# wwPDB EM Validation Summary Report (i)

Oct 22, 2024 – 08:14 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 3JAH |
| EMDB ID | : | EMD-3039 |
| Title | : | Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAG stop codon |
| Authors | : | Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V. |
| Deposited on | : | 2015-06-10 |
| Resolution | : | 3.45 Å(reported) |
| Based on initial models | : | 1DT9, 3J92, 4V51, 3J7P, 3BK7 |

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

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

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

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The following versions of software and data (see references (1)) were used in the production of this report:

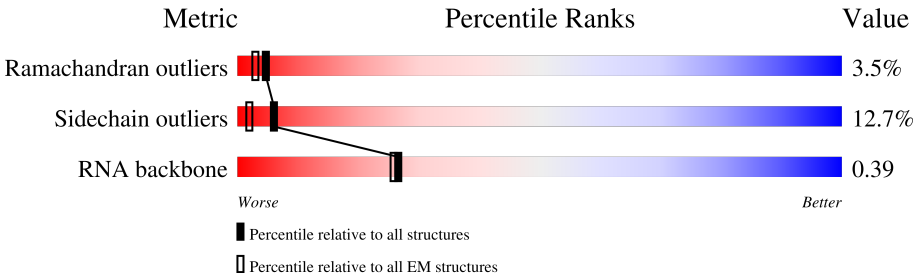
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 244 | 88% 11% |
| 2 | B | 394 | 87% 12% |
| 3 | C | 362 | 84% 15% |
| 4 | D | 292 | 89% 11% |
| 5 | E | 248 | 10% 78% 17% 5% |
| 6 | F | 225 | 87% 12% |
| 7 | G | 241 | 13% 88% 12% |
| 8 | H | 190 | 87% 13% |

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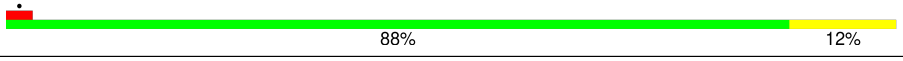
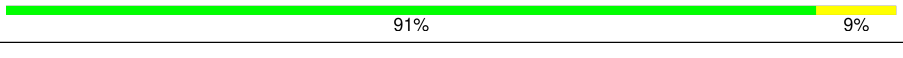
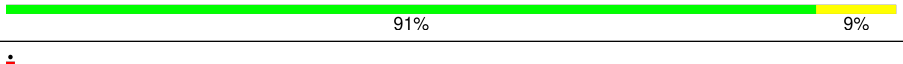
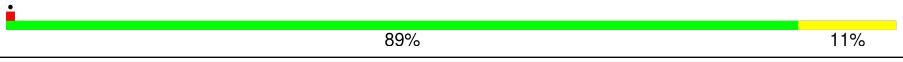
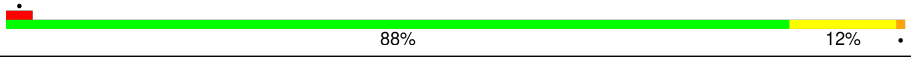
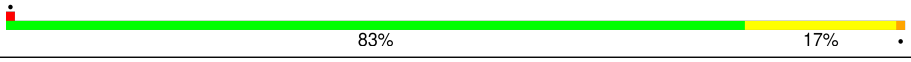
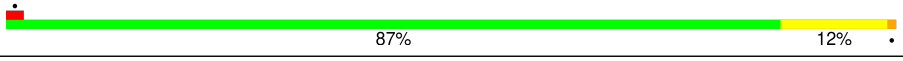
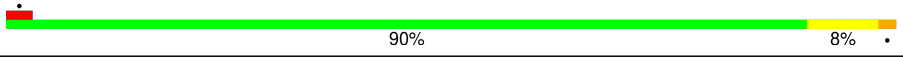
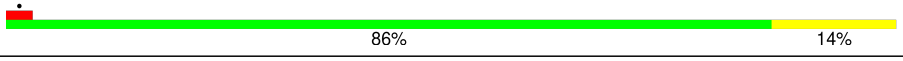
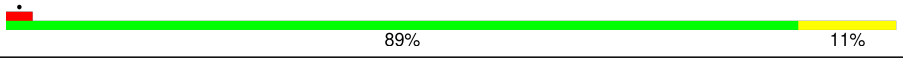
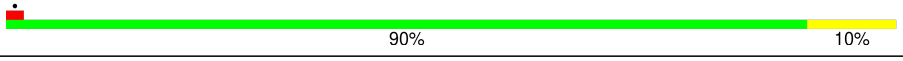
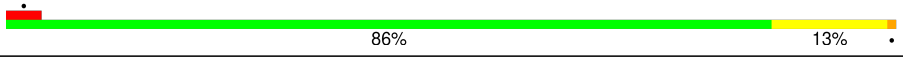
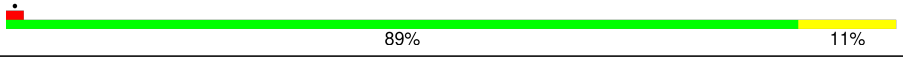
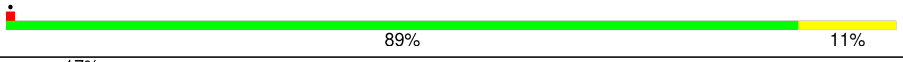
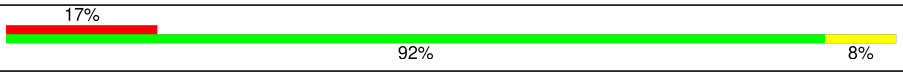
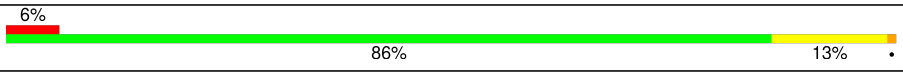
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | I | 213 |   |
| 10 | J | 169 |   |
| 11 | L | 210 |   |
| 12 | M | 138 |   |
| 13 | N | 203 |   |
| 14 | O | 199 |   |
| 15 | P | 153 |   |
| 16 | Q | 187 |   |
| 17 | R | 180 |   |
| 18 | S | 175 |   |
| 19 | T | 159 |   |
| 20 | U | 99 |   |
| 21 | V | 131 |   |
| 22 | W | 63 |   |
| 23 | X | 119 |   |
| 24 | Y | 134 |   |
| 25 | Z | 135 |   |
| 26 | a | 147 |   |
| 27 | b | 75 |   |
| 28 | c | 94 |   |
| 29 | d | 107 |   |
| 30 | e | 128 |   |
| 31 | f | 109 |   |
| 32 | g | 114 |   |
| 33 | h | 122 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | i | 102 | 91% 9% |
| 35 | j | 86 | 83% 15% |
| 36 | k | 69 | 7% 84% 14% |
| 37 | l | 50 | 84% 16% |
| 38 | m | 52 | 83% 17% |
| 39 | n | 23 | 83% 17% |
| 40 | o | 104 | 86% 13% |
| 41 | p | 91 | 92% 8% |
| 42 | r | 125 | 78% 18% |
| 43 | s | 198 | 72% 90% 10% |
| 44 | t | 163 | 69% 80% 20% |
| 45 | 1 | 15 | 20% 80% 20% |
| 46 | 2 | 76 | 72% 26% |
| 47 | 3 | 75 | 20% 51% 41% 8% |
| 48 | 5 | 3662 | 7% 66% 32% |
| 49 | 7 | 120 | 83% 17% |
| 50 | 8 | 156 | 67% 33% |
| 51 | 9 | 1719 | 6% 63% 35% |
| 52 | AA | 208 | 85% 15% |
| 53 | BB | 213 | 83% 16% |
| 54 | CC | 218 | 84% 15% |
| 55 | DD | 227 | 7% 85% 15% |
| 56 | EE | 262 | 78% 21% |
| 57 | FF | 191 | 6% 77% 22% |
| 58 | GG | 237 | 11% 86% 14% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 59 | HH | 189 | 13% 83% 16% |
| 60 | II | 206 | 10% 84% 16% |
| 61 | JJ | 185 | 84% 14% |
| 62 | KK | 98 | 11% 79% 19% |
| 63 | LL | 152 | 11% 81% 17% |
| 64 | MM | 124 | 55% 80% 19% |
| 65 | NN | 150 | 82% 18% |
| 66 | OO | 136 | 75% 21% |
| 67 | PP | 127 | 12% 83% 17% |
| 68 | QQ | 141 | 85% 15% |
| 69 | RR | 129 | 11% 85% 13% |
| 70 | SS | 137 | 84% 13% |
| 71 | TT | 141 | 84% 15% |
| 72 | UU | 104 | 11% 81% 16% |
| 73 | VV | 83 | 87% 13% |
| 74 | WW | 129 | 85% 14% |
| 75 | XX | 141 | 81% 18% |
| 76 | YY | 126 | 6% 78% 22% |
| 77 | ZZ | 75 | 88% 12% |
| 78 | aa | 98 | 81% 19% |
| 79 | bb | 83 | 5% 80% 20% |
| 80 | cc | 61 | 8% 80% 20% |
| 81 | dd | 53 | 81% 19% |
| 82 | ee | 57 | 16% 82% 16% |
| 83 | ff | 68 | 35% 87% 9% |

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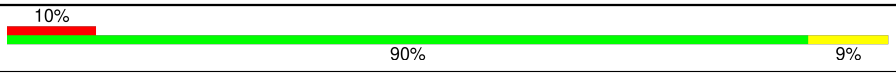
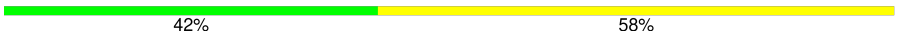
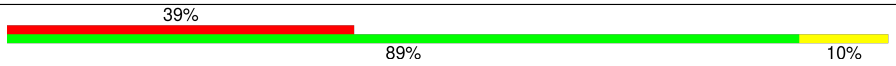
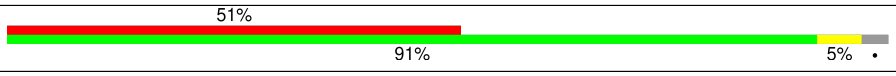
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 84 | gg | 313 |   |
| 85 | hh | 12 |   |
| 86 | ii | 416 |   |
| 87 | jj | 594 |   |

# 2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 226454 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 protein called uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1868 | 1171 | 382 | 309 | 6 | | |

- Molecule 2 is a protein called uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 394 | Total | C | N | O | S | 0 | 0 |
| | | | 3148 | 2007 | 591 | 537 | 13 | | |

- Molecule 3 is a protein called uL4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 362 | Total | C | N | O | S | 0 | 0 |
| | | | 2884 | 1814 | 578 | 478 | 14 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 361 | LYS | - | expression tag | UNP G1SVW5 |
| C | 362 | LYS | - | expression tag | UNP G1SVW5 |
| C | 363 | SER | - | expression tag | UNP G1SVW5 |

- Molecule 4 is a protein called uL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2386 | 1509 | 437 | 426 | 14 | | |

- Molecule 5 is a protein called eL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 236 | Total | C | N | O | S | 0 | 0 |
| | | | 1898 | 1215 | 362 | 318 | 3 | | |

- Molecule 6 is a protein called uL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1870 | 1202 | 358 | 301 | 9 | | |

- Molecule 7 is a protein called eL8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1934 | 1233 | 371 | 326 | 4 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 191 | GLY | CYS | conflict | UNP G1STW0 |

- Molecule 8 is a protein called uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1516 | 954 | 284 | 272 | 6 | | |

- Molecule 9 is a protein called uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1655 | 1051 | 319 | 272 | 13 | | |

- Molecule 10 is a protein called uL5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1353 | 855 | 252 | 240 | 6 | | |

- Molecule 11 is a protein called eL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | L | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1703 | 1065 | 354 | 280 | 4 | | |

- Molecule 12 is a protein called eL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | M | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1137 | 727 | 221 | 182 | 7 | | |

- Molecule 13 is a protein called eL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | N | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1701 | 1072 | 359 | 266 | 4 | | |

- Molecule 14 is a protein called uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | O | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1638 | 1056 | 321 | 256 | 5 | | |

- Molecule 15 is a protein called uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | P | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1242 | 776 | 241 | 216 | 9 | | |

- Molecule 16 is a protein called uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | Q | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1506 | 941 | 311 | 249 | 5 | | |

- Molecule 17 is a protein called eL19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | R | 180 | Total | C | N | O | S | 0 | 0 |
| | | | 1508 | 933 | 328 | 238 | 9 | | |

- Molecule 18 is a protein called eL20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | S | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1454 | 925 | 284 | 235 | 10 | | |

- Molecule 19 is a protein called eL21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | T | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1298 | 823 | 252 | 217 | 6 | | |

- Molecule 20 is a protein called eL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | U | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 518 | 141 | 147 | 2 | | |

- Molecule 21 is a protein called uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | V | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 618 | 184 | 172 | 5 | | |

- Molecule 22 is a protein called eL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | W | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 528 | 337 | 103 | 85 | 3 | | |

- Molecule 23 is a protein called uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | X | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 976 | 624 | 183 | 168 | 1 | | |

- Molecule 24 is a protein called uL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | Y | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1115 | 700 | 226 | 186 | 3 | | |

- Molecule 25 is a protein called eL27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Z | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1107 | 714 | 208 | 182 | 3 | | |

- Molecule 26 is a protein called uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | a | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 734 | 239 | 185 | 4 | | |

- Molecule 27 is a protein called eL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | b | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 609 | 378 | 130 | 98 | 3 | | |

- Molecule 28 is a protein called eL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | c | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 732 | 465 | 130 | 131 | 6 | | |

- Molecule 29 is a protein called eL31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | d | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 888 | 560 | 171 | 155 | 2 | | |

- Molecule 30 is a protein called eL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | e | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 667 | 216 | 165 | 5 | | |

- Molecule 31 is a protein called eL33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | f | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 876 | 555 | 174 | 143 | 4 | | |

- Molecule 32 is a protein called eL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | g | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 906 | 566 | 187 | 147 | 6 | | |

- Molecule 33 is a protein called uL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | h | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 1013 | 640 | 204 | 168 | 1 | | |

- Molecule 34 is a protein called eL36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | i | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 830 | 520 | 176 | 129 | 5 | | |

- Molecule 35 is a protein called eL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | j | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 705 | 434 | 155 | 111 | 5 | | |

- Molecule 36 is a protein called eL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | k | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 569 | 366 | 103 | 99 | 1 | | |

- Molecule 37 is a protein called eL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | l | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 281 | 98 | 64 | 1 | | |

- Molecule 38 is a protein called eL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | m | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 429 | 266 | 90 | 67 | 6 | | |

- Molecule 39 is a protein called eL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | n | 23 | Total | C | N | O | S | 0 | 0 |
| | | | 222 | 134 | 61 | 25 | 2 | | |

- Molecule 40 is a protein called eL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | o | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 851 | 533 | 174 | 138 | 6 | | |

- Molecule 41 is a protein called eL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | p | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 708 | 445 | 136 | 120 | 7 | | |

- Molecule 42 is a protein called eL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | r | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 1001 | 621 | 206 | 168 | 6 | | |

- Molecule 43 is a protein called uL10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | s | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1523 | 969 | 265 | 280 | 9 | | |

- Molecule 44 is a protein called uL11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | t | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1238 | 773 | 230 | 230 | 5 | | |

- Molecule 45 is a protein called peptide.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | 1 | 15 | Total | C | N | O | S | 0 | 0 |
| | | | 125 | 82 | 20 | 22 | 1 | | |

- Molecule 46 is a RNA chain called tRNA(Val).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | 2 | 76 | Total | C | N | O | P | 0 | 0 |
| | | | 1616 | 723 | 291 | 527 | 75 | | |

- Molecule 47 is a RNA chain called tRNA(Lys).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | 3 | 75 | Total | C | N | O | P | 0 | 0 |
| | | | 1593 | 712 | 281 | 526 | 74 | | |

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | 5 | 3662 | Total | C | N | O | P | 0 | 0 |
| | | | 78486 | 34947 | 14363 | 25515 | 3661 | | |

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | 7 | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2558 | 1141 | 456 | 842 | 119 | | |

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | 8 | 156 | Total | C | N | O | P | 0 | 0 |
| | | | 3314 | 1480 | 585 | 1094 | 155 | | |

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | 9 | 1719 | Total | C | N | O | P | 0 | 0 |
| | | | 36680 | 16371 | 6586 | 12005 | 1718 | | |

- Molecule 52 is a protein called uS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | AA | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1642 | 1045 | 289 | 300 | 8 | | |

- Molecule 53 is a protein called eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | BB | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1729 | 1098 | 309 | 308 | 14 | | |

- Molecule 54 is a protein called uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | CC | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1692 | 1102 | 287 | 296 | 7 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| CC | 194 | ARG | HIS | conflict | UNP G1TUT9 |
| CC | 228 | GLY | SER | conflict | UNP G1TUT9 |

- Molecule 55 is a protein called uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | DD | 227 | Total | C | N | O | S | 0 | 0 |
| | | | 1764 | 1124 | 317 | 315 | 8 | | |

- Molecule 56 is a protein called eS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | EE | 262 | Total | C | N | O | S | 0 | 0 |
| | | | 2073 | 1323 | 384 | 357 | 9 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| EE | 25 | GLY | SER | conflict | UNP G1TK17 |

- Molecule 57 is a protein called uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | FF | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 943 | 286 | 273 | 7 | | |

- Molecule 58 is a protein called eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | GG | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1923 | 1200 | 387 | 329 | 7 | | |

- Molecule 59 is a protein called eS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | HH | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1521 | 969 | 280 | 271 | 1 | | |

- Molecule 60 is a protein called eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | II | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1686 | 1058 | 332 | 291 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| II | 47 | ARG | GLY | conflict | UNP G1TJW1 |

- Molecule 61 is a protein called uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | JJ | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 969 | 306 | 248 | 2 | | |

- Molecule 62 is a protein called eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | KK | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 827 | 539 | 148 | 134 | 6 | | |

- Molecule 63 is a protein called uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | LL | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1238 | 788 | 232 | 212 | 6 | | |

- Molecule 64 is a protein called eS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | MM | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 958 | 600 | 170 | 179 | 9 | | |

- Molecule 65 is a protein called uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | NN | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1208 | 773 | 229 | 205 | 1 | | |

- Molecule 66 is a protein called uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | OO | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1016 | 621 | 199 | 190 | 6 | | |

- Molecule 67 is a protein called uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | PP | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1060 | 673 | 201 | 179 | 7 | | |

- Molecule 68 is a protein called uS9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | QQ | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1124 | 715 | 212 | 194 | 3 | | |

- Molecule 69 is a protein called eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | RR | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1047 | 658 | 193 | 191 | 5 | | |

- Molecule 70 is a protein called uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | SS | 137 | Total | C | N | O | S | 0 | 0 |
| | | | 1139 | 714 | 231 | 193 | 1 | | |

- Molecule 71 is a protein called eS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | TT | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1102 | 692 | 212 | 195 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| TT | 119 | GLY | TRP | conflict | UNP G1TN62 |

- Molecule 72 is a protein called uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | UU | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 821 | 514 | 155 | 148 | 4 | | |

- Molecule 73 is a protein called eS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | VV | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 636 | 394 | 118 | 119 | 5 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| VV | 3 | ASN | SER | conflict | UNP G1TM82 |
| VV | 4 | ASP | ASN | conflict | UNP G1TM82 |
| VV | 50 | PHE | SER | conflict | UNP G1TM82 |
| VV | 75 | ALA | SER | conflict | UNP G1TM82 |

- Molecule 74 is a protein called uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | WW | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1034 | 659 | 193 | 176 | 6 | | |

- Molecule 75 is a protein called uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | XX | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 693 | 219 | 183 | 3 | | |

- Molecule 76 is a protein called eS24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | YY | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1023 | 646 | 200 | 172 | 5 | | |

- Molecule 77 is a protein called eS25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | ZZ | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 598 | 382 | 111 | 104 | 1 | | |

- Molecule 78 is a protein called eS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | aa | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 781 | 486 | 161 | 129 | 5 | | |

- Molecule 79 is a protein called eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 79 | bb | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 651 | 408 | 121 | 115 | 7 | | |

- Molecule 80 is a protein called eS28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 80 | cc | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 475 | 290 | 92 | 91 | 2 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| cc | 18 | ILE | LEU | conflict | UNP G1TIB4 |
| cc | 20 | LYS | ARG | conflict | UNP G1TIB4 |
| cc | 40 | HIS | ARG | conflict | UNP G1TIB4 |
| cc | 42 | THR | ILE | conflict | UNP G1TIB4 |

- Molecule 81 is a protein called uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 81 | dd | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 445 | 278 | 90 | 72 | 5 | | |

- Molecule 82 is a protein called eS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 82 | ee | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 457 | 282 | 101 | 73 | 1 | | |

- Molecule 83 is a protein called eS31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 83 | ff | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 520 | 331 | 98 | 85 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| ff | ? | - | VAL | deletion | UNP G1SK22 |

- Molecule 84 is a protein called RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 84 | gg | 313 | Total | C | N | O | S | 0 | 0 |
| | | | 2436 | 1535 | 424 | 465 | 12 | | |

- Molecule 85 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 85 | hh | 12 | Total | C | N | O | P | 0 | 0 |
| | | | 257 | 115 | 46 | 84 | 12 | | |

- Molecule 86 is a protein called eRF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 86 | ii | 416 | Total | C | N | O | S | 0 | 0 |
| | | | 3280 | 2087 | 559 | 623 | 11 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| ii | 183 | ALA | GLY | engineered mutation | UNP P62495 |
| ii | 184 | ALA | GLY | engineered mutation | UNP P62495 |

- Molecule 87 is a protein called ABCE1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 87 | jj | 576 | Total | C | N | O | S | 0 | 0 |
| | | | 4543 | 2904 | 779 | 829 | 31 | | |

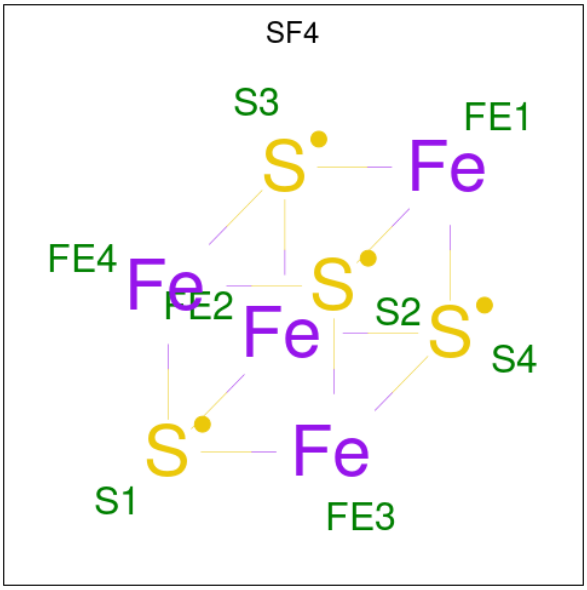
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 88 | B | 1 | Total Mg<br>1 1 | 0 |
| 88 | C | 1 | Total Mg<br>1 1 | 0 |
| 88 | I | 1 | Total Mg<br>1 1 | 0 |
| 88 | P | 1 | Total Mg<br>1 1 | 0 |
| 88 | V | 1 | Total Mg<br>1 1 | 0 |
| 88 | g | 1 | Total Mg<br>1 1 | 0 |
| 88 | 5 | 146 | Total Mg<br>146 146 | 0 |
| 88 | 7 | 5 | Total Mg<br>5 5 | 0 |
| 88 | 8 | 2 | Total Mg<br>2 2 | 0 |
| 88 | 9 | 34 | Total Mg<br>34 34 | 0 |
| 88 | LL | 1 | Total Mg<br>1 1 | 0 |
| 88 | hh | 1 | Total Mg<br>1 1 | 0 |

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

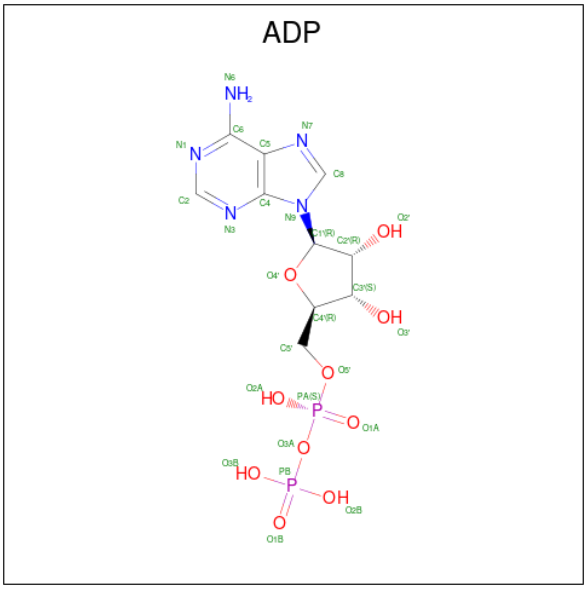
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 89 | g | 1 | Total Zn<br>1 1 | 0 |
| 89 | j | 1 | Total Zn<br>1 1 | 0 |
| 89 | m | 1 | Total Zn<br>1 1 | 0 |
| 89 | o | 1 | Total Zn<br>1 1 | 0 |
| 89 | p | 1 | Total Zn<br>1 1 | 0 |
| 89 | aa | 1 | Total Zn<br>1 1 | 0 |
| 89 | dd | 1 | Total Zn<br>1 1 | 0 |
| 89 | ff | 1 | Total Zn<br>1 1 | 0 |

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 90 | jj | 1 | Total Fe S<br>8 4 4 | 0 |
| 90 | jj | 1 | Total Fe S<br>8 4 4 | 0 |

- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



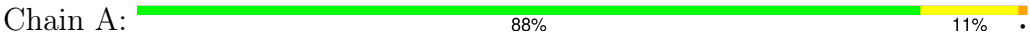
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 91 | jj | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 91 | jj | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

# 3 Residue-property plots (i)

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

• Molecule 1: uL2

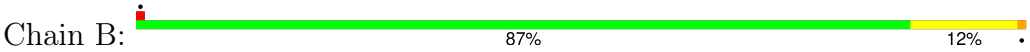
Chain A:

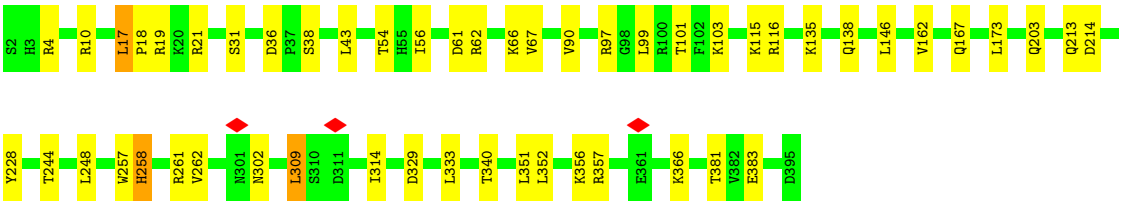




• Molecule 2: uL3

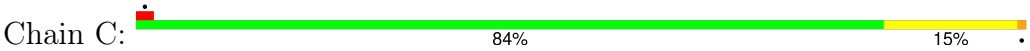
Chain B:

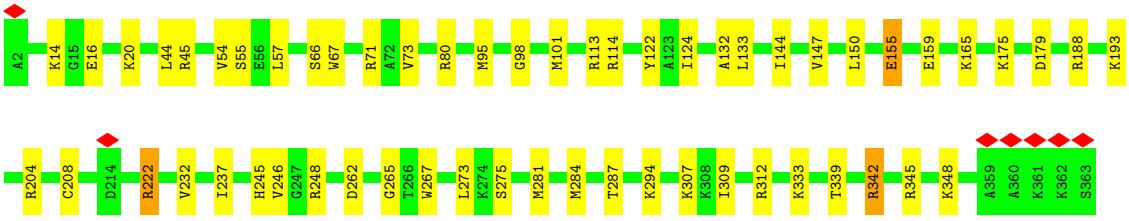



• Molecule 3: uL4

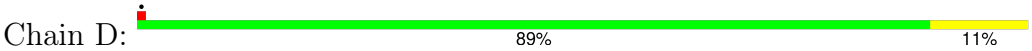
Chain C:

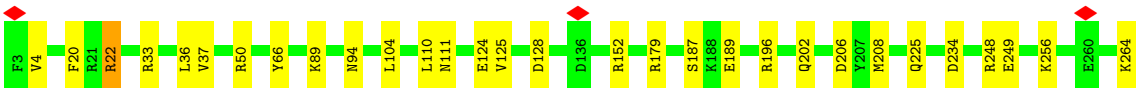


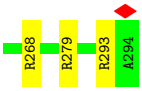




• Molecule 4: uL18

Chain D:

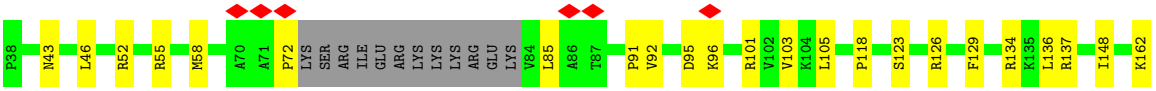


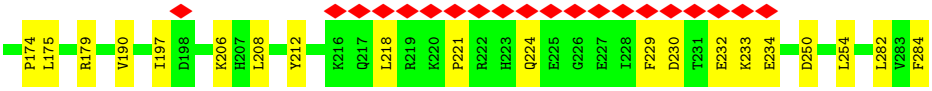






• Molecule 5: eL6

Chain E:

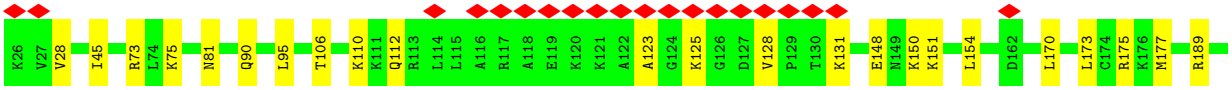

• Molecule 6: uL30

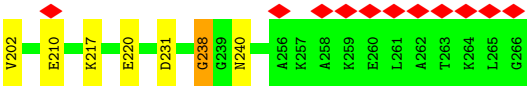
Chain F:



• Molecule 7: eL8

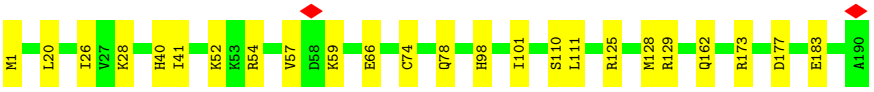
Chain G:

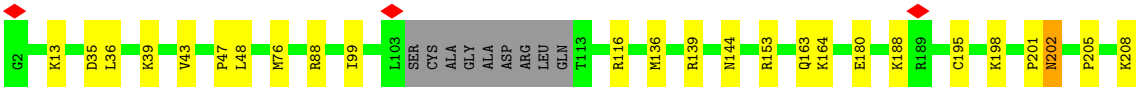

• Molecule 8: uL6

Chain H:


• Molecule 9: uL16

Chain I:


• Molecule 10: uL5

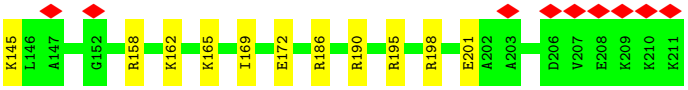
Chain J:



• Molecule 11: eL13

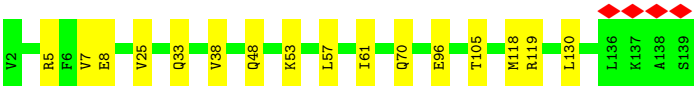
Chain L:





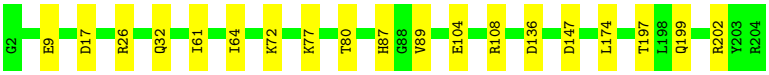

• Molecule 12: eL14

Chain M:

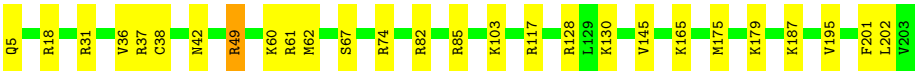

• Molecule 13: eL15

Chain N:


• Molecule 14: uL13

Chain O:

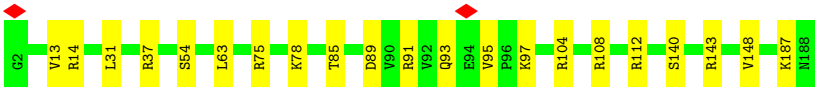




• Molecule 15: uL22

Chain P:


• Molecule 16: uL14

Chain Q:

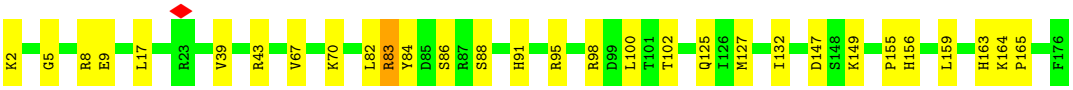

• Molecule 17: eL19

Chain R:



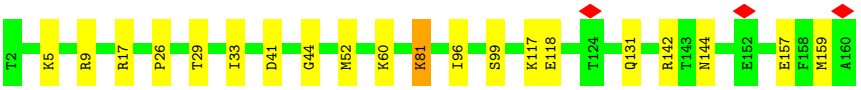
• Molecule 18: eL20

Chain S:

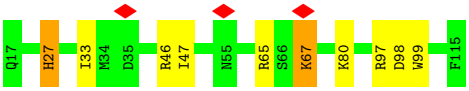

• Molecule 19: eL21

Chain T:

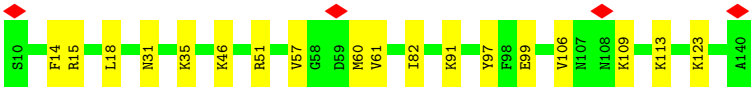

• Molecule 20: eL22

Chain U:

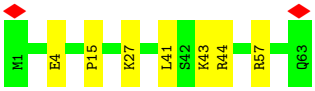

• Molecule 21: uL14

Chain V:


• Molecule 22: eL24

Chain W:



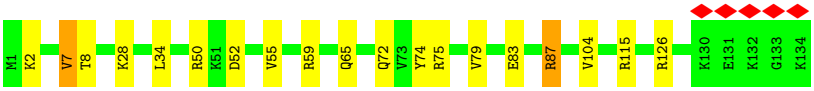

• Molecule 23: uL23

Chain X:



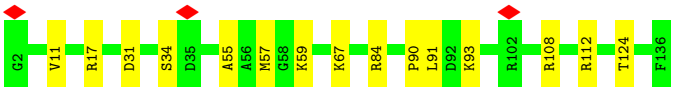
• Molecule 24: uL24

Chain Y:

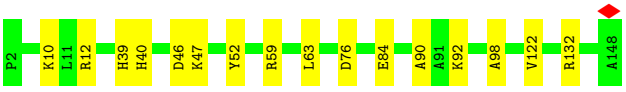

• Molecule 25: eL27

Chain Z:

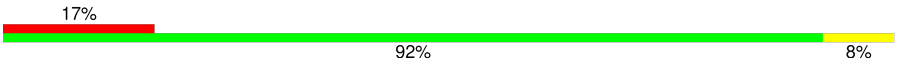

• Molecule 26: uL15

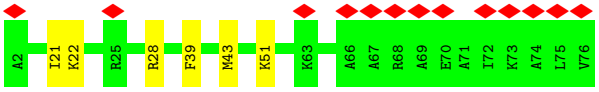
Chain a:


• Molecule 27: eL29

Chain b:



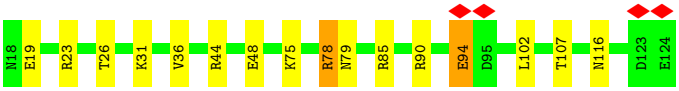

• Molecule 28: eL30

Chain c:



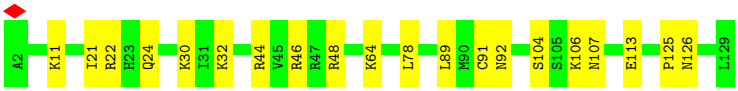
• Molecule 29: eL31

Chain d:



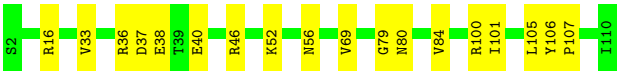

• Molecule 30: eL32

Chain e:

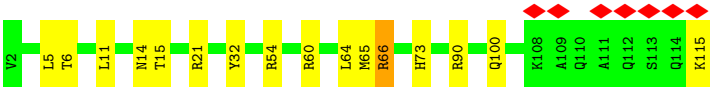

• Molecule 31: eL33

Chain f:

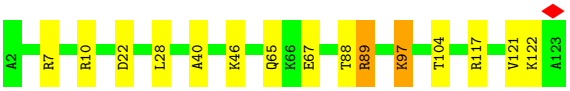

• Molecule 32: eL34

Chain g:

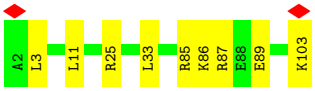

• Molecule 33: uL29

Chain h:

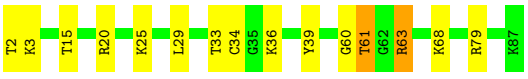

• Molecule 34: eL36

Chain i:

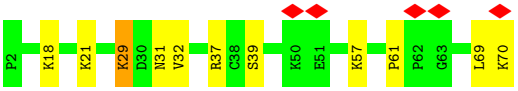

• Molecule 35: eL37

Chain j:

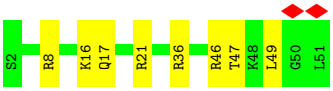

• Molecule 36: eL38

Chain k:



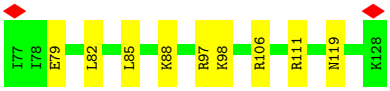

• Molecule 37: eL39

Chain l:

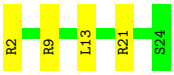

• Molecule 38: eL40

Chain m:

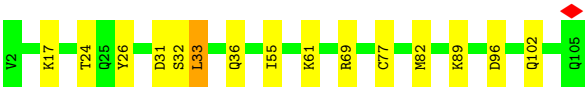

• Molecule 39: eL41

Chain n:

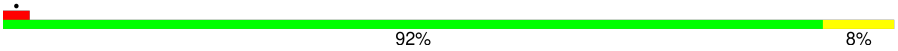

• Molecule 40: eL42

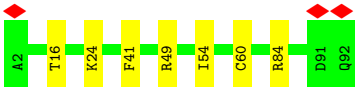
Chain o:


• Molecule 41: eL43

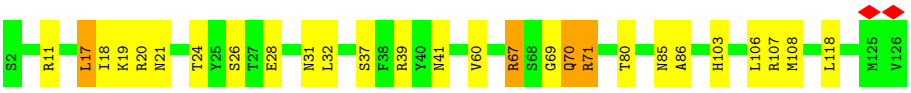
Chain p:



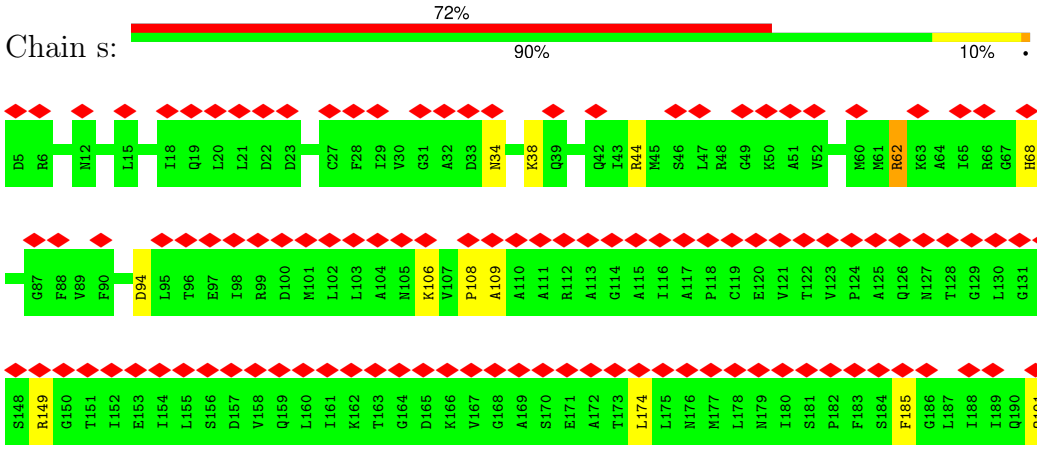

• Molecule 42: eL28

Chain r:

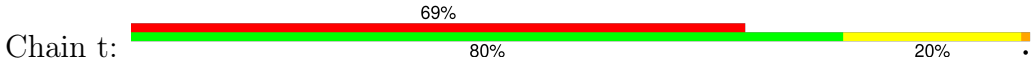

• Molecule 43: uL10

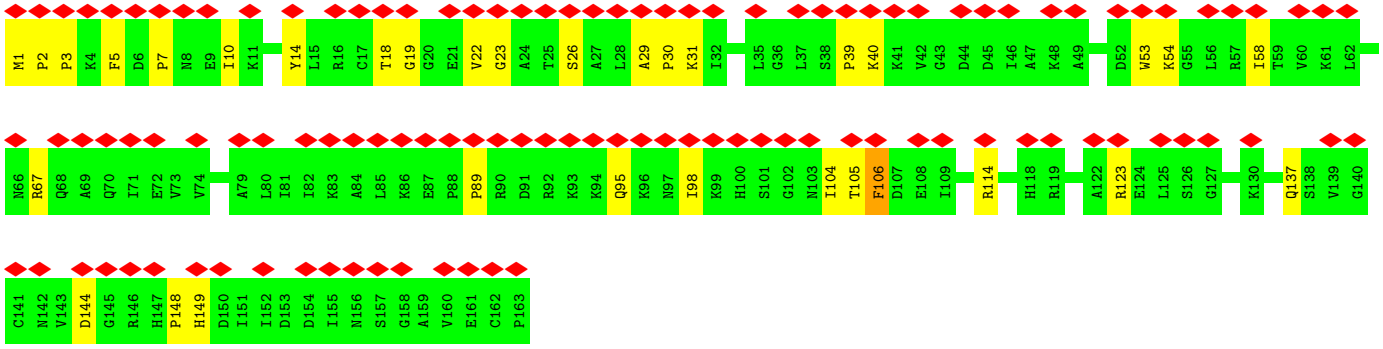
Chain s:




- Molecule 44: uL11

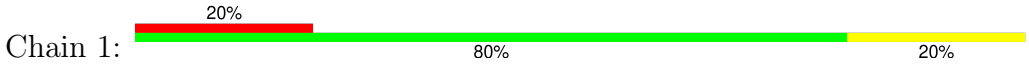
Chain t:

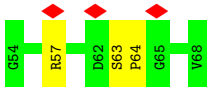



- Molecule 45: peptide

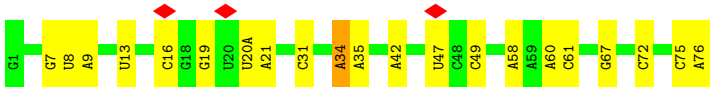
Chain 1:



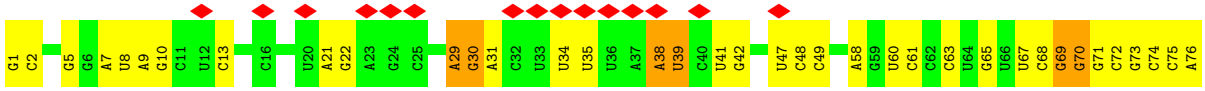

- Molecule 46: tRNA(Val)

Chain 2:

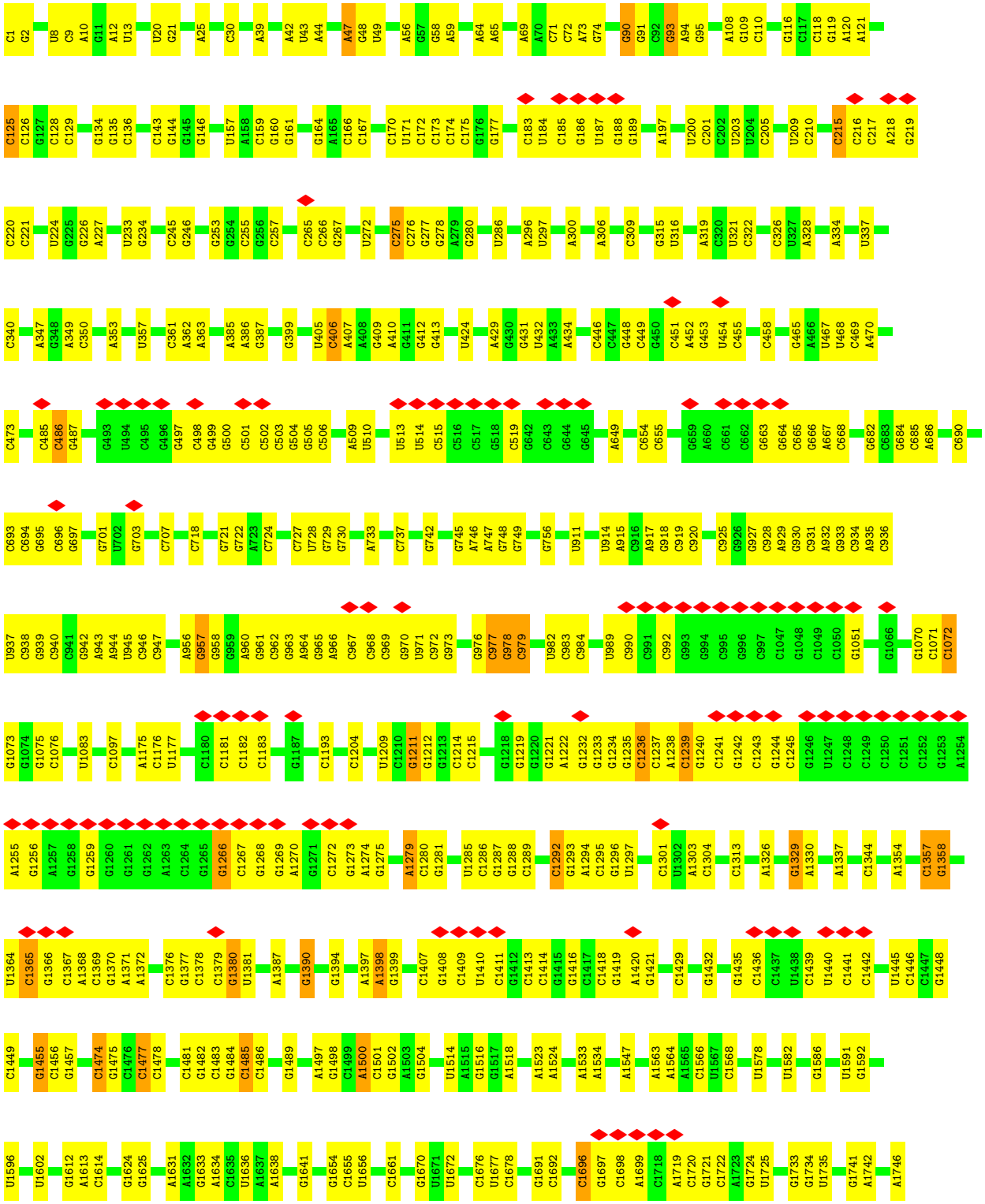

- Molecule 47: tRNA(Lys)

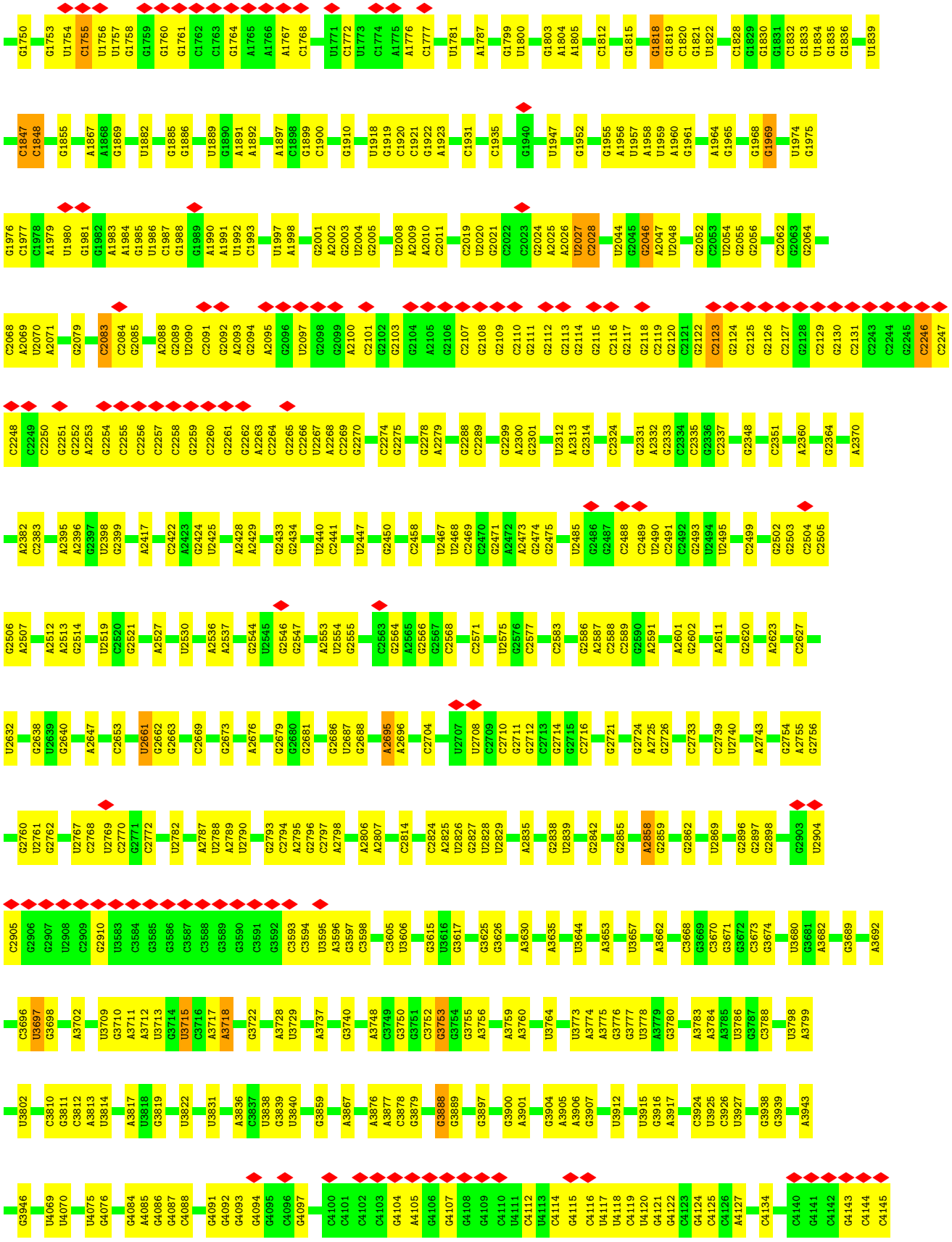
Chain 3:

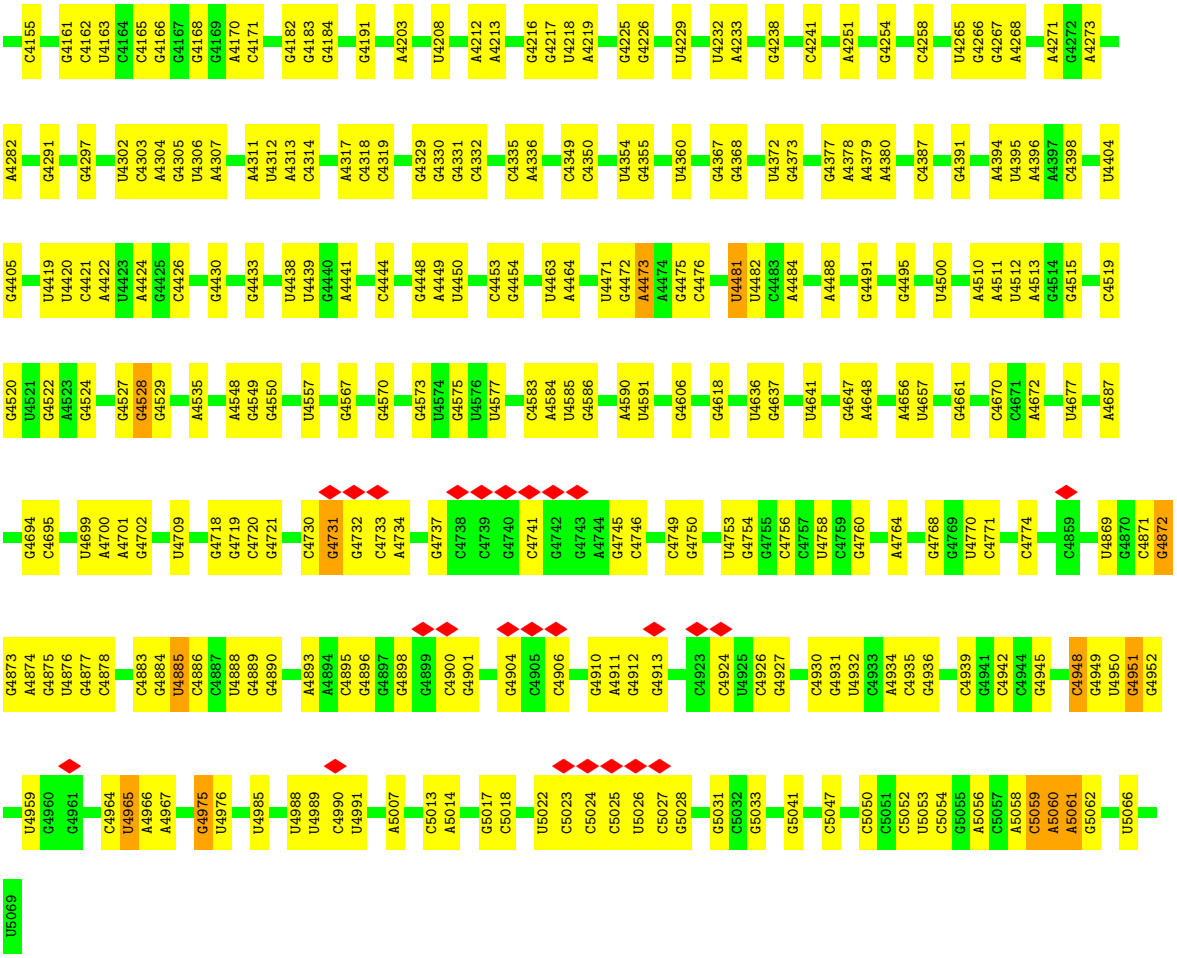



• Molecule 48: 28S ribosomal RNA

Chain 5:

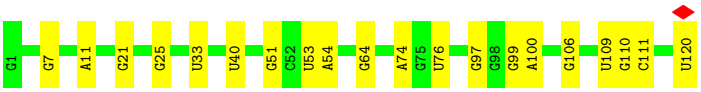




G1750 G1753 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 U1771 C1772 U1773 C1774 A1775 A1776 C1777 U1781 A1787 G1799 U1800 G1803 A1804 A1805 C1812 G1815 G1818 G1819 C1820 G1821 U1822 C1828 G1829 G1830 G1831 C1832 G1833 U1834 G1835 G1836 U1839
C1847 C1848 G1855 A1867 A1868 G1869 U1882 G1885 G1886 U1889 G1890 A1891 A1892 A1897 C1898 G1899 C1900 G1910 U1918 G1919 C1920 C1921 G1922 A1923 C1931 C1935 G1940 U1947 G1952 G1955 A1956 U1957 A1958 U1959 A1960 G1961 A1964 G1965 G1968 G1969 U1974 G1975
G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 G1988 G1989 A1990 A1991 U1992 C1993 U1997 A1998 G2001 A2002 G2003 U2004 G2005 U2008 A2009 A2010 C2011 C2019 U2020 G2021 C2022 C2023 G2024 A2025 A2026 U2027 C2028 U2044 G2045 G2046 A2047 U2048 G2052 C2053 U2054 G2055 G2056 C2062 G2063 G2064
C2068 A2069 U2070 A2071 G2079 C2083 C2084 G2085 A2088 G2089 U2090 C2091 G2092 A2093 G2094 A2095 G2096 U2097 G2098 G2099 A2100 C2101 G2102 G2103 G2104 A2105 G2106 C2107 G2108 G2109 C2110 G2111 G2112 G2113 G2114 G2115 C2116 G2117 G2118 C2119 G2120 C2121 G2122 C2123 G2124 C2125 G2126 C2127 G2128 C2129 G2130 C2131 C2243 C2244 G2245 C2246 C2247
C2248 C2249 C2250 G2251 G2252 A2253 G2254 C2255 C2256 C2257 C2258 G2259 C2260 G2261 G2262 A2263 C2264 G2265 C2266 U2267 A2268 C2269 G2270 C2274 G2275 G2278 A2279 G2288 C2289 G2299 A2300 G2301 U2312 A2313 G2314 C2324 G2331 A2332 G2333 C2334 C2335 G2336 C2337 G2348 C2351 A2360 G2364 A2370
A2382 C2383 A2395 A2396 G2397 U2398 G2399 A2417 C2422 A2423 G2424 U2425 A2428 A2429 G2433 G2434 U2440 C2441 U2447 G2450 C2458 U2467 U2468 C2469 C2470 G2471 A2472 A2473 G2474 G2475 U2485 G2486 G2487 C2488 C2489 U2490 C2491 C2492 G2493 U2494 U2495 C2499 G2502 G2503 C2504 C2505
G2506 A2507 A2512 A2513 G2514 U2519 C2520 G2521 A2527 U2530 A2536 A2537 G2544 U2545 G2546 G2547 A2553 U2554 G2555 C2563 G2564 A2565 G2566 G2567 C2568 C2571 U2575 G2576 C2577 C2583 G2586 A2587 C2588 C2589 G2590 A2591 A2601 G2602 A2611 G2620 A2623 C2627
U2632 G2638 U2639 G2640 A2647 C2653 U2661 G2662 G2663 C2669 G2673 A2676 G2679 G2680 G2681 G2686 U2687 G2688 A2695 A2696 C2704 U2707 U2708 C2709 C2710 G2711 G2712 C2713 G2714 G2715 C2716 G2721 G2724 A2725 G2726 C2733 C2739 U2740 A2743 G2754 A2755 G2756
G2760 U2761 G2762 U2767 C2768 U2769 C2770 G2771 C2772 U2782 A2787 U2788 A2789 U2790 G2793 C2794 A2795 G2796 C2797 A2798 A2806 A2807 C2814 C2824 A2825 U2826 G2827 U2828 U2829 A2835 G2838 U2839 G2842 G2855 A2858 G2859 G2862 U2869 G2896 G2897 G2898 G2903 U2904
C2905 G2906 G2907 U2908 C2909 G2910 U3583 C3584 G3585 G3586 C3587 C3588 G3589 G3590 C3591 G3592 C3593 C3594 U3595 A3596 G3597 C3598 C3605 U3606 G3615 U3616 G3617 G3625 G3626 A3630 A3635 U3644 A3653 U3657 A3662 C3668 G3669 C3670 G3671 G3672 C3673 G3674 U3680 G3681 A3682 G3689 A3692
C3696 U3697 G3698 A3702 U3709 G3710 A3711 A3712 U3713 G3714 U3715 C3716 A3717 A3718 G3722 A3728 U3729 A3737 G3740 A3748 C3749 G3750 G3751 C3752 G3753 G3754 G3755 A3756 A3759 A3760 U3764 U3773 A3774 A3775 G3776 G3777 U3778 A3779 G3780 A3783 A3784 A3785 U3786 G3787 C3788 U3798 A3799
U3802 C3810 G3811 C3812 A3813 U3814 A3817 U3818 G3819 U3822 U3831 A3836 C3837 U3838 G3839 U3840 G3859 A3867 A3876 A3877 C3878 G3879 G3888 G3889 G3897 G3900 A3901 G3904 A3905 A3906 G3907 U3912 U3915 G3916 A3917 C3924 U3925 C3926 U3927 G3938 G3939 A3943
G3946 U4069 U4070 U4075 G4076 G4084 A4085 G4086 G4087 C4088 G4091 G4092 G4093 G4094 G4095 C4096 G4097 C4100 C4101 C4102 C4103 G4104 A4105 G4106 G4107 G4108 G4109 C4110 U4111 C4112 U4113 C4114 G4115 C4116 U4117 U4118 C4119 U4120 G4121 G4122 G4123 G4124 C4125 C4126 A4127 C4134 C4140 G4141 C4142 G4143 C4144 C4145



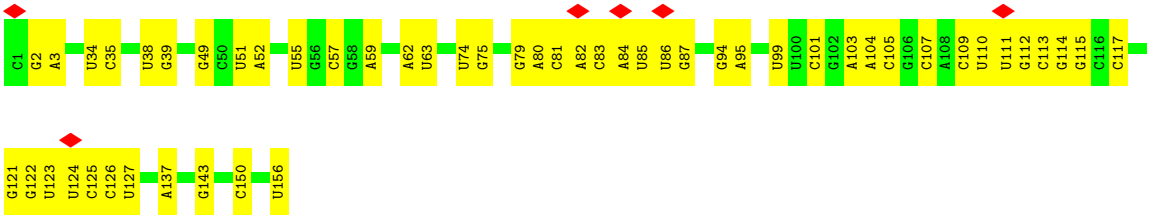

• Molecule 49: 5S ribosomal RNA

Chain 7:

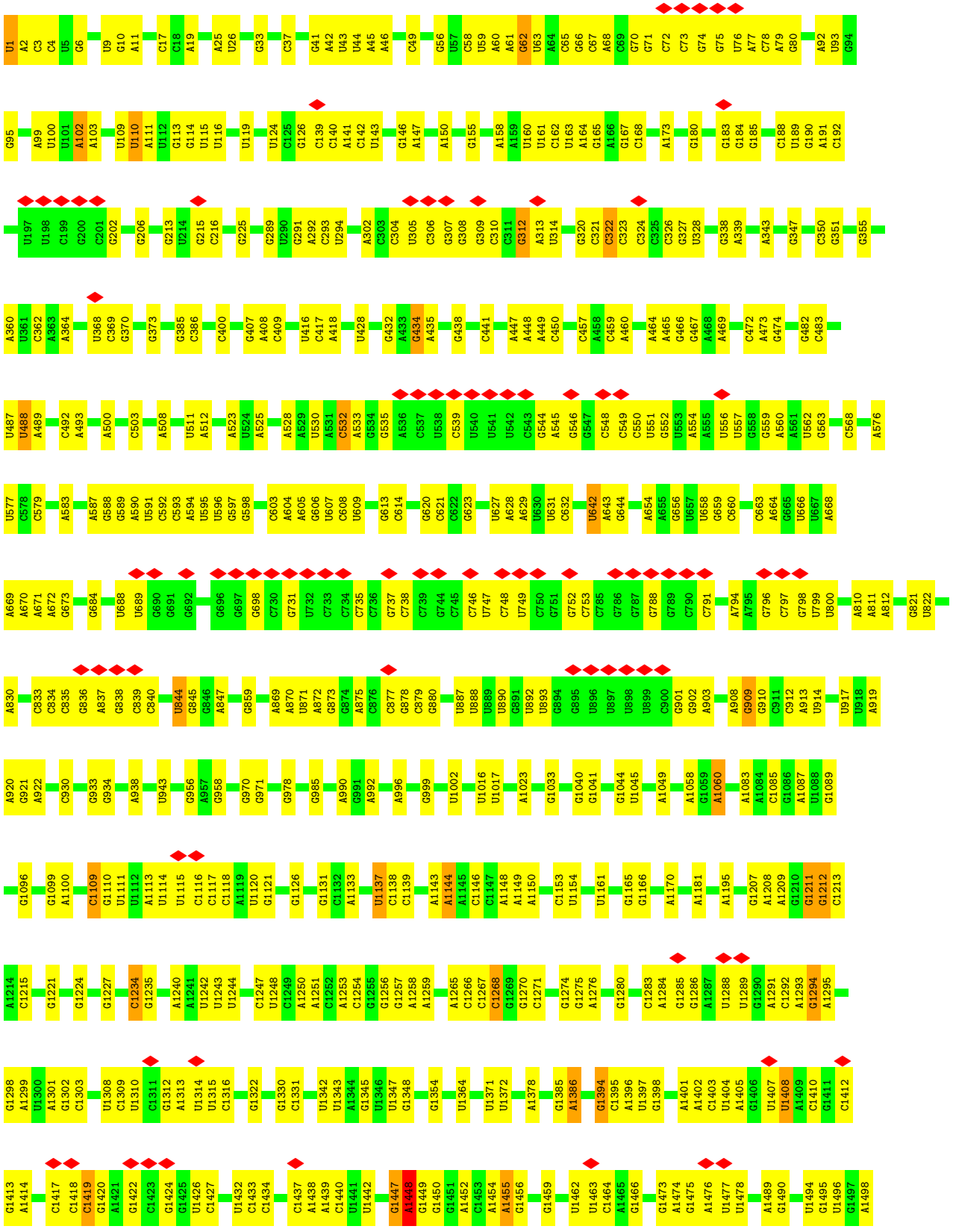

• Molecule 50: 5.8S ribosomal RNA

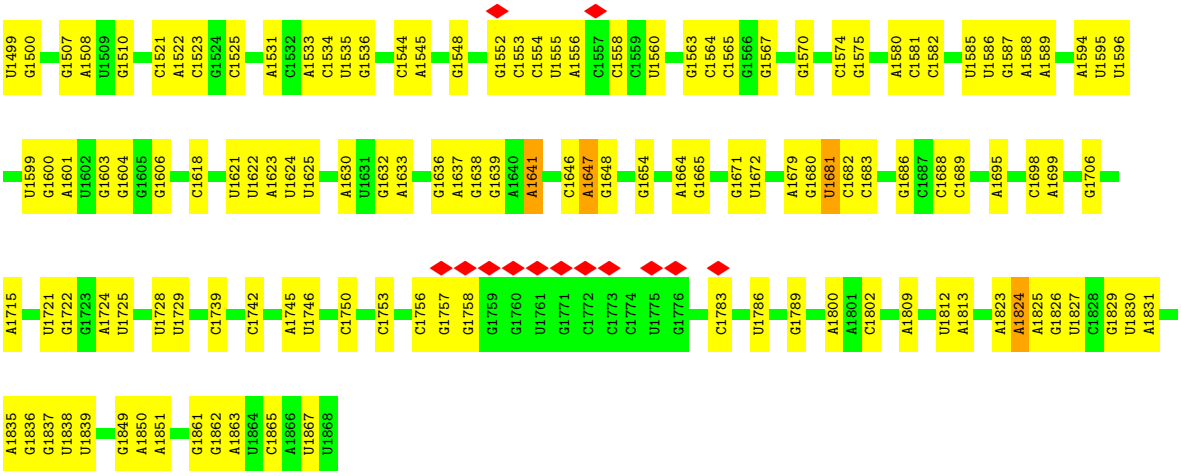
Chain 8:


• Molecule 51: 18S ribosomal RNA

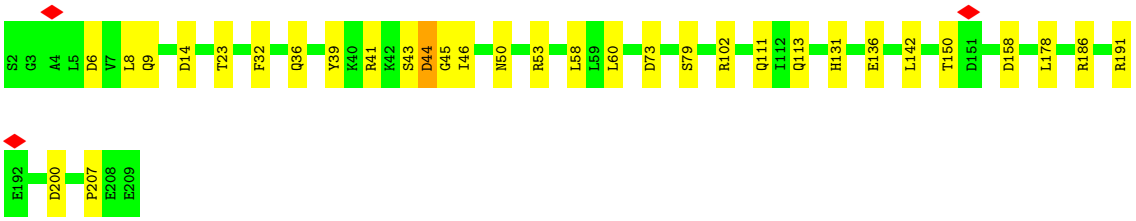
Chain 9:





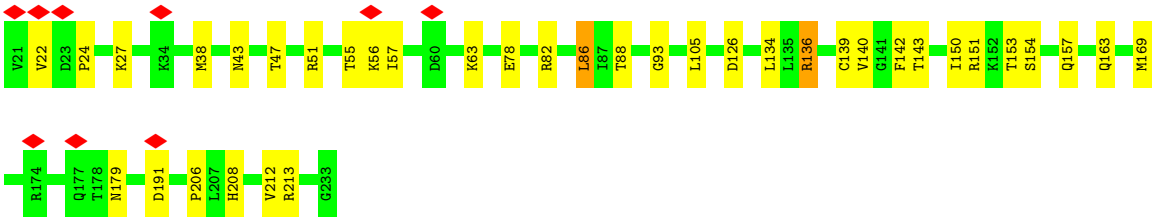

- Molecule 52: uS2

Chain AA:


- Molecule 53: eS1

Chain BB:

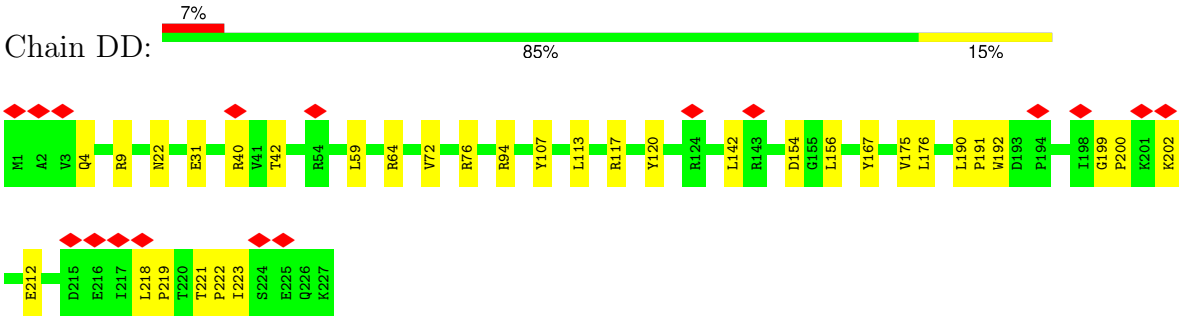

- Molecule 54: uS5

Chain CC:



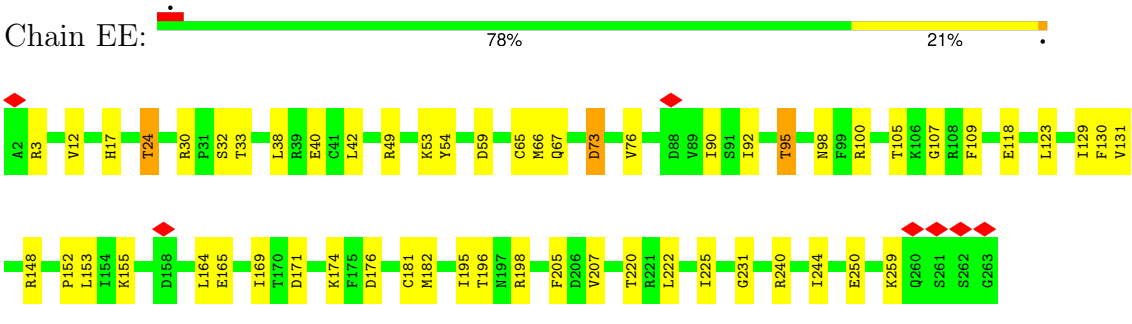
- Molecule 55: uS3

Chain DD:



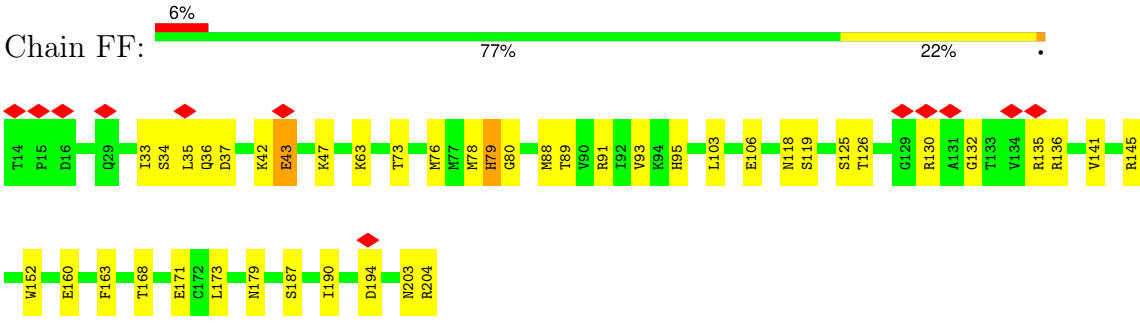

• Molecule 56: eS4

Chain EE:



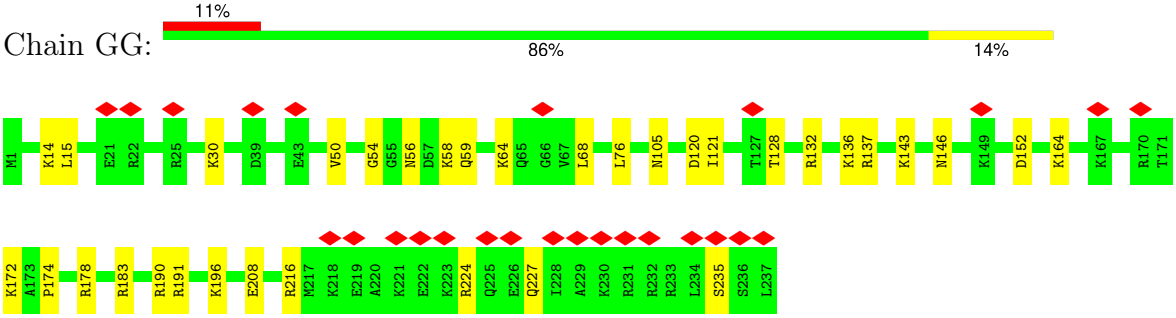

• Molecule 57: uS7

Chain FF:



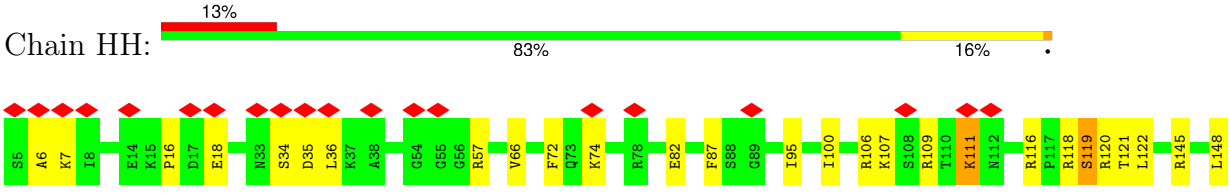

• Molecule 58: eS6

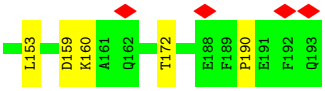
Chain GG:




• Molecule 59: eS7

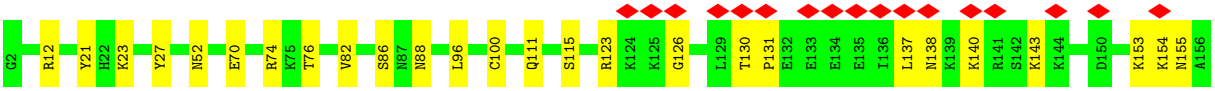
Chain HH:

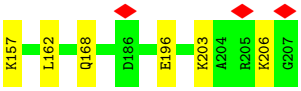





• Molecule 60: eS8

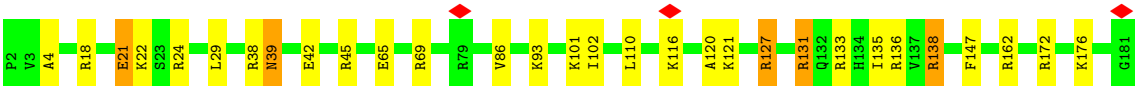
Chain II:

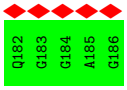




• Molecule 61: uS4

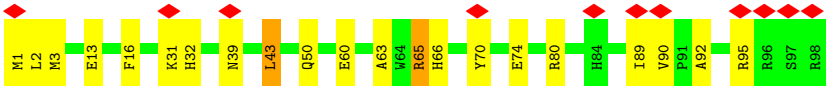
Chain JJ:

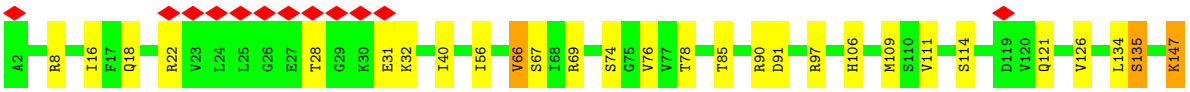

• Molecule 62: eS10

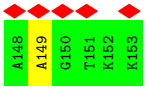
Chain KK:


• Molecule 63: uS17

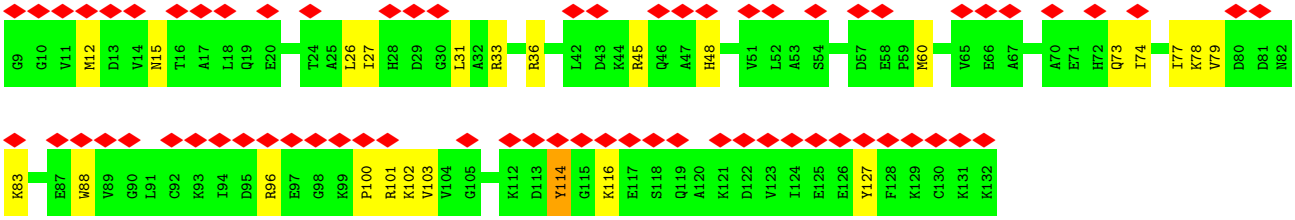
Chain LL:

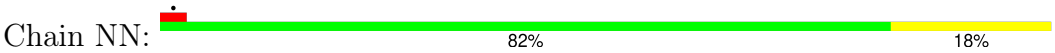



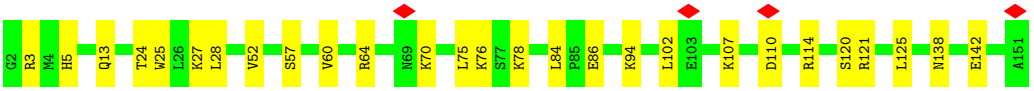

• Molecule 64: eS12

Chain MM:

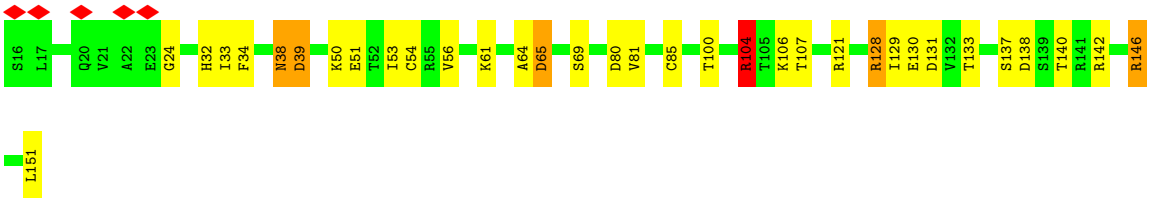



• Molecule 65: uS15

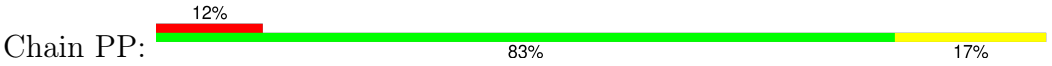


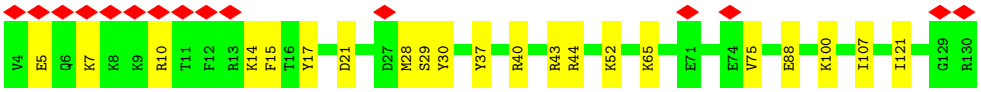




• Molecule 66: uS11

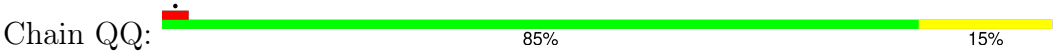



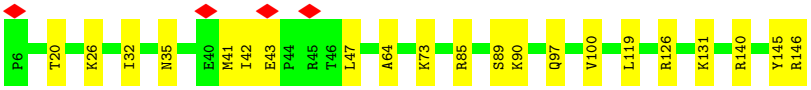

• Molecule 67: uS19



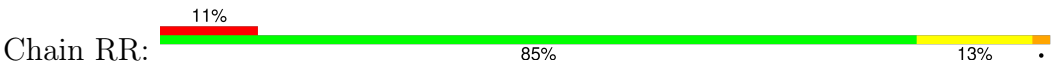



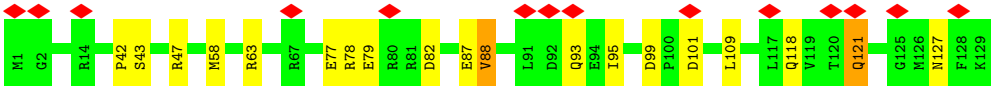

• Molecule 68: uS9



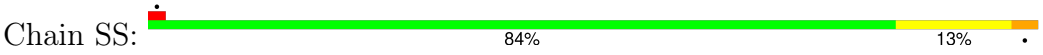




• Molecule 69: eS17



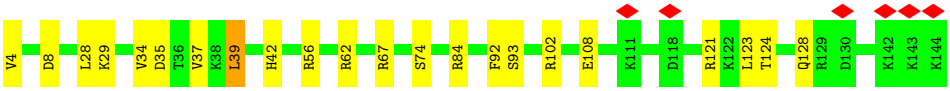




• Molecule 70: uS13




• Molecule 71: eS19

Chain TT:

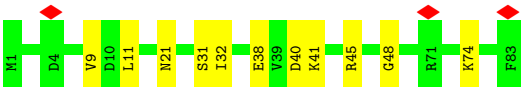

• Molecule 72: uS10

Chain UU:



• Molecule 73: eS21

Chain VV:

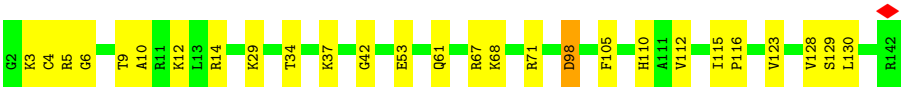

• Molecule 74: uS8

Chain WW:



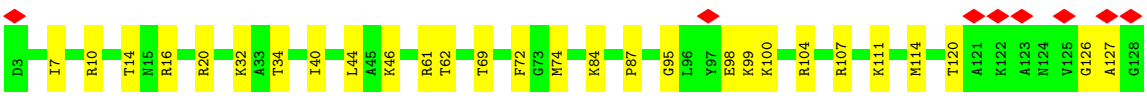
• Molecule 75: uS12

Chain XX:

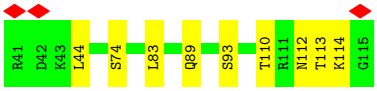

• Molecule 76: eS24

Chain YY:

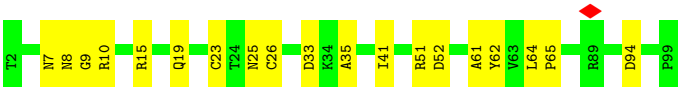

• Molecule 77: eS25

Chain ZZ:



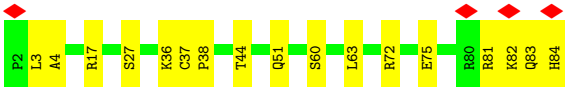

• Molecule 78: eS26

Chain aa:

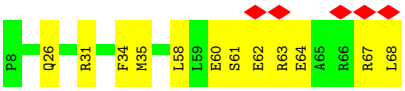

• Molecule 79: eS27

Chain bb:

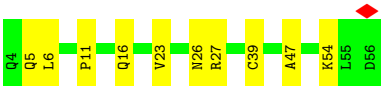

• Molecule 80: eS28

Chain cc:

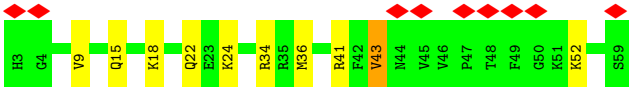

• Molecule 81: uS14

Chain dd:

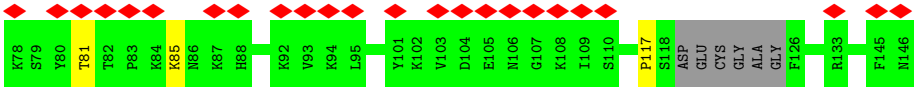

• Molecule 82: eS30

Chain ee:

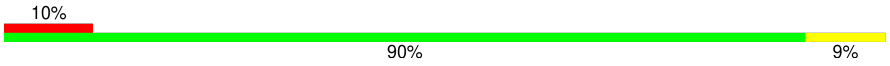

• Molecule 83: eS31

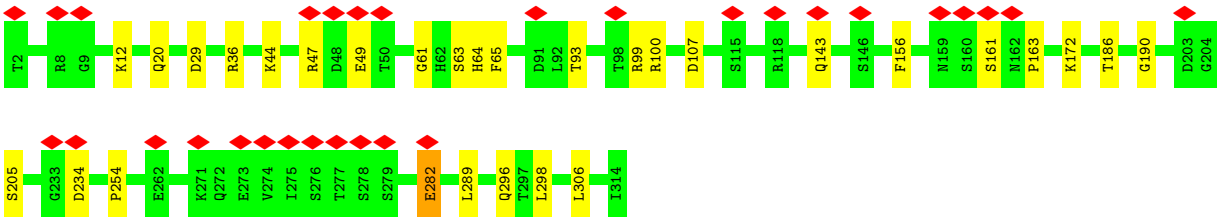
Chain ff:


• Molecule 84: RACK1

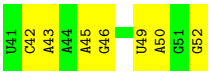
Chain gg:



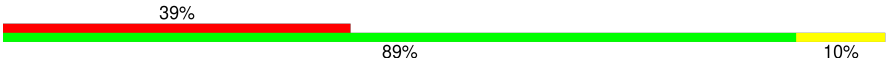

• Molecule 85: mRNA

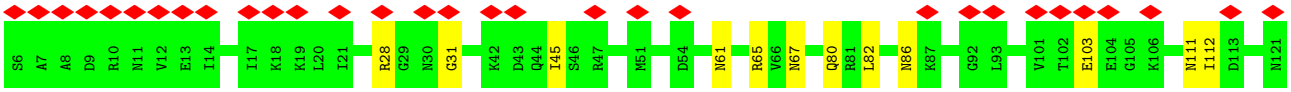
Chain hh:

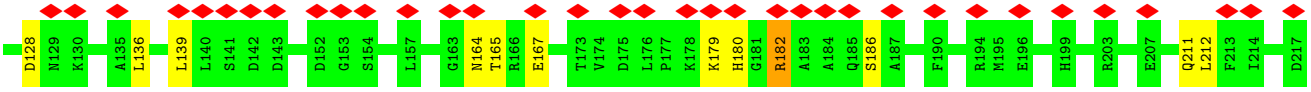



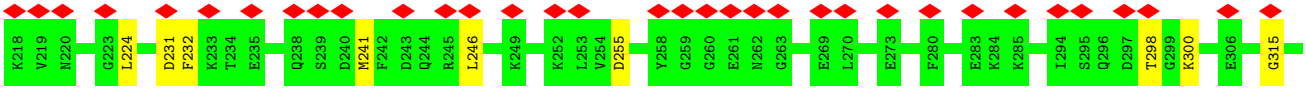

• Molecule 86: eRF1

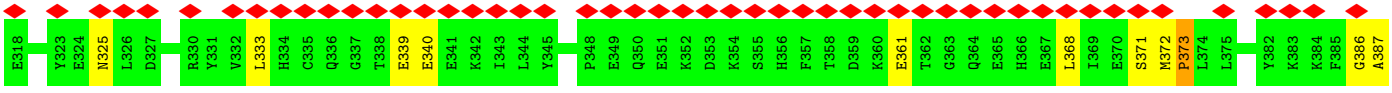
Chain ii:

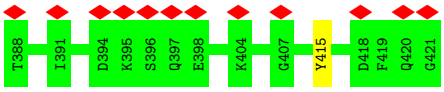


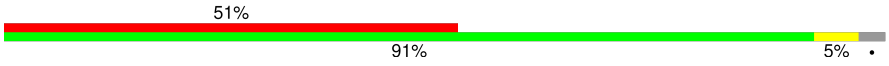



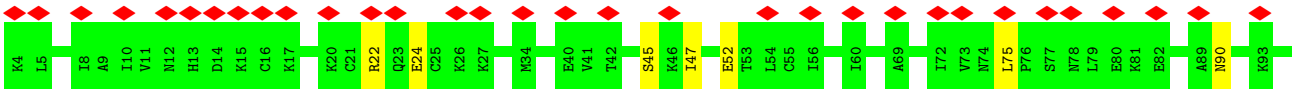



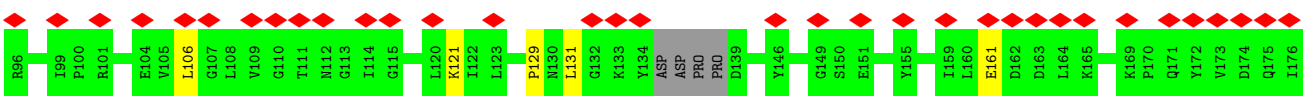



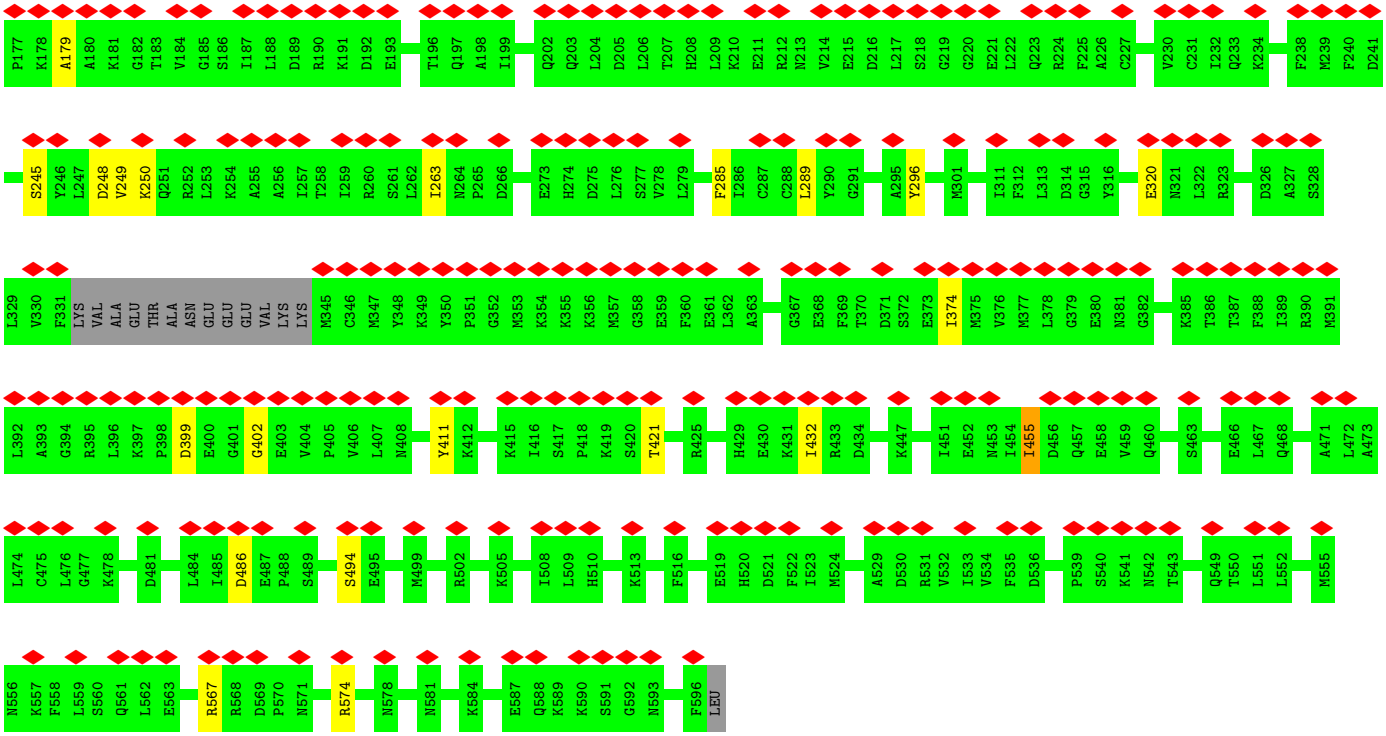

• Molecule 87: ABCE1

Chain jj:




P177 K178 A179 A180 K181 G182 T183 V184 G185 S186 I187 L188 D189 R190 K191 D192 E193 T196 Q197 A198 I199 Q202 Q203 L204 D205 L206 T207 H208 L209 K210 E211 R212 N213 V214 E215 D216 L217 S218 G219 G220 E221 L222 Q223 R224 F225 A226 C227 V230 C231 I232 Q233 K234 F238 M239 F240 D241
S245 Y246 L247 D248 V249 K250 Q251 R252 L253 K254 A255 A256 I257 T258 I259 R260 S261 L262 I263 N264 P265 D266 E273 H274 D275 L276 S277 V278 L279 F285 I286 C287 C288 L289 Y290 G291 A295 Y296 M301 I311 F312 L313 D314 G315 Y316 E320 N321 L322 R323 D326 A327 S328
L329 V330 F331 LYS VAL ALA GLU THR ALA ASN GLU GLU GLU VAL LYS LYS M345 C346 M347 Y348 K349 Y350 P351 G352 M353 K354 K355 K356 M357 G358 E359 F360 E361 L362 A363 G367 E368 F369 T370 D371 S372 E373 I374 M375 V376 M377 L378 G379 E380 N381 G382 K385 T386 T387 F388 I389 R390 M391
L392 A393 G394 R395 L396 K397 P398 D399 E400 G401 G402 E403 V404 P405 V406 L407 N408 Y411 K412 K415 I416 S417 P418 K419 S420 T421 R425 H429 E430 K431 I432 R433 D434 K447 I451 E452 N453 I454 I455 D456 Q457 E458 V459 Q460 S463 E466 L467 Q468 A471 L472 A473
L474 C475 L476 G477 K478 D481 L484 I485 D486 E487 P488 S489 S494 E495 M499 R502 K505 I508 L509 H510 K513 F516 E519 H520 D521 F522 I523 M524 A529 D530 R531 V532 I533 V534 F535 D536 P539 S540 K541 N542 T543 Q549 T550 L551 L552 M555
N556 K557 F558 L559 S560 Q561 L562 E563 R567 R568 D569 P570 N571 R574 N578 N581 K584 E587 Q588 K589 K590 S591 G592 N593 F596 LEU

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 20515 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 30 | Depositor |
| Minimum defocus (nm) | 1700 | Depositor |
| Maximum defocus (nm) | 3600 | Depositor |
| Magnification | 104478 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.528 | Depositor |
| Minimum map value | -0.315 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.017 | Depositor |
| Recommended contour level | 0.07 | Depositor |
| Map size (Å) | 562.8, 562.8, 562.8 | wwPDB |
| Map dimensions | 420, 420, 420 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.3399999, 1.3399999, 1.3399999 | 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: SF4, MG, ADP, ZN

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 | 0.46 | 0/1906 | 0.79 | 0/2556 |
| 2 | B | 0.40 | 0/3216 | 0.78 | 1/4311 (0.0%) |
| 3 | C | 0.43 | 0/2938 | 0.80 | 5/3946 (0.1%) |
| 4 | D | 0.37 | 0/2432 | 0.70 | 2/3257 (0.1%) |
| 5 | E | 0.46 | 0/1936 | 0.82 | 2/2600 (0.1%) |
| 6 | F | 0.40 | 0/1905 | 0.75 | 1/2539 (0.0%) |
| 7 | G | 0.38 | 0/1967 | 0.73 | 1/2647 (0.0%) |
| 8 | H | 0.37 | 0/1535 | 0.71 | 0/2063 |
| 9 | I | 0.41 | 0/1693 | 0.69 | 0/2260 |
| 10 | J | 0.38 | 0/1376 | 0.73 | 0/1841 |
| 11 | L | 0.41 | 0/1734 | 0.79 | 0/2317 |
| 12 | M | 0.37 | 0/1158 | 0.74 | 0/1547 |
| 13 | N | 0.43 | 0/1746 | 0.83 | 0/2338 |
| 14 | O | 0.40 | 0/1671 | 0.77 | 0/2234 |
| 15 | P | 0.42 | 0/1268 | 0.75 | 0/1701 |
| 16 | Q | 0.41 | 0/1530 | 0.81 | 1/2041 (0.0%) |
| 17 | R | 0.41 | 0/1524 | 0.79 | 0/2013 |
| 18 | S | 0.40 | 0/1493 | 0.85 | 3/2002 (0.1%) |
| 19 | T | 0.41 | 0/1326 | 0.72 | 0/1770 |
| 20 | U | 0.41 | 0/822 | 0.68 | 0/1103 |
| 21 | V | 0.40 | 0/993 | 0.73 | 0/1332 |
| 22 | W | 0.48 | 0/541 | 0.83 | 1/720 (0.1%) |
| 23 | X | 0.42 | 0/993 | 0.74 | 0/1334 |
| 24 | Y | 0.37 | 0/1132 | 0.80 | 2/1504 (0.1%) |
| 25 | Z | 0.39 | 0/1130 | 0.72 | 0/1507 |
| 26 | a | 0.40 | 0/1191 | 0.79 | 0/1590 |
| 27 | b | 0.44 | 0/619 | 0.73 | 0/818 |
| 28 | c | 0.36 | 0/742 | 0.69 | 0/996 |
| 29 | d | 0.38 | 0/903 | 0.81 | 1/1216 (0.1%) |
| 30 | e | 0.47 | 0/1071 | 0.85 | 0/1429 |
| 31 | f | 0.52 | 0/895 | 0.87 | 0/1198 |
| 32 | g | 0.42 | 0/916 | 0.81 | 1/1220 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | h | 0.36 | 0/1021 | 0.77 | 1/1348 (0.1%) |
| 34 | i | 0.40 | 0/841 | 0.82 | 2/1112 (0.2%) |
| 35 | j | 0.45 | 0/720 | 0.93 | 1/952 (0.1%) |
| 36 | k | 0.37 | 0/575 | 0.68 | 0/761 |
| 37 | l | 0.50 | 0/454 | 0.84 | 0/599 |
| 38 | m | 0.37 | 0/435 | 0.76 | 0/575 |
| 39 | n | 0.41 | 0/223 | 0.91 | 0/284 |
| 40 | o | 0.39 | 0/864 | 0.75 | 0/1140 |
| 41 | p | 0.42 | 0/718 | 0.71 | 0/953 |
| 42 | r | 0.48 | 0/1017 | 0.80 | 1/1364 (0.1%) |
| 43 | s | 0.38 | 0/1547 | 0.58 | 0/2088 |
| 44 | t | 0.41 | 0/1257 | 0.69 | 0/1697 |
| 45 | 1 | 0.45 | 0/129 | 0.72 | 0/173 |
| 46 | 2 | 0.26 | 0/1805 | 0.72 | 1/2809 (0.0%) |
| 47 | 3 | 0.36 | 0/1777 | 0.97 | 10/2763 (0.4%) |
| 48 | 5 | 0.37 | 4/87790 (0.0%) | 0.79 | 75/136937 (0.1%) |
| 49 | 7 | 0.30 | 0/2858 | 0.69 | 0/4455 |
| 50 | 8 | 0.36 | 0/3701 | 0.74 | 0/5766 |
| 51 | 9 | 0.32 | 1/41013 (0.0%) | 0.79 | 45/63919 (0.1%) |
| 52 | AA | 0.36 | 0/1679 | 0.70 | 0/2283 |
| 53 | BB | 0.38 | 0/1756 | 0.77 | 4/2350 (0.2%) |
| 54 | CC | 0.41 | 0/1730 | 0.76 | 1/2344 (0.0%) |
| 55 | DD | 0.37 | 0/1792 | 0.72 | 0/2412 |
| 56 | EE | 0.39 | 0/2115 | 0.78 | 0/2843 |
| 57 | FF | 0.49 | 0/1531 | 0.78 | 1/2059 (0.0%) |
| 58 | GG | 0.37 | 0/1946 | 0.78 | 0/2590 |
| 59 | HH | 0.44 | 0/1544 | 0.72 | 1/2068 (0.0%) |
| 60 | II | 0.41 | 0/1715 | 0.78 | 0/2287 |
| 61 | JJ | 0.41 | 0/1550 | 0.88 | 4/2069 (0.2%) |
| 62 | KK | 0.47 | 0/851 | 0.73 | 0/1147 |
| 63 | LL | 0.40 | 0/1259 | 0.78 | 0/1684 |
| 64 | MM | 0.42 | 0/968 | 0.64 | 0/1296 |
| 65 | NN | 0.39 | 0/1232 | 0.77 | 0/1656 |
| 66 | OO | 0.42 | 0/1029 | 0.88 | 1/1380 (0.1%) |
| 67 | PP | 0.39 | 0/1079 | 0.76 | 0/1437 |
| 68 | QQ | 0.37 | 0/1142 | 0.70 | 0/1528 |
| 69 | RR | 0.42 | 0/1060 | 0.71 | 0/1421 |
| 70 | SS | 0.38 | 0/1157 | 0.84 | 1/1548 (0.1%) |
| 71 | TT | 0.43 | 0/1120 | 0.78 | 2/1499 (0.1%) |
| 72 | UU | 0.36 | 0/831 | 0.71 | 0/1115 |
| 73 | VV | 0.39 | 0/645 | 0.75 | 0/865 |
| 74 | WW | 0.38 | 0/1051 | 0.79 | 0/1406 |
| 75 | XX | 0.38 | 0/1116 | 0.80 | 0/1490 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | YY | 0.39 | 0/1040 | 0.74 | 0/1382 |
| 77 | ZZ | 0.37 | 0/604 | 0.75 | 0/810 |
| 78 | aa | 0.39 | 0/794 | 0.83 | 0/1065 |
| 79 | bb | 0.37 | 0/665 | 0.67 | 0/891 |
| 80 | cc | 0.36 | 0/478 | 0.78 | 0/640 |
| 81 | dd | 0.40 | 0/455 | 0.80 | 0/603 |
| 82 | ee | 0.46 | 0/462 | 0.75 | 0/607 |
| 83 | ff | 0.39 | 0/531 | 0.62 | 0/703 |
| 84 | gg | 0.37 | 0/2493 | 0.65 | 0/3394 |
| 85 | hh | 0.29 | 0/287 | 0.76 | 0/445 |
| 86 | ii | 0.39 | 0/3333 | 0.63 | 2/4483 (0.0%) |
| 87 | jj | 0.47 | 1/4625 (0.0%) | 0.58 | 0/6238 |
| All | All | 0.38 | 6/242712 (0.0%) | 0.78 | 174/355683 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 2 | B | 0 | 4 |
| 3 | C | 0 | 2 |
| 4 | D | 0 | 1 |
| 5 | E | 0 | 1 |
| 7 | G | 0 | 1 |
| 9 | I | 0 | 2 |
| 11 | L | 0 | 3 |
| 17 | R | 0 | 1 |
| 18 | S | 0 | 2 |
| 19 | T | 0 | 1 |
| 20 | U | 0 | 1 |
| 24 | Y | 0 | 1 |
| 31 | f | 0 | 1 |
| 42 | r | 0 | 2 |
| 48 | 5 | 0 | 1 |
| 51 | 9 | 0 | 1 |
| 52 | AA | 0 | 1 |
| 56 | EE | 0 | 2 |
| 57 | FF | 0 | 2 |
| 59 | HH | 0 | 1 |
| 60 | II | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 61 | JJ | 0 | 2 |
| 66 | OO | 0 | 1 |
| 68 | QQ | 0 | 1 |
| 70 | SS | 0 | 1 |
| 71 | TT | 0 | 1 |
| 72 | UU | 0 | 2 |
| 73 | VV | 0 | 1 |
| 74 | WW | 0 | 2 |
| 75 | XX | 0 | 1 |
| 78 | aa | 0 | 1 |
| 86 | ii | 0 | 3 |
| All | All | 0 | 49 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 5 | 1965 | G | O3'-P | -23.01 | 1.33 | 1.61 |
| 87 | jj | 121 | LYS | CE-NZ | 19.94 | 1.99 | 1.49 |
| 51 | 9 | 908 | A | O3'-P | 8.98 | 1.72 | 1.61 |
| 48 | 5 | 1847 | C | O3'-P | -6.16 | 1.53 | 1.61 |
| 48 | 5 | 957 | G | O3'-P | 5.62 | 1.67 | 1.61 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 51 | 9 | 909 | G | O5'-P-OP2 | -16.21 | 91.11 | 105.70 |
| 47 | 3 | 70 | G | N9-C1'-C2' | -13.18 | 96.87 | 114.00 |
| 48 | 5 | 3753 | G | N9-C1'-C2' | -11.91 | 98.52 | 114.00 |
| 51 | 9 | 1235 | G | N9-C1'-C2' | -11.46 | 99.11 | 114.00 |
| 48 | 5 | 3718 | A | N9-C1'-C2' | -10.30 | 100.61 | 114.00 |

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 196 | TRP | Peptide |
| 2 | B | 17 | LEU | Peptide |
| 2 | B | 257 | TRP | Peptide |
| 2 | B | 258 | HIS | Peptide |
| 2 | B | 351 | LEU | Peptide |

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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 | 242/244 (99%) | 209 (86%) | 28 (12%) | 5 (2%) | 5 32 |
| 2 | B | 392/394 (100%) | 345 (88%) | 42 (11%) | 5 (1%) | 10 41 |
| 3 | C | 360/362 (99%) | 322 (89%) | 27 (8%) | 11 (3%) | 3 26 |
| 4 | D | 290/292 (99%) | 262 (90%) | 25 (9%) | 3 (1%) | 13 46 |
| 5 | E | 232/248 (94%) | 179 (77%) | 36 (16%) | 17 (7%) | 1 10 |
| 6 | F | 223/225 (99%) | 204 (92%) | 17 (8%) | 2 (1%) | 14 48 |
| 7 | G | 239/241 (99%) | 203 (85%) | 31 (13%) | 5 (2%) | 5 32 |
| 8 | H | 188/190 (99%) | 165 (88%) | 20 (11%) | 3 (2%) | 8 37 |
| 9 | I | 200/213 (94%) | 181 (90%) | 15 (8%) | 4 (2%) | 6 33 |
| 10 | J | 167/169 (99%) | 147 (88%) | 13 (8%) | 7 (4%) | 2 19 |
| 11 | L | 208/210 (99%) | 180 (86%) | 16 (8%) | 12 (6%) | 1 13 |
| 12 | M | 136/138 (99%) | 123 (90%) | 12 (9%) | 1 (1%) | 19 53 |
| 13 | N | 201/203 (99%) | 181 (90%) | 20 (10%) | 0 | 100 100 |
| 14 | O | 197/199 (99%) | 184 (93%) | 12 (6%) | 1 (0%) | 25 59 |
| 15 | P | 151/153 (99%) | 135 (89%) | 16 (11%) | 0 | 100 100 |
| 16 | Q | 185/187 (99%) | 169 (91%) | 14 (8%) | 2 (1%) | 12 44 |
| 17 | R | 178/180 (99%) | 166 (93%) | 9 (5%) | 3 (2%) | 7 36 |
| 18 | S | 173/175 (99%) | 157 (91%) | 12 (7%) | 4 (2%) | 5 31 |
| 19 | T | 157/159 (99%) | 139 (88%) | 15 (10%) | 3 (2%) | 6 34 |
| 20 | U | 97/99 (98%) | 82 (84%) | 11 (11%) | 4 (4%) | 2 20 |
| 21 | V | 129/131 (98%) | 115 (89%) | 13 (10%) | 1 (1%) | 16 50 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 22 | W | 61/63 (97%) | 56 (92%) | 4 (7%) | 1 (2%) | 8 37 |
| 23 | X | 117/119 (98%) | 109 (93%) | 6 (5%) | 2 (2%) | 7 36 |
| 24 | Y | 132/134 (98%) | 114 (86%) | 17 (13%) | 1 (1%) | 16 50 |
| 25 | Z | 133/135 (98%) | 113 (85%) | 13 (10%) | 7 (5%) | 1 15 |
| 26 | a | 145/147 (99%) | 122 (84%) | 19 (13%) | 4 (3%) | 4 27 |
| 27 | b | 73/75 (97%) | 67 (92%) | 5 (7%) | 1 (1%) | 9 40 |
| 28 | c | 92/94 (98%) | 89 (97%) | 3 (3%) | 0 | 100 100 |
| 29 | d | 105/107 (98%) | 91 (87%) | 13 (12%) | 1 (1%) | 13 46 |
| 30 | e | 126/128 (98%) | 115 (91%) | 6 (5%) | 5 (4%) | 2 20 |
| 31 | f | 107/109 (98%) | 94 (88%) | 8 (8%) | 5 (5%) | 2 17 |
| 32 | g | 112/114 (98%) | 103 (92%) | 8 (7%) | 1 (1%) | 14 48 |
| 33 | h | 120/122 (98%) | 107 (89%) | 9 (8%) | 4 (3%) | 3 25 |
| 34 | i | 100/102 (98%) | 92 (92%) | 6 (6%) | 2 (2%) | 6 33 |
| 35 | j | 84/86 (98%) | 70 (83%) | 9 (11%) | 5 (6%) | 1 13 |
| 36 | k | 67/69 (97%) | 56 (84%) | 7 (10%) | 4 (6%) | 1 13 |
| 37 | l | 48/50 (96%) | 40 (83%) | 7 (15%) | 1 (2%) | 5 32 |
| 38 | m | 50/52 (96%) | 44 (88%) | 6 (12%) | 0 | 100 100 |
| 39 | n | 21/23 (91%) | 21 (100%) | 0 | 0 | 100 100 |
| 40 | o | 102/104 (98%) | 92 (90%) | 7 (7%) | 3 (3%) | 3 27 |
| 41 | p | 89/91 (98%) | 80 (90%) | 8 (9%) | 1 (1%) | 12 44 |
| 42 | r | 123/125 (98%) | 102 (83%) | 14 (11%) | 7 (6%) | 1 14 |
| 43 | s | 196/198 (99%) | 164 (84%) | 22 (11%) | 10 (5%) | 1 16 |
| 44 | t | 161/163 (99%) | 102 (63%) | 33 (20%) | 26 (16%) | 0 2 |
| 45 | 1 | 13/15 (87%) | 11 (85%) | 0 | 2 (15%) | 0 2 |
| 52 | AA | 206/208 (99%) | 173 (84%) | 23 (11%) | 10 (5%) | 2 16 |
| 53 | BB | 211/213 (99%) | 165 (78%) | 33 (16%) | 13 (6%) | 1 12 |
| 54 | CC | 216/218 (99%) | 184 (85%) | 26 (12%) | 6 (3%) | 4 27 |
| 55 | DD | 225/227 (99%) | 181 (80%) | 33 (15%) | 11 (5%) | 2 16 |
| 56 | EE | 260/262 (99%) | 200 (77%) | 42 (16%) | 18 (7%) | 1 10 |
| 57 | FF | 189/191 (99%) | 160 (85%) | 21 (11%) | 8 (4%) | 2 19 |
| 58 | GG | 235/237 (99%) | 198 (84%) | 31 (13%) | 6 (3%) | 4 29 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 59 | HH | 187/189 (99%) | 148 (79%) | 25 (13%) | 14 (8%) | 1 9 |
| 60 | II | 204/206 (99%) | 168 (82%) | 28 (14%) | 8 (4%) | 2 21 |
| 61 | JJ | 183/185 (99%) | 153 (84%) | 20 (11%) | 10 (6%) | 1 14 |
| 62 | KK | 96/98 (98%) | 65 (68%) | 21 (22%) | 10 (10%) | 0 6 |
| 63 | LL | 150/152 (99%) | 125 (83%) | 19 (13%) | 6 (4%) | 2 20 |
| 64 | MM | 122/124 (98%) | 87 (71%) | 28 (23%) | 7 (6%) | 1 14 |
| 65 | NN | 148/150 (99%) | 126 (85%) | 17 (12%) | 5 (3%) | 3 24 |
| 66 | OO | 134/136 (98%) | 99 (74%) | 21 (16%) | 14 (10%) | 0 6 |
| 67 | PP | 125/127 (98%) | 107 (86%) | 15 (12%) | 3 (2%) | 5 30 |
| 68 | QQ | 139/141 (99%) | 116 (84%) | 18 (13%) | 5 (4%) | 3 23 |
| 69 | RR | 127/129 (98%) | 106 (84%) | 15 (12%) | 6 (5%) | 2 17 |
| 70 | SS | 135/137 (98%) | 114 (84%) | 16 (12%) | 5 (4%) | 2 22 |
| 71 | TT | 139/141 (99%) | 126 (91%) | 10 (7%) | 3 (2%) | 5 32 |
| 72 | UU | 102/104 (98%) | 87 (85%) | 9 (9%) | 6 (6%) | 1 13 |
| 73 | VV | 81/83 (98%) | 67 (83%) | 10 (12%) | 4 (5%) | 2 16 |
| 74 | WW | 127/129 (98%) | 106 (84%) | 16 (13%) | 5 (4%) | 2 21 |
| 75 | XX | 139/141 (99%) | 118 (85%) | 13 (9%) | 8 (6%) | 1 13 |
| 76 | YY | 124/126 (98%) | 99 (80%) | 17 (14%) | 8 (6%) | 1 12 |
| 77 | ZZ | 73/75 (97%) | 59 (81%) | 12 (16%) | 2 (3%) | 4 28 |
| 78 | aa | 96/98 (98%) | 73 (76%) | 13 (14%) | 10 (10%) | 0 6 |
| 79 | bb | 81/83 (98%) | 61 (75%) | 16 (20%) | 4 (5%) | 2 16 |
| 80 | cc | 59/61 (97%) | 47 (80%) | 10 (17%) | 2 (3%) | 3 24 |
| 81 | dd | 51/53 (96%) | 45 (88%) | 3 (6%) | 3 (6%) | 1 13 |
| 82 | ee | 55/57 (96%) | 40 (73%) | 12 (22%) | 3 (6%) | 1 14 |
| 83 | ff | 58/68 (85%) | 50 (86%) | 6 (10%) | 2 (3%) | 3 24 |
| 84 | gg | 311/313 (99%) | 269 (86%) | 33 (11%) | 9 (3%) | 3 27 |
| 86 | ii | 414/416 (100%) | 380 (92%) | 26 (6%) | 8 (2%) | 6 34 |
| 87 | jj | 568/594 (96%) | 513 (90%) | 41 (7%) | 14 (2%) | 4 29 |
| All | All | 12492/12709 (98%) | 10717 (86%) | 1333 (11%) | 442 (4%) | 5 24 |

5 of 442 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 196 | TRP |
| 3 | C | 273 | LEU |
| 5 | E | 91 | PRO |
| 5 | E | 95 | ASP |
| 5 | E | 118 | PRO |

### 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 | 187/187 (100%) | 161 (86%) | 26 (14%) | 3 17 |
| 2 | B | 336/342 (98%) | 291 (87%) | 45 (13%) | 3 18 |
| 3 | C | 302/302 (100%) | 260 (86%) | 42 (14%) | 3 17 |
| 4 | D | 247/247 (100%) | 218 (88%) | 29 (12%) | 4 22 |
| 5 | E | 208/221 (94%) | 185 (89%) | 23 (11%) | 5 24 |
| 6 | F | 194/195 (100%) | 165 (85%) | 29 (15%) | 2 15 |
| 7 | G | 206/206 (100%) | 182 (88%) | 24 (12%) | 4 22 |
| 8 | H | 169/169 (100%) | 148 (88%) | 21 (12%) | 4 20 |
| 9 | I | 174/180 (97%) | 153 (88%) | 21 (12%) | 4 20 |
| 10 | J | 142/142 (100%) | 126 (89%) | 16 (11%) | 4 23 |
| 11 | L | 176/176 (100%) | 145 (82%) | 31 (18%) | 1 8 |
| 12 | M | 117/117 (100%) | 102 (87%) | 15 (13%) | 3 19 |
| 13 | N | 171/171 (100%) | 152 (89%) | 19 (11%) | 5 24 |
| 14 | O | 171/171 (100%) | 144 (84%) | 27 (16%) | 2 13 |
| 15 | P | 134/134 (100%) | 120 (90%) | 14 (10%) | 5 26 |
| 16 | Q | 163/163 (100%) | 145 (89%) | 18 (11%) | 5 24 |
| 17 | R | 159/159 (100%) | 140 (88%) | 19 (12%) | 4 21 |
| 18 | S | 156/156 (100%) | 132 (85%) | 24 (15%) | 2 14 |
| 19 | T | 139/139 (100%) | 122 (88%) | 17 (12%) | 4 20 |
| 20 | U | 89/89 (100%) | 82 (92%) | 7 (8%) | 10 35 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 21 | V | 101/101 (100%) | 84 (83%) | 17 (17%) | 1 10 |
| 22 | W | 55/55 (100%) | 50 (91%) | 5 (9%) | 7 30 |
| 23 | X | 107/107 (100%) | 97 (91%) | 10 (9%) | 7 30 |
| 24 | Y | 124/124 (100%) | 107 (86%) | 17 (14%) | 3 17 |
| 25 | Z | 117/117 (100%) | 109 (93%) | 8 (7%) | 13 41 |
| 26 | a | 119/119 (100%) | 107 (90%) | 12 (10%) | 6 27 |
| 27 | b | 62/62 (100%) | 57 (92%) | 5 (8%) | 9 34 |
| 28 | c | 79/79 (100%) | 66 (84%) | 13 (16%) | 2 11 |
| 29 | d | 98/98 (100%) | 82 (84%) | 16 (16%) | 2 11 |
| 30 | e | 114/114 (100%) | 99 (87%) | 15 (13%) | 3 18 |
| 31 | f | 88/88 (100%) | 76 (86%) | 12 (14%) | 3 18 |
| 32 | g | 98/98 (100%) | 83 (85%) | 15 (15%) | 2 14 |
| 33 | h | 109/109 (100%) | 97 (89%) | 12 (11%) | 5 24 |
| 34 | i | 86/86 (100%) | 81 (94%) | 5 (6%) | 17 45 |
| 35 | j | 73/73 (100%) | 62 (85%) | 11 (15%) | 2 14 |
| 36 | k | 64/64 (100%) | 56 (88%) | 8 (12%) | 3 20 |
| 37 | l | 47/47 (100%) | 40 (85%) | 7 (15%) | 2 15 |
| 38 | m | 48/48 (100%) | 39 (81%) | 9 (19%) | 1 7 |
| 39 | n | 22/22 (100%) | 18 (82%) | 4 (18%) | 1 7 |
| 40 | o | 92/92 (100%) | 79 (86%) | 13 (14%) | 3 17 |
| 41 | p | 74/74 (100%) | 68 (92%) | 6 (8%) | 9 34 |
| 42 | r | 109/109 (100%) | 88 (81%) | 21 (19%) | 1 6 |
| 43 | s | 166/166 (100%) | 155 (93%) | 11 (7%) | 14 42 |
| 44 | t | 136/136 (100%) | 128 (94%) | 8 (6%) | 16 45 |
| 45 | 1 | 13/13 (100%) | 12 (92%) | 1 (8%) | 10 36 |
| 52 | AA | 174/174 (100%) | 152 (87%) | 22 (13%) | 3 19 |
| 53 | BB | 194/194 (100%) | 169 (87%) | 25 (13%) | 3 19 |
| 54 | CC | 183/183 (100%) | 155 (85%) | 28 (15%) | 2 14 |
| 55 | DD | 190/190 (100%) | 168 (88%) | 22 (12%) | 4 22 |
| 56 | EE | 223/223 (100%) | 183 (82%) | 40 (18%) | 1 8 |
| 57 | FF | 161/161 (100%) | 126 (78%) | 35 (22%) | 1 4 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 58 | GG | 207/207 (100%) | 179 (86%) | 28 (14%) | 3 18 |
| 59 | HH | 169/169 (100%) | 151 (89%) | 18 (11%) | 5 25 |
| 60 | II | 178/178 (100%) | 155 (87%) | 23 (13%) | 3 19 |
| 61 | JJ | 161/161 (100%) | 141 (88%) | 20 (12%) | 4 20 |
| 62 | KK | 89/89 (100%) | 76 (85%) | 13 (15%) | 2 16 |
| 63 | LL | 136/136 (100%) | 110 (81%) | 26 (19%) | 1 6 |
| 64 | MM | 104/104 (100%) | 85 (82%) | 19 (18%) | 1 7 |
| 65 | NN | 130/130 (100%) | 108 (83%) | 22 (17%) | 1 10 |
| 66 | OO | 106/106 (100%) | 81 (76%) | 25 (24%) | 0 3 |
| 67 | PP | 116/116 (100%) | 98 (84%) | 18 (16%) | 2 13 |
| 68 | QQ | 117/117 (100%) | 102 (87%) | 15 (13%) | 3 19 |
| 69 | RR | 117/117 (100%) | 102 (87%) | 15 (13%) | 3 19 |
| 70 | SS | 119/119 (100%) | 100 (84%) | 19 (16%) | 2 12 |
| 71 | TT | 112/112 (100%) | 94 (84%) | 18 (16%) | 2 12 |
| 72 | UU | 94/94 (100%) | 79 (84%) | 15 (16%) | 2 12 |
| 73 | VV | 67/67 (100%) | 61 (91%) | 6 (9%) | 8 31 |
| 74 | WW | 112/112 (100%) | 99 (88%) | 13 (12%) | 4 22 |
| 75 | XX | 113/113 (100%) | 94 (83%) | 19 (17%) | 1 10 |
| 76 | YY | 108/108 (100%) | 88 (82%) | 20 (18%) | 1 7 |
| 77 | ZZ | 66/66 (100%) | 59 (89%) | 7 (11%) | 5 25 |
| 78 | aa | 85/85 (100%) | 77 (91%) | 8 (9%) | 7 29 |
| 79 | bb | 75/75 (100%) | 62 (83%) | 13 (17%) | 1 9 |
| 80 | cc | 54/54 (100%) | 44 (82%) | 10 (18%) | 1 7 |
| 81 | dd | 47/47 (100%) | 40 (85%) | 7 (15%) | 2 15 |
| 82 | ee | 47/47 (100%) | 39 (83%) | 8 (17%) | 1 10 |
| 83 | ff | 58/61 (95%) | 57 (98%) | 1 (2%) | 56 75 |
| 84 | gg | 272/272 (100%) | 250 (92%) | 22 (8%) | 9 34 |
| 86 | ii | 358/358 (100%) | 324 (90%) | 34 (10%) | 7 29 |
| 87 | jj | 506/522 (97%) | 487 (96%) | 19 (4%) | 28 58 |
| All | All | 10889/10934 (100%) | 9508 (87%) | 1381 (13%) | 6 19 |

5 of 1381 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 58 | GG | 227 | GLN |
| 70 | SS | 17 | ASN |
| 60 | II | 82 | VAL |
| 58 | GG | 224 | ARG |
| 64 | MM | 78 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 217 | GLN |
| 7 | G | 29 | ASN |
| 42 | r | 103 | HIS |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 46 | 2 | 74/76 (97%) | 20 (27%) | 1 (1%) |
| 47 | 3 | 72/75 (96%) | 36 (50%) | 7 (9%) |
| 48 | 5 | 3645/3662 (99%) | 1179 (32%) | 269 (7%) |
| 49 | 7 | 119/120 (99%) | 19 (15%) | 1 (0%) |
| 50 | 8 | 155/156 (99%) | 52 (33%) | 6 (3%) |
| 51 | 9 | 1711/1719 (99%) | 608 (35%) | 129 (7%) |
| 85 | hh | 11/12 (91%) | 7 (63%) | 0 |
| All | All | 5787/5820 (99%) | 1921 (33%) | 413 (7%) |

5 of 1921 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | 2 | 7 | G |
| 46 | 2 | 8 | U |
| 46 | 2 | 9 | A |
| 46 | 2 | 13 | U |
| 46 | 2 | 16 | C |

5 of 413 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | 5 | 4124 | G |
| 51 | 9 | 3 | C |
| 51 | 9 | 1646 | C |
| 48 | 5 | 4378 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | 5 | 4889 | G |

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 207 ligands modelled in this entry, 203 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 90 | SF4 | jj | 600 | 87 | 0,12,12 | - | - | - | | |
| 91 | ADP | jj | 602 | - | 24,29,29 | 1.04 | 3 (12%) | 29,45,45 | 1.29 | 2 (6%) |
| 90 | SF4 | jj | 601 | 87 | 0,12,12 | - | - | - | | |
| 91 | ADP | jj | 603 | - | 24,29,29 | 1.03 | 3 (12%) | 29,45,45 | 1.29 | 2 (6%) |

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 |
|---|---|---|---|---|---|---|---|
| 90 | SF4 | jj | 600 | 87 | - | - | 0/6/5/5 |
| 91 | ADP | jj | 602 | - | - | 1/12/32/32 | 0/3/3/3 |
| 90 | SF4 | jj | 601 | 87 | - | - | 0/6/5/5 |
| 91 | ADP | jj | 603 | - | - | 1/12/32/32 | 0/3/3/3 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 91 | jj | 603 | ADP | C2-N3 | 2.39 | 1.35 | 1.32 |
| 91 | jj | 602 | ADP | C2-N3 | 2.29 | 1.35 | 1.32 |
| 91 | jj | 602 | ADP | PA-O3A | 2.27 | 1.61 | 1.59 |
| 91 | jj | 602 | ADP | O4'-C1' | 2.14 | 1.43 | 1.40 |
| 91 | jj | 603 | ADP | PA-O3A | 2.13 | 1.61 | 1.59 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 91 | jj | 602 | ADP | N3-C2-N1 | -4.33 | 122.80 | 128.67 |
| 91 | jj | 603 | ADP | N3-C2-N1 | -4.32 | 122.81 | 128.67 |
| 91 | jj | 603 | ADP | C4-C5-N7 | -2.74 | 106.45 | 109.34 |
| 91 | jj | 602 | ADP | C4-C5-N7 | -2.74 | 106.45 | 109.34 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

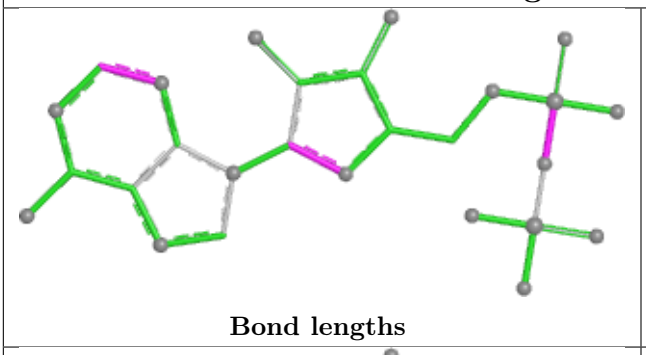
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 91 | jj | 603 | ADP | O4'-C4'-C5'-O5' |
| 91 | jj | 602 | ADP | PB-O3A-PA-O1A |

There are no ring outliers.

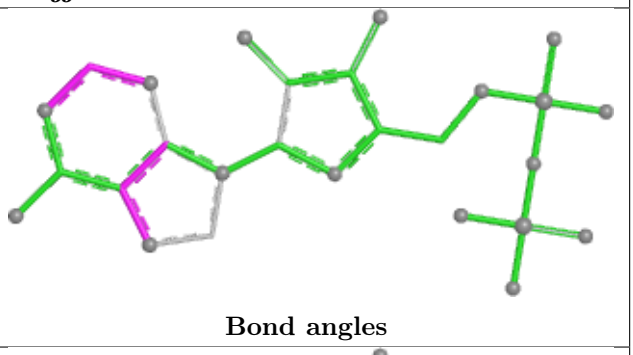
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

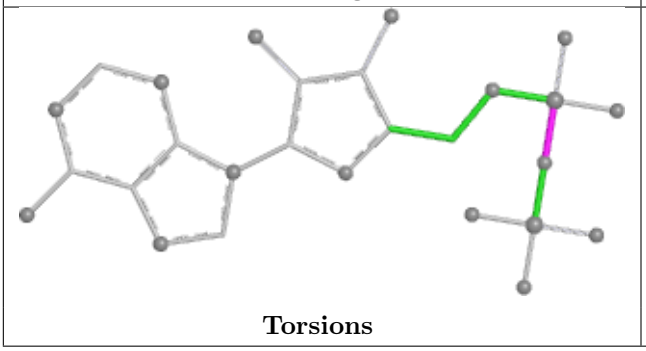
**Ligand ADP jj 602**



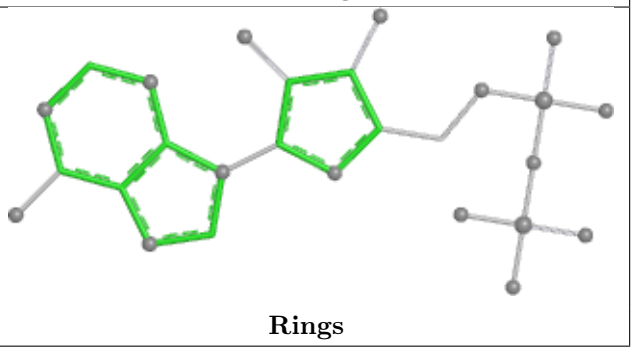
Bond lengths



Bond angles

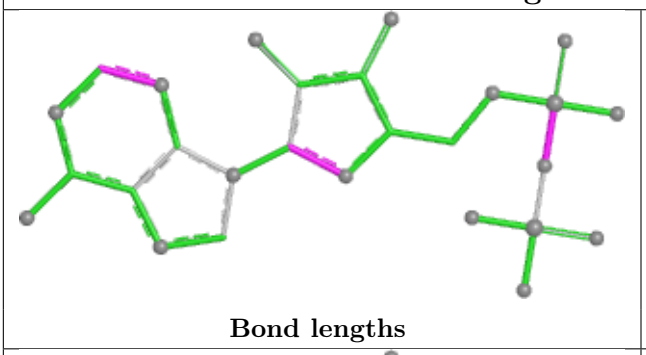


Torsions

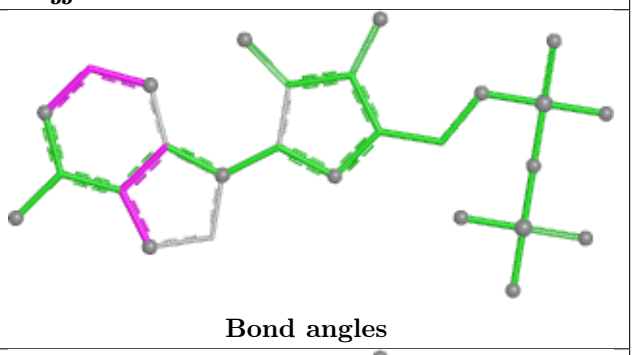


Rings

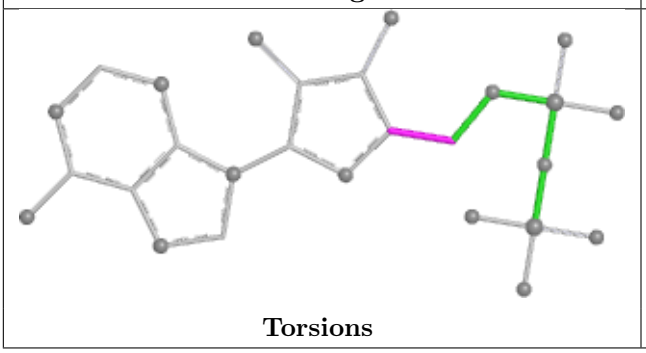
**Ligand ADP jj 603**



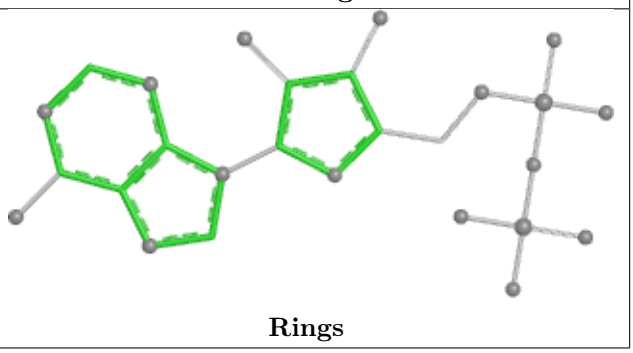
Bond lengths



Bond angles



Torsions



Rings

## 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 |
|---|---|---|
| 48 | 5 | 17 |
| 51 | 9 | 8 |
| 47 | 3 | 2 |
| 46 | 2 | 1 |
| 87 | jj | 1 |

The worst 5 of 29 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | 9 | 753:C | O3' | 785:C | P | 23.16 |
| 1 | 9 | 126:G | O3' | 139:C | P | 22.33 |
| 1 | 9 | 698:G | O3' | 730:C | P | 19.62 |
| 1 | 5 | 4776:G | O3' | 4859:C | P | 17.95 |
| 1 | 9 | 1761:U | O3' | 1771:G | P | 17.55 |

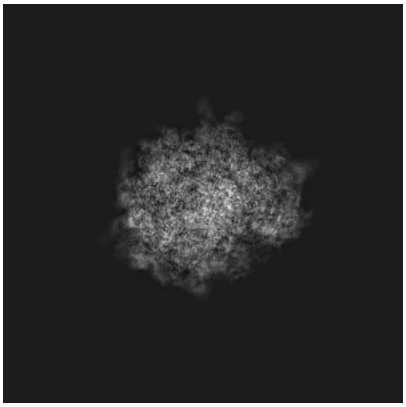
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3039. These allow visual inspection of the internal detail of the map and identification of artifacts.

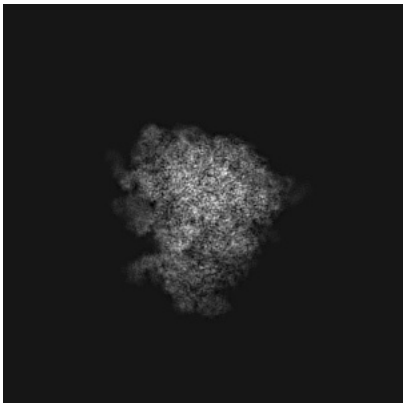
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

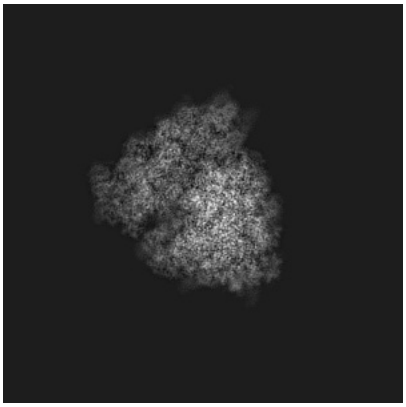
### 6.1.1 Primary map



X



Y

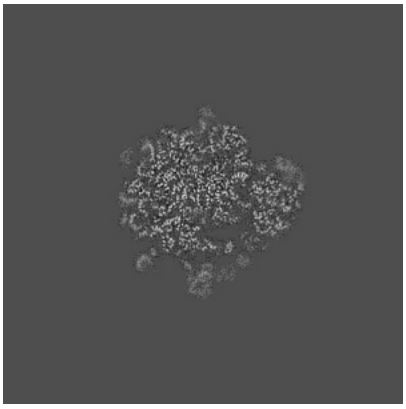


Z

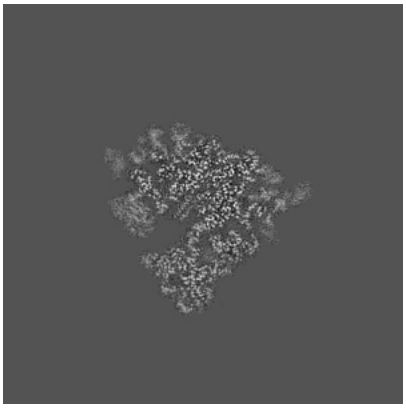
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

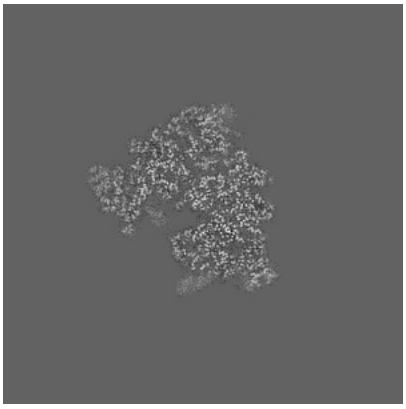
### 6.2.1 Primary map



X Index: 210



Y Index: 210

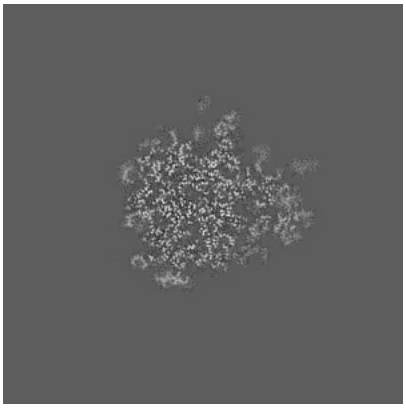


Z Index: 210

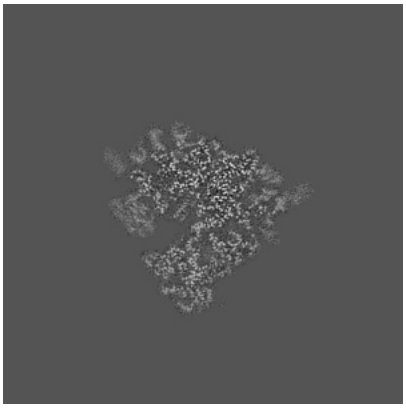
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

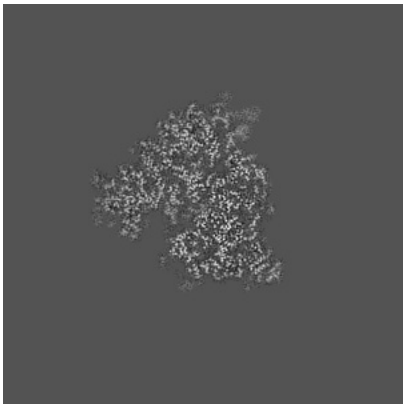
### 6.3.1 Primary map



X Index: 228



Y Index: 211

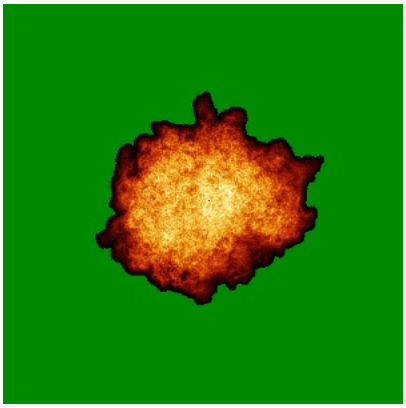


Z Index: 203

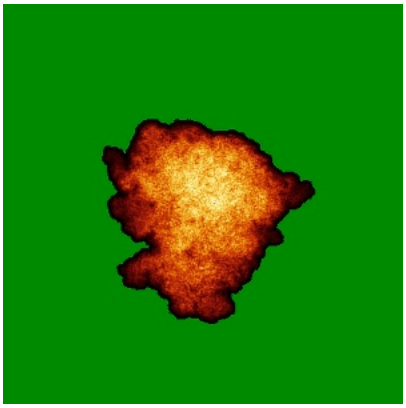
The images above show the largest variance slices of the map in three orthogonal directions.

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

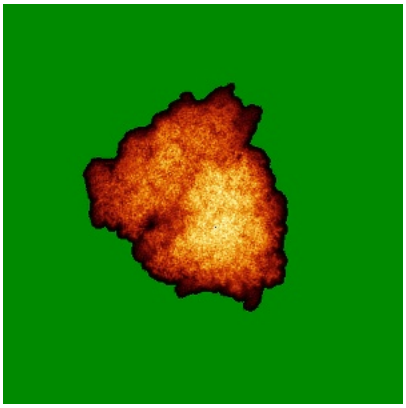
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

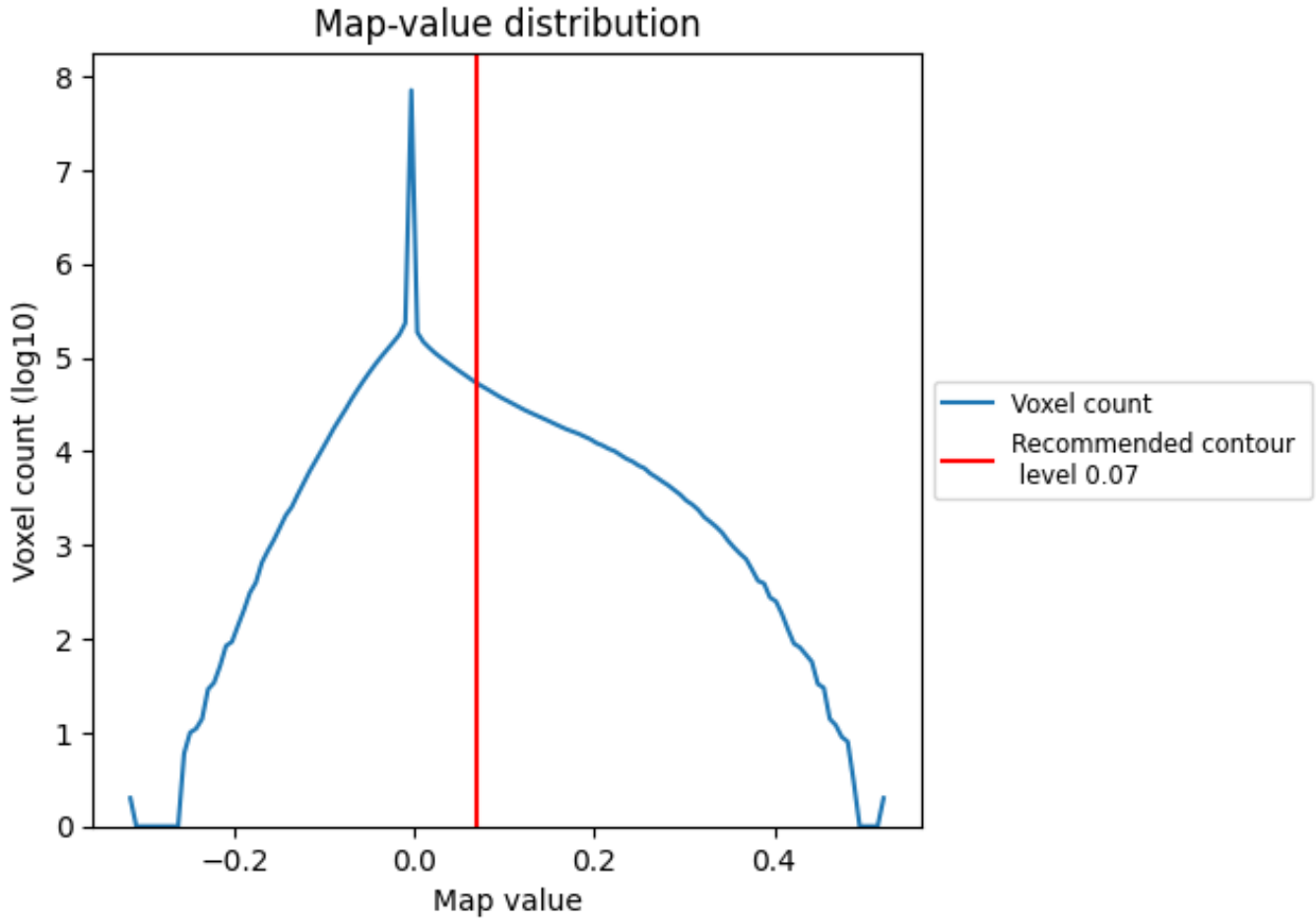
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

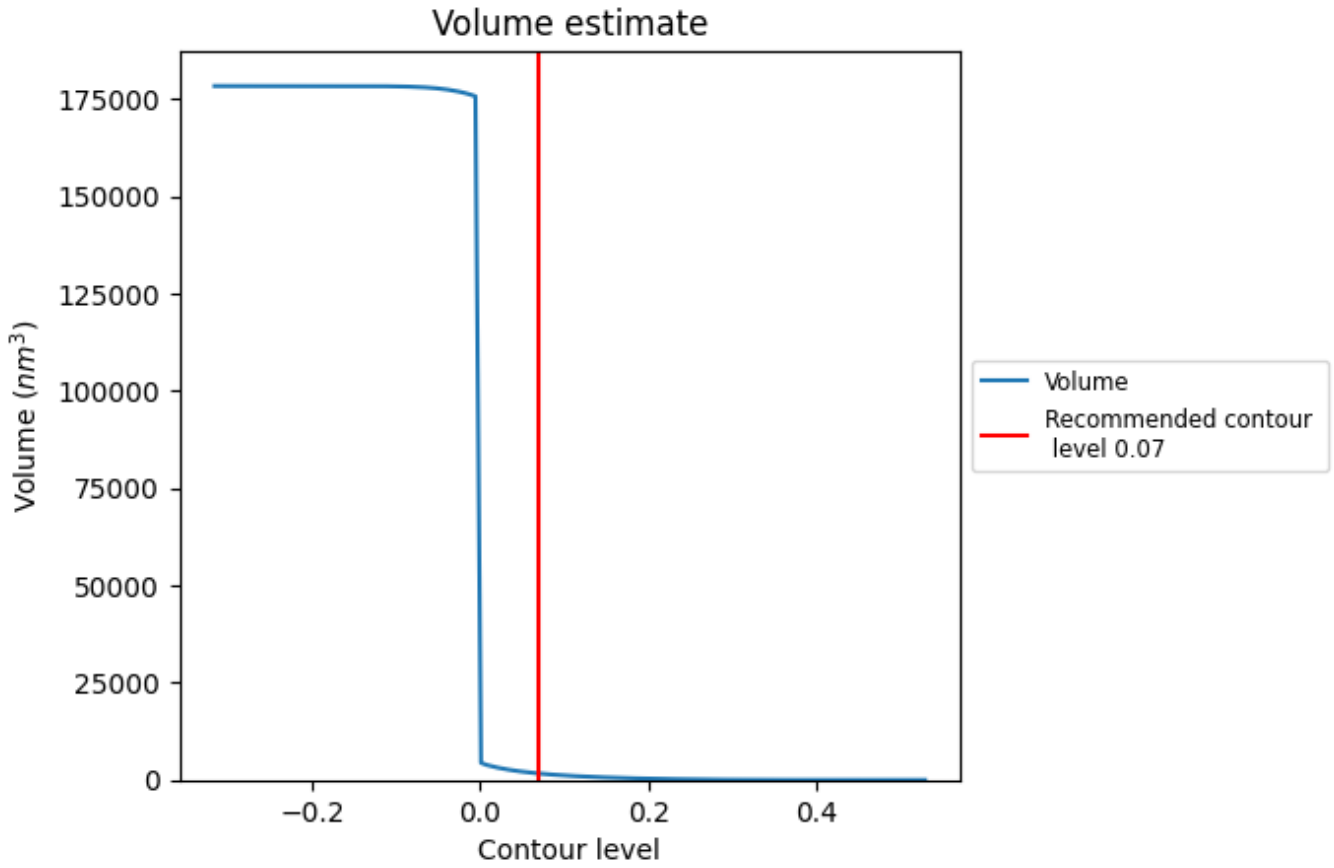
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

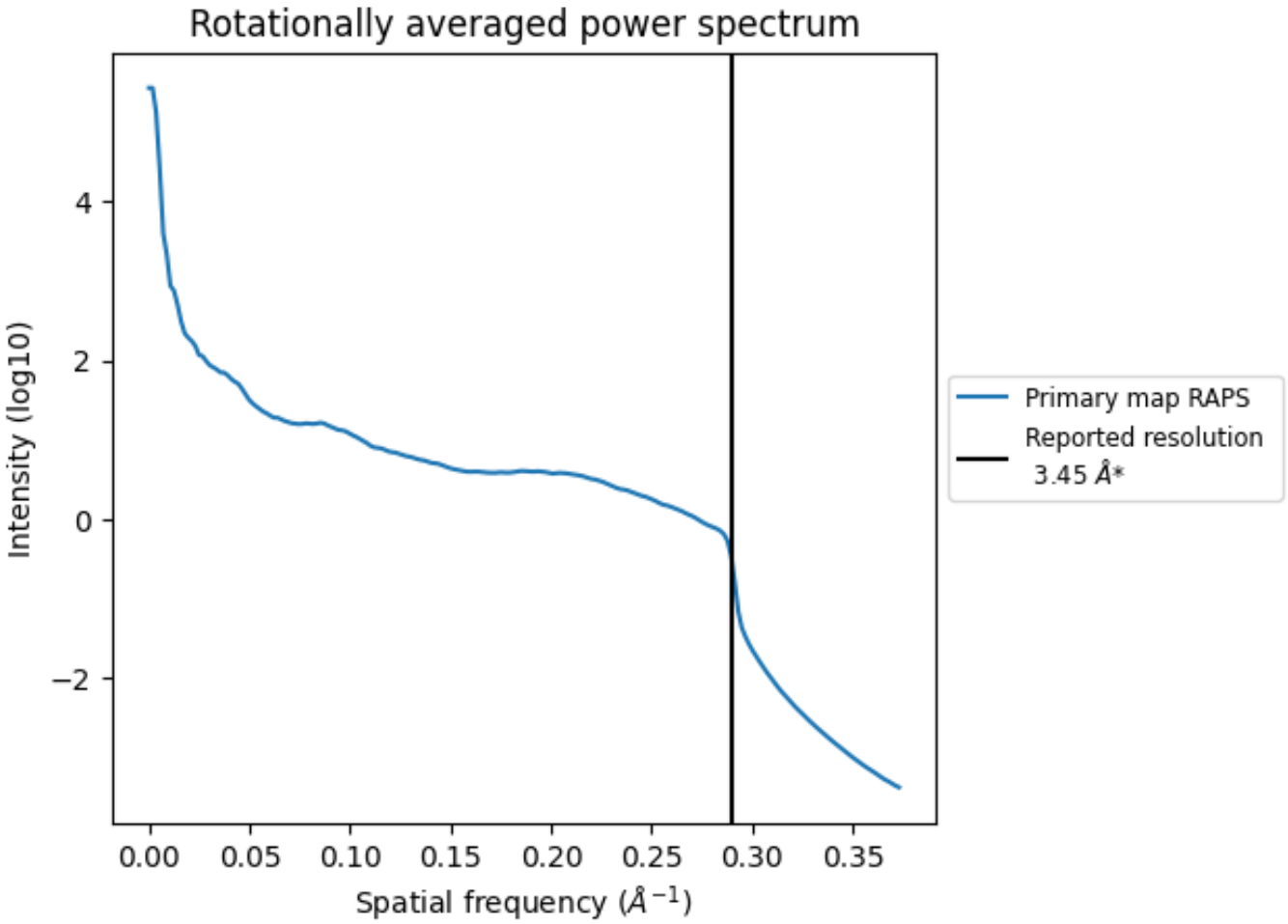
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1656 $nm^3$; this corresponds to an approximate mass of 1496 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)

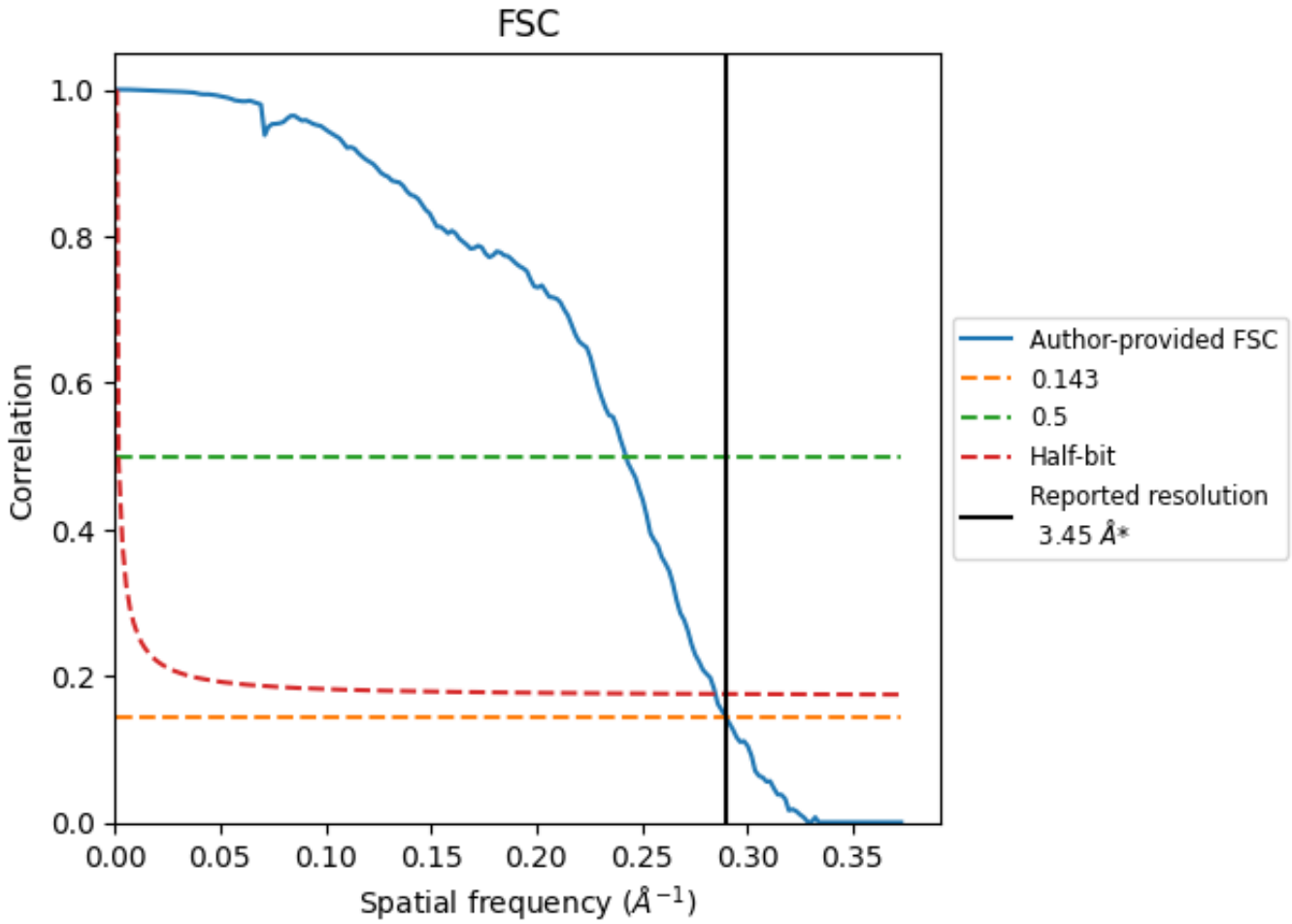



*Reported resolution corresponds to spatial frequency of 0.290 Å$^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.290 Å$^{-1}$

## 8.2 Resolution estimates (i)

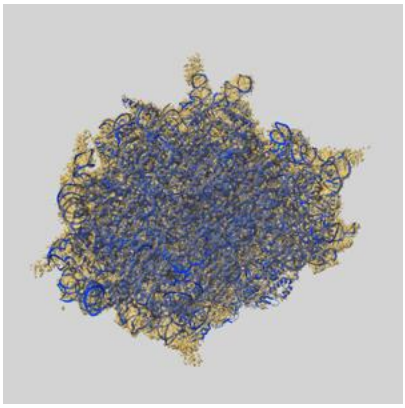
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.45 | - | - |
| Author-provided FSC curve | 3.45 | 4.12 | 3.51 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

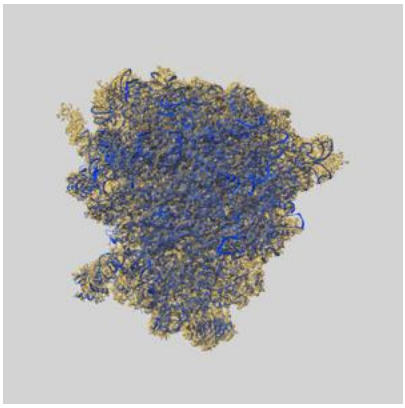
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3039 and PDB model 3JAH. Per-residue inclusion information can be found in section 3 on page 24.

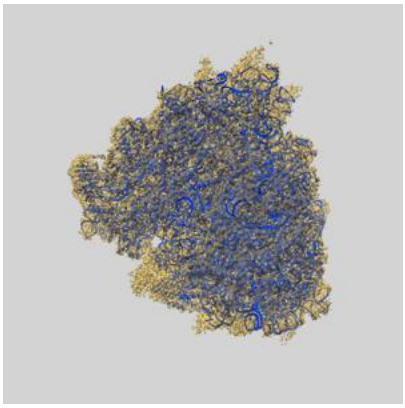
## 9.1 Map-model overlay



X



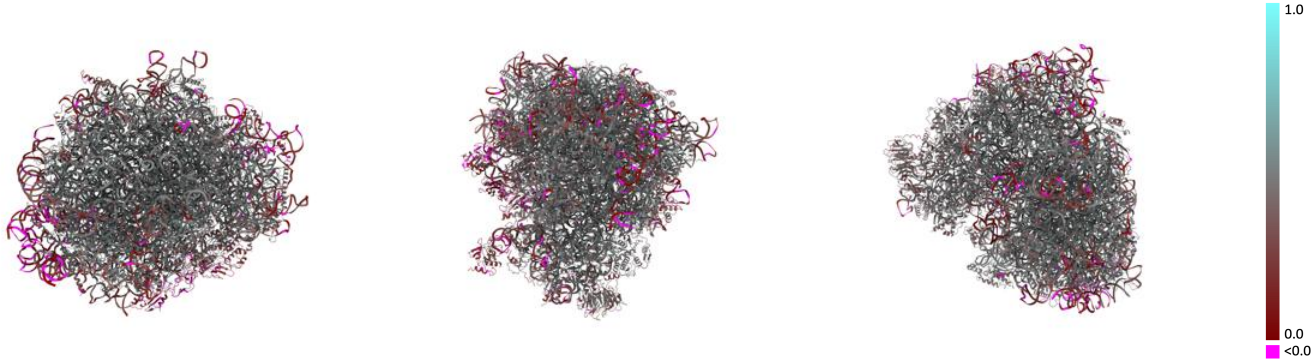
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

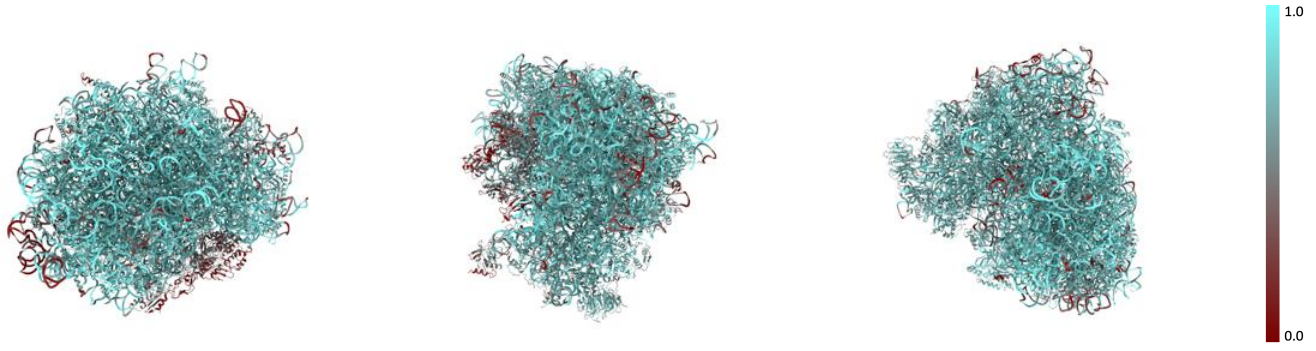
## 9.2 Q-score mapped to coordinate model




X Y Z

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

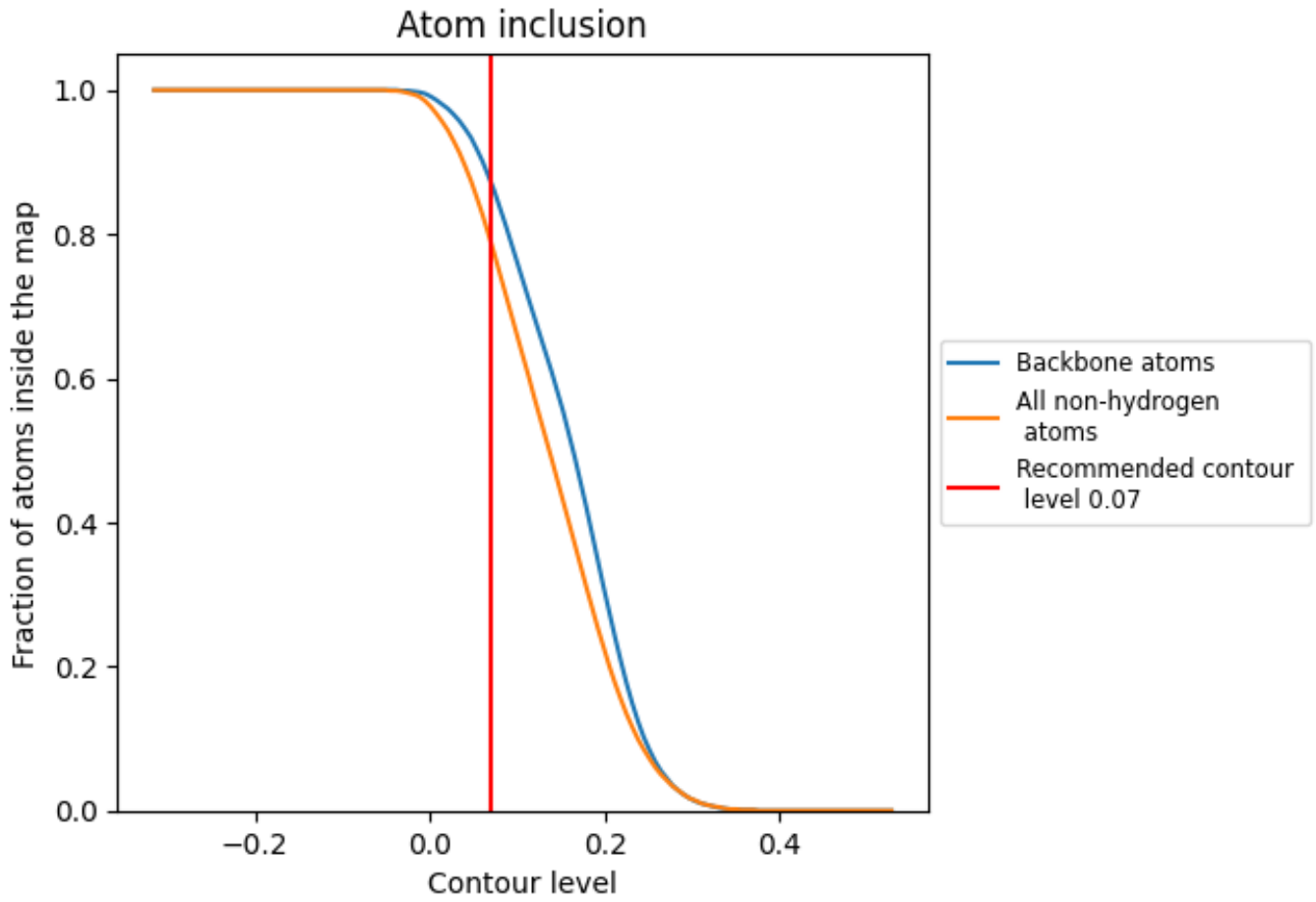
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

## 9.4 Atom inclusion (i)




At the recommended contour level, 87% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7880 | 0.4220 |
| 1 | 0.5790 | 0.4150 |
| 2 | 0.8210 | 0.3920 |
| 3 | 0.5400 | 0.2310 |
| 5 | 0.8440 | 0.4100 |
| 7 | 0.9450 | 0.4810 |
| 8 | 0.8850 | 0.4360 |
| 9 | 0.8580 | 0.4170 |
| A | 0.8160 | 0.5110 |
| AA | 0.7530 | 0.4540 |
| B | 0.8160 | 0.4980 |
| BB | 0.7450 | 0.4630 |
| C | 0.8040 | 0.4910 |
| CC | 0.7680 | 0.4710 |
| D | 0.7990 | 0.4550 |
| DD | 0.6680 | 0.4010 |
| E | 0.7210 | 0.4160 |
| EE | 0.7630 | 0.4700 |
| F | 0.8050 | 0.4870 |
| FF | 0.6990 | 0.4280 |
| G | 0.6970 | 0.4080 |
| GG | 0.6780 | 0.3660 |
| H | 0.7670 | 0.4690 |
| HH | 0.6430 | 0.3800 |
| I | 0.7880 | 0.4810 |
| II | 0.7330 | 0.4270 |
| J | 0.7620 | 0.4350 |
| JJ | 0.7600 | 0.4550 |
| KK | 0.6450 | 0.3440 |
| L | 0.7780 | 0.4530 |
| LL | 0.7180 | 0.4460 |
| M | 0.8000 | 0.4560 |
| MM | 0.3720 | 0.1710 |
| N | 0.8380 | 0.5080 |
| NN | 0.7830 | 0.4750 |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| Chain | Atom inclusion | Q-score |
|---|---|---|
| O | 0.8120 | 0.4870 |
| OO | 0.7710 | 0.4790 |
| P | 0.8190 | 0.5040 |
| PP | 0.6510 | 0.3750 |
| Q | 0.7960 | 0.5000 |
| QQ | 0.7350 | 0.4470 |
| R | 0.7630 | 0.4520 |
| RR | 0.6690 | 0.3950 |
| S | 0.8120 | 0.4910 |
| SS | 0.7430 | 0.4190 |
| T | 0.7930 | 0.4790 |
| TT | 0.7360 | 0.4240 |
| U | 0.7490 | 0.4220 |
| UU | 0.6610 | 0.4020 |
| V | 0.7630 | 0.4940 |
| VV | 0.7350 | 0.4630 |
| W | 0.8050 | 0.4840 |
| WW | 0.7900 | 0.4880 |
| X | 0.7780 | 0.4670 |
| XX | 0.7700 | 0.4960 |
| Y | 0.7910 | 0.4670 |
| YY | 0.7370 | 0.4160 |
| Z | 0.8100 | 0.4740 |
| ZZ | 0.6930 | 0.3830 |
| a | 0.8430 | 0.5100 |
| aa | 0.7910 | 0.4860 |
| b | 0.6880 | 0.4000 |
| bb | 0.7140 | 0.4450 |
| c | 0.8040 | 0.4690 |
| cc | 0.6750 | 0.4260 |
| d | 0.7950 | 0.4660 |
| dd | 0.7780 | 0.4520 |
| e | 0.8040 | 0.5000 |
| ee | 0.6540 | 0.4090 |
| f | 0.8280 | 0.5090 |
| ff | 0.4820 | 0.2530 |
| g | 0.7780 | 0.4700 |
| gg | 0.6610 | 0.3850 |
| h | 0.7890 | 0.4630 |
| hh | 0.8100 | 0.4440 |
| i | 0.7760 | 0.4520 |
| ii | 0.4330 | 0.3710 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| j | 0.8440 | 0.5000 |
| jj | 0.3780 | 0.3410 |
| k | 0.7240 | 0.4200 |
| l | 0.8180 | 0.4960 |
| m | 0.7840 | 0.4770 |
| n | 0.7960 | 0.4730 |
| o | 0.7680 | 0.4860 |
| p | 0.7920 | 0.4850 |
| r | 0.8220 | 0.4860 |
| s | 0.2520 | 0.1220 |
| t | 0.2800 | 0.1180 |