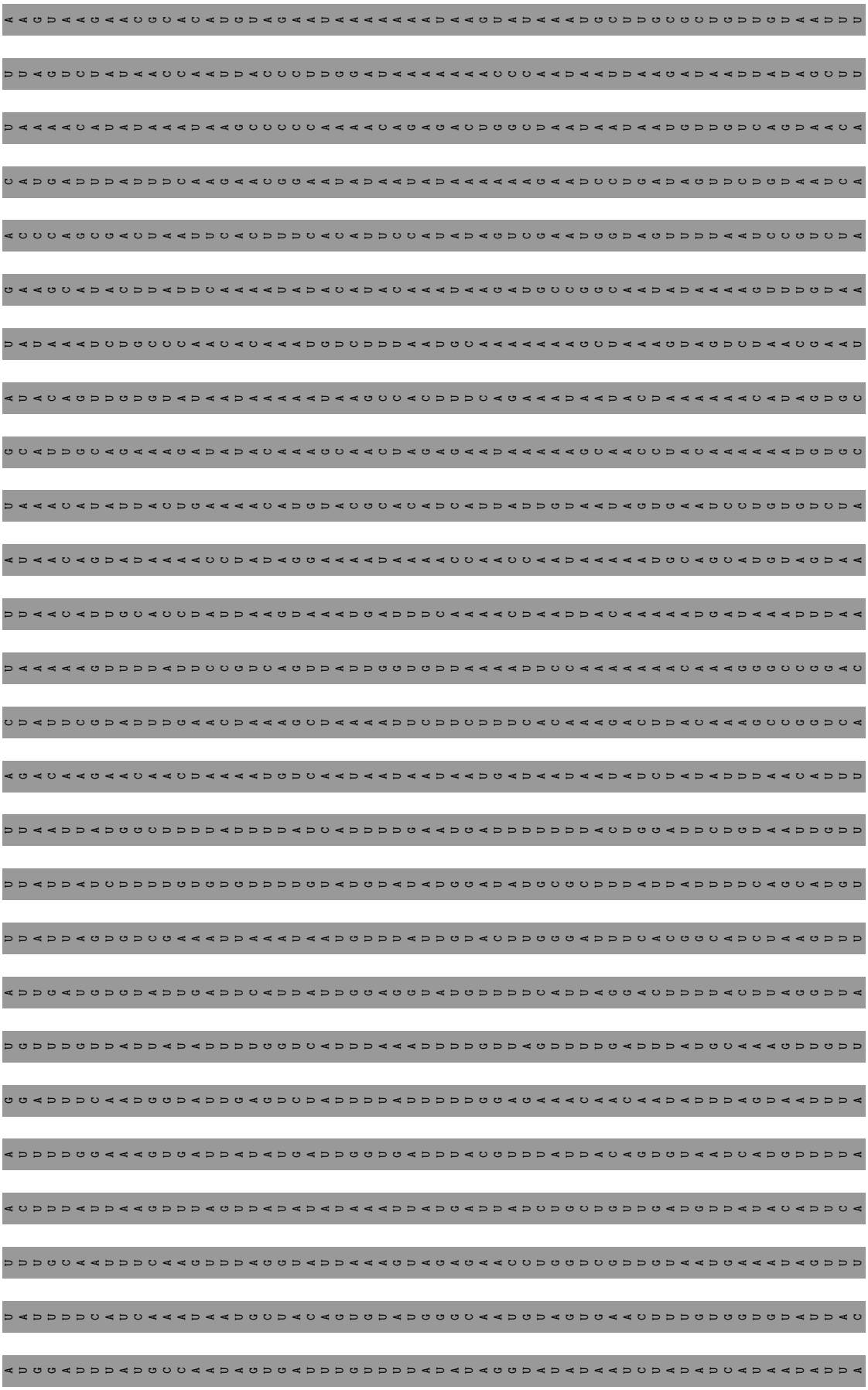


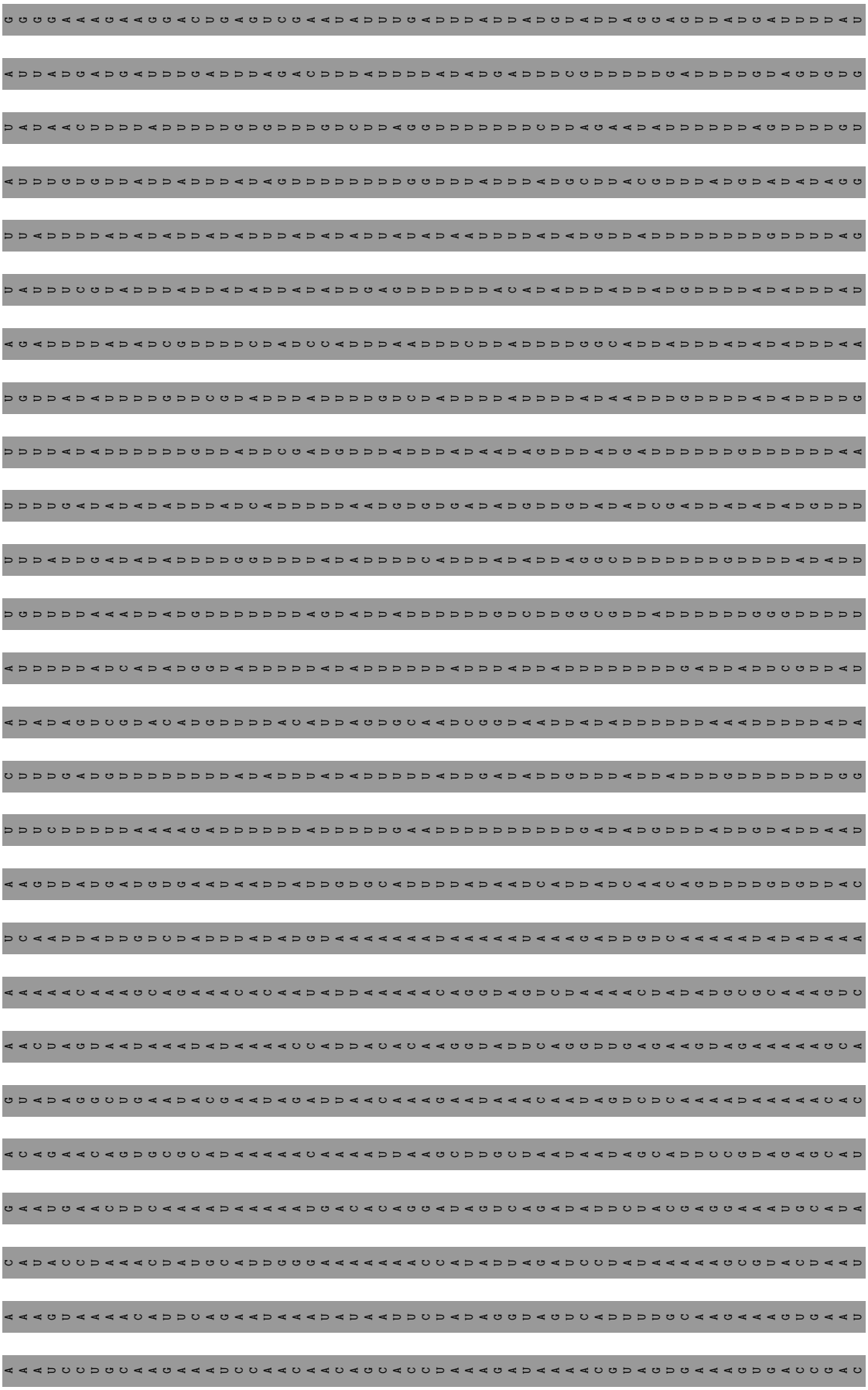


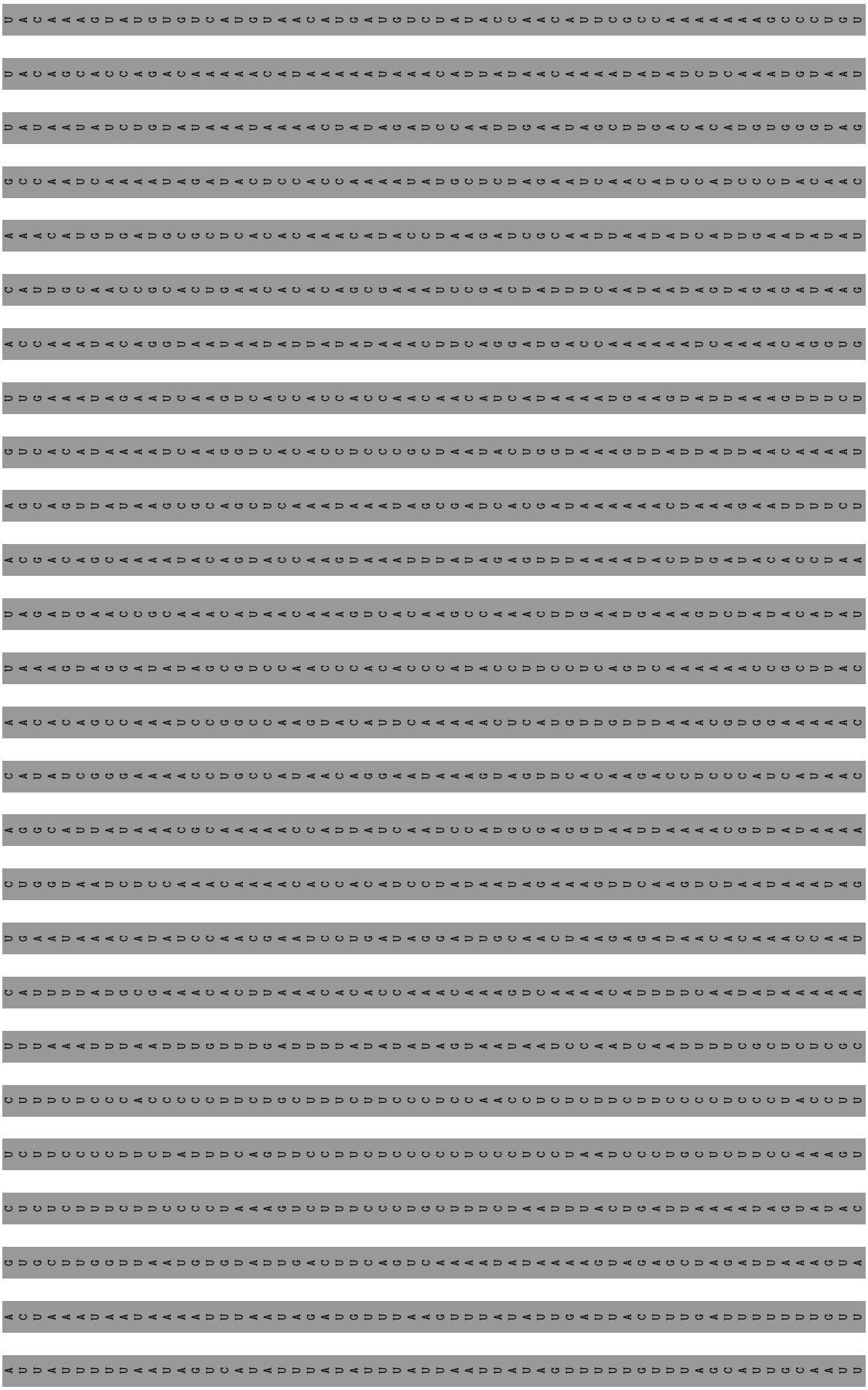


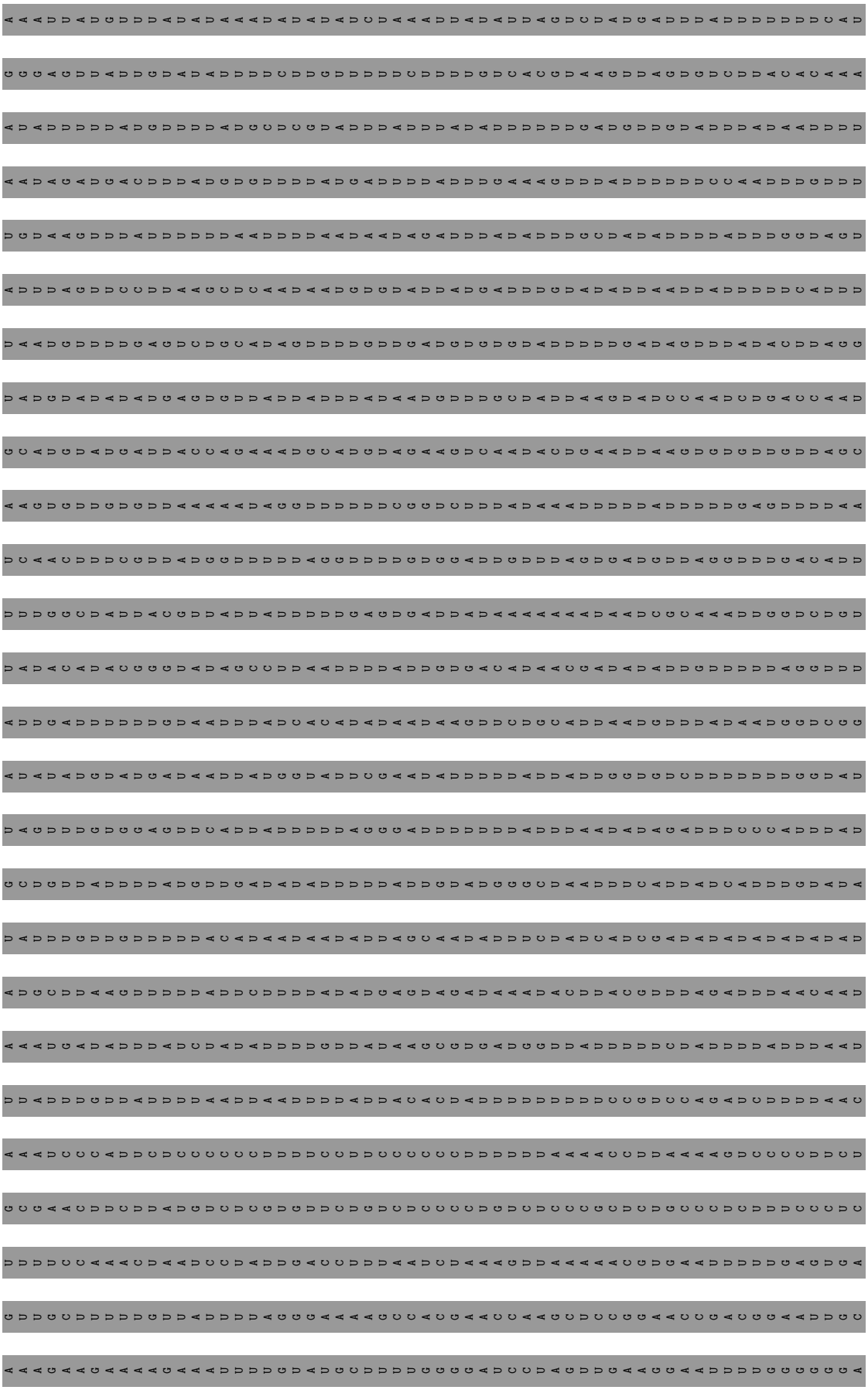


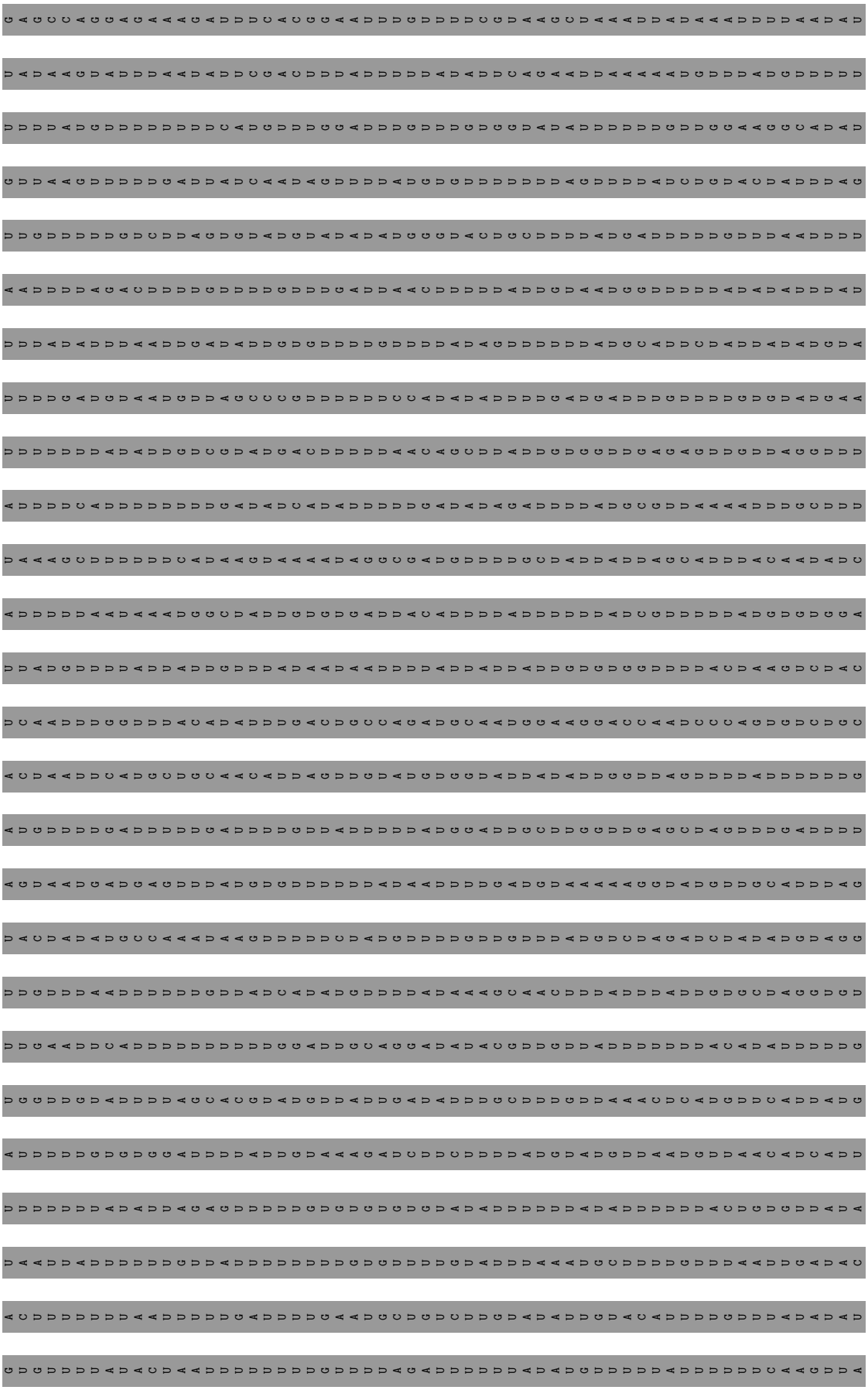


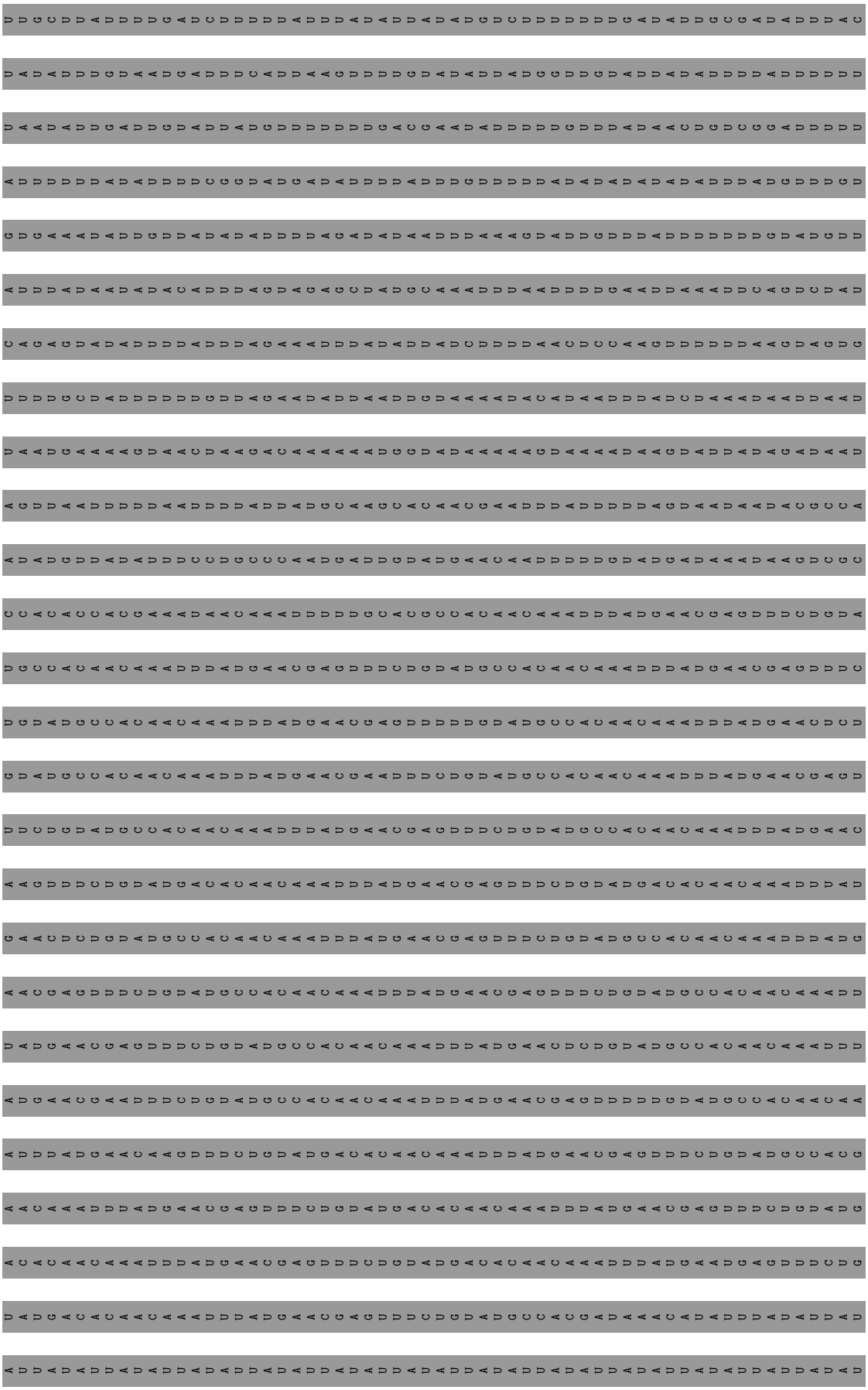


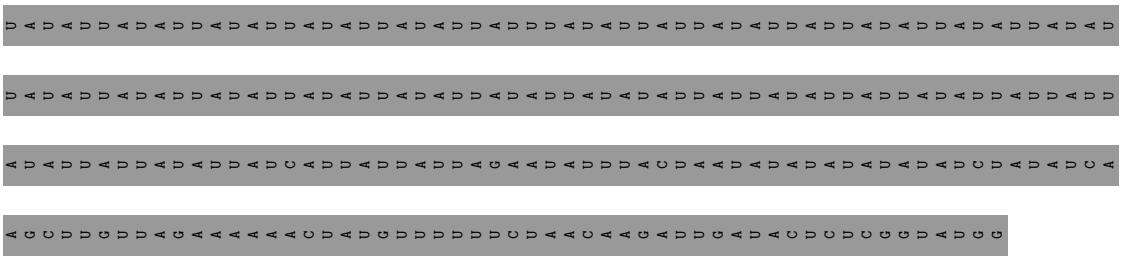












- Molecule 74: R1

Chain R1:



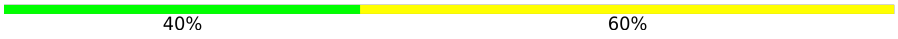
- Molecule 75: R2

Chain R2:



- Molecule 76: R5

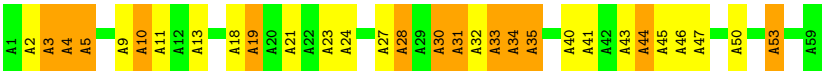
Chain R5:





- Molecule 77: U8

Chain U8:

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 59200 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (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: ATP, GTP

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 | 0.48 | 0/3011 | 0.49 | 0/4097 |
| 2 | B | 1.07 | 1/3623 (0.0%) | 0.49 | 1/4931 (0.0%) |
| 3 | C | 0.41 | 0/1831 | 0.48 | 0/2498 |
| 4 | E | 0.32 | 0/1864 | 0.46 | 0/2512 |
| 5 | F | 0.47 | 0/1272 | 0.51 | 0/1730 |
| 6 | G | 0.48 | 0/2857 | 0.64 | 5/3879 (0.1%) |
| 7 | I | 0.41 | 0/2220 | 0.46 | 0/2998 |
| 8 | J | 0.47 | 0/1175 | 0.70 | 0/1582 |
| 9 | K | 0.40 | 0/1499 | 0.47 | 0/2026 |
| 10 | L | 0.42 | 0/1452 | 0.52 | 0/1970 |
| 11 | M | 0.44 | 0/2168 | 0.51 | 0/2928 |
| 12 | N | 0.43 | 0/1650 | 0.55 | 0/2242 |
| 13 | O | 0.39 | 0/2529 | 0.48 | 0/3422 |
| 14 | Q | 0.41 | 0/1827 | 0.51 | 0/2463 |
| 15 | R | 0.37 | 0/3852 | 0.46 | 0/5243 |
| 16 | S | 0.41 | 0/1271 | 0.48 | 0/1712 |
| 17 | T | 0.46 | 0/501 | 0.47 | 0/665 |
| 18 | V | 0.48 | 0/1231 | 0.47 | 0/1645 |
| 19 | Z | 0.39 | 0/940 | 0.49 | 0/1279 |
| 20 | BA | 0.29 | 0/797 | 0.50 | 0/1084 |
| 21 | CA | 0.38 | 0/4341 | 0.56 | 2/5889 (0.0%) |
| 22 | UA | 0.23 | 0/1014 | 0.56 | 0/1418 |
| 23 | BB | 0.49 | 0/922 | 0.53 | 0/1248 |
| 24 | CB | 0.31 | 0/1092 | 0.52 | 0/1477 |
| 25 | BK | 0.38 | 0/5536 | 0.52 | 2/7536 (0.0%) |
| 26 | BQ | 0.36 | 0/3310 | 0.47 | 0/4478 |
| 27 | BN | 0.39 | 0/1539 | 0.58 | 0/2093 |
| 28 | BE | 0.44 | 0/337 | 0.53 | 0/458 |
| 29 | BO | 0.38 | 0/1311 | 0.54 | 0/1766 |
| 30 | At | 0.40 | 0/1373 | 0.47 | 0/1848 |
| 31 | Au | 0.34 | 0/702 | 0.41 | 0/943 |
| 32 | Ae | 0.39 | 0/2436 | 0.47 | 0/3316 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | Af | 0.43 | 0/1228 | 0.52 | 0/1671 |
| 34 | Ah | 0.30 | 0/3327 | 0.44 | 0/4518 |
| 35 | Ap | 0.32 | 0/1819 | 0.43 | 0/2458 |
| 36 | Al | 0.39 | 0/1909 | 0.49 | 0/2606 |
| 37 | Ab | 0.46 | 0/1454 | 0.46 | 0/1966 |
| 38 | Aa | 0.37 | 0/1103 | 0.49 | 0/1498 |
| 39 | BP | 0.41 | 0/1109 | 0.48 | 0/1507 |
| 40 | Az | 0.47 | 0/1192 | 0.43 | 0/1613 |
| 41 | Am | 0.41 | 0/2508 | 0.48 | 0/3392 |
| 42 | As | 0.34 | 0/1204 | 0.49 | 0/1622 |
| 43 | BG | 0.31 | 0/692 | 0.51 | 0/935 |
| 44 | Ad | 0.49 | 0/1547 | 0.63 | 2/2097 (0.1%) |
| 45 | Aw | 0.89 | 2/1552 (0.1%) | 0.73 | 3/2107 (0.1%) |
| 46 | BH | 0.39 | 0/1430 | 0.47 | 0/1937 |
| 47 | Aj | 0.41 | 0/2837 | 0.46 | 0/3821 |
| 48 | Ar | 0.38 | 0/1689 | 0.54 | 1/2280 (0.0%) |
| 49 | An | 0.32 | 0/1990 | 0.49 | 0/2701 |
| 50 | BF | 0.35 | 0/675 | 0.50 | 0/907 |
| 51 | Av | 0.31 | 0/853 | 0.51 | 0/1152 |
| 52 | BM | 0.27 | 0/3136 | 0.46 | 0/4259 |
| 53 | Ag | 0.44 | 0/1063 | 0.46 | 0/1442 |
| 54 | Bl | 0.31 | 0/1440 | 0.46 | 0/1953 |
| 55 | Ax | 0.31 | 0/1439 | 0.54 | 0/1952 |
| 56 | BS | 0.37 | 0/1016 | 0.49 | 0/1388 |
| 57 | BX | 0.34 | 0/2126 | 0.59 | 1/2892 (0.0%) |
| 57 | BY | 0.29 | 0/2152 | 0.51 | 0/2927 |
| 58 | BZ | 0.44 | 0/2911 | 0.67 | 2/3954 (0.1%) |
| 59 | CC | 0.28 | 0/679 | 0.43 | 0/921 |
| 60 | CD | 0.31 | 0/774 | 0.49 | 0/1034 |
| 61 | BT | 0.30 | 0/2399 | 0.51 | 0/3255 |
| 62 | BU | 0.37 | 0/3739 | 0.56 | 1/5052 (0.0%) |
| 63 | BW | 0.43 | 0/3658 | 0.57 | 1/4940 (0.0%) |
| 64 | BV | 0.31 | 0/1634 | 0.56 | 0/2212 |
| 66 | U6 | 0.40 | 0/934 | 0.69 | 0/1306 |
| 67 | U1 | 0.42 | 0/229 | 0.65 | 0/319 |
| 68 | U3 | 0.31 | 0/374 | 0.61 | 0/522 |
| 69 | U4 | 0.25 | 0/679 | 0.36 | 0/949 |
| 70 | U5 | 0.27 | 0/469 | 0.60 | 0/655 |
| 71 | BR | 0.32 | 0/1745 | 0.49 | 0/2370 |
| 72 | U2 | 0.23 | 0/184 | 0.58 | 0/256 |
| 73 | 1 | 1.25 | 16/18754 (0.1%) | 1.12 | 83/29135 (0.3%) |
| 74 | R1 | 0.65 | 0/68 | 1.38 | 0/103 |
| 75 | R2 | 0.42 | 0/729 | 1.21 | 1/1111 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | R5 | 0.28 | 0/109 | 0.71 | 0/166 |
| 77 | U8 | 0.74 | 0/294 | 1.19 | 0/410 |
| All | All | 0.60 | 19/144335 (0.0%) | 0.65 | 105/199647 (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 |
|---|---|---|---|
| 6 | G | 1 | 0 |
| 14 | Q | 0 | 1 |
| 57 | BX | 0 | 1 |
| 66 | U6 | 0 | 2 |
| 70 | U5 | 0 | 3 |
| All | All | 1 | 7 |

The worst 5 of 19 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 73 | 1 | 106 | A | N3-C4 | 70.07 | 1.76 | 1.34 |
| 73 | 1 | 106 | A | C6-N1 | 62.10 | 1.79 | 1.35 |
| 2 | B | 194 | LYS | CE-NZ | 58.85 | 2.96 | 1.49 |
| 73 | 1 | 106 | A | N1-C2 | 47.98 | 1.77 | 1.34 |
| 73 | 1 | 106 | A | C2-N3 | 45.12 | 1.74 | 1.33 |

The worst 5 of 105 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 73 | 1 | 106 | A | N1-C2-N3 | -50.07 | 104.26 | 129.30 |
| 73 | 1 | 106 | A | C2-N3-C4 | 36.61 | 128.91 | 110.60 |
| 45 | Aw | 81 | ARG | CD-NE-CZ | 21.68 | 153.95 | 123.60 |
| 73 | 1 | 106 | A | C6-N1-C2 | 21.24 | 131.34 | 118.60 |
| 45 | Aw | 81 | ARG | NE-CZ-NH1 | 12.11 | 126.35 | 120.30 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 6 | G | 310 | HIS | CA |

5 of 7 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 57 | BX | 295 | PHE | Peptide |
| 14 | Q | 23 | PRO | Mainchain |
| 70 | U5 | 6 | ALA | Peptide |
| 66 | U6 | 34 | ALA | Peptide |
| 66 | U6 | 68 | ALA | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2909 | 0 | 2723 | 99 | 0 |
| 2 | B | 3513 | 0 | 3413 | 122 | 0 |
| 3 | C | 1772 | 0 | 1734 | 68 | 0 |
| 4 | E | 1818 | 0 | 1867 | 112 | 0 |
| 5 | F | 1231 | 0 | 1205 | 60 | 0 |
| 6 | G | 2767 | 0 | 2676 | 144 | 0 |
| 7 | I | 2153 | 0 | 2089 | 101 | 0 |
| 8 | J | 1146 | 0 | 1148 | 104 | 0 |
| 9 | K | 1467 | 0 | 1469 | 50 | 0 |
| 10 | L | 1419 | 0 | 1443 | 41 | 0 |
| 11 | M | 2116 | 0 | 2150 | 116 | 0 |
| 12 | N | 1599 | 0 | 1591 | 124 | 0 |
| 13 | O | 2477 | 0 | 2477 | 135 | 0 |
| 14 | Q | 1785 | 0 | 1784 | 90 | 0 |
| 15 | R | 3755 | 0 | 3722 | 152 | 0 |
| 16 | S | 1244 | 0 | 1272 | 51 | 0 |
| 17 | T | 487 | 0 | 495 | 32 | 0 |
| 18 | V | 1202 | 0 | 1224 | 65 | 0 |
| 19 | Z | 907 | 0 | 896 | 40 | 0 |
| 20 | BA | 786 | 0 | 812 | 45 | 0 |
| 21 | CA | 4230 | 0 | 4140 | 235 | 0 |
| 22 | UA | 1015 | 0 | 1017 | 32 | 0 |
| 23 | BB | 894 | 0 | 872 | 47 | 0 |
| 24 | CB | 1074 | 0 | 1076 | 67 | 0 |
| 25 | BK | 5419 | 0 | 5423 | 253 | 0 |
| 26 | BQ | 3230 | 0 | 3136 | 162 | 0 |
| 27 | BN | 1507 | 0 | 1479 | 106 | 0 |
| 28 | BE | 325 | 0 | 296 | 3 | 0 |
| 29 | BO | 1281 | 0 | 1287 | 92 | 0 |

*Continued on next page...*

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 30 | At | 1346 | 0 | 1299 | 0 | 0 |
| 31 | Au | 681 | 0 | 673 | 0 | 0 |
| 32 | Ae | 2354 | 0 | 2324 | 0 | 0 |
| 33 | Af | 1192 | 0 | 1165 | 0 | 0 |
| 34 | Ah | 3242 | 0 | 3132 | 0 | 0 |
| 35 | Ap | 1775 | 0 | 1699 | 0 | 0 |
| 36 | Al | 1857 | 0 | 1823 | 0 | 0 |
| 37 | Ab | 1413 | 0 | 1353 | 0 | 0 |
| 38 | Aa | 1076 | 0 | 1058 | 0 | 0 |
| 39 | BP | 1070 | 0 | 1019 | 46 | 0 |
| 40 | Az | 1150 | 0 | 1082 | 0 | 0 |
| 41 | Am | 2435 | 0 | 2356 | 0 | 0 |
| 42 | As | 1187 | 0 | 1203 | 0 | 0 |
| 43 | BG | 675 | 0 | 675 | 37 | 0 |
| 44 | Ad | 1502 | 0 | 1488 | 0 | 0 |
| 45 | Aw | 1509 | 0 | 1470 | 0 | 0 |
| 46 | BH | 1394 | 0 | 1350 | 49 | 0 |
| 47 | Aj | 2777 | 0 | 2778 | 0 | 0 |
| 48 | Ar | 1644 | 0 | 1608 | 0 | 0 |
| 49 | An | 1946 | 0 | 1905 | 0 | 0 |
| 50 | BF | 661 | 0 | 655 | 25 | 0 |
| 51 | Av | 828 | 0 | 811 | 0 | 0 |
| 52 | BM | 3069 | 0 | 3105 | 173 | 0 |
| 53 | Ag | 1031 | 0 | 999 | 0 | 0 |
| 54 | Bl | 1409 | 0 | 1400 | 0 | 0 |
| 55 | Ax | 1388 | 0 | 1305 | 0 | 0 |
| 56 | BS | 978 | 0 | 941 | 67 | 0 |
| 57 | BX | 2086 | 0 | 2075 | 151 | 0 |
| 57 | BY | 2111 | 0 | 2093 | 143 | 0 |
| 58 | BZ | 2829 | 0 | 2808 | 224 | 0 |
| 59 | CC | 668 | 0 | 668 | 31 | 0 |
| 60 | CD | 761 | 0 | 775 | 44 | 0 |
| 61 | BT | 2346 | 0 | 2366 | 99 | 0 |
| 62 | BU | 3680 | 0 | 3731 | 233 | 0 |
| 63 | BW | 3589 | 0 | 3714 | 184 | 0 |
| 64 | BV | 1596 | 0 | 1586 | 81 | 0 |
| 65 | U7 | 200 | 0 | 48 | 5 | 0 |
| 66 | U6 | 935 | 0 | 937 | 25 | 0 |
| 67 | U1 | 230 | 0 | 232 | 14 | 0 |
| 68 | U3 | 375 | 0 | 377 | 16 | 0 |
| 69 | U4 | 680 | 0 | 682 | 11 | 0 |
| 70 | U5 | 470 | 0 | 472 | 24 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 71 | BR | 1703 | 0 | 1703 | 90 | 0 |
| 72 | U2 | 185 | 0 | 187 | 16 | 0 |
| 73 | 1 | 16777 | 0 | 8400 | 700 | 0 |
| 74 | R1 | 62 | 0 | 32 | 10 | 0 |
| 75 | R2 | 665 | 0 | 344 | 43 | 0 |
| 76 | R5 | 100 | 0 | 51 | 5 | 0 |
| 77 | U8 | 295 | 0 | 297 | 50 | 0 |
| 78 | BU | 32 | 0 | 12 | 9 | 0 |
| 79 | BW | 31 | 12 | 12 | 2 | 0 |
| All | All | 139523 | 12 | 129194 | 4568 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 4568 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 73:1:106:A:N3 | 73:1:106:A:C2 | 1.74 | 1.55 |
| 73:1:106:A:C6 | 73:1:106:A:N1 | 1.79 | 1.49 |
| 73:1:106:A:N3 | 73:1:106:A:C4 | 1.76 | 1.49 |
| 73:1:106:A:C2 | 73:1:106:A:N1 | 1.77 | 1.49 |
| 2:B:194:LYS:NZ | 73:1:208:U:C2 | 1.88 | 1.42 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 354/467 (76%) | 298 (84%) | 55 (16%) | 1 (0%) | 41 72 |
| 2 | B | 433/436 (99%) | 387 (89%) | 46 (11%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | C | 210/262 (80%) | 182 (87%) | 27 (13%) | 1 (0%) | 29 61 |
| 4 | E | 223/346 (64%) | 192 (86%) | 30 (14%) | 1 (0%) | 34 67 |
| 5 | F | 145/171 (85%) | 125 (86%) | 20 (14%) | 0 | 100 100 |
| 6 | G | 332/374 (89%) | 289 (87%) | 36 (11%) | 7 (2%) | 7 30 |
| 7 | I | 255/305 (84%) | 218 (86%) | 37 (14%) | 0 | 100 100 |
| 8 | J | 139/144 (96%) | 108 (78%) | 27 (19%) | 4 (3%) | 4 24 |
| 9 | K | 177/194 (91%) | 159 (90%) | 18 (10%) | 0 | 100 100 |
| 10 | L | 176/186 (95%) | 159 (90%) | 17 (10%) | 0 | 100 100 |
| 11 | M | 257/279 (92%) | 218 (85%) | 39 (15%) | 0 | 100 100 |
| 12 | N | 187/252 (74%) | 154 (82%) | 29 (16%) | 4 (2%) | 7 30 |
| 13 | O | 298/476 (63%) | 267 (90%) | 30 (10%) | 1 (0%) | 41 72 |
| 14 | Q | 215/234 (92%) | 191 (89%) | 23 (11%) | 1 (0%) | 29 61 |
| 15 | R | 470/480 (98%) | 410 (87%) | 59 (13%) | 1 (0%) | 47 78 |
| 16 | S | 148/409 (36%) | 135 (91%) | 13 (9%) | 0 | 100 100 |
| 17 | T | 53/83 (64%) | 47 (89%) | 6 (11%) | 0 | 100 100 |
| 18 | V | 139/151 (92%) | 114 (82%) | 25 (18%) | 0 | 100 100 |
| 19 | Z | 111/197 (56%) | 95 (86%) | 16 (14%) | 0 | 100 100 |
| 20 | BA | 104/167 (62%) | 85 (82%) | 19 (18%) | 0 | 100 100 |
| 21 | CA | 535/618 (87%) | 417 (78%) | 113 (21%) | 5 (1%) | 17 49 |
| 22 | UA | 201/203 (99%) | 167 (83%) | 30 (15%) | 4 (2%) | 7 30 |
| 23 | BB | 104/156 (67%) | 87 (84%) | 17 (16%) | 0 | 100 100 |
| 24 | CB | 133/202 (66%) | 95 (71%) | 38 (29%) | 0 | 100 100 |
| 25 | BK | 690/893 (77%) | 608 (88%) | 78 (11%) | 4 (1%) | 25 57 |
| 26 | BQ | 409/445 (92%) | 362 (88%) | 46 (11%) | 1 (0%) | 47 78 |
| 27 | BN | 192/344 (56%) | 163 (85%) | 27 (14%) | 2 (1%) | 15 46 |
| 28 | BE | 35/118 (30%) | 26 (74%) | 9 (26%) | 0 | 100 100 |
| 29 | BO | 154/190 (81%) | 108 (70%) | 44 (29%) | 2 (1%) | 12 39 |
| 30 | At | 163/183 (89%) | 136 (83%) | 27 (17%) | 0 | 100 100 |
| 31 | Au | 78/186 (42%) | 72 (92%) | 6 (8%) | 0 | 100 100 |
| 32 | Ae | 288/311 (93%) | 243 (84%) | 45 (16%) | 0 | 100 100 |
| 33 | Af | 143/155 (92%) | 126 (88%) | 17 (12%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 34 | Ah | 395/570 (69%) | 347 (88%) | 46 (12%) | 2 (0%) | 29 61 |
| 35 | Ap | 212/240 (88%) | 193 (91%) | 19 (9%) | 0 | 100 100 |
| 36 | Al | 226/346 (65%) | 197 (87%) | 27 (12%) | 2 (1%) | 17 49 |
| 37 | Ab | 166/262 (63%) | 148 (89%) | 18 (11%) | 0 | 100 100 |
| 38 | Aa | 133/195 (68%) | 106 (80%) | 23 (17%) | 4 (3%) | 4 23 |
| 39 | BP | 129/254 (51%) | 105 (81%) | 23 (18%) | 1 (1%) | 19 51 |
| 40 | Az | 128/152 (84%) | 121 (94%) | 7 (6%) | 0 | 100 100 |
| 41 | Am | 294/340 (86%) | 265 (90%) | 29 (10%) | 0 | 100 100 |
| 42 | As | 142/249 (57%) | 125 (88%) | 17 (12%) | 0 | 100 100 |
| 43 | BG | 83/1347 (6%) | 64 (77%) | 17 (20%) | 2 (2%) | 6 28 |
| 44 | Ad | 185/237 (78%) | 165 (89%) | 20 (11%) | 0 | 100 100 |
| 45 | Aw | 183/187 (98%) | 160 (87%) | 23 (13%) | 0 | 100 100 |
| 46 | BH | 179/229 (78%) | 158 (88%) | 20 (11%) | 1 (1%) | 25 57 |
| 47 | Aj | 338/503 (67%) | 303 (90%) | 35 (10%) | 0 | 100 100 |
| 48 | Ar | 193/205 (94%) | 148 (77%) | 45 (23%) | 0 | 100 100 |
| 49 | An | 236/331 (71%) | 206 (87%) | 28 (12%) | 2 (1%) | 19 51 |
| 50 | BF | 77/109 (71%) | 65 (84%) | 12 (16%) | 0 | 100 100 |
| 51 | Av | 98/192 (51%) | 75 (76%) | 23 (24%) | 0 | 100 100 |
| 52 | BM | 387/457 (85%) | 345 (89%) | 42 (11%) | 0 | 100 100 |
| 53 | Ag | 122/244 (50%) | 105 (86%) | 17 (14%) | 0 | 100 100 |
| 54 | Bl | 184/266 (69%) | 164 (89%) | 20 (11%) | 0 | 100 100 |
| 55 | Ax | 165/216 (76%) | 122 (74%) | 39 (24%) | 4 (2%) | 6 28 |
| 56 | BS | 121/416 (29%) | 100 (83%) | 21 (17%) | 0 | 100 100 |
| 57 | BX | 270/569 (48%) | 202 (75%) | 64 (24%) | 4 (2%) | 10 36 |
| 57 | BY | 273/569 (48%) | 214 (78%) | 58 (21%) | 1 (0%) | 34 67 |
| 58 | BZ | 347/413 (84%) | 277 (80%) | 60 (17%) | 10 (3%) | 4 24 |
| 59 | CC | 82/150 (55%) | 76 (93%) | 6 (7%) | 0 | 100 100 |
| 60 | CD | 88/126 (70%) | 70 (80%) | 17 (19%) | 1 (1%) | 14 44 |
| 61 | BT | 298/464 (64%) | 235 (79%) | 62 (21%) | 1 (0%) | 41 72 |
| 62 | BU | 461/497 (93%) | 373 (81%) | 85 (18%) | 3 (1%) | 22 55 |
| 63 | BW | 443/776 (57%) | 359 (81%) | 76 (17%) | 8 (2%) | 8 32 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 64 | BV | 195/787 (25%) | 151 (77%) | 42 (22%) | 2 (1%) | 15 46 |
| 66 | U6 | 185/187 (99%) | 138 (75%) | 43 (23%) | 4 (2%) | 6 29 |
| 67 | U1 | 44/46 (96%) | 34 (77%) | 8 (18%) | 2 (4%) | 2 16 |
| 68 | U3 | 73/75 (97%) | 55 (75%) | 17 (23%) | 1 (1%) | 11 37 |
| 69 | U4 | 134/136 (98%) | 120 (90%) | 14 (10%) | 0 | 100 100 |
| 70 | U5 | 92/94 (98%) | 52 (56%) | 38 (41%) | 2 (2%) | 6 29 |
| 71 | BR | 210/301 (70%) | 178 (85%) | 32 (15%) | 0 | 100 100 |
| 72 | U2 | 35/37 (95%) | 24 (69%) | 11 (31%) | 0 | 100 100 |
| 77 | U8 | 57/59 (97%) | 34 (60%) | 8 (14%) | 15 (26%) | 0 0 |
| All | All | 15214/22450 (68%) | 12822 (84%) | 2281 (15%) | 111 (1%) | 26 55 |

5 of 111 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | G | 310 | HIS |
| 6 | G | 311 | PRO |
| 6 | G | 333 | ILE |
| 8 | J | 60 | ASN |
| 12 | N | 77 | ASN |

### 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 |
|---|---|---|---|---|---|
| 1 | A | 305/394 (77%) | 289 (95%) | 16 (5%) | 23 53 |
| 2 | B | 380/381 (100%) | 359 (94%) | 21 (6%) | 21 51 |
| 3 | C | 190/227 (84%) | 178 (94%) | 12 (6%) | 18 47 |
| 4 | E | 193/301 (64%) | 181 (94%) | 12 (6%) | 18 48 |
| 5 | F | 130/152 (86%) | 126 (97%) | 4 (3%) | 40 68 |
| 6 | G | 290/323 (90%) | 266 (92%) | 24 (8%) | 11 36 |
| 7 | I | 223/262 (85%) | 212 (95%) | 11 (5%) | 25 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 8 | J | 119/122 (98%) | 103 (87%) | 16 (13%) | 4 | 15 |
| 9 | K | 151/162 (93%) | 143 (95%) | 8 (5%) | 22 | 52 |
| 10 | L | 151/158 (96%) | 132 (87%) | 19 (13%) | 4 | 17 |
| 11 | M | 226/242 (93%) | 210 (93%) | 16 (7%) | 14 | 44 |
| 12 | N | 175/220 (80%) | 155 (89%) | 20 (11%) | 5 | 21 |
| 13 | O | 272/397 (68%) | 257 (94%) | 15 (6%) | 21 | 51 |
| 14 | Q | 191/204 (94%) | 175 (92%) | 16 (8%) | 11 | 36 |
| 15 | R | 406/412 (98%) | 379 (93%) | 27 (7%) | 16 | 46 |
| 16 | S | 135/336 (40%) | 126 (93%) | 9 (7%) | 16 | 46 |
| 17 | T | 52/74 (70%) | 49 (94%) | 3 (6%) | 20 | 50 |
| 18 | V | 125/135 (93%) | 121 (97%) | 4 (3%) | 39 | 67 |
| 19 | Z | 97/172 (56%) | 90 (93%) | 7 (7%) | 14 | 43 |
| 20 | BA | 86/135 (64%) | 82 (95%) | 4 (5%) | 26 | 57 |
| 21 | CA | 446/501 (89%) | 403 (90%) | 43 (10%) | 8 | 29 |
| 23 | BB | 91/140 (65%) | 88 (97%) | 3 (3%) | 38 | 66 |
| 24 | CB | 118/179 (66%) | 106 (90%) | 12 (10%) | 7 | 26 |
| 25 | BK | 582/739 (79%) | 539 (93%) | 43 (7%) | 13 | 42 |
| 26 | BQ | 347/375 (92%) | 330 (95%) | 17 (5%) | 25 | 55 |
| 27 | BN | 159/280 (57%) | 142 (89%) | 17 (11%) | 6 | 24 |
| 28 | BE | 35/100 (35%) | 32 (91%) | 3 (9%) | 10 | 35 |
| 29 | BO | 136/158 (86%) | 125 (92%) | 11 (8%) | 11 | 38 |
| 30 | At | 140/153 (92%) | 132 (94%) | 8 (6%) | 20 | 50 |
| 31 | Au | 69/164 (42%) | 65 (94%) | 4 (6%) | 20 | 50 |
| 32 | Ae | 249/261 (95%) | 233 (94%) | 16 (6%) | 17 | 47 |
| 33 | Af | 125/135 (93%) | 117 (94%) | 8 (6%) | 17 | 47 |
| 34 | Ah | 337/485 (70%) | 317 (94%) | 20 (6%) | 19 | 49 |
| 35 | Ap | 189/208 (91%) | 173 (92%) | 16 (8%) | 10 | 35 |
| 36 | Al | 204/299 (68%) | 189 (93%) | 15 (7%) | 13 | 42 |
| 37 | Ab | 150/235 (64%) | 141 (94%) | 9 (6%) | 19 | 49 |
| 38 | Aa | 118/166 (71%) | 109 (92%) | 9 (8%) | 13 | 41 |
| 39 | BP | 110/215 (51%) | 101 (92%) | 9 (8%) | 11 | 37 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 40 | Az | 123/143 (86%) | 116 (94%) | 7 (6%) | 20 50 |
| 41 | Am | 250/287 (87%) | 237 (95%) | 13 (5%) | 23 53 |
| 42 | As | 131/204 (64%) | 124 (95%) | 7 (5%) | 22 52 |
| 43 | BG | 77/1047 (7%) | 69 (90%) | 8 (10%) | 7 25 |
| 44 | Ad | 159/193 (82%) | 151 (95%) | 8 (5%) | 24 54 |
| 45 | Aw | 157/159 (99%) | 154 (98%) | 3 (2%) | 57 78 |
| 46 | BH | 150/189 (79%) | 145 (97%) | 5 (3%) | 38 66 |
| 47 | Aj | 287/420 (68%) | 274 (96%) | 13 (4%) | 27 58 |
| 48 | Ar | 169/179 (94%) | 159 (94%) | 10 (6%) | 19 49 |
| 49 | An | 208/289 (72%) | 196 (94%) | 12 (6%) | 20 50 |
| 50 | BF | 68/95 (72%) | 63 (93%) | 5 (7%) | 13 42 |
| 51 | Av | 90/169 (53%) | 82 (91%) | 8 (9%) | 9 33 |
| 52 | BM | 319/370 (86%) | 283 (89%) | 36 (11%) | 6 21 |
| 53 | Ag | 106/211 (50%) | 98 (92%) | 8 (8%) | 13 41 |
| 54 | Bl | 153/221 (69%) | 144 (94%) | 9 (6%) | 19 49 |
| 55 | Ax | 150/190 (79%) | 140 (93%) | 10 (7%) | 16 46 |
| 56 | BS | 103/328 (31%) | 98 (95%) | 5 (5%) | 25 55 |
| 57 | BX | 226/483 (47%) | 205 (91%) | 21 (9%) | 9 31 |
| 57 | BY | 229/483 (47%) | 211 (92%) | 18 (8%) | 12 39 |
| 58 | BZ | 305/363 (84%) | 276 (90%) | 29 (10%) | 8 29 |
| 59 | CC | 77/129 (60%) | 73 (95%) | 4 (5%) | 23 53 |
| 60 | CD | 83/112 (74%) | 78 (94%) | 5 (6%) | 19 49 |
| 61 | BT | 257/398 (65%) | 242 (94%) | 15 (6%) | 20 50 |
| 62 | BU | 401/431 (93%) | 361 (90%) | 40 (10%) | 7 27 |
| 63 | BW | 386/661 (58%) | 352 (91%) | 34 (9%) | 10 33 |
| 64 | BV | 172/644 (27%) | 166 (96%) | 6 (4%) | 36 65 |
| 71 | BR | 177/241 (73%) | 171 (97%) | 6 (3%) | 37 65 |
| All | All | 12515/18241 (69%) | 11643 (93%) | 872 (7%) | 19 44 |

5 of 872 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | Ah | 350 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | BH | 54 | ARG |
| 62 | BU | 263 | THR |
| 35 | Ap | 157 | THR |
| 34 | Ah | 336 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 291 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | BM | 384 | HIS |
| 64 | BV | 324 | GLN |
| 57 | BY | 84 | HIS |
| 58 | BZ | 372 | GLN |
| 25 | BK | 424 | GLN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 73 | 1 | 790/19000 (4%) | 465 (58%) | 77 (9%) |
| 74 | R1 | 2/3 (66%) | 2 (100%) | 1 (50%) |
| 75 | R2 | 32/35 (91%) | 24 (75%) | 10 (31%) |
| 76 | R5 | 4/5 (80%) | 0 | 0 |
| All | All | 828/19043 (4%) | 491 (59%) | 88 (10%) |

5 of 491 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 73 | 1 | 35 | U |
| 73 | 1 | 36 | U |
| 73 | 1 | 39 | U |
| 73 | 1 | 41 | A |
| 73 | 1 | 42 | A |

5 of 88 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 73 | 1 | 590 | A |
| 73 | 1 | 1097 | A |
| 73 | 1 | 594 | U |
| 73 | 1 | 916 | G |
| 73 | 1 | 1172 | A |

## 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)

2 ligands 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 | $\#\|Z\| > 2$ |
| 78 | GTP | BU | 501 | - | 26,34,34 | 0.97 | 2 (7%) | 32,54,54 | 0.99 | 3 (9%) |
| 79 | ATP | BW | 801 | - | 26,33,33 | 0.70 | 0 | 31,52,52 | 0.82 | 1 (3%) |

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 |
|---|---|---|---|---|---|---|---|
| 78 | GTP | BU | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 79 | ATP | BW | 801 | - | - | 1/18/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | BU | 501 | GTP | C5-C6 | -2.61 | 1.42 | 1.47 |
| 78 | BU | 501 | GTP | C8-N7 | -2.13 | 1.31 | 1.35 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | BU | 501 | GTP | O4'-C4'-C3' | -2.58 | 100.02 | 105.11 |
| 79 | BW | 801 | ATP | C5-C6-N6 | 2.32 | 123.87 | 120.35 |
| 78 | BU | 501 | GTP | PB-O3B-PG | 2.24 | 140.51 | 132.83 |
| 78 | BU | 501 | GTP | O6-C6-C5 | 2.01 | 128.30 | 124.37 |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 78 | BU | 501 | GTP | PB-O3A-PA-O5' |
| 78 | BU | 501 | GTP | C5'-O5'-PA-O3A |
| 78 | BU | 501 | GTP | C5'-O5'-PA-O2A |
| 78 | BU | 501 | GTP | O4'-C4'-C5'-O5' |
| 78 | BU | 501 | GTP | C4'-C5'-O5'-PA |

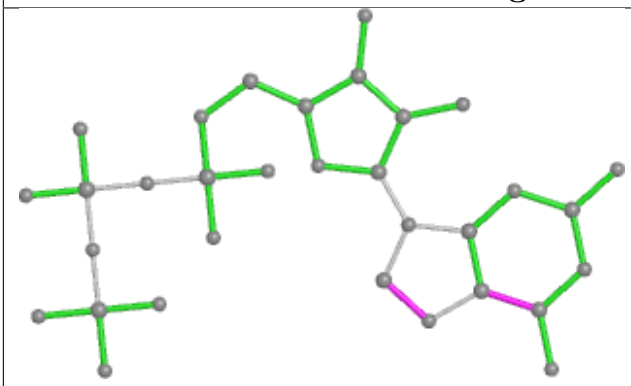
There are no ring outliers.

2 monomers are involved in 11 short contacts:

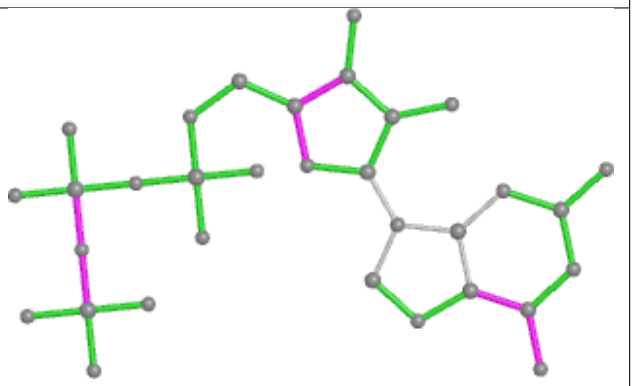
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 78 | BU | 501 | GTP | 9 | 0 |
| 79 | BW | 801 | ATP | 2 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight $> 250$ and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

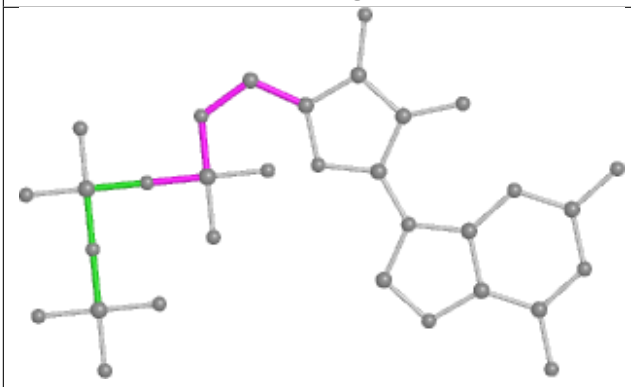
**Ligand GTP BU 501**



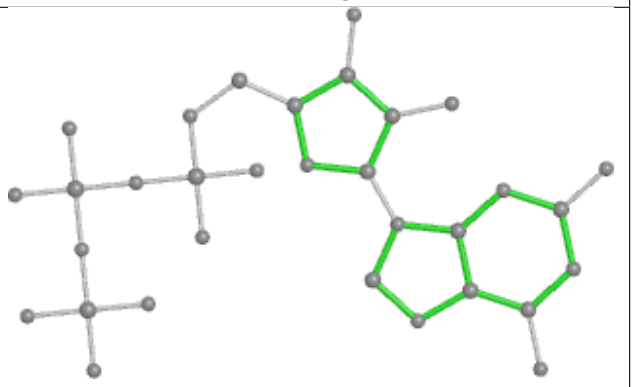
**Bond lengths**



**Bond angles**

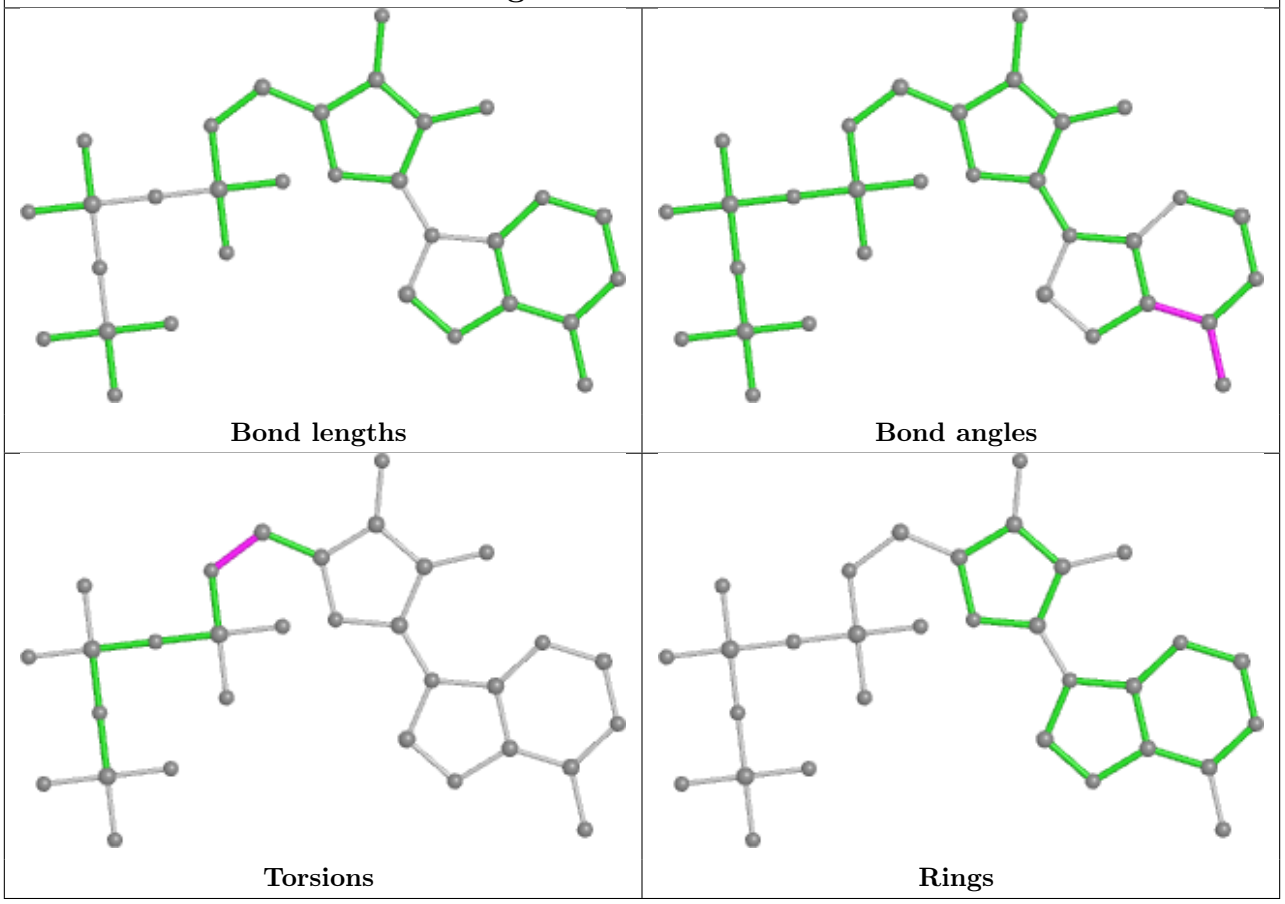


**Torsions**



**Rings**

**Ligand ATP BW 801**




## 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 |
|---|---|---|
| 75 | R2 | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | R2 | 21:U | O3' | 122:U | P | 84.98 |
| 1 | R2 | 134:U | O3' | 235:U | P | 16.60 |

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11821. 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.