# wwPDB EM Map/Model Validation Report (i)

Jul 19, 2016 – 02:45 PM EDT

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|---|---|---|
| PDB ID | : | 3JCS |
| EMDB ID: | : | EMD-6583 |
| Title | : | 2.8 Angstrom cryo-EM structure of the large ribosomal subunit from the eukaryotic parasite Leishmania |
| Authors | : | Shalev-Benami, M.; Zhang, Y.; Matzov, D.; Halfon, Y.; Zackay, A.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G. |
| Deposited on | : | 2016-01-21 |
| Resolution | : | 2.80 Å(reported) |

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

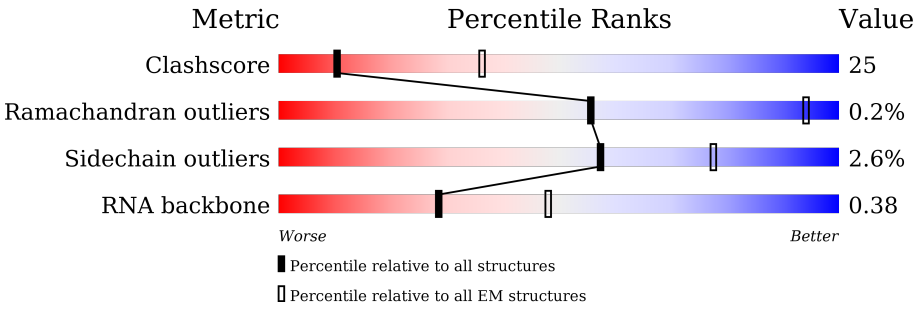
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20027790 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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 | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |
| RNA backbone | 3027 | 244 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 | 1 | 1782 | 25% 38% 22% • 13% |
| 2 | 2 | 1527 | 21% 34% 18% 27% |
| 3 | 3 | 213 | 22% 38% 26% 14% |
| 4 | 4 | 183 | 28% 35% 19% 19% |
| 5 | 5 | 133 | 16% 28% 15% • 40% |
| 6 | 6 | 76 | • 20% 53% 5% 20% |
| 7 | 7 | 171 | 28% 44% 16% • 10% |
| 8 | 8 | 121 | 13% 46% 39% • |

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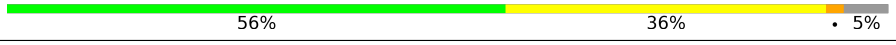
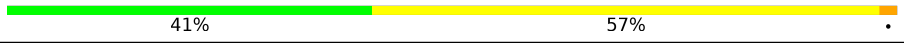
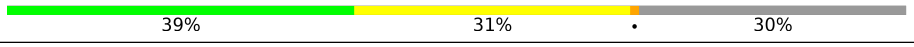
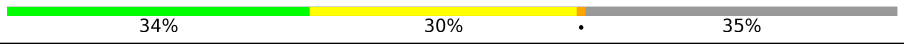
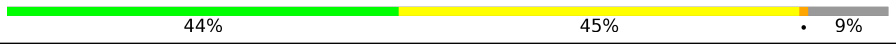
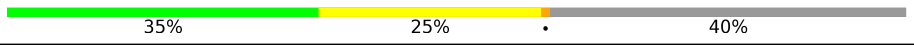
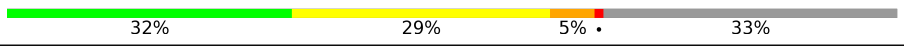
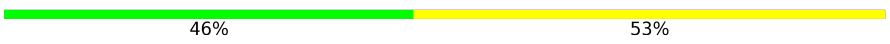
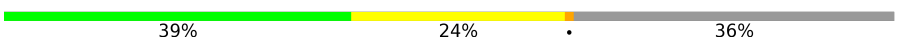
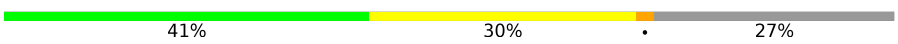
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | A | 260 |   |
| 10 | B | 419 |   |
| 11 | C | 373 |   |
| 12 | D | 188 |   |
| 13 | E | 190 |   |
| 14 | F | 195 |   |
| 15 | G | 348 |   |
| 16 | H | 222 |   |
| 17 | I | 220 |   |
| 18 | J | 139 |   |
| 19 | K | 233 |   |
| 20 | L | 145 |   |
| 21 | M | 204 |   |
| 22 | N | 213 |   |
| 23 | O | 305 |   |
| 24 | P | 198 |   |
| 25 | Q | 245 |   |
| 26 | R | 179 |   |
| 27 | S | 159 |   |
| 28 | T | 166 |   |
| 29 | U | 129 |   |
| 30 | V | 145 |   |
| 31 | W | 143 |   |
| 32 | X | 124 |   |
| 33 | Y | 134 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | Z | 147 | 41% 12% 46% |
| 35 | a | 127 | 92% 6% |
| 36 | b | 70 | 87% 6% 7% |
| 37 | c | 252 | 87% 12% |
| 38 | d | 104 | 69% 28% |
| 39 | e | 183 | 61% 39% |
| 40 | f | 133 | 92% 5% |
| 41 | g | 144 | 85% 13% |
| 42 | h | 168 | 64% 35% |
| 43 | i | 105 | 57% 40% |
| 44 | j | 83 | 90% 6% |
| 45 | k | 83 | 69% 30% |
| 46 | l | 51 | 92% 6% |
| 47 | m | 92 | 91% 7% |
| 48 | n | 106 | 80% 19% |

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 |
|---|---|---|---|---|---|---|---|
| 1 | OMU | 1 | 36 | - | - | X | - |
| 1 | OMG | 1 | 959 | - | - | X | - |
| 2 | OMU | 2 | 1078 | - | - | X | - |
| 2 | OMG | 2 | 1079 | - | - | X | - |
| 2 | OMG | 2 | 1254 | - | - | X | - |
| 2 | OMC | 2 | 1318 | - | - | X | - |
| 2 | OMC | 2 | 443 | - | - | X | - |
| 2 | A2M | 2 | 527 | - | - | X | - |
| 2 | OMG | 2 | 71 | - | - | X | - |
| 7 | OMU | 7 | 7 | - | - | X | - |

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 117257 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 26S alpha ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | 1 | 1554 | 33313 | 14886 | 6081 | 10792 | 1554 | 0 | 0 |

- Molecule 2 is a RNA chain called 26S delta ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | 2 | 1119 | 23926 | 10702 | 4308 | 7797 | 1119 | 0 | 0 |

- Molecule 3 is a RNA chain called 26S gamma ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | 3 | 184 | 3893 | 1740 | 662 | 1307 | 184 | 0 | 0 |

- Molecule 4 is a RNA chain called 26S delta ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | 4 | 149 | 3177 | 1418 | 570 | 1040 | 149 | 0 | 0 |

- Molecule 5 is a RNA chain called 26S epsilon ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | 5 | 80 | 1708 | 763 | 310 | 555 | 80 | 0 | 0 |

- Molecule 6 is a RNA chain called 26S zeta ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | 6 | 61 | 1288 | 577 | 225 | 425 | 61 | 0 | 0 |

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 7 | 154 | Total | C | N | O | P | 0 | 0 |
| | | | 3280 | 1469 | 584 | 1074 | 153 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 8 | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2531 | 1132 | 450 | 830 | 119 | | |

- Molecule 9 is a protein called ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | A | 245 | Total | C | N | O | S | 2 | 0 |
| | | | 1859 | 1158 | 384 | 307 | 10 | | |

- Molecule 10 is a protein called ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | B | 396 | Total | C | N | O | S | 2 | 0 |
| | | | 3020 | 1908 | 592 | 508 | 12 | | |

- Molecule 11 is a protein called ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | C | 301 | Total | C | N | O | S | 1 | 0 |
| | | | 2237 | 1413 | 428 | 384 | 12 | | |

- Molecule 12 is a protein called ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 12 | D | 161 | Total | C | N | O | 0 | 0 |
| | | | 799 | 476 | 161 | 162 | | |

- Molecule 13 is a protein called ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | E | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 953 | 276 | 272 | 8 | | |

- Molecule 14 is a protein called ribosomal protein L6e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | F | 137 | Total | C | N | O | S | 1 | 0 |
| | | | 1002 | 641 | 192 | 167 | 2 | | |

- Molecule 15 is a protein called ribosomal protein L8e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | G | 226 | Total | C | N | O | S | 1 | 0 |
| | | | 1772 | 1113 | 353 | 299 | 7 | | |

- Molecule 16 is a protein called ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | H | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1596 | 1019 | 307 | 263 | 7 | | |

- Molecule 17 is a protein called ribosomal protein L13e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | I | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1061 | 666 | 221 | 169 | 5 | | |

- Molecule 18 is a protein called ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | J | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 924 | 588 | 171 | 160 | 5 | | |

- Molecule 19 is a protein called ribosomal protein L14e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | K | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1061 | 661 | 212 | 184 | 4 | | |

- Molecule 20 is a protein called ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | L | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1096 | 691 | 223 | 177 | 5 | | |

- Molecule 21 is a protein called ribosomal protein L15e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | M | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1714 | 1080 | 362 | 264 | 8 | | |

- Molecule 22 is a protein called ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | N | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1714 | 1077 | 340 | 281 | 16 | | |

- Molecule 23 is a protein called ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | O | 235 | Total | C | N | O | S | 0 | 0 |
| | | | 1557 | 986 | 300 | 268 | 3 | | |

- Molecule 24 is a protein called ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | P | 195 | Total | C | N | O | S | 1 | 0 |
| | | | 1494 | 942 | 299 | 247 | 6 | | |

- Molecule 25 is a protein called ribosomal protein L19e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Q | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 730 | 243 | 186 | 3 | | |

- Molecule 26 is a protein called ribosomal protein L20e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | R | 131 | Total | C | N | O | S | 1 | 0 |
| | | | 1019 | 651 | 197 | 167 | 4 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| R | 158 | ILE | LEU | VARIANT | UNP E9BRT7 |

- Molecule 27 is a protein called ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | S | 149 | Total | C | N | O | S | 2 | 0 |
| | | | 1112 | 704 | 218 | 187 | 3 | | |

- Molecule 28 is a protein called ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | T | 154 | Total | C | N | O | S | 2 | 0 |
| | | | 1221 | 763 | 241 | 206 | 11 | | |

- Molecule 29 is a protein called ribosomal protein L22e.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 29 | U | 100 | Total | C | N | O | 0 | 0 |
| | | | 541 | 331 | 101 | 109 | | |

- Molecule 30 is a protein called ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | V | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 892 | 566 | 171 | 153 | 2 | | |

- Molecule 31 is a protein called ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | W | 117 | Total | C | N | O | S | 1 | 0 |
| | | | 896 | 562 | 187 | 144 | 3 | | |

- Molecule 32 is a protein called ribosomal protein L24e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | X | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 508 | 333 | 96 | 76 | 3 | | |

- Molecule 33 is a protein called ribosomal protein L27e.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 33 | Y | 132 | Total | C | N | O | 0 | 0 |
| | | | 914 | 589 | 174 | 151 | | |

- Molecule 34 is a protein called ribosomal protein L28e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | Z | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 329 | 111 | 95 | 3 | | |

- Molecule 35 is a protein called ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | a | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 982 | 613 | 203 | 163 | 3 | | |

- Molecule 36 is a protein called ribosomal protein L29e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | b | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 503 | 309 | 113 | 80 | 1 | | |

- Molecule 37 is a protein called ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | c | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1732 | 1105 | 327 | 289 | 11 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| c | 49 | ALA | GLY | VARIANT | UNP E9BI29 |

- Molecule 38 is a protein called ribosomal protein L30e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | d | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 518 | 325 | 93 | 97 | 3 | | |

- Molecule 39 is a protein called ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | e | 112 | Total | C | N | O | S | 1 | 0 |
| | | | 824 | 531 | 155 | 136 | 2 | | |

- Molecule 40 is a protein called ribosomal protein L32e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | f | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 982 | 616 | 195 | 167 | 4 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| f | 105 | LYS | THR | VARIANT | UNP E9BFJ5 |

- Molecule 41 is a protein called ribosomal protein L33e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | g | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 983 | 612 | 205 | 161 | 5 | | |

- Molecule 42 is a protein called ribosomal protein L34e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | h | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 856 | 529 | 182 | 140 | 5 | | |

- Molecule 43 is a protein called ribosomal protein L36e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | i | 63 | Total | C | N | O | S | 1 | 0 |
| | | | 494 | 316 | 100 | 76 | 2 | | |

- Molecule 44 is a protein called ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | j | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 639 | 385 | 149 | 99 | 6 | | |

- Molecule 45 is a protein called ribosomal protein L38e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | k | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 373 | 234 | 71 | 66 | 2 | | |

- Molecule 46 is a protein called ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | l | 50 | Total | C | N | O | S | 1 | 0 |
| | | | 457 | 294 | 98 | 64 | 1 | | |

- Molecule 47 is a protein called ribosomal protein L43e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | m | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 668 | 414 | 135 | 113 | 6 | | |

- Molecule 48 is a protein called ribosomal protein L44e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | n | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 659 | 418 | 129 | 110 | 2 | | |

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 49 | g | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 49 | j | 4 | Total | Mg | 0 |
| | | | 4 | 4 | |
| 49 | 1 | 51 | Total | Mg | 0 |
| | | | 51 | 51 | |
| 49 | K | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 49 | h | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 49 | C | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 49 | V | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 49 | 7 | 9 | Total | Mg | 0 |
| | | | 9 | 9 | |
| 49 | a | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 49 | 4 | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 49 | 5 | 4 | Total | Mg | 0 |
| | | | 4 | 4 | |
| 49 | 2 | 25 | Total | Mg | 0 |
| | | | 25 | 25 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 49 | 3 | 3 | Total Mg<br>3 3 | 0 |
| 49 | f | 2 | Total Mg<br>2 2 | 0 |
| 49 | M | 3 | Total Mg<br>3 3 | 0 |

- Molecule 50 is water.

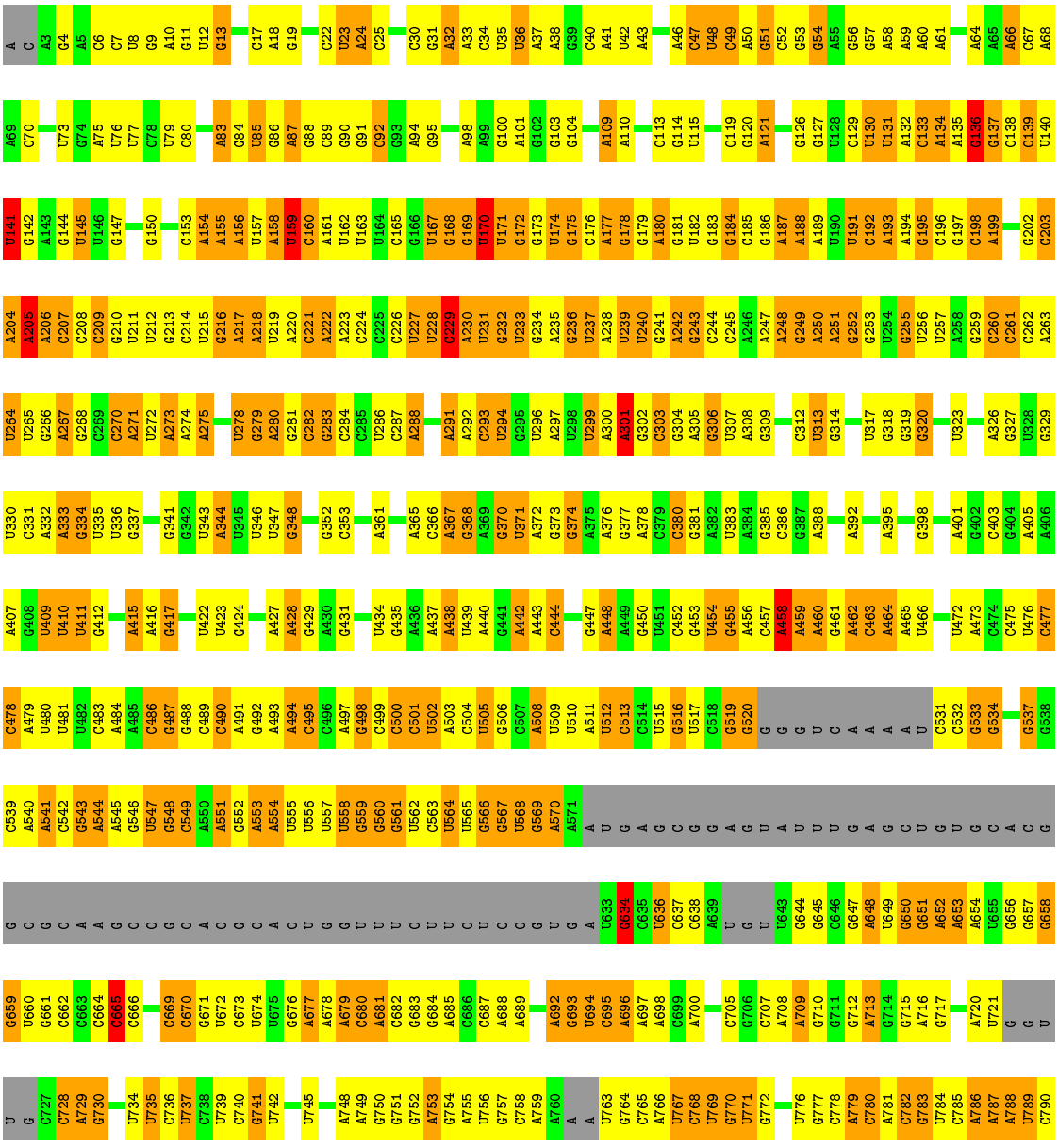
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 50 | 1 | 72 | Total O<br>72 72 | 0 |
| 50 | 2 | 40 | Total O<br>40 40 | 0 |
| 50 | 4 | 4 | Total O<br>4 4 | 0 |
| 50 | 5 | 4 | Total O<br>4 4 | 0 |
| 50 | 7 | 16 | Total O<br>16 16 | 0 |
| 50 | 8 | 1 | Total O<br>1 1 | 0 |
| 50 | A | 2 | Total O<br>2 2 | 0 |
| 50 | G | 1 | Total O<br>1 1 | 0 |
| 50 | M | 2 | Total O<br>2 2 | 0 |
| 50 | i | 1 | Total O<br>1 1 | 0 |
| 50 | j | 1 | Total O<br>1 1 | 0 |

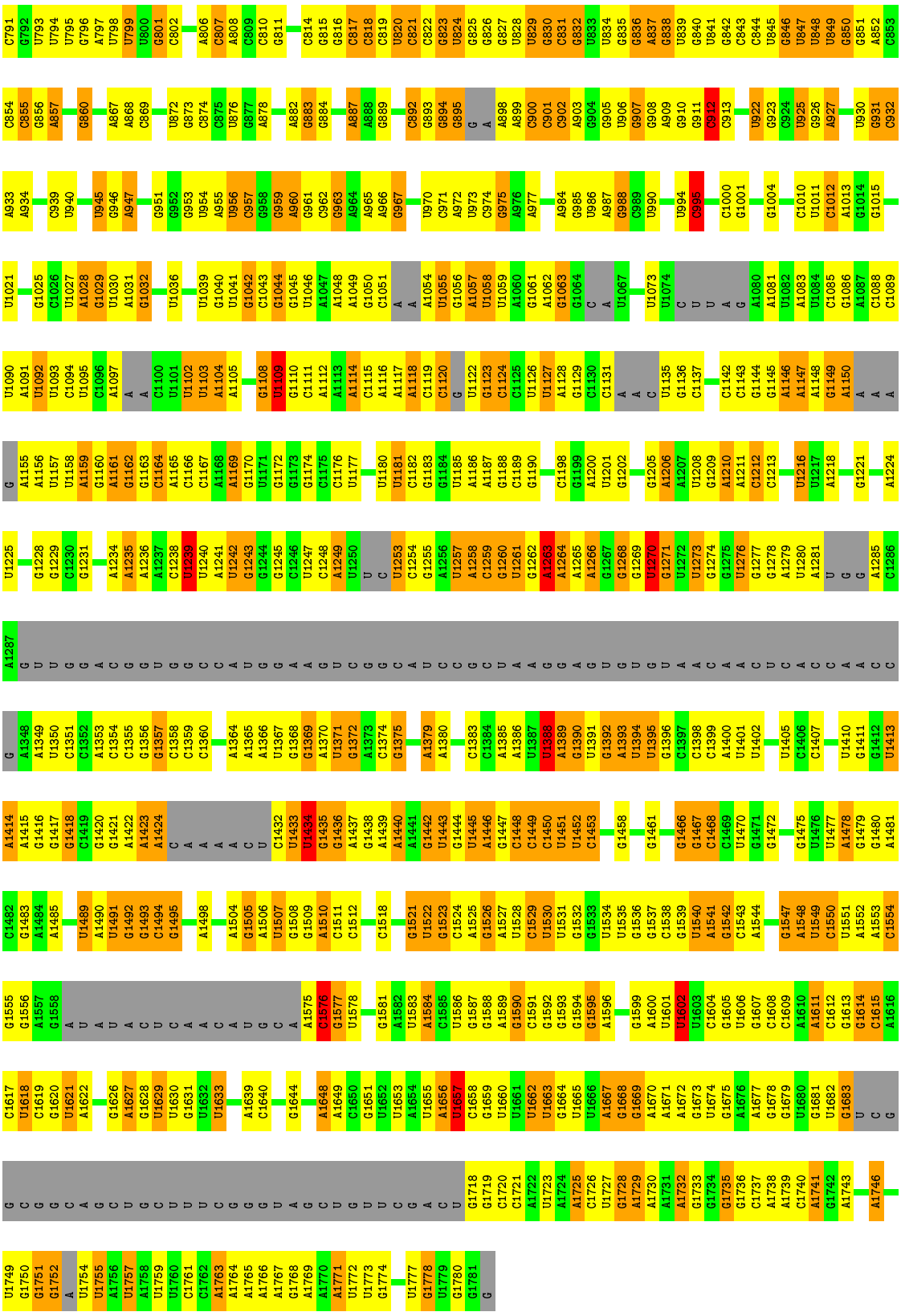
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 26S alpha ribosomal RNA

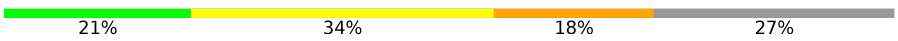
Chain 1: 25% 38% 22% 13%

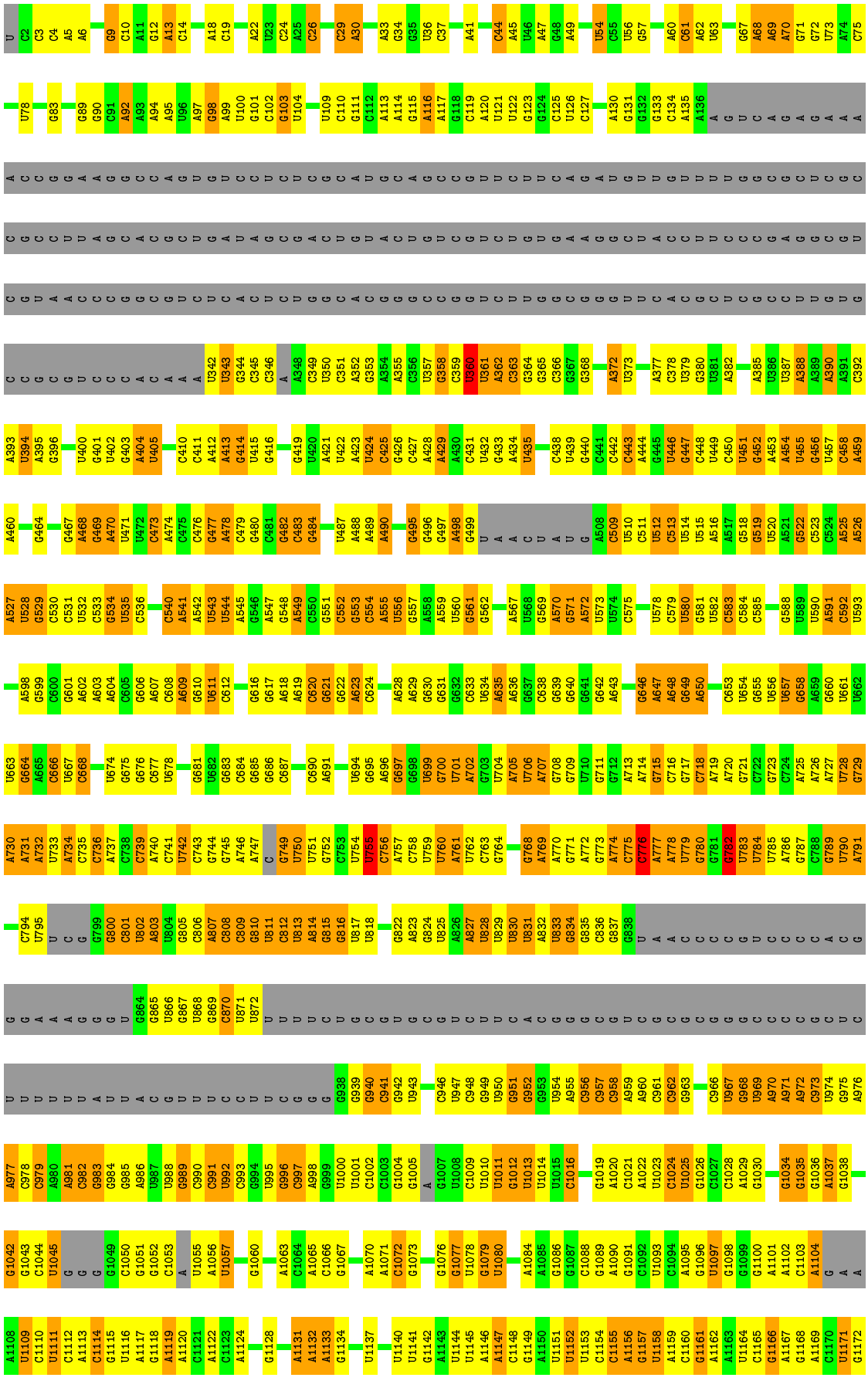


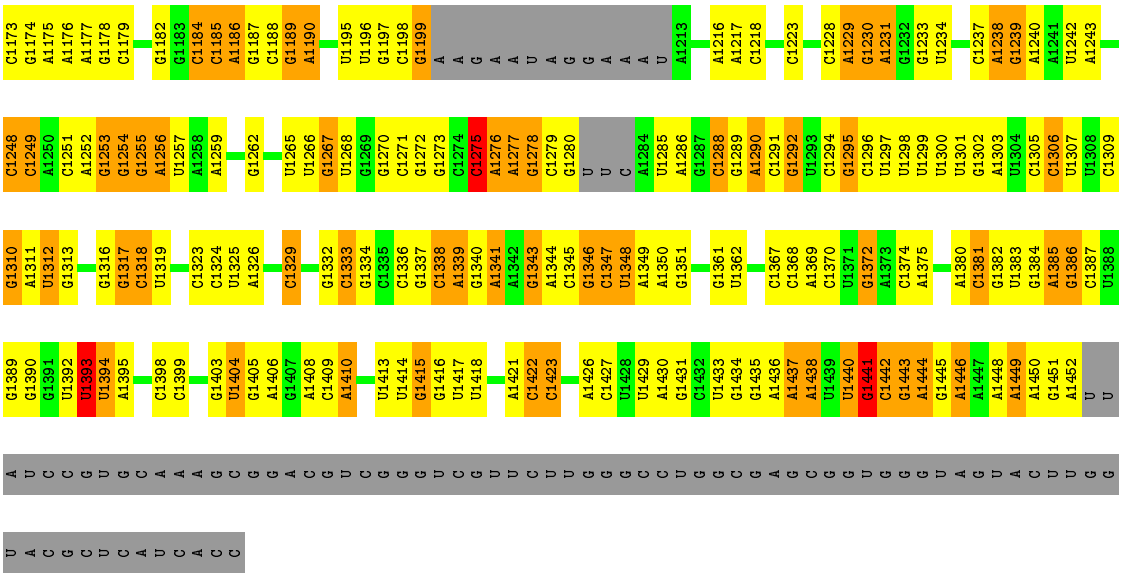


- Molecule 2: 26S delta ribosomal RNA

Chain 2:

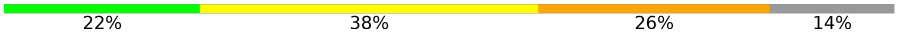


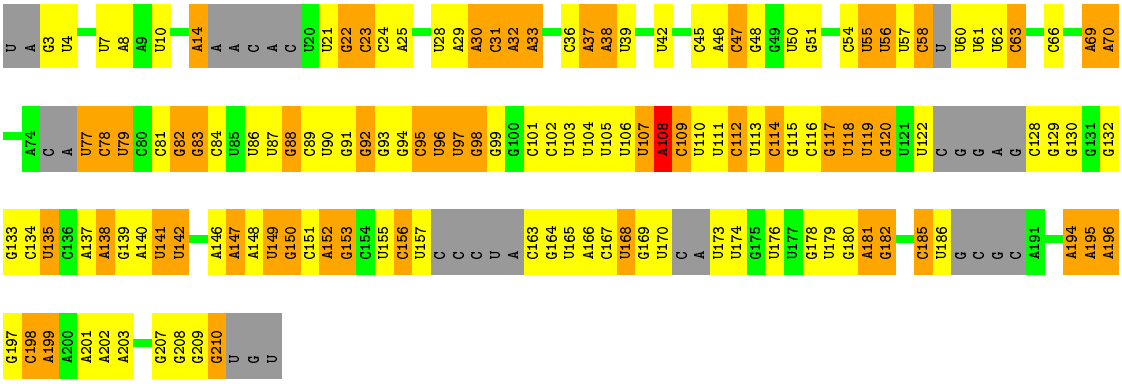




• Molecule 3: 26S gamma ribosomal RNA

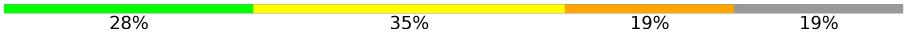
Chain 3:

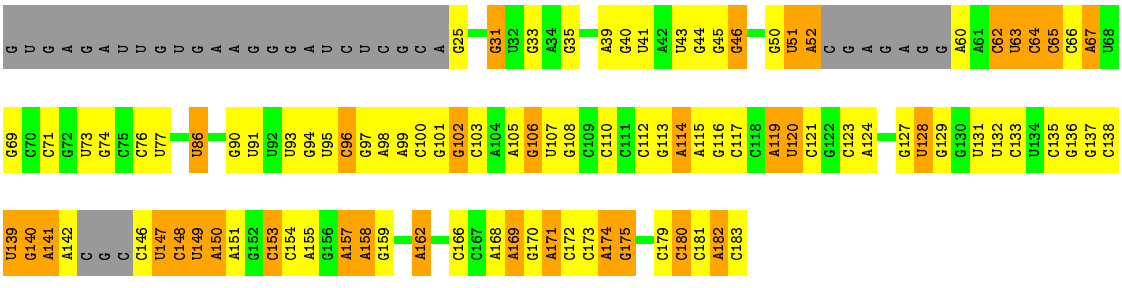


• Molecule 4: 26S delta ribosomal RNA

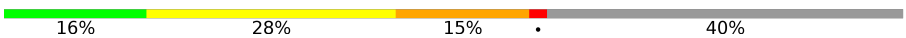
Chain 4:

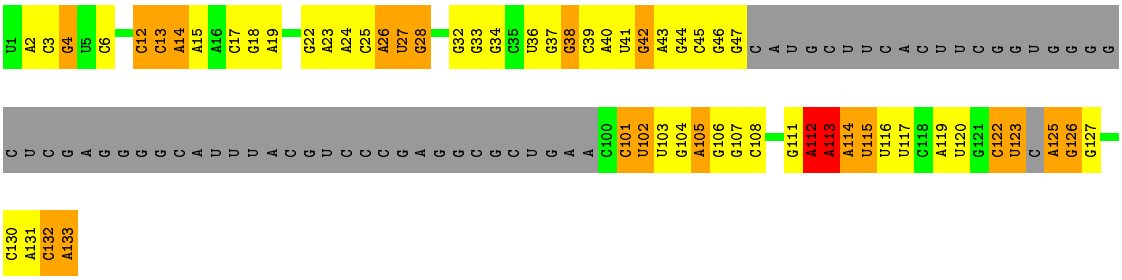


• Molecule 5: 26S epsilon ribosomal RNA

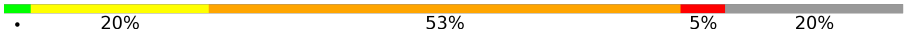
Chain 5:

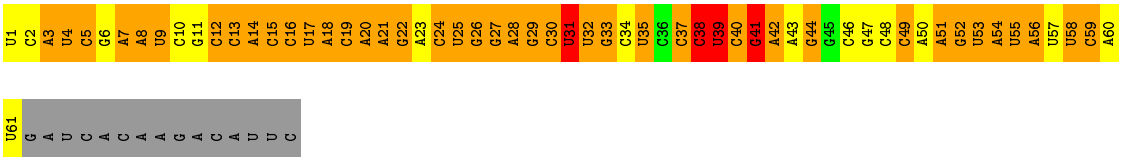




• Molecule 6: 26S zeta ribosomal RNA

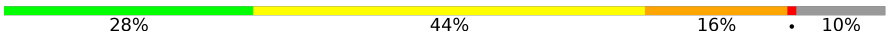
Chain 6:

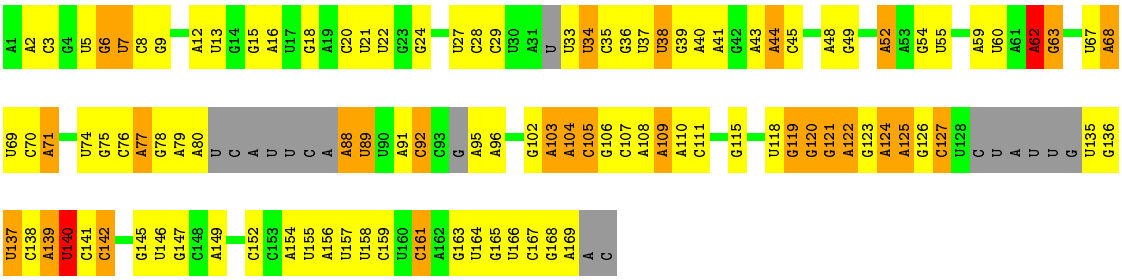


• Molecule 7: 5.8S ribosomal RNA

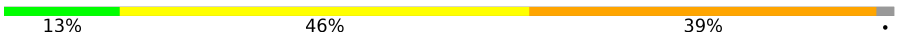
Chain 7:

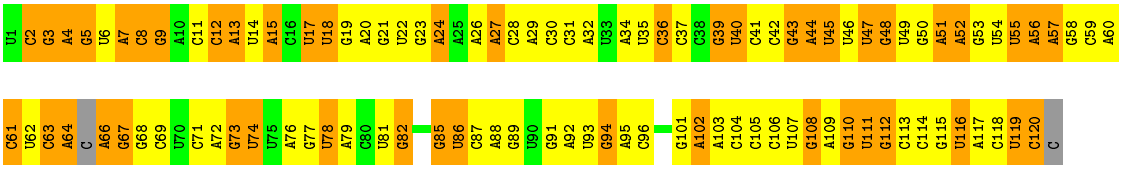


• Molecule 8: 5S ribosomal RNA

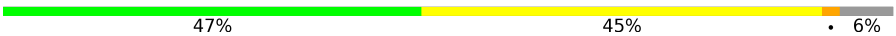
Chain 8:

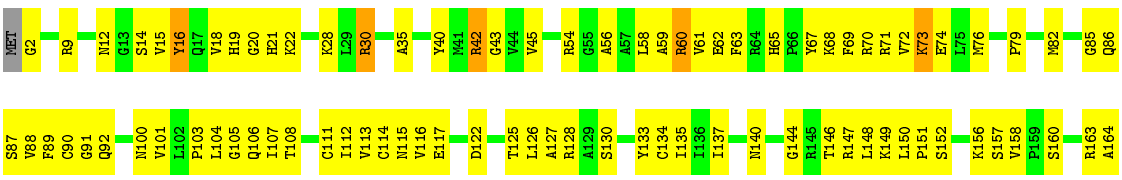


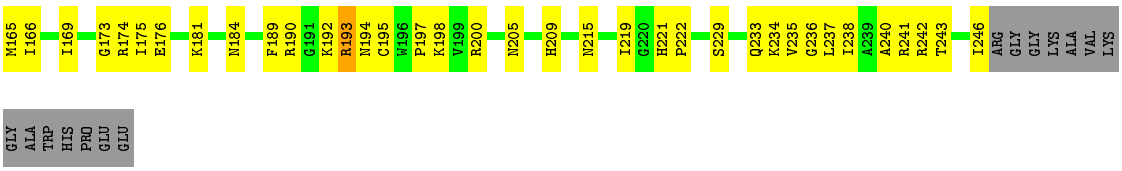



• Molecule 9: ribosomal protein L2

Chain A:



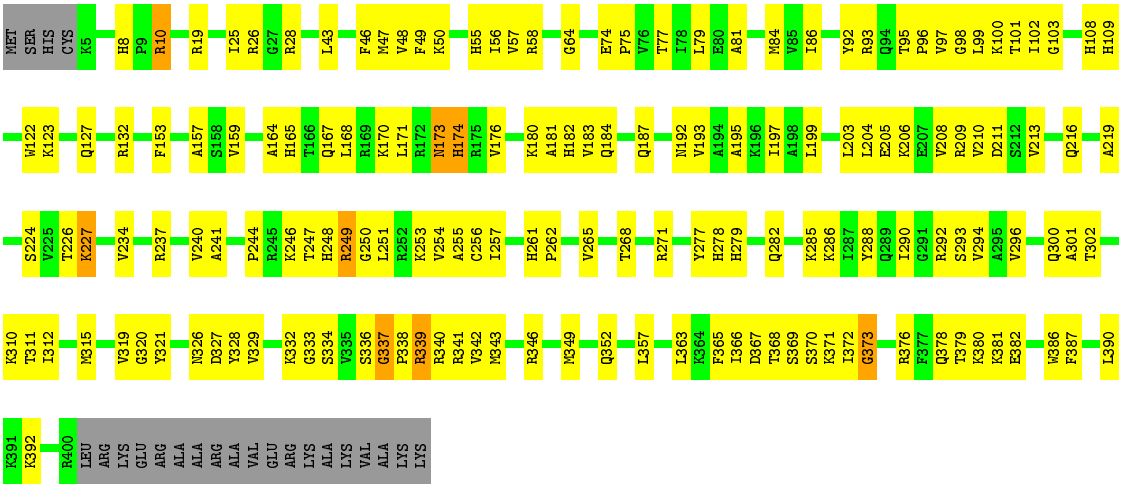







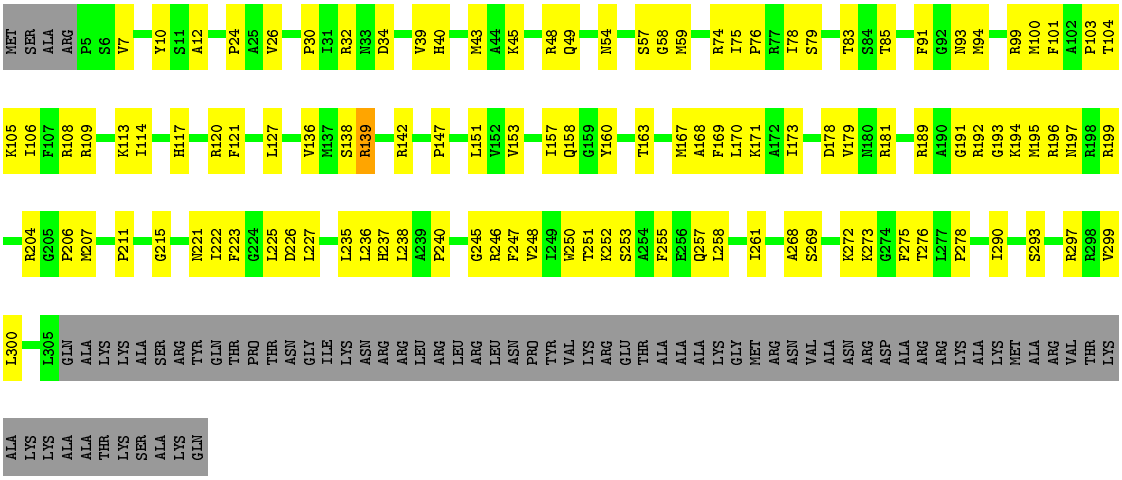
• Molecule 10: ribosomal protein L3

Chain B:

• Molecule 11: ribosomal protein L4

Chain C:

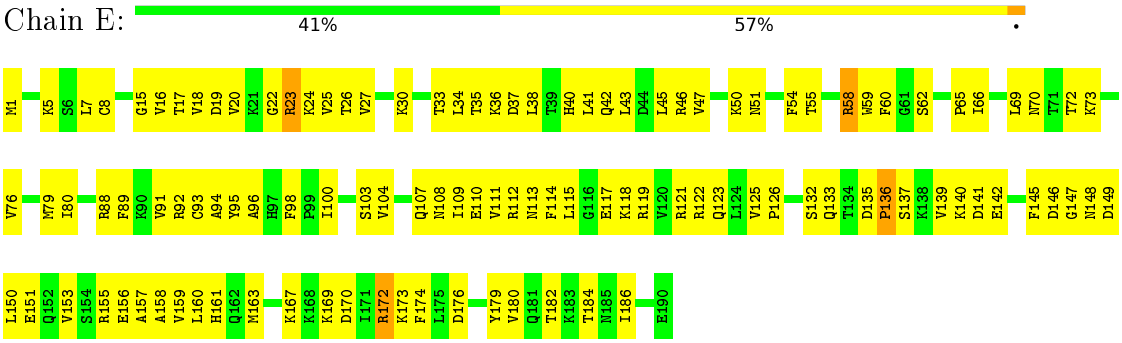



• Molecule 12: ribosomal protein L5

Chain D:

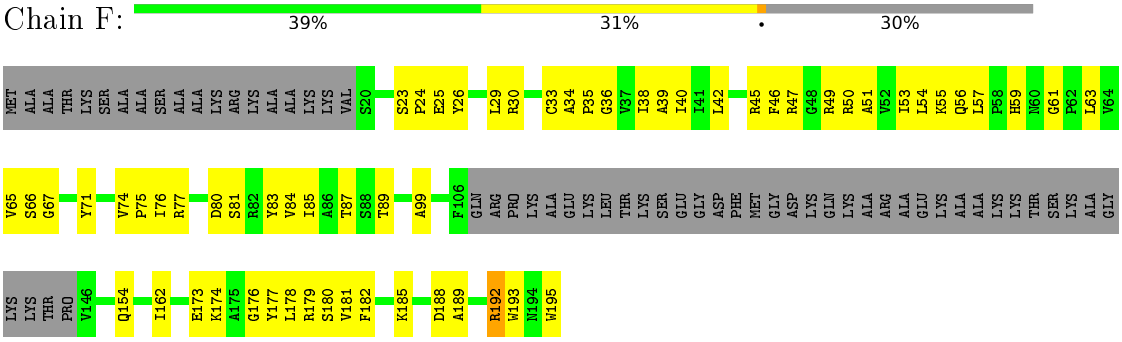

• Molecule 13: ribosomal protein L6

Chain E:



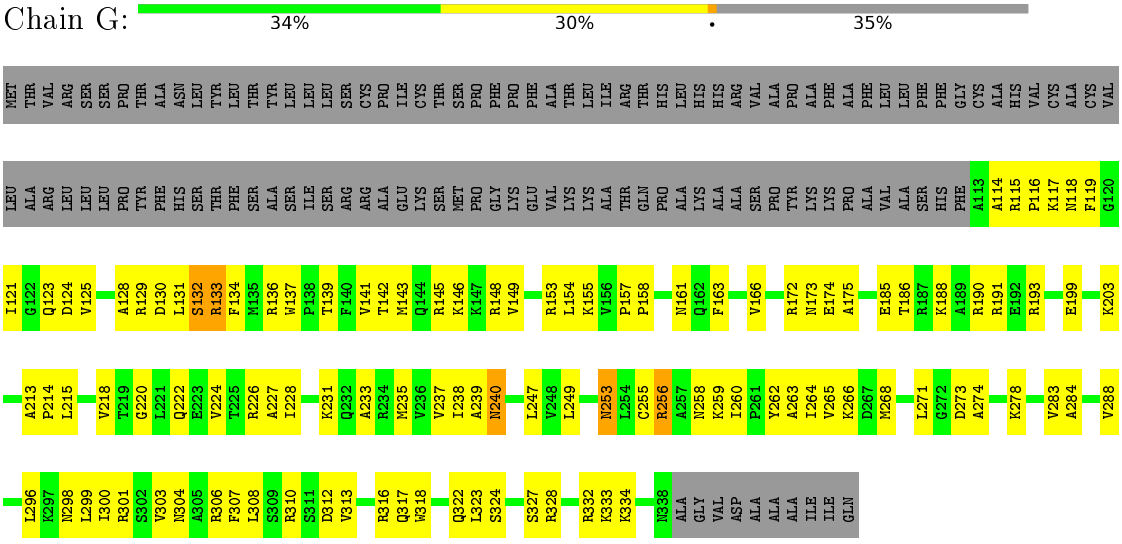

- Molecule 14: ribosomal protein L6e

Chain F:



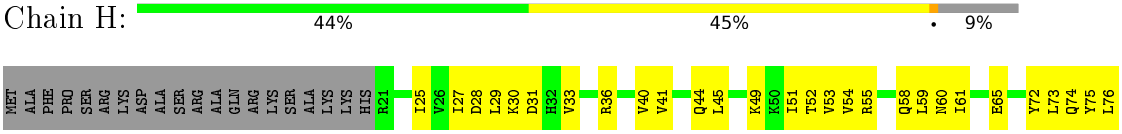

- Molecule 15: ribosomal protein L8e

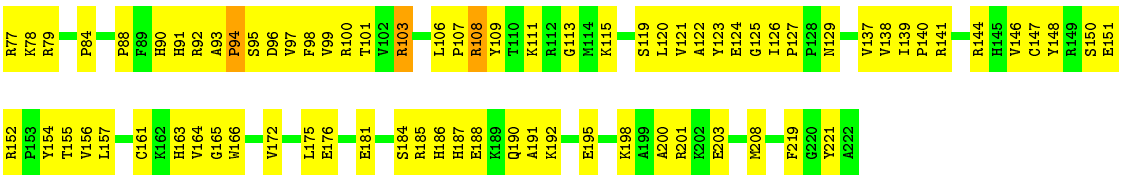
Chain G:




- Molecule 16: ribosomal protein L13

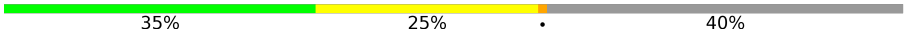
Chain H:

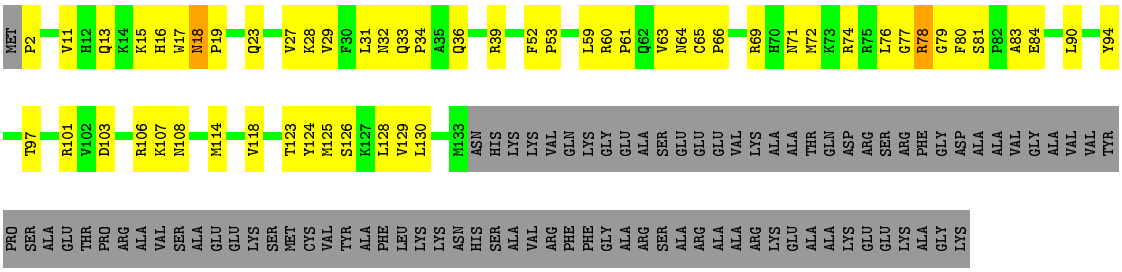





- Molecule 17: ribosomal protein L13e

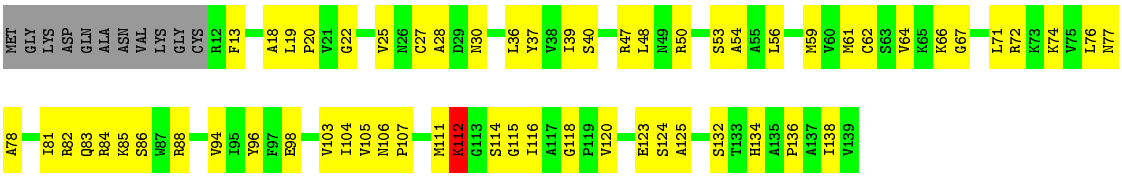
Chain I:



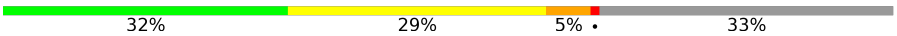

- Molecule 18: ribosomal protein L14

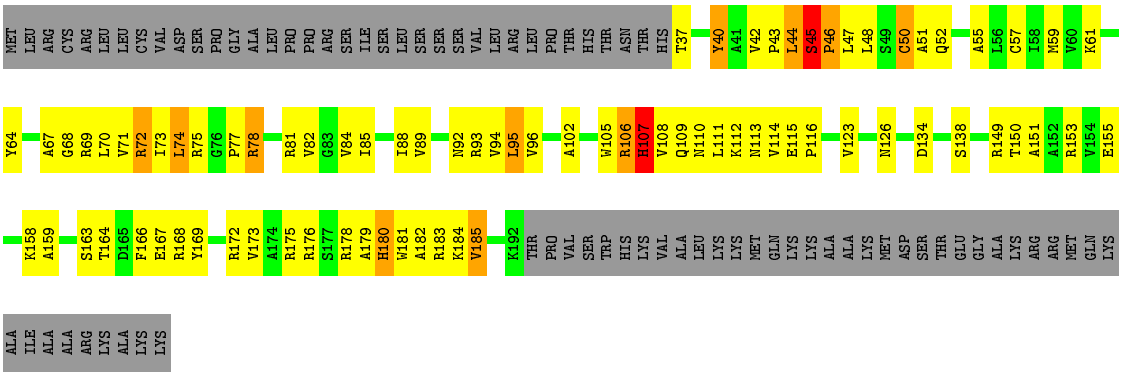
Chain J:


- Molecule 19: ribosomal protein L14e

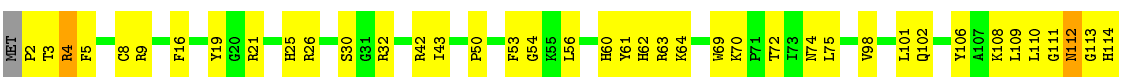
Chain K:

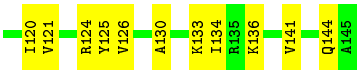



- Molecule 20: ribosomal protein L15

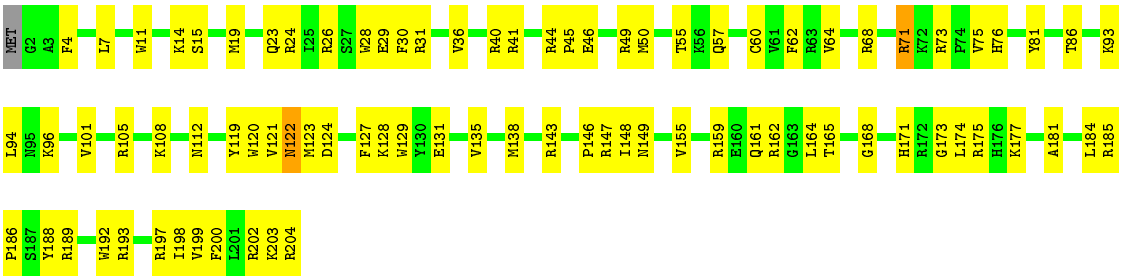
Chain L:



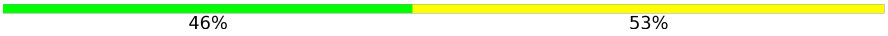

• Molecule 21: ribosomal protein L15e

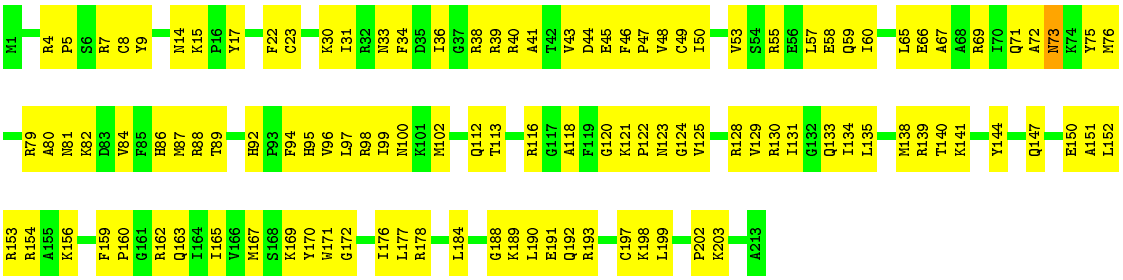
Chain M:


• Molecule 22: ribosomal protein L16

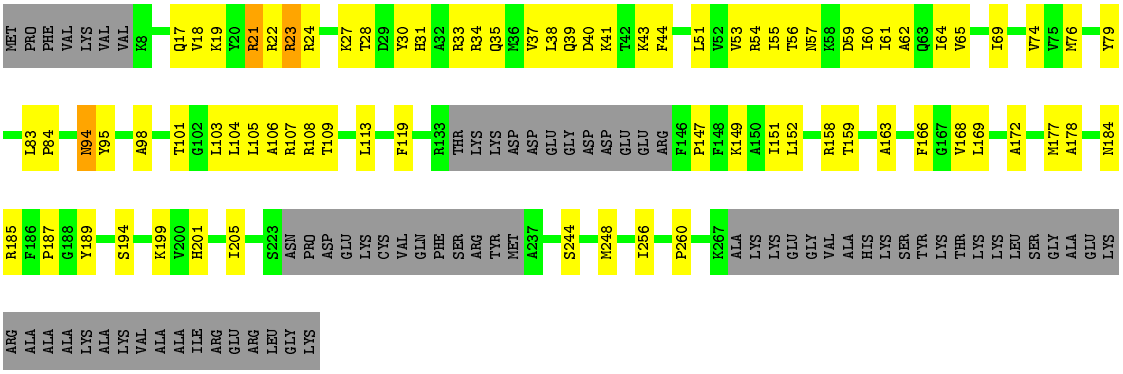
Chain N:



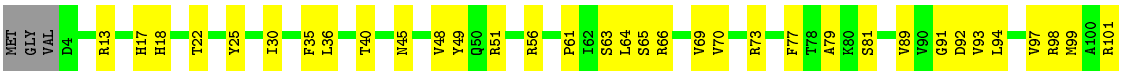

• Molecule 23: ribosomal protein L18

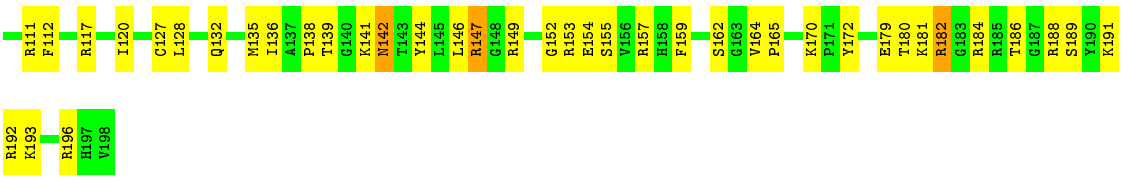
Chain O:


• Molecule 24: ribosomal protein L18e

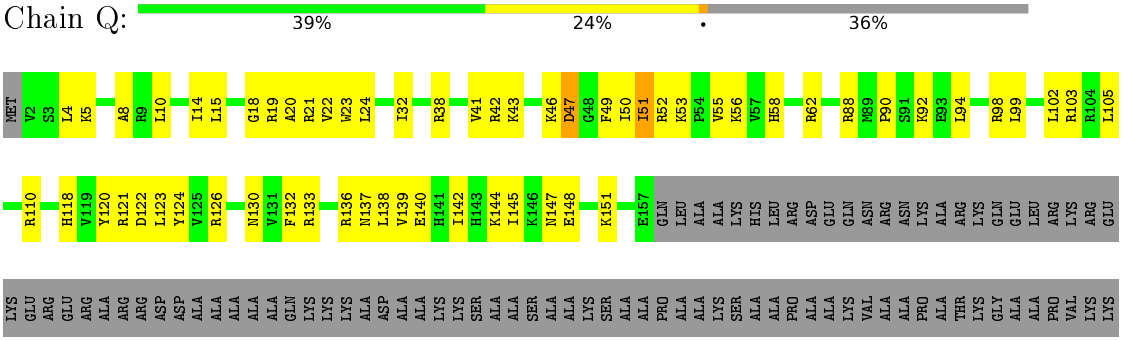
Chain P:



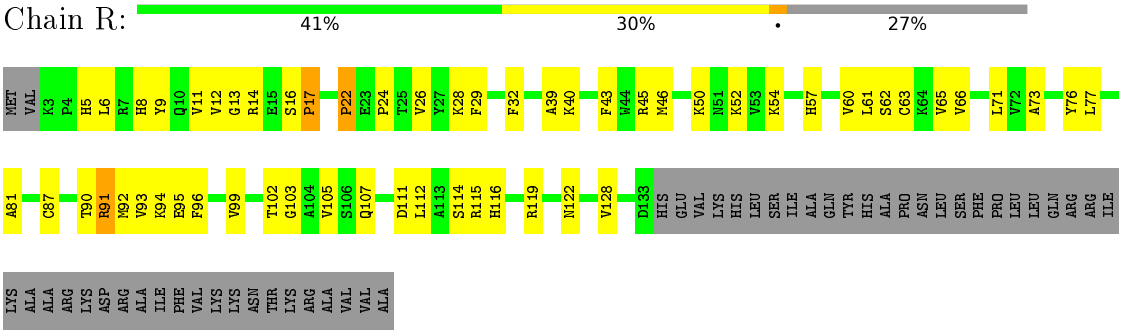

• Molecule 25: ribosomal protein L19e

Chain Q:



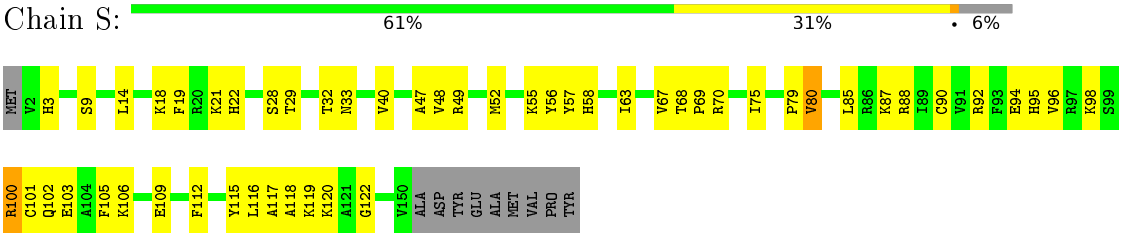

• Molecule 26: ribosomal protein L20e

Chain R:



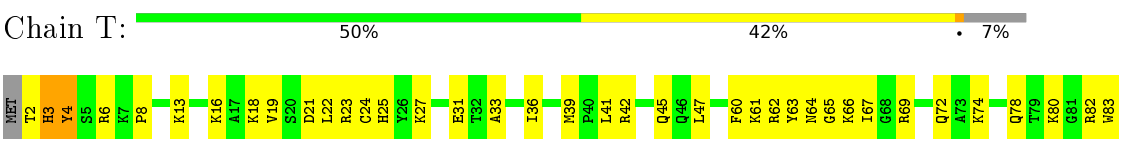

• Molecule 27: ribosomal protein L21e

Chain S:



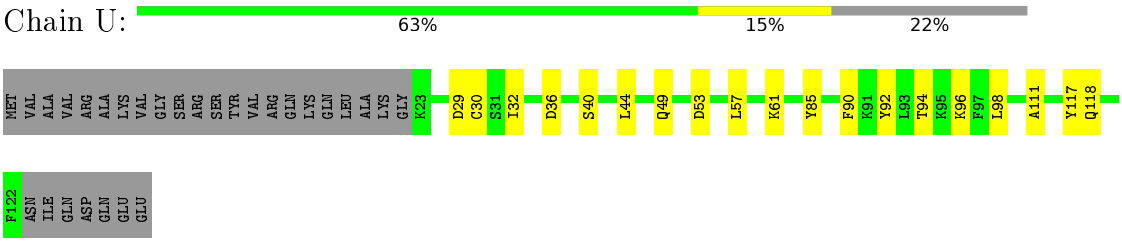

• Molecule 28: ribosomal protein L22

Chain T:



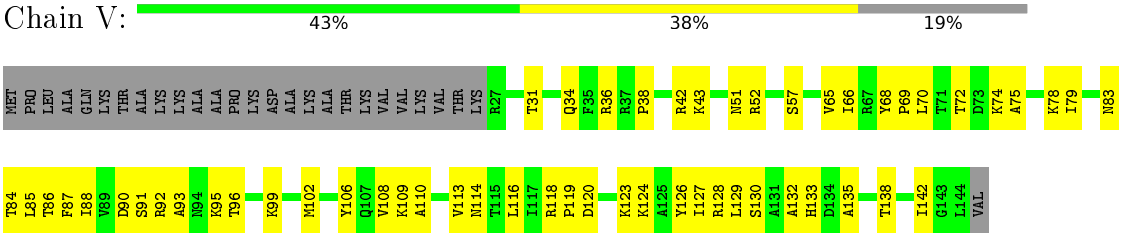

- Molecule 29: ribosomal protein L22e

Chain U:



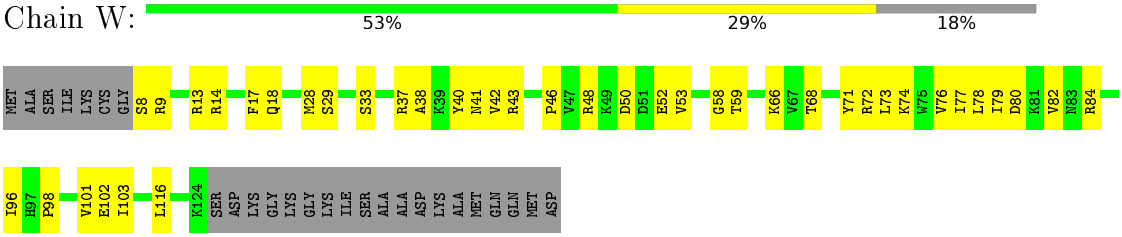

- Molecule 30: ribosomal protein L23

Chain V:



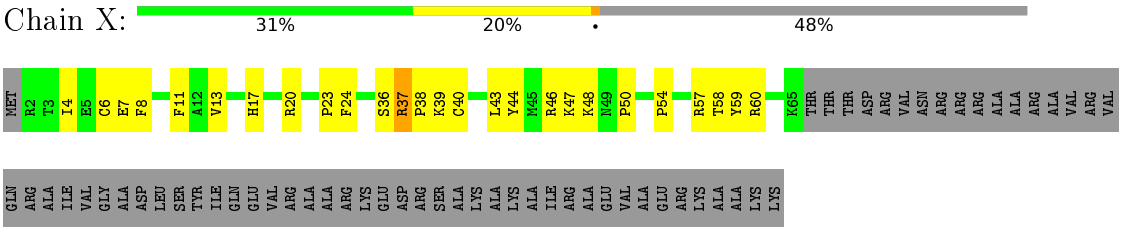

- Molecule 31: ribosomal protein L24

Chain W:



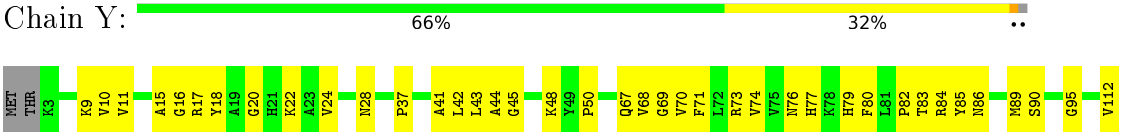

- Molecule 32: ribosomal protein L24e

Chain X:



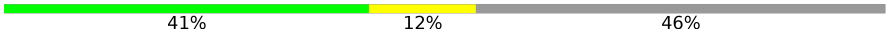

- Molecule 33: ribosomal protein L27e

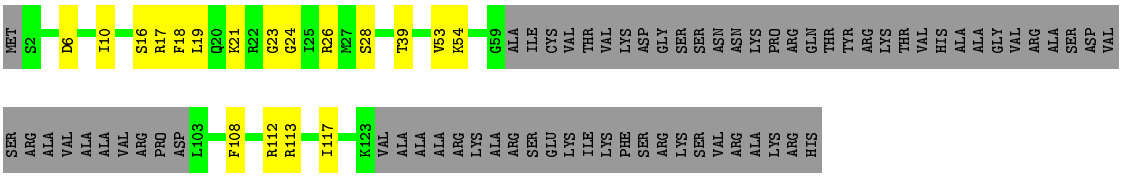
Chain Y:




• Molecule 34: ribosomal protein L28e

Chain Z:




• Molecule 35: ribosomal protein L29

Chain a:



• Molecule 36: ribosomal protein L29e

Chain b:



• Molecule 37: ribosomal protein L30

Chain c:



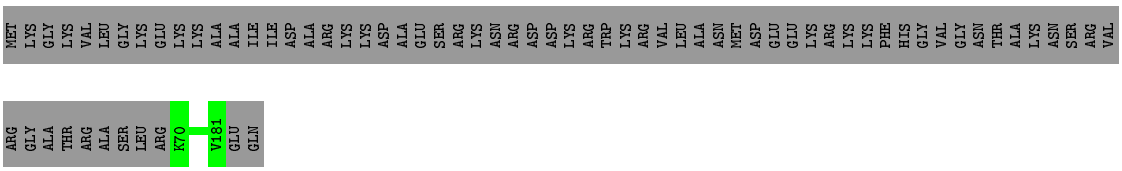
• Molecule 38: ribosomal protein L30e

Chain d:



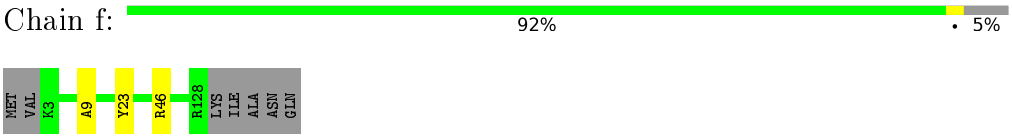
• Molecule 39: ribosomal protein L31e

Chain e:

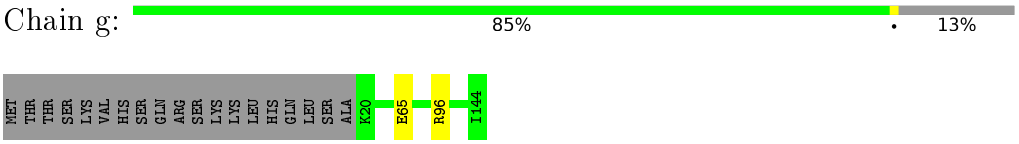

• Molecule 40: ribosomal protein L32e

Chain f:



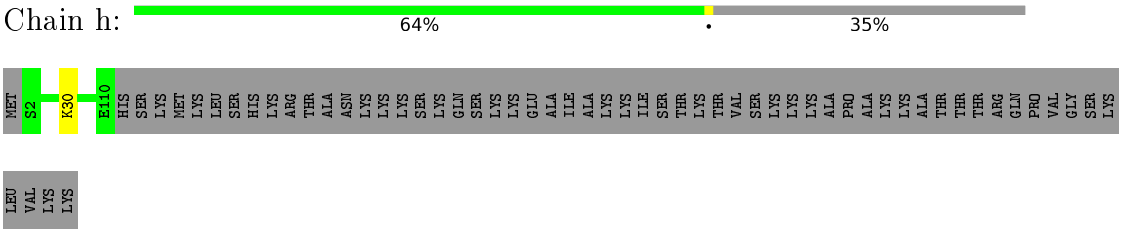

- Molecule 41: ribosomal protein L33e

Chain g:



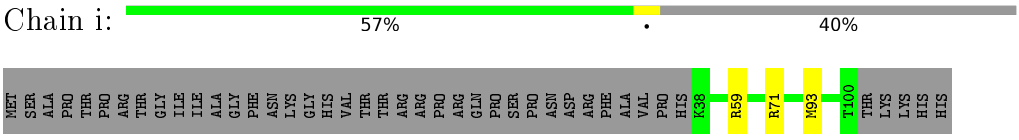

- Molecule 42: ribosomal protein L34e

Chain h:



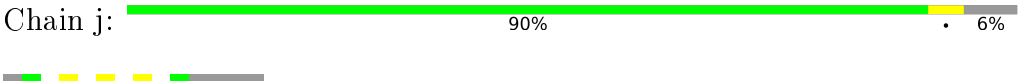

- Molecule 43: ribosomal protein L36e

Chain i:



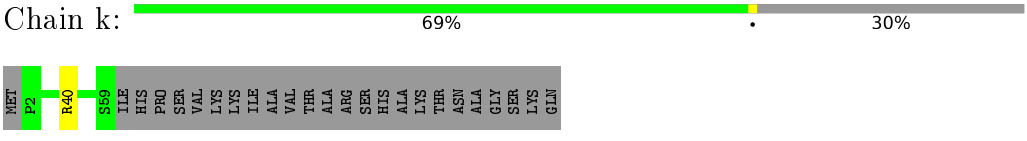

- Molecule 44: ribosomal protein L37e

Chain j:



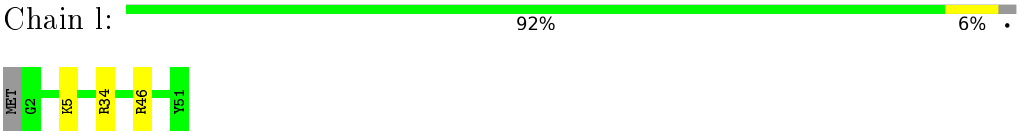

- Molecule 45: ribosomal protein L38e

Chain k:



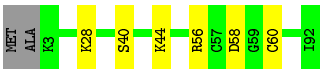

- Molecule 46: ribosomal protein L39e

Chain l:



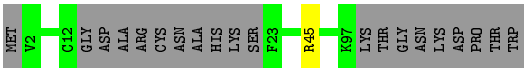

- Molecule 47: ribosomal protein L43e

Chain m:


- Molecule 48: ribosomal protein L44e

Chain n:

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 107134 | Depositor |
| Resolution determination method | FSC 0.143 | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 30 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | 29000 | Depositor |
| Image detector | K2 Summit direct electron detector | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, MG, OMG, H2U, OMU, A2M

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 | #$\|Z\|>2$ | RMSZ | #$\|Z\|>2$ |
| 1 | 1 | 0.75 | 8/36881 (0.0%) | 0.90 | 48/57466 (0.1%) |
| 10 | B | 0.44 | 0/3086 | 0.55 | 0/4176 |
| 11 | C | 0.45 | 0/2284 | 0.60 | 0/3092 |
| 12 | D | 0.25 | 0/800 | 0.49 | 0/1111 |
| 13 | E | 0.29 | 0/1529 | 0.56 | 0/2056 |
| 14 | F | 0.40 | 0/1023 | 0.56 | 0/1390 |
| 15 | G | 0.38 | 0/1798 | 0.59 | 1/2423 (0.0%) |
| 16 | H | 0.42 | 0/1628 | 0.60 | 0/2194 |
| 17 | I | 0.40 | 0/1084 | 0.57 | 0/1454 |
| 18 | J | 0.39 | 0/941 | 0.61 | 2/1277 (0.2%) |
| 19 | K | 0.27 | 0/1077 | 0.59 | 1/1475 (0.1%) |
| 2 | 2 | 0.60 | 0/26109 | 0.86 | 28/40668 (0.1%) |
| 20 | L | 0.43 | 0/1123 | 0.56 | 0/1505 |
| 21 | M | 0.49 | 0/1754 | 0.57 | 0/2342 |
| 22 | N | 0.27 | 0/1747 | 0.54 | 0/2338 |
| 23 | O | 0.32 | 0/1583 | 0.50 | 0/2157 |
| 24 | P | 0.42 | 0/1519 | 0.57 | 0/2040 |
| 25 | Q | 0.35 | 0/1179 | 0.53 | 0/1588 |
| 26 | R | 0.42 | 0/1044 | 0.59 | 1/1415 (0.1%) |
| 27 | S | 0.43 | 0/1142 | 0.60 | 0/1547 |
| 28 | T | 0.45 | 0/1249 | 0.65 | 1/1679 (0.1%) |
| 29 | U | 0.26 | 0/545 | 0.49 | 0/754 |
| 3 | 3 | 0.48 | 0/4337 | 0.84 | 1/6734 (0.0%) |
| 30 | V | 0.42 | 0/907 | 0.51 | 0/1227 |
| 31 | W | 0.37 | 0/910 | 0.56 | 0/1224 |
| 32 | X | 0.40 | 0/527 | 0.53 | 0/716 |
| 33 | Y | 0.37 | 0/934 | 0.51 | 0/1274 |
| 34 | Z | 0.28 | 0/545 | 0.52 | 0/739 |
| 35 | a | 0.32 | 0/992 | 0.53 | 0/1326 |
| 36 | b | 0.34 | 0/514 | 0.50 | 0/690 |
| 37 | c | 0.42 | 0/1763 | 0.52 | 0/2374 |
| 38 | d | 0.31 | 0/525 | 0.50 | 0/719 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >2 | RMSZ | #\|Z\| >2 |
| 39 | e | 0.37 | 0/838 | 0.57 | 0/1131 |
| 4 | 4 | 0.69 | 0/3549 | 0.88 | 3/5525 (0.1%) |
| 40 | f | 0.46 | 0/1002 | 0.55 | 0/1346 |
| 41 | g | 0.49 | 0/1003 | 0.53 | 0/1352 |
| 42 | h | 0.38 | 0/868 | 0.55 | 0/1160 |
| 43 | i | 0.38 | 0/499 | 0.56 | 0/662 |
| 44 | j | 0.50 | 0/651 | 0.61 | 0/869 |
| 45 | k | 0.30 | 0/378 | 0.57 | 0/518 |
| 46 | l | 0.43 | 0/470 | 0.51 | 0/627 |
| 47 | m | 0.43 | 0/680 | 0.53 | 0/913 |
| 48 | n | 0.34 | 0/667 | 0.56 | 0/889 |
| 5 | 5 | 0.69 | 0/1908 | 0.91 | 3/2967 (0.1%) |
| 6 | 6 | 0.39 | 2/1437 (0.1%) | 0.79 | 4/2234 (0.2%) |
| 7 | 7 | 0.76 | 0/3615 | 0.87 | 2/5622 (0.0%) |
| 8 | 8 | 0.47 | 0/2828 | 0.82 | 0/4401 |
| 9 | A | 0.47 | 0/1903 | 0.56 | 0/2559 |
| All | All | 0.59 | 10/125375 (0.0%) | 0.79 | 95/185945 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 10 | B | 0 | 2 |
| 13 | E | 0 | 1 |
| 15 | G | 0 | 1 |
| 16 | H | 0 | 1 |
| 19 | K | 0 | 3 |
| 26 | R | 0 | 1 |
| 27 | S | 0 | 1 |
| 28 | T | 0 | 1 |
| 40 | f | 0 | 1 |
| 9 | A | 0 | 1 |
| All | All | 0 | 13 |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 634 | G | C1'-N9 | -6.69 | 1.37 | 1.46 |
| 1 | 1 | 159 | U | C1'-N1 | 6.17 | 1.58 | 1.48 |
| 1 | 1 | 568 | U | C1'-N1 | 6.06 | 1.57 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 564 | U | C1'-N1 | 5.95 | 1.57 | 1.48 |
| 1 | 1 | 565 | U | C1'-N1 | 5.91 | 1.57 | 1.48 |

The worst 5 of 95 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | K | 45 | SER | C-N-CD | -11.87 | 94.48 | 120.60 |
| 1 | 1 | 1575 | A | OP1-P-O3' | -11.81 | 79.22 | 105.20 |
| 1 | 1 | 1757 | U | C2-N1-C1' | 8.96 | 128.45 | 117.70 |
| 2 | 2 | 776 | C | N1-C2-O2 | 8.91 | 124.25 | 118.90 |
| 2 | 2 | 776 | C | C2-N1-C1' | 8.72 | 128.39 | 118.80 |

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 9 | A | 60[B] | ARG | Mainchain |
| 10 | B | 337 | GLY | Peptide |
| 10 | B | 373 | GLY | Peptide |
| 13 | E | 136 | PRO | Peptide |
| 15 | G | 114 | 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 | 1 | 33313 | 0 | 16798 | 1118 | 0 |
| 2 | 2 | 23926 | 0 | 12113 | 740 | 0 |
| 3 | 3 | 3893 | 0 | 1971 | 147 | 0 |
| 4 | 4 | 3177 | 0 | 1611 | 112 | 0 |
| 5 | 5 | 1708 | 0 | 867 | 59 | 0 |
| 6 | 6 | 1288 | 0 | 657 | 184 | 0 |
| 7 | 7 | 3280 | 0 | 1664 | 103 | 0 |
| 8 | 8 | 2531 | 0 | 1281 | 155 | 0 |
| 9 | A | 1859 | 0 | 1901 | 128 | 0 |
| 10 | B | 3020 | 0 | 3003 | 172 | 0 |
| 11 | C | 2237 | 0 | 2231 | 118 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 12 | D | 799 | 0 | 374 | 5 | 0 |
| 13 | E | 1509 | 0 | 1595 | 122 | 0 |
| 14 | F | 1002 | 0 | 994 | 55 | 0 |
| 15 | G | 1772 | 0 | 1853 | 108 | 0 |
| 16 | H | 1596 | 0 | 1683 | 143 | 0 |
| 17 | I | 1061 | 0 | 1123 | 64 | 0 |
| 18 | J | 924 | 0 | 934 | 60 | 0 |
| 19 | K | 1061 | 0 | 939 | 196 | 0 |
| 20 | L | 1096 | 0 | 1096 | 52 | 0 |
| 21 | M | 1714 | 0 | 1793 | 95 | 0 |
| 22 | N | 1714 | 0 | 1786 | 111 | 0 |
| 23 | O | 1557 | 0 | 1351 | 84 | 0 |
| 24 | P | 1494 | 0 | 1554 | 83 | 0 |
| 25 | Q | 1162 | 0 | 1130 | 74 | 0 |
| 26 | R | 1019 | 0 | 981 | 52 | 0 |
| 27 | S | 1112 | 0 | 1051 | 57 | 0 |
| 28 | T | 1221 | 0 | 1230 | 98 | 0 |
| 29 | U | 541 | 0 | 295 | 10 | 0 |
| 30 | V | 892 | 0 | 903 | 48 | 0 |
| 31 | W | 896 | 0 | 915 | 36 | 0 |
| 32 | X | 508 | 0 | 477 | 25 | 0 |
| 33 | Y | 914 | 0 | 813 | 40 | 0 |
| 34 | Z | 538 | 0 | 479 | 18 | 0 |
| 35 | a | 982 | 0 | 1029 | 0 | 0 |
| 36 | b | 503 | 0 | 500 | 0 | 0 |
| 37 | c | 1732 | 0 | 1768 | 0 | 0 |
| 38 | d | 518 | 0 | 462 | 0 | 0 |
| 39 | e | 824 | 0 | 839 | 0 | 0 |
| 40 | f | 982 | 0 | 985 | 0 | 0 |
| 41 | g | 983 | 0 | 1006 | 0 | 0 |
| 42 | h | 856 | 0 | 873 | 0 | 0 |
| 43 | i | 494 | 0 | 535 | 0 | 0 |
| 44 | j | 639 | 0 | 641 | 0 | 0 |
| 45 | k | 373 | 0 | 302 | 0 | 0 |
| 46 | l | 457 | 0 | 484 | 0 | 0 |
| 47 | m | 668 | 0 | 648 | 0 | 0 |
| 48 | n | 659 | 0 | 672 | 0 | 0 |
| 49 | 1 | 51 | 0 | 0 | 0 | 0 |
| 49 | 2 | 25 | 0 | 0 | 0 | 0 |
| 49 | 3 | 3 | 0 | 0 | 0 | 0 |
| 49 | 4 | 2 | 0 | 0 | 0 | 0 |
| 49 | 5 | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 49 | 7 | 9 | 0 | 0 | 0 | 0 |
| 49 | C | 1 | 0 | 0 | 0 | 0 |
| 49 | K | 1 | 0 | 0 | 0 | 0 |
| 49 | M | 3 | 0 | 0 | 0 | 0 |
| 49 | V | 1 | 0 | 0 | 0 | 0 |
| 49 | a | 1 | 0 | 0 | 0 | 0 |
| 49 | f | 2 | 0 | 0 | 0 | 0 |
| 49 | g | 1 | 0 | 0 | 0 | 0 |
| 49 | h | 1 | 0 | 0 | 0 | 0 |
| 49 | j | 4 | 0 | 0 | 0 | 0 |
| 50 | 1 | 72 | 0 | 0 | 18 | 0 |
| 50 | 2 | 40 | 0 | 0 | 17 | 0 |
| 50 | 4 | 4 | 0 | 0 | 1 | 0 |
| 50 | 5 | 4 | 0 | 0 | 0 | 0 |
| 50 | 7 | 16 | 0 | 0 | 2 | 0 |
| 50 | 8 | 1 | 0 | 0 | 1 | 0 |
| 50 | A | 2 | 0 | 0 | 1 | 0 |
| 50 | G | 1 | 0 | 0 | 0 | 0 |
| 50 | M | 2 | 0 | 0 | 0 | 0 |
| 50 | i | 1 | 0 | 0 | 0 | 0 |
| 50 | j | 1 | 0 | 0 | 0 | 0 |
| All | All | 117257 | 0 | 80190 | 3902 | 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 25.

The worst 5 of 3902 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) |
|---|---|---|---|
| 3:3:57:U:H2' | 3:3:58:C:C5 | 1.26 | 1.62 |
| 19:K:89:VAL:CG1 | 26:R:73:ALA:HB2 | 1.26 | 1.56 |
| 19:K:89:VAL:HG12 | 26:R:73:ALA:CB | 1.38 | 1.50 |
| 24:P:17:HIS:CE1 | 24:P:18:HIS:HD1 | 1.29 | 1.50 |
| 25:Q:23:TRP:CE3 | 25:Q:51:ILE:CD1 | 2.02 | 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 | |
|---|---|---|---|---|---|---|---|
| 9 | A | 245/260 (94%) | 220 (90%) | 25 (10%) | 0 | 100 | 100 |
| 10 | B | 396/419 (94%) | 352 (89%) | 43 (11%) | 1 (0%) | 46 | 79 |
| 11 | C | 300/373 (80%) | 269 (90%) | 31 (10%) | 0 | 100 | 100 |
| 12 | D | 159/188 (85%) | 136 (86%) | 23 (14%) | 0 | 100 | 100 |
| 13 | E | 188/190 (99%) | 160 (85%) | 28 (15%) | 0 | 100 | 100 |
| 14 | F | 134/195 (69%) | 112 (84%) | 22 (16%) | 0 | 100 | 100 |
| 15 | G | 225/348 (65%) | 205 (91%) | 18 (8%) | 2 (1%) | 21 | 55 |
| 16 | H | 200/222 (90%) | 175 (88%) | 24 (12%) | 1 (0%) | 34 | 69 |
| 17 | I | 130/220 (59%) | 120 (92%) | 10 (8%) | 0 | 100 | 100 |
| 18 | J | 126/139 (91%) | 115 (91%) | 11 (9%) | 0 | 100 | 100 |
| 19 | K | 154/233 (66%) | 136 (88%) | 17 (11%) | 1 (1%) | 30 | 65 |
| 20 | L | 142/145 (98%) | 127 (89%) | 15 (11%) | 0 | 100 | 100 |
| 21 | M | 201/204 (98%) | 187 (93%) | 14 (7%) | 0 | 100 | 100 |
| 22 | N | 211/213 (99%) | 186 (88%) | 25 (12%) | 0 | 100 | 100 |
| 23 | O | 229/305 (75%) | 205 (90%) | 24 (10%) | 0 | 100 | 100 |
| 24 | P | 194/198 (98%) | 179 (92%) | 15 (8%) | 0 | 100 | 100 |
| 25 | Q | 154/245 (63%) | 141 (92%) | 13 (8%) | 0 | 100 | 100 |
| 26 | R | 130/179 (73%) | 104 (80%) | 25 (19%) | 1 (1%) | 24 | 58 |
| 27 | S | 149/159 (94%) | 125 (84%) | 22 (15%) | 2 (1%) | 15 | 44 |
| 28 | T | 154/166 (93%) | 127 (82%) | 27 (18%) | 0 | 100 | 100 |
| 29 | U | 98/129 (76%) | 81 (83%) | 17 (17%) | 0 | 100 | 100 |
| 30 | V | 116/145 (80%) | 99 (85%) | 17 (15%) | 0 | 100 | 100 |
| 31 | W | 116/143 (81%) | 106 (91%) | 10 (9%) | 0 | 100 | 100 |
| 32 | X | 62/124 (50%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 33 | Y | 130/134 (97%) | 111 (85%) | 19 (15%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 34 | Z | 75/147 (51%) | 65 (87%) | 10 (13%) | 0 | 100 100 |
| 35 | a | 122/127 (96%) | 105 (86%) | 17 (14%) | 0 | 100 100 |
| 36 | b | 63/70 (90%) | 53 (84%) | 10 (16%) | 0 | 100 100 |
| 37 | c | 220/252 (87%) | 190 (86%) | 30 (14%) | 0 | 100 100 |
| 38 | d | 71/104 (68%) | 63 (89%) | 8 (11%) | 0 | 100 100 |
| 39 | e | 111/183 (61%) | 92 (83%) | 19 (17%) | 0 | 100 100 |
| 40 | f | 124/133 (93%) | 110 (89%) | 14 (11%) | 0 | 100 100 |
| 41 | g | 123/144 (85%) | 112 (91%) | 11 (9%) | 0 | 100 100 |
| 42 | h | 106/168 (63%) | 91 (86%) | 15 (14%) | 0 | 100 100 |
| 43 | i | 62/105 (59%) | 57 (92%) | 5 (8%) | 0 | 100 100 |
| 44 | j | 76/83 (92%) | 68 (90%) | 8 (10%) | 0 | 100 100 |
| 45 | k | 56/83 (68%) | 52 (93%) | 4 (7%) | 0 | 100 100 |
| 46 | l | 49/51 (96%) | 46 (94%) | 2 (4%) | 1 (2%) | 9 30 |
| 47 | m | 88/92 (96%) | 71 (81%) | 16 (18%) | 1 (1%) | 17 50 |
| 48 | n | 82/106 (77%) | 66 (80%) | 16 (20%) | 0 | 100 100 |
| All | All | 5771/7124 (81%) | 5078 (88%) | 683 (12%) | 10 (0%) | 56 84 |

5 of 10 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | G | 132 | SER |
| 26 | R | 22 | PRO |
| 27 | S | 101 | CYS |
| 47 | m | 40 | SER |
| 10 | B | 380 | LYS |

### 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 |
|---|---|---|---|---|---|
| 9 | A | 188/204 (92%) | 181 (96%) | 7 (4%) | 41 76 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 10 | B | 296/352 (84%) | 288 (97%) | 8 (3%) | 52 85 |
| 11 | C | 222/302 (74%) | 221 (100%) | 1 (0%) | 92 98 |
| 12 | D | 4/163 (2%) | 4 (100%) | 0 | 100 100 |
| 13 | E | 172/172 (100%) | 169 (98%) | 3 (2%) | 68 92 |
| 14 | F | 92/154 (60%) | 91 (99%) | 1 (1%) | 80 95 |
| 15 | G | 179/292 (61%) | 173 (97%) | 6 (3%) | 44 78 |
| 16 | H | 166/188 (88%) | 164 (99%) | 2 (1%) | 78 95 |
| 17 | I | 114/181 (63%) | 110 (96%) | 4 (4%) | 43 77 |
| 18 | J | 91/111 (82%) | 88 (97%) | 3 (3%) | 45 79 |
| 19 | K | 79/195 (40%) | 68 (86%) | 11 (14%) | 4 13 |
| 20 | L | 105/115 (91%) | 103 (98%) | 2 (2%) | 65 91 |
| 21 | M | 179/180 (99%) | 176 (98%) | 3 (2%) | 68 92 |
| 22 | N | 178/179 (99%) | 175 (98%) | 3 (2%) | 68 92 |
| 23 | O | 103/242 (43%) | 100 (97%) | 3 (3%) | 50 83 |
| 24 | P | 149/164 (91%) | 145 (97%) | 4 (3%) | 52 85 |
| 25 | Q | 100/196 (51%) | 98 (98%) | 2 (2%) | 63 90 |
| 26 | R | 98/158 (62%) | 96 (98%) | 2 (2%) | 63 90 |
| 27 | S | 100/133 (75%) | 100 (100%) | 0 | 100 100 |
| 28 | T | 125/144 (87%) | 125 (100%) | 0 | 100 100 |
| 29 | U | 13/114 (11%) | 13 (100%) | 0 | 100 100 |
| 30 | V | 86/124 (69%) | 84 (98%) | 2 (2%) | 58 88 |
| 31 | W | 87/122 (71%) | 87 (100%) | 0 | 100 100 |
| 32 | X | 48/104 (46%) | 46 (96%) | 2 (4%) | 36 71 |
| 33 | Y | 70/115 (61%) | 69 (99%) | 1 (1%) | 74 94 |
| 34 | Z | 44/119 (37%) | 44 (100%) | 0 | 100 100 |
| 35 | a | 99/117 (85%) | 92 (93%) | 7 (7%) | 18 46 |
| 36 | b | 48/58 (83%) | 44 (92%) | 4 (8%) | 14 38 |
| 37 | c | 168/209 (80%) | 164 (98%) | 4 (2%) | 57 87 |
| 38 | d | 47/90 (52%) | 44 (94%) | 3 (6%) | 22 52 |
| 39 | e | 79/156 (51%) | 79 (100%) | 0 | 100 100 |
| 40 | f | 97/114 (85%) | 95 (98%) | 2 (2%) | 61 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 41 | g | 98/121 (81%) | 96 (98%) | 2 (2%) | 63 90 |
| 42 | h | 85/145 (59%) | 84 (99%) | 1 (1%) | 78 95 |
| 43 | i | 47/89 (53%) | 44 (94%) | 3 (6%) | 22 52 |
| 44 | j | 63/70 (90%) | 60 (95%) | 3 (5%) | 31 66 |
| 45 | k | 26/74 (35%) | 25 (96%) | 1 (4%) | 40 74 |
| 46 | l | 46/47 (98%) | 44 (96%) | 2 (4%) | 35 70 |
| 47 | m | 63/74 (85%) | 58 (92%) | 5 (8%) | 15 40 |
| 48 | n | 64/92 (70%) | 63 (98%) | 1 (2%) | 70 93 |
| All | All | 4118/5979 (69%) | 4010 (97%) | 108 (3%) | 57 86 |

5 of 108 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | M | 60 | CYS |
| 24 | P | 182 | ARG |
| 45 | k | 40 | ARG |
| 21 | M | 122 | ASN |
| 23 | O | 21 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | N | 71 | GLN |
| 25 | Q | 130 | ASN |
| 42 | h | 62 | HIS |
| 22 | N | 163 | GLN |
| 23 | O | 94 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1 | 1535/1782 (86%) | 588 (38%) | 57 (3%) |
| 2 | 2 | 1106/1527 (72%) | 445 (40%) | 28 (2%) |
| 3 | 3 | 177/213 (83%) | 83 (46%) | 10 (5%) |
| 4 | 4 | 146/183 (79%) | 48 (32%) | 5 (3%) |
| 5 | 5 | 78/133 (58%) | 30 (38%) | 4 (5%) |
| 6 | 6 | 60/76 (78%) | 48 (80%) | 15 (25%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 7 | 7 | 150/171 (87%) | 50 (33%) | 2 (1%) |
| 8 | 8 | 118/121 (97%) | 54 (45%) | 5 (4%) |
| All | All | 3370/4206 (80%) | 1346 (39%) | 126 (3%) |

5 of 1346 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 4 | G |
| 1 | 1 | 10 | A |
| 1 | 1 | 13 | G |
| 1 | 1 | 23 | U |
| 1 | 1 | 24 | A |

5 of 126 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1763 | A |
| 2 | 2 | 782 | G |
| 6 | 6 | 41 | G |
| 2 | 2 | 68 | A |
| 2 | 2 | 512 | U |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 1 | OMG | 1 | 1526 | 1 | 18,26,27 | 1.11 | 2 (11%) | 21,38,41 | 2.07 | 5 (23%) |
| 1 | OMC | 1 | 1529 | 1 | 15,22,23 | 0.86 | 0 | 20,31,34 | 1.65 | 2 (10%) |
| 1 | A2M | 1 | 1541 | 1,2 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.77 | 1 (5%) |
| 1 | OMG | 1 | 1542 | 1,2 | 18,26,27 | 1.12 | 2 (11%) | 21,38,41 | 2.06 | 4 (19%) |
| 1 | OMG | 1 | 1628 | 1 | 18,26,27 | 1.14 | 2 (11%) | 21,38,41 | 2.22 | 6 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | OMU | 1 | 36 | 1 | 14,22,23 | 0.92 | 1 (7%) | 19,31,34 | 1.58 | 2 (10%) |
| 1 | OMU | 1 | 48 | 1 | 14,22,23 | 1.02 | 1 (7%) | 19,31,34 | 1.68 | 1 (5%) |
| 1 | A2M | 1 | 678 | 1,2 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.82 | 1 (5%) |
| 1 | A2M | 1 | 681 | 1 | 18,25,26 | 0.96 | 1 (5%) | 18,36,39 | 1.82 | 1 (5%) |
| 1 | OMC | 1 | 695 | 1 | 15,22,23 | 0.95 | 1 (6%) | 20,31,34 | 1.61 | 4 (20%) |
| 1 | OMU | 1 | 845 | 1 | 14,22,23 | 1.03 | 2 (14%) | 19,31,34 | 1.64 | 2 (10%) |
| 1 | OMU | 1 | 847 | 1 | 14,22,23 | 0.93 | 1 (7%) | 19,31,34 | 1.56 | 1 (5%) |
| 1 | OMG | 1 | 856 | 1 | 18,26,27 | 1.06 | 2 (11%) | 21,38,41 | 2.23 | 6 (28%) |
| 1 | A2M | 1 | 927 | 1 | 18,25,26 | 1.04 | 1 (5%) | 18,36,39 | 1.94 | 1 (5%) |
| 1 | A2M | 1 | 955 | 1 | 18,25,26 | 0.97 | 1 (5%) | 18,36,39 | 1.92 | 2 (11%) |
| 1 | OMG | 1 | 959 | 1 | 18,26,27 | 1.22 | 2 (11%) | 21,38,41 | 2.02 | 5 (23%) |
| 2 | OMU | 2 | 1078 | 2 | 14,22,23 | 0.87 | 1 (7%) | 19,31,34 | 1.63 | 1 (5%) |
| 2 | OMG | 2 | 1079 | 2 | 18,26,27 | 1.21 | 2 (11%) | 21,38,41 | 2.13 | 6 (28%) |
| 2 | OMU | 2 | 1153 | 2 | 14,22,23 | 0.97 | 1 (7%) | 19,31,34 | 1.73 | 2 (10%) |
| 2 | OMC | 2 | 1160 | 2 | 15,22,23 | 0.84 | 0 | 20,31,34 | 1.69 | 2 (10%) |
| 2 | A2M | 2 | 1186 | 2 | 18,25,26 | 0.97 | 1 (5%) | 18,36,39 | 1.82 | 2 (11%) |
| 2 | OMG | 2 | 1230 | 2 | 18,26,27 | 1.17 | 2 (11%) | 21,38,41 | 2.04 | 5 (23%) |
| 2 | OMC | 2 | 1249 | 2 | 15,22,23 | 0.81 | 0 | 20,31,34 | 1.64 | 3 (15%) |
| 2 | OMG | 2 | 1254 | 2 | 18,26,27 | 1.13 | 2 (11%) | 21,38,41 | 1.94 | 4 (19%) |
| 2 | OMC | 2 | 1318 | 2 | 15,22,23 | 0.82 | 0 | 20,31,34 | 1.52 | 2 (10%) |
| 2 | OMC | 2 | 1398 | 2 | 15,22,23 | 0.86 | 0 | 20,31,34 | 1.55 | 2 (10%) |
| 2 | H2U | 2 | 1404 | 2 | 17,21,22 | 1.10 | 2 (11%) | 23,30,33 | 1.79 | 4 (17%) |
| 2 | A2M | 2 | 382 | 2 | 18,25,26 | 0.95 | 1 (5%) | 18,36,39 | 1.73 | 1 (5%) |
| 2 | OMC | 2 | 443 | 2 | 15,22,23 | 0.84 | 0 | 20,31,34 | 1.61 | 1 (5%) |
| 2 | A2M | 2 | 527 | 2 | 18,25,26 | 0.97 | 1 (5%) | 18,36,39 | 2.01 | 2 (11%) |
| 2 | OMG | 2 | 534 | 2 | 18,26,27 | 1.19 | 2 (11%) | 21,38,41 | 2.14 | 6 (28%) |
| 2 | OMC | 2 | 554 | 2 | 15,22,23 | 0.81 | 0 | 20,31,34 | 1.67 | 2 (10%) |
| 2 | OMG | 2 | 571 | 2 | 18,26,27 | 1.15 | 2 (11%) | 21,38,41 | 2.21 | 6 (28%) |
| 2 | A2M | 2 | 572 | 2 | 18,25,26 | 1.00 | 1 (5%) | 18,36,39 | 1.71 | 1 (5%) |
| 2 | OMC | 2 | 583 | 2 | 15,22,23 | 0.89 | 0 | 20,31,34 | 1.66 | 1 (5%) |
| 2 | A2M | 2 | 591 | 2 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.86 | 1 (5%) |
| 2 | A2M | 2 | 628 | 2 | 18,25,26 | 0.97 | 1 (5%) | 18,36,39 | 1.91 | 2 (11%) |
| 2 | OMG | 2 | 641 | 2 | 18,26,27 | 1.13 | 2 (11%) | 21,38,41 | 2.15 | 6 (28%) |
| 2 | OMG | 2 | 655 | 2 | 18,26,27 | 1.16 | 2 (11%) | 21,38,41 | 1.94 | 4 (19%) |
| 2 | OMU | 2 | 656 | 2 | 14,22,23 | 0.89 | 1 (7%) | 19,31,34 | 1.64 | 2 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | OMU | 2 | 667 | 2 | 14,22,23 | 0.88 | 1 (7%) | 19,31,34 | 1.70 | 1 (5%) |
| 2 | OMG | 2 | 71 | 2 | 18,26,27 | 1.15 | 2 (11%) | 21,38,41 | 1.98 | 5 (23%) |
| 7 | A2M | 7 | 162 | 1,7 | 18,25,26 | 1.03 | 1 (5%) | 18,36,39 | 2.06 | 3 (16%) |
| 7 | OMU | 7 | 7 | 1,7 | 14,22,23 | 0.94 | 1 (7%) | 19,31,34 | 1.79 | 2 (10%) |

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 |
|---|---|---|---|---|---|---|---|
| 1 | OMG | 1 | 1526 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMC | 1 | 1529 | 1 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | A2M | 1 | 1541 | 1,2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | 1 | 1542 | 1,2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | 1 | 1628 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMU | 1 | 36 | 1 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | OMU | 1 | 48 | 1 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | A2M | 1 | 678 | 1,2 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | 1 | 681 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMC | 1 | 695 | 1 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | OMU | 1 | 845 | 1 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | OMU | 1 | 847 | 1 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | OMG | 1 | 856 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | 1 | 927 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | A2M | 1 | 955 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | 1 | 959 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMU | 2 | 1078 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMG | 2 | 1079 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMU | 2 | 1153 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMC | 2 | 1160 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 1186 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 1230 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 1249 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMG | 2 | 1254 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 1318 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMC | 2 | 1398 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | H2U | 2 | 1404 | 2 | - | 0/7/38/39 | 0/2/2/2 |
| 2 | A2M | 2 | 382 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 443 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 527 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 534 | 2 | - | 0/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | OMC | 2 | 554 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMG | 2 | 571 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 572 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 583 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 591 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 628 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 641 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 655 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMU | 2 | 656 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMU | 2 | 667 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMG | 2 | 71 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 7 | A2M | 7 | 162 | 1,7 | - | 0/5/27/28 | 0/3/3/3 |
| 7 | OMU | 7 | 7 | 1,7 | - | 0/5/27/28 | 0/2/2/2 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 2 | 1404 | H2U | C4-N3 | -2.68 | 1.33 | 1.37 |
| 2 | 2 | 1404 | H2U | C2-N3 | -2.57 | 1.33 | 1.38 |
| 1 | 1 | 845 | OMU | C2-N3 | -2.37 | 1.33 | 1.38 |
| 1 | 1 | 48 | OMU | C2-N3 | -2.32 | 1.33 | 1.38 |
| 1 | 1 | 36 | OMU | C2-N3 | -2.21 | 1.33 | 1.38 |

The worst 5 of 123 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 927 | A2M | N3-C2-N1 | -7.00 | 123.37 | 128.87 |
| 1 | 1 | 678 | A2M | N3-C2-N1 | -6.92 | 123.43 | 128.87 |
| 1 | 1 | 955 | A2M | N3-C2-N1 | -6.88 | 123.47 | 128.87 |
| 2 | 2 | 628 | A2M | N3-C2-N1 | -6.83 | 123.50 | 128.87 |
| 2 | 2 | 591 | A2M | N3-C2-N1 | -6.72 | 123.59 | 128.87 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

41 monomers are involved in 186 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | 1 | 1526 | OMG | 2 | 0 |
| 1 | 1 | 1529 | OMC | 6 | 0 |
| 1 | 1 | 1541 | A2M | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | 1 | 1542 | OMG | 2 | 0 |
| 1 | 1 | 1628 | OMG | 1 | 0 |
| 1 | 1 | 36 | OMU | 14 | 0 |
| 1 | 1 | 48 | OMU | 4 | 0 |
| 1 | 1 | 678 | A2M | 2 | 0 |
| 1 | 1 | 681 | A2M | 2 | 0 |
| 1 | 1 | 695 | OMC | 3 | 0 |
| 1 | 1 | 845 | OMU | 2 | 0 |
| 1 | 1 | 847 | OMU | 3 | 0 |
| 1 | 1 | 856 | OMG | 2 | 0 |
| 1 | 1 | 927 | A2M | 3 | 0 |
| 1 | 1 | 955 | A2M | 2 | 0 |
| 1 | 1 | 959 | OMG | 9 | 0 |
| 2 | 2 | 1078 | OMU | 11 | 0 |
| 2 | 2 | 1079 | OMG | 9 | 0 |
| 2 | 2 | 1153 | OMU | 6 | 0 |
| 2 | 2 | 1160 | OMC | 3 | 0 |
| 2 | 2 | 1186 | A2M | 3 | 0 |
| 2 | 2 | 1230 | OMG | 2 | 0 |
| 2 | 2 | 1249 | OMC | 1 | 0 |
| 2 | 2 | 1254 | OMG | 10 | 0 |
| 2 | 2 | 1318 | OMC | 7 | 0 |
| 2 | 2 | 1398 | OMC | 4 | 0 |
| 2 | 2 | 1404 | H2U | 2 | 0 |
| 2 | 2 | 382 | A2M | 2 | 0 |
| 2 | 2 | 443 | OMC | 7 | 0 |
| 2 | 2 | 527 | A2M | 13 | 0 |
| 2 | 2 | 534 | OMG | 4 | 0 |
| 2 | 2 | 554 | OMC | 3 | 0 |
| 2 | 2 | 571 | OMG | 1 | 0 |
| 2 | 2 | 572 | A2M | 2 | 0 |
| 2 | 2 | 583 | OMC | 1 | 0 |
| 2 | 2 | 591 | A2M | 7 | 0 |
| 2 | 2 | 628 | A2M | 4 | 0 |
| 2 | 2 | 655 | OMG | 7 | 0 |
| 2 | 2 | 667 | OMU | 5 | 0 |
| 2 | 2 | 71 | OMG | 11 | 0 |
| 7 | 7 | 7 | OMU | 10 | 0 |

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 109 ligands modelled in this entry, 109 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.