# wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2024 – 01:57 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 4V8A |
| Title | : | The structure of thermorubin in complex with the 70S ribosome from Thermus thermophilus. |
| Authors | : | Bulkley, D.; Johnson, F.A.; Steitz, T.A. |
| Deposited on | : | 2011-12-05 |
| Resolution | : | 3.20 Å(reported) |

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

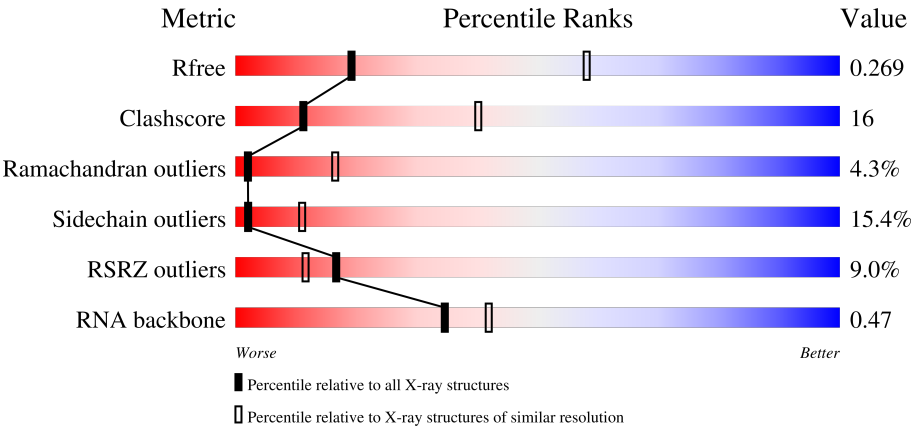
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 1.20.1 |
| EDS | : | 3.0 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4 | : | 9.0.003 (Gargrove) |
| Density-Fitness | : | 1.0.11 |
| 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:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 164625 | 1370 (3.20-3.20) |
| Clashscore | 180529 | 1497 (3.20-3.20) |
| Ramachandran outliers | 177936 | 1479 (3.20-3.20) |
| Sidechain outliers | 177891 | 1478 (3.20-3.20) |
| RSRZ outliers | 164620 | 1371 (3.20-3.20) |
| RNA backbone | 3690 | 1111 (3.50-2.90) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AA | 2915 | 4% 36% 43% 15% |
| 1 | BA | 2915 | 3% 45% 34% 15% |
| 2 | AB | 122 | 9% 27% 52% 16% |
| 2 | BB | 122 | 2% 49% 35% 13% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | AD | 276 | 3% 64% 28% 7% |
| 3 | BD | 276 | 2% 64% 29% 6% |
| 4 | AE | 206 | 2% 48% 43% 8% |
| 4 | BE | 206 | 2% 60% 29% 10% |
| 5 | AF | 205 | % 56% 36% 7% |
| 5 | BF | 205 | % 60% 32% 6% |
| 6 | AG | 182 | 27% 47% 45% 7% |
| 6 | BG | 182 | 12% 48% 46% 5% |
| 7 | AH | 180 | 8% 44% 47% 6% |
| 7 | BH | 180 | 8% 61% 33% |
| 8 | AI | 148 | 22% 43% 40% 14% |
| 8 | BI | 148 | 2% 51% 30% 16% |
| 9 | AN | 140 | 2% 44% 44% 11% |
| 9 | BN | 140 | 3% 54% 40% 6% |
| 10 | AO | 122 | 2% 60% 37% |
| 10 | BO | 122 | 3% 67% 30% |
| 11 | AP | 150 | 7% 60% 31% 7% |
| 11 | BP | 150 | 6% 64% 27% 7% |
| 12 | AQ | 141 | 4% 55% 36% 9% |
| 12 | BQ | 141 | % 56% 33% 11% |
| 13 | AR | 118 | 3% 50% 38% 12% |
| 13 | BR | 118 | 3% 57% 32% 11% |
| 14 | AS | 112 | 18% 45% 43% 11% |
| 14 | BS | 112 | 5% 44% 46% 9% |
| 15 | AT | 146 | 2% 47% 38% 5% 10% |

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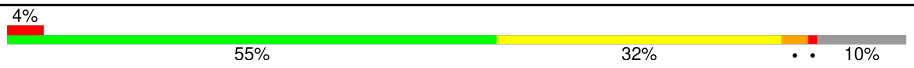
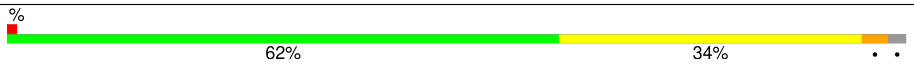
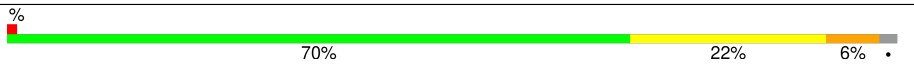
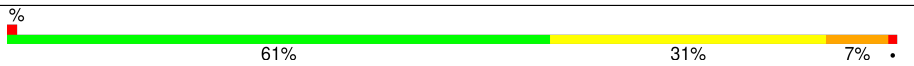
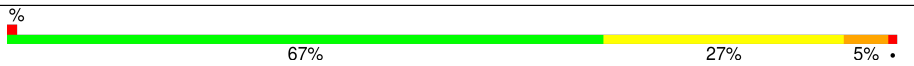
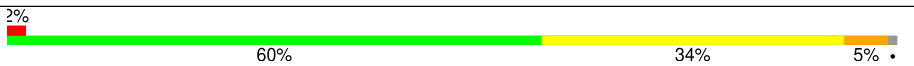
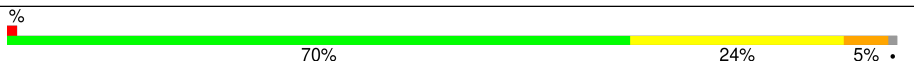
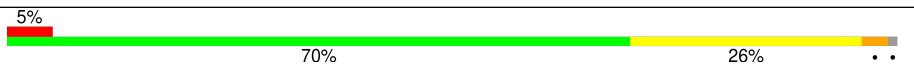
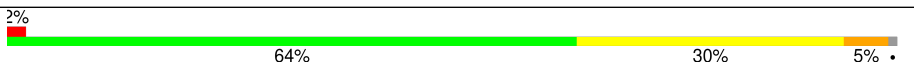
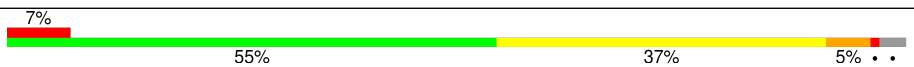
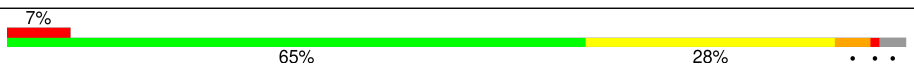
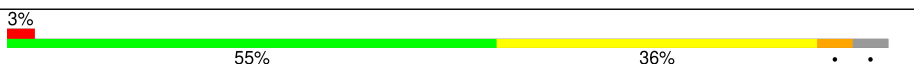
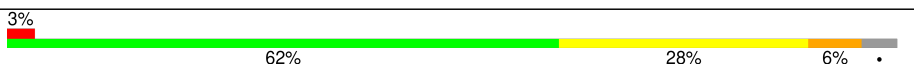
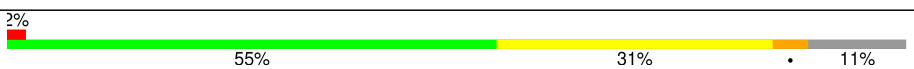
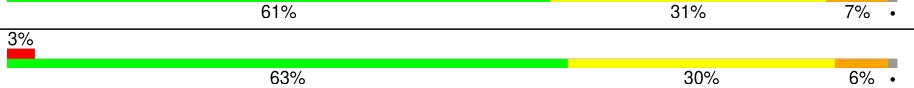
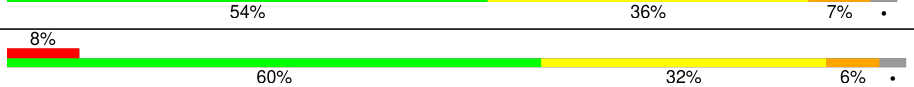
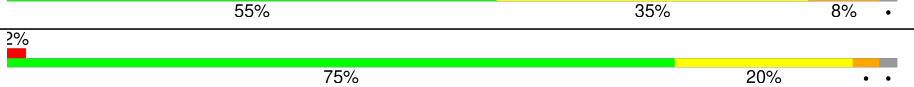
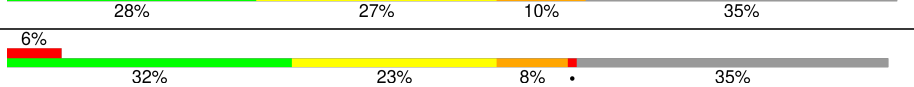
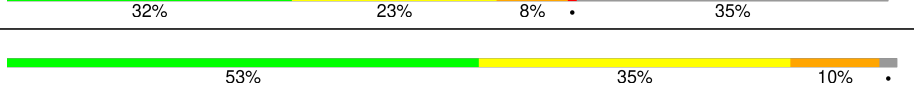
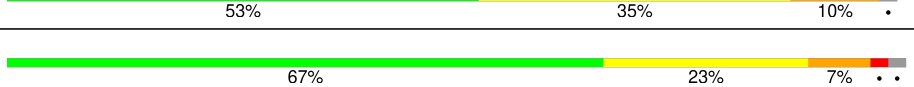
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | BT | 146 |   |
| 16 | AU | 118 |   |
| 16 | BU | 118 |   |
| 17 | AV | 101 |   |
| 17 | BV | 101 |   |
| 18 | AW | 113 |   |
| 18 | BW | 113 |   |
| 19 | AX | 96 |   |
| 19 | BX | 96 |   |
| 20 | AY | 110 |   |
| 20 | BY | 110 |   |
| 21 | AZ | 206 |   |
| 21 | BZ | 206 |   |
| 22 | A0 | 85 |   |
| 22 | B0 | 85 |   |
| 23 | A1 | 98 |   |
| 23 | B1 | 98 |   |
| 24 | A2 | 72 |   |
| 24 | B2 | 72 |   |
| 25 | A3 | 60 |   |
| 25 | B3 | 60 |   |
| 26 | A4 | 71 |   |
| 26 | B4 | 71 |   |
| 27 | A5 | 60 |   |
| 27 | B5 | 60 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | A6 | 54 | 7% 44% 43% 9% |
| 28 | B6 | 54 | 50% 39% 9% |
| 29 | A7 | 49 | 8% 53% 43% |
| 29 | B7 | 49 | 4% 57% 33% 8% |
| 30 | A8 | 65 | 9% 54% 42% |
| 30 | B8 | 65 | 3% 66% 29% |
| 31 | CA | 1521 | 11% 29% 53% 14% |
| 31 | DA | 1521 | 9% 31% 51% 14% |
| 32 | CB | 256 | 5% 38% 40% 11% 11% |
| 32 | DB | 256 | 10% 38% 42% 9% 11% |
| 33 | CC | 239 | 14% 54% 28% 5% 14% |
| 33 | DC | 239 | 16% 47% 33% 6% 14% |
| 34 | CD | 209 | 20% 48% 41% 9% |
| 34 | DD | 209 | 19% 51% 40% 8% |
| 35 | CE | 162 | 2% 41% 42% 8% 9% |
| 35 | DE | 162 | 7% 44% 40% 6% 9% |
| 36 | CF | 101 | 4% 57% 35% 7% |
| 36 | DF | 101 | 6% 60% 31% 7% |
| 37 | CG | 156 | 38% 57% 33% 8% |
| 37 | DG | 156 | 29% 52% 42% |
| 38 | CH | 138 | 4% 57% 35% 8% |
| 38 | DH | 138 | 6% 52% 37% 10% |
| 39 | CI | 128 | 46% 52% 38% 9% |
| 39 | DI | 128 | 61% 53% 37% 8% |
| 40 | CJ | 105 | 37% 54% 28% 9% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | DJ | 105 | 43% 43% 38% 10% 9% |
| 41 | CK | 129 | 5% 56% 29% • 12% |
| 41 | DK | 129 | 5% 51% 33% • 12% |
| 42 | CL | 132 | 9% 53% 31% 8% 8% |
| 42 | DL | 132 | 9% 53% 33% 6% 8% |
| 43 | CM | 126 | 44% 50% 32% 9% 10% |
| 43 | DM | 126 | 34% 43% 35% 12% • 10% |
| 44 | CN | 61 | 46% 33% 51% 15% • |
| 44 | DN | 61 | 61% 49% 34% 13% • • |
| 45 | CO | 89 | 6% 49% 39% 10% • |
| 45 | DO | 89 | 8% 54% 36% 9% • |
| 46 | CP | 88 | 13% 47% 34% 13% 7% |
| 46 | DP | 88 | 20% 44% 45% • 7% |
| 47 | CQ | 105 | 4% 54% 35% 5% 6% |
| 47 | DQ | 105 | 6% 64% 25% 6% 6% |
| 48 | CR | 88 | 7% 51% 23% • • 23% |
| 48 | DR | 88 | % 53% 22% • 23% |
| 49 | CS | 93 | 51% 39% 34% 10% • 16% |
| 49 | DS | 93 | 35% 39% 42% • 16% |
| 50 | CT | 106 | 15% 40% 42% 8% • 9% |
| 50 | DT | 106 | 12% 52% 34% • • 9% |
| 51 | CU | 27 | 81% 52% 26% 7% 15% |
| 51 | DU | 27 | 78% 48% 30% 7% 15% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 52 | T8B | AA | 3001 | - | - | X | - |
| 52 | T8B | BA | 3001 | - | - | X | - |

# 2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 279316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | AA | 2827 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60900 | 27102 | 11403 | 19569 | 2826 | | | |
| 1 | BA | 2827 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60900 | 27102 | 11403 | 19569 | 2826 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AA | 272A | G | U | conflict | GB AP008226.1 |
| BA | 272A | G | U | conflict | GB AP008226.1 |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | AB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2574 | 1146 | 476 | 833 | 119 | | | |
| 2 | BB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2574 | 1146 | 476 | 833 | 119 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AB | 120 | G | A | conflict | GB AP008226.1 |
| BB | 120 | G | A | conflict | GB AP008226.1 |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | AD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |
| 3 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | AE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 982 | 297 | 270 | 6 | | | |
| 4 | BE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 982 | 297 | 270 | 6 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | AF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1576 | 1005 | 297 | 272 | 2 | | | |
| 5 | BF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1576 | 1005 | 297 | 272 | 2 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | AG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1368 | 879 | 242 | 244 | 3 | | | |
| 6 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1368 | 879 | 242 | 244 | 3 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | AH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1317 | 837 | 243 | 236 | 1 | | | |
| 7 | BH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1317 | 837 | 243 | 236 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | AI | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1046 | 674 | 180 | 191 | 1 | | | |
| 8 | BI | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1046 | 674 | 180 | 191 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AI | 110 | GLU | ASP | conflict | UNP Q5SLQ1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BI | 110 | GLU | ASP | conflict | UNP Q5SLQ1 |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | AN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 717 | 207 | 184 | 4 | | | |
| 9 | BN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 717 | 207 | 184 | 4 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | AO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 923 | 583 | 168 | 168 | 4 | | | |
| 10 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 923 | 583 | 168 | 168 | 4 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | AP | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1119 | 695 | 227 | 194 | 3 | | | |
| 11 | BP | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1119 | 695 | 227 | 194 | 3 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | AQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 12 | BQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | AR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 13 | BR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | AS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 865 | 544 | 172 | 149 | | | |
| 14 | BS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 865 | 544 | 172 | 149 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | AT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1063 | 666 | 213 | 183 | 1 | | | |
| 15 | BT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1063 | 666 | 213 | 183 | 1 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | AU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 16 | BU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | AV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |
| 17 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | AW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 554 | 172 | 153 | 2 | | | |
| 18 | BW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 554 | 172 | 153 | 2 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | AX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 483 | 134 | 124 | 1 | | | |
| 19 | BX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 483 | 134 | 124 | 1 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | AY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 503 | 145 | 131 | 6 | | | |
| 20 | BY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 503 | 145 | 131 | 6 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | AZ | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1522 | 972 | 269 | 279 | 2 | | | |
| 21 | BZ | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1522 | 972 | 269 | 279 | 2 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | A0 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 594 | 368 | 125 | 100 | 1 | | | |
| 22 | B0 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 594 | 368 | 125 | 100 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | A1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 745 | 469 | 144 | 131 | 1 | | | |
| 23 | B1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 745 | 469 | 144 | 131 | 1 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | A2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | B2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | A3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 458 | 293 | 87 | 78 | | | |
| 25 | B3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 458 | 293 | 87 | 78 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | A4 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 349 | 223 | 57 | 64 | 5 | | | |
| 26 | B4 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 349 | 223 | 57 | 64 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | A5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 286 | 90 | 74 | 5 | | | |
| 27 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 286 | 90 | 74 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | A6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 278 | 90 | 77 | 4 | | | |
| 28 | B6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 278 | 90 | 77 | 4 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | A7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 29 | B7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | A8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 326 | 99 | 82 | 2 | | | |
| 30 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 326 | 99 | 82 | 2 | | | |

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | CA | 1498 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32208 | 14334 | 5974 | 10402 | 1498 | | | |
| 31 | DA | 1498 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32208 | 14334 | 5974 | 10402 | 1498 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| CA | ? | - | U | deletion | GB AP008226.1 |
| DA | ? | - | U | deletion | GB AP008226.1 |

- Molecule 32 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | CB | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1777 | 1134 | 318 | 320 | 5 | | | |
| 32 | DB | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1777 | 1134 | 318 | 320 | 5 | | | |

- Molecule 33 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1450 | 906 | 279 | 264 | 1 | | | |
| 33 | DC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1450 | 906 | 279 | 264 | 1 | | | |

- Molecule 34 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | CD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1520 | 960 | 283 | 272 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | DD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1520 | 960 | 283 | 272 | 5 | | | |

- Molecule 35 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | CE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 699 | 204 | 198 | 4 | | | |
| 35 | DE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 699 | 204 | 198 | 4 | | | |

- Molecule 36 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 781 | 495 | 137 | 146 | 3 | | | |
| 36 | DF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 781 | 495 | 137 | 146 | 3 | | | |

- Molecule 37 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | CG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1167 | 727 | 224 | 210 | 6 | | | |
| 37 | DG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1167 | 727 | 224 | 210 | 6 | | | |

- Molecule 38 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 38 | CH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 665 | 188 | 190 | 2 | | | |
| 38 | DH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 665 | 188 | 190 | 2 | | | |

- Molecule 39 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | CI | 125 | Total | C | N | O | 0 | 0 | 0 |
| | | | 852 | 533 | 163 | 156 | | | |
| 39 | DI | 125 | Total | C | N | O | 0 | 0 | 0 |
| | | | 852 | 533 | 163 | 156 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| CI | 58 | ARG | HIS | conflict | UNP P80374 |
| DI | 58 | ARG | HIS | conflict | UNP P80374 |

- Molecule 40 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | CJ | 96 | Total | C | N | O | 0 | 0 | 0 |
| | | | 659 | 408 | 131 | 120 | | | |
| 40 | DJ | 96 | Total | C | N | O | 0 | 0 | 0 |
| | | | 659 | 408 | 131 | 120 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| CJ | 75 | LEU | ILE | conflict | UNP Q5SHN7 |
| DJ | 75 | LEU | ILE | conflict | UNP Q5SHN7 |

- Molecule 41 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | CK | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 828 | 516 | 155 | 154 | 3 | | | |
| 41 | DK | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 828 | 516 | 155 | 154 | 3 | | | |

- Molecule 42 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | CL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 909 | 570 | 179 | 159 | 1 | | | |
| 42 | DL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 909 | 570 | 179 | 159 | 1 | | | |

- Molecule 43 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 43 | CM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 494 | 164 | 142 | 1 | | | |
| 43 | DM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 494 | 164 | 142 | 1 | | | |

- Molecule 44 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | CN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 478 | 303 | 99 | 72 | 4 | | | |
| 44 | DN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 478 | 303 | 99 | 72 | 4 | | | |

- Molecule 45 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 45 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 724 | 453 | 143 | 126 | 2 | | | |
| 45 | DO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 724 | 453 | 143 | 126 | 2 | | | |

- Molecule 46 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 46 | CP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 651 | 416 | 123 | 111 | 1 | | | |
| 46 | DP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 651 | 416 | 123 | 111 | 1 | | | |

- Molecule 47 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | CQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |
| 47 | DQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

- Molecule 48 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | CR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 514 | 329 | 98 | 87 | | | |
| 48 | DR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 514 | 329 | 98 | 87 | | | |

- Molecule 49 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 49 | CS | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 544 | 342 | 105 | 95 | 2 | | | |
| 49 | DS | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 544 | 342 | 105 | 95 | 2 | | | |

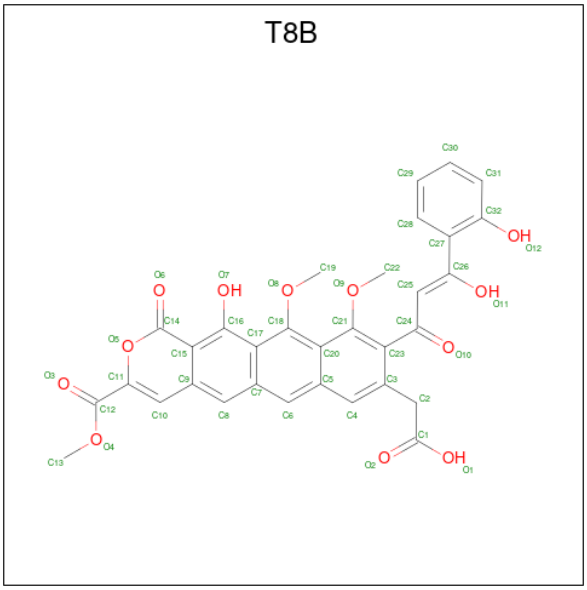
- Molecule 50 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | CT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 708 | 435 | 151 | 120 | 2 | | | |
| 50 | DT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 708 | 435 | 151 | 120 | 2 | | | |

- Molecule 51 is a protein called 30S ribosomal protein THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | CU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |
| 51 | DU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |

- Molecule 52 is Thermorubin (three-letter code: T8B) (formula: $C_{32}H_{24}O_{12}$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 52 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 44 | 32 | 12 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 52 | BA | 1 | Total C O<br>44 32 12 | 0 | 0 |

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

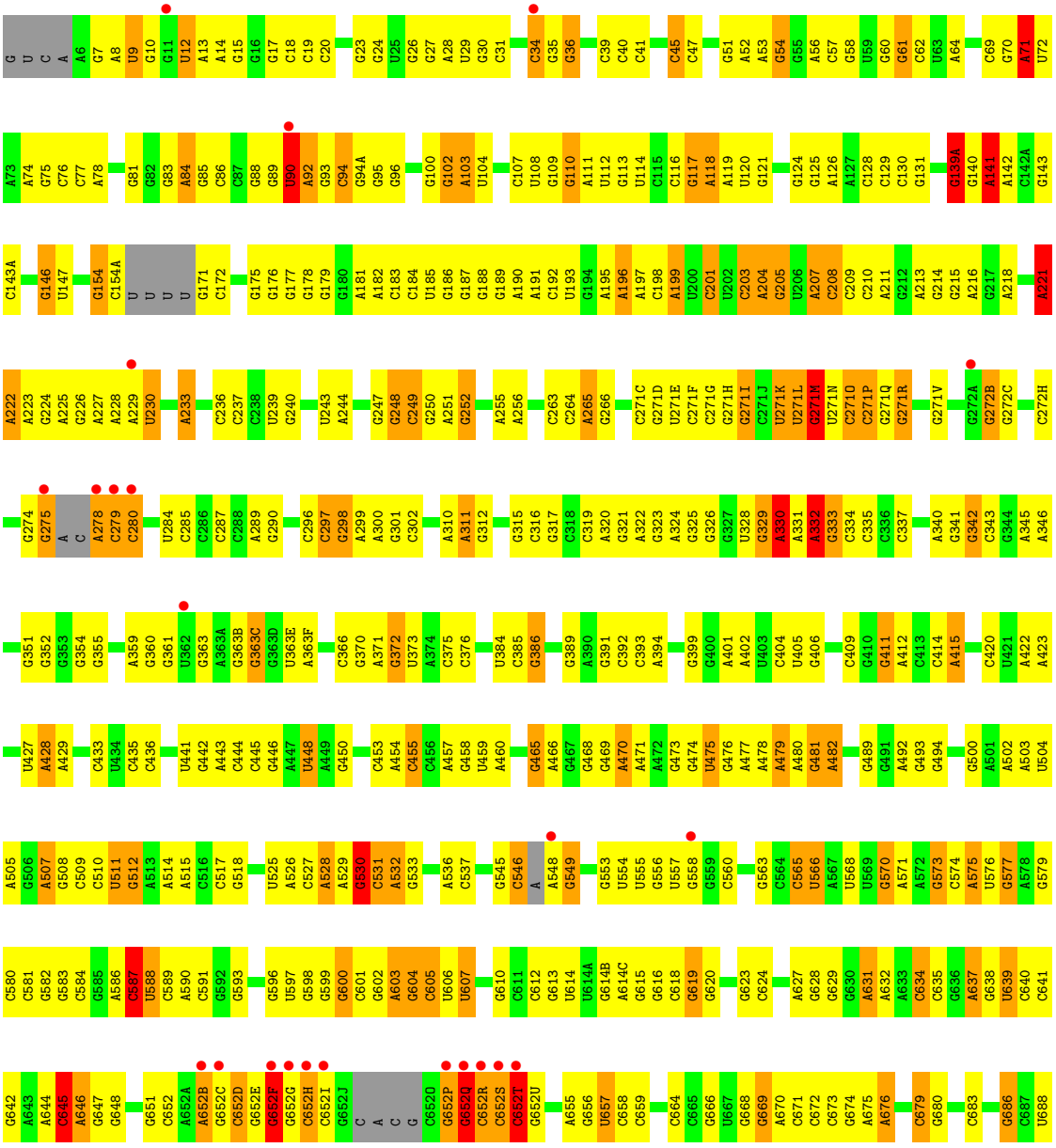
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 53 | AA | 2 | Total Mg<br>2 2 | 0 | 0 |
| 53 | BA | 2 | Total Mg<br>2 2 | 0 | 0 |

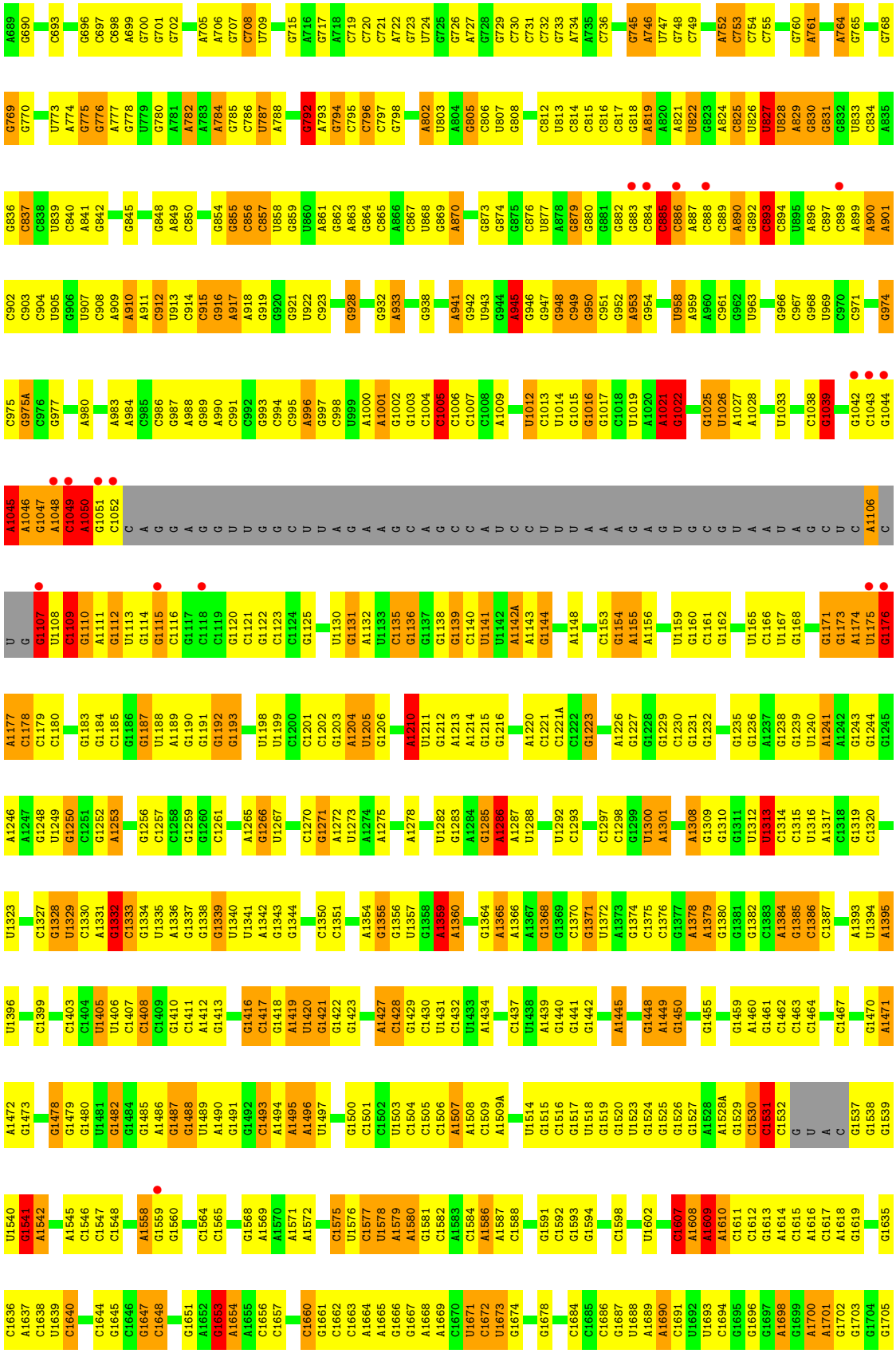
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: 23S ribosomal RNA

Chain AA:


A689 G690 C693 G696 C697 C698 A699 G700 G701 G702 A705 A706 G707 C708 U709 G715 A716 G717 A718 C719 C720 C721 A722 G723 U724 G725 G726 A727 G728 G729 C730 C731 C732 G733 A734 A735 C736 G745 A746 U747 G748 C749 A752 C753 C754 C755 G760 A761 A764 G765 G768
G769 G770 U773 A774 G775 G776 A777 C778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 G792 A793 G794 C795 C796 C797 G798 A802 U803 A804 G805 C806 U807 G808 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 U822 G823 A824 C825 U826 U827 U828 A829 G830 G831 G832 U833 C834 A835
G836 C837 C838 U839 C840 A841 G842 G845 G848 A849 C850 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 A870 G873 G874 G875 C876 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901
C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 G920 G921 U922 C923 G928 G932 A933 G938 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 C951 G952 A953 G954 U958 A959 A960 C961 G962 U963 G966 C967 G968 U969 C970 C971 G974
C975 G975A G976 G977 A980 A983 A984 C985 C986 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 G1025 U1026 A1027 A1028 U1033 C1038 G1039 G1042 C1043 C1044
A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C A G G A G U U U G G C U U A G A A G C C A G C C A C C U U U A A A G A G U G C C A G U A A C G C U C A1106 C
U G G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1119 G1120 C1121 G1122 C1123 C1124 G1125 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144 A1148 C1153 G1154 A1155 A1156 U1159 G1160 C1161 G1162 U1165 C1166 U1167 G1168 G1171 G1173 A1174 U1175 G1176
A1177 C1178 C1179 C1180 G1183 G1184 C1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1193 U1198 U1199 C1200 C1201 C1202 G1203 A1204 U1205 G1206 A1210 U1211 G1212 A1213 A1214 G1215 G1216 A1220 C1221 C1221A C1222 G1223 A1226 G1227 G1228 G1229 C1230 G1231 G1232 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1245
A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 G1256 C1257 C1258 G1259 G1260 C1261 A1265 G1266 U1267 C1270 G1271 A1272 U1273 A1274 A1275 A1278 U1282 G1283 A1284 G1285 A1286 A1287 U1288 U1292 C1293 C1297 C1298 G1299 U1300 A1301 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 C1318 G1319 C1320
U1323 C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1350 C1351 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 C1375 C1376 G1377 A1378 A1379 G1380 G1381 U1382 C1383 A1384 G1385 C1386 C1387 A1393 U1394 A1395
U1396 C1399 C1403 C1404 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 C1437 U1438 A1439 G1440 G1441 G1442 A1445 G1448 A1449 G1450 G1455 G1459 A1460 G1461 C1462 C1463 C1464 C1467 G1470 A1471
A1472 G1473 G1478 G1479 G1480 U1481 G1482 G1484 G1485 A1486 G1487 G1488 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 G1500 C1501 C1502 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A U1514 G1515 C1516 G1517 U1518 G1519 G1520 U1523 G1524 G1525 G1526 G1527 A1528 A1528A G1529 C1530 C1631 C1532 G U A C G1537 G1538 G1539
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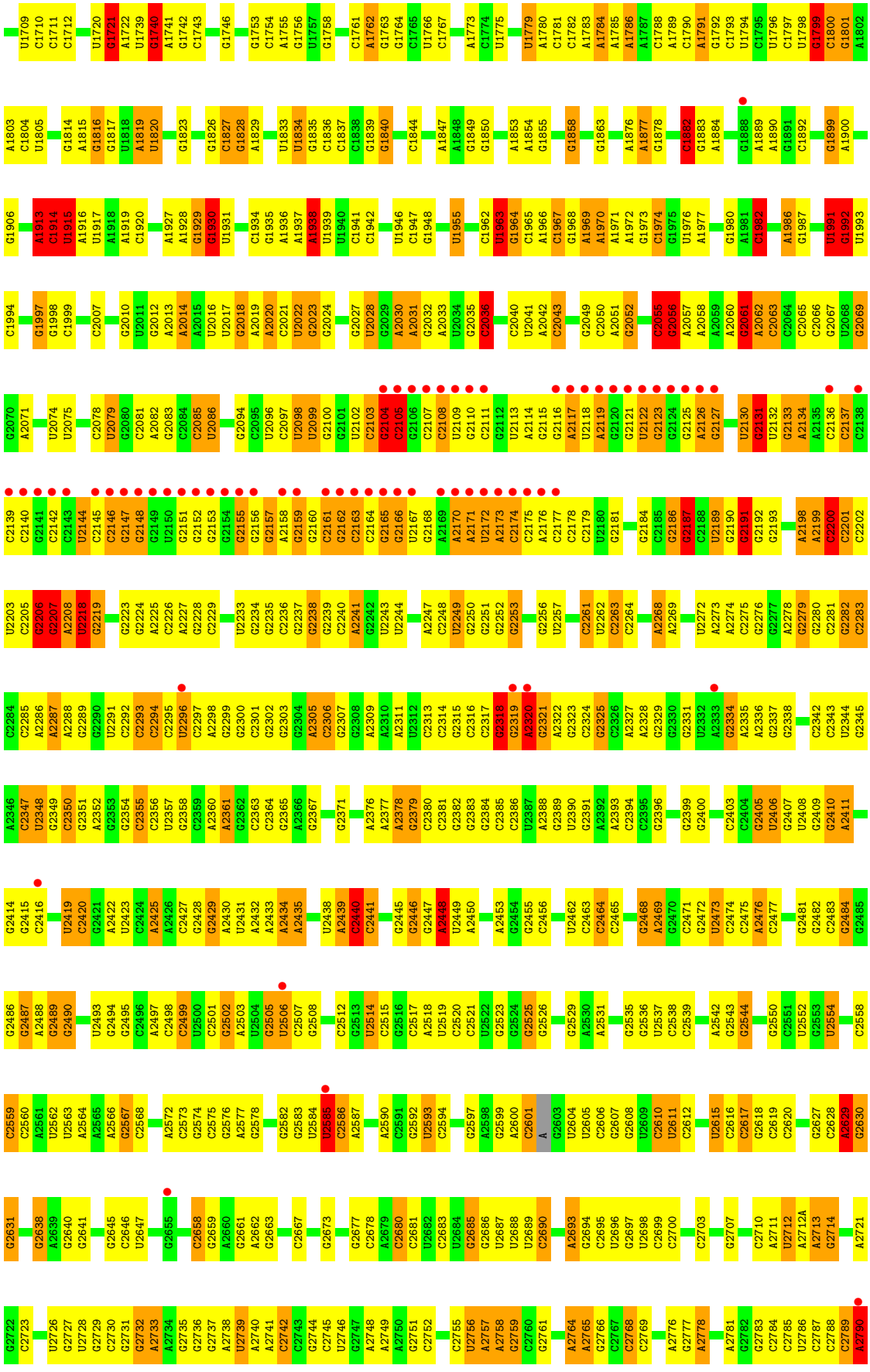
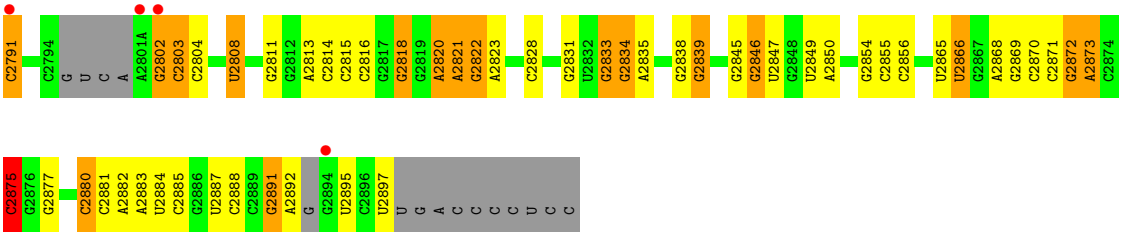
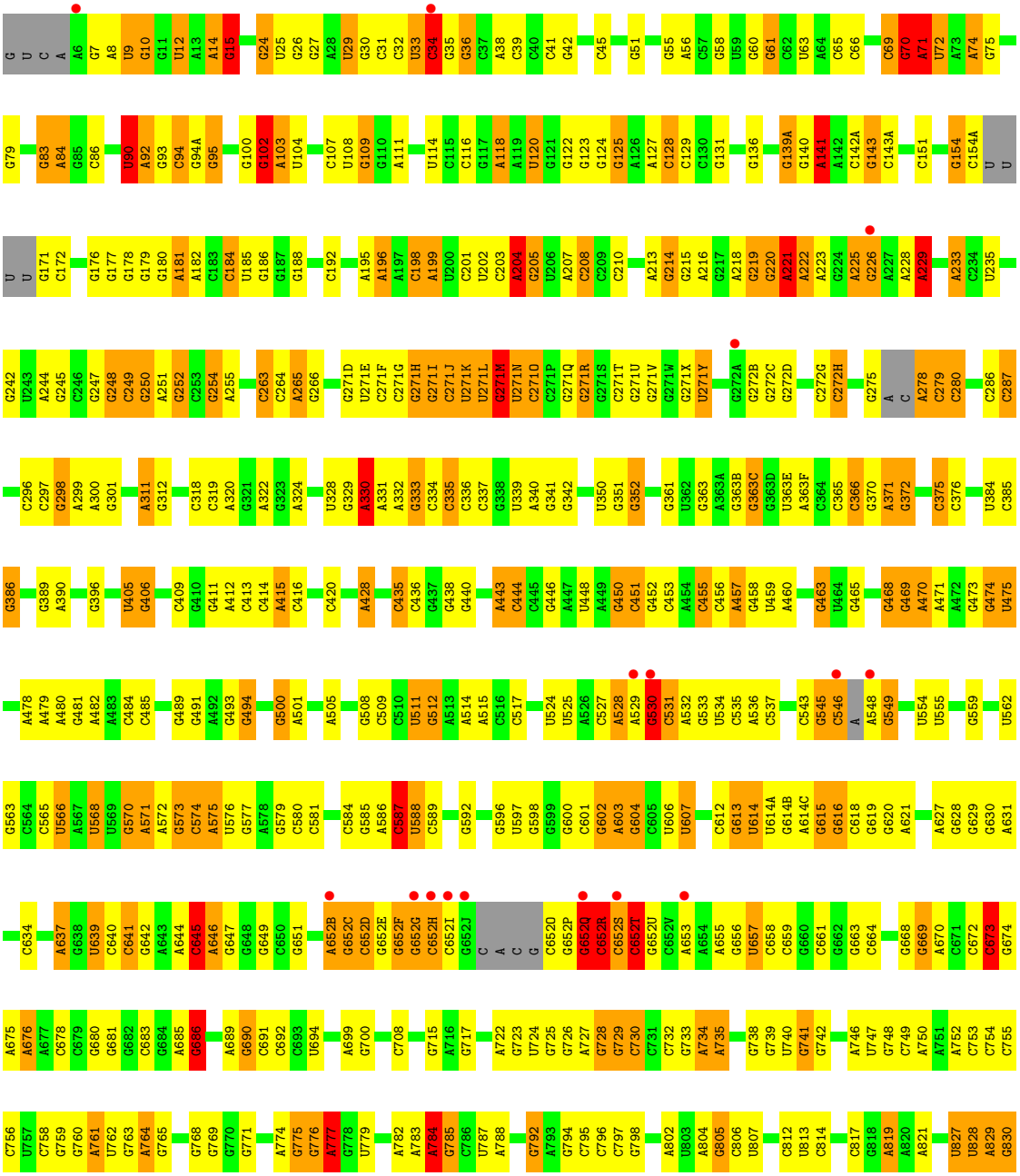
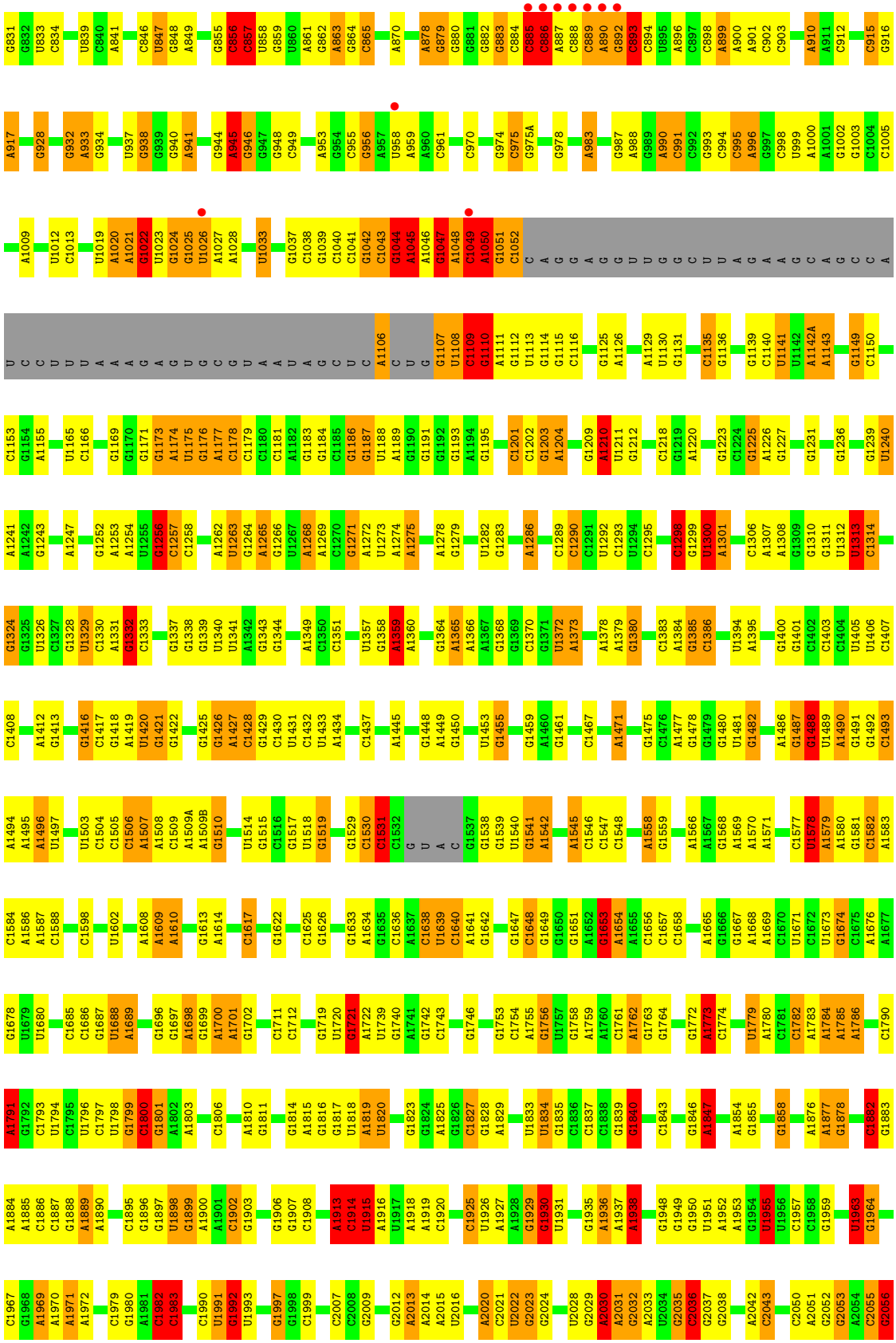


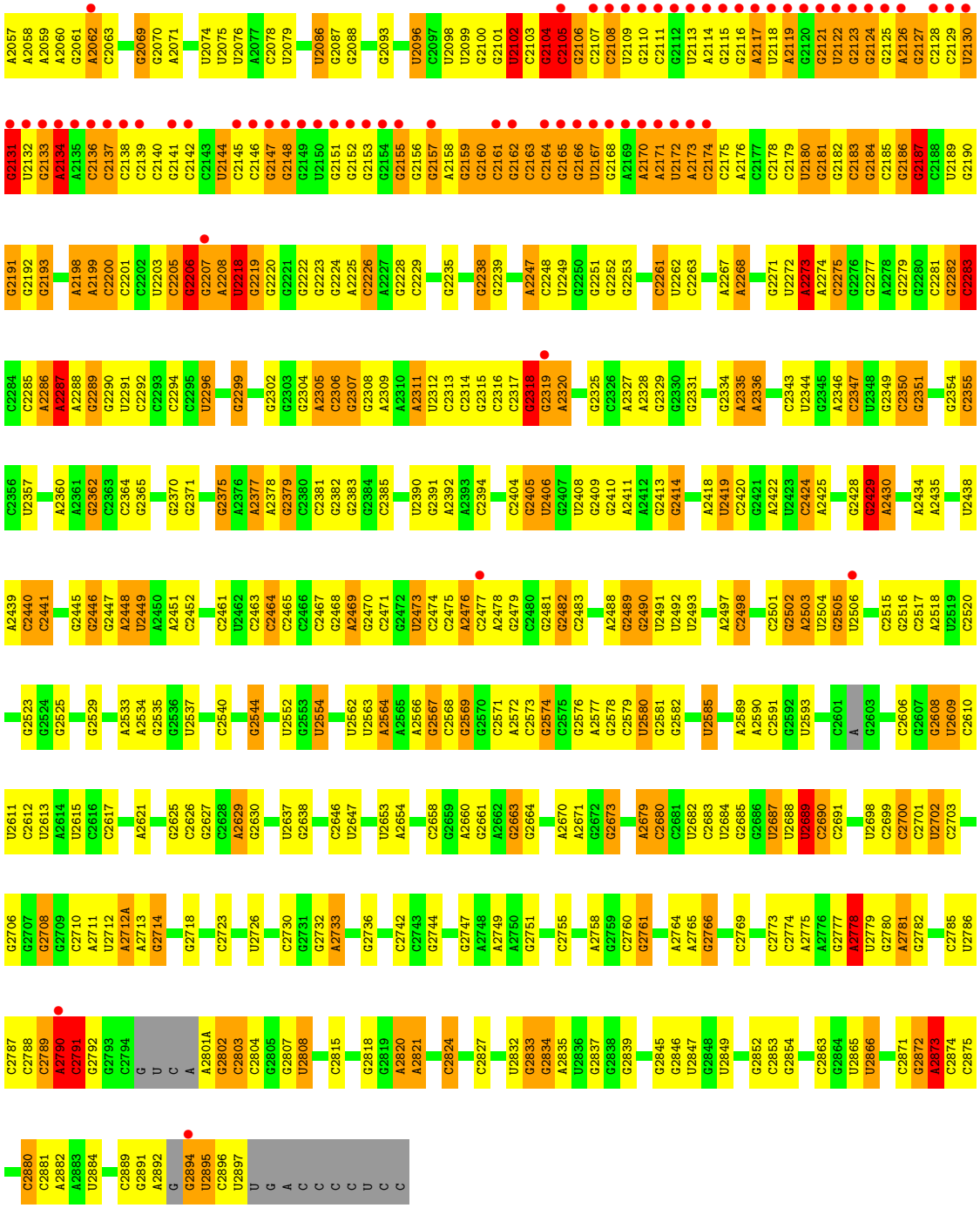


• Molecule 1: 23S ribosomal RNA

Chain BA:

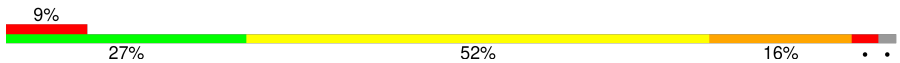



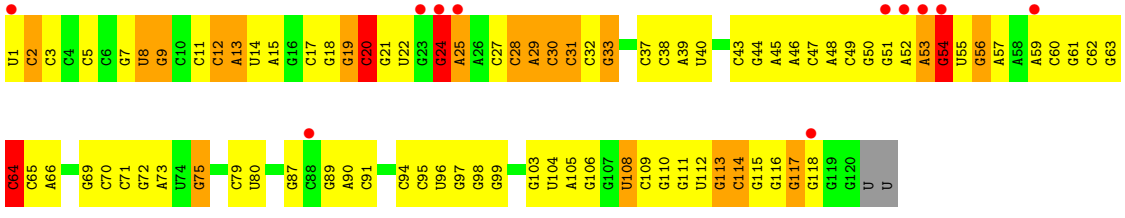




• Molecule 2: 5S ribosomal RNA

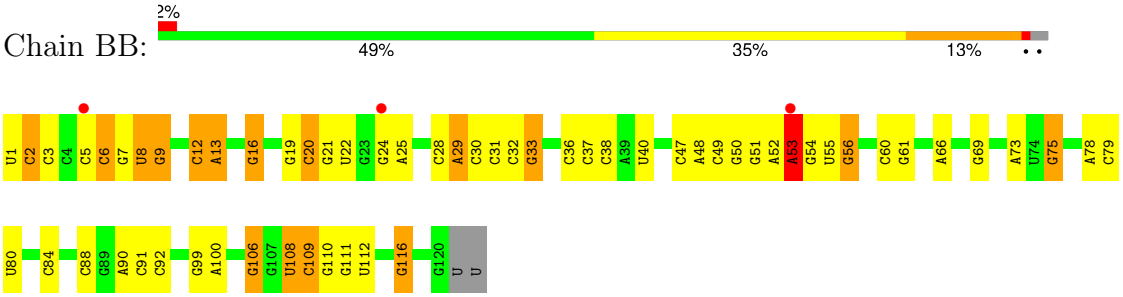
Chain AB:



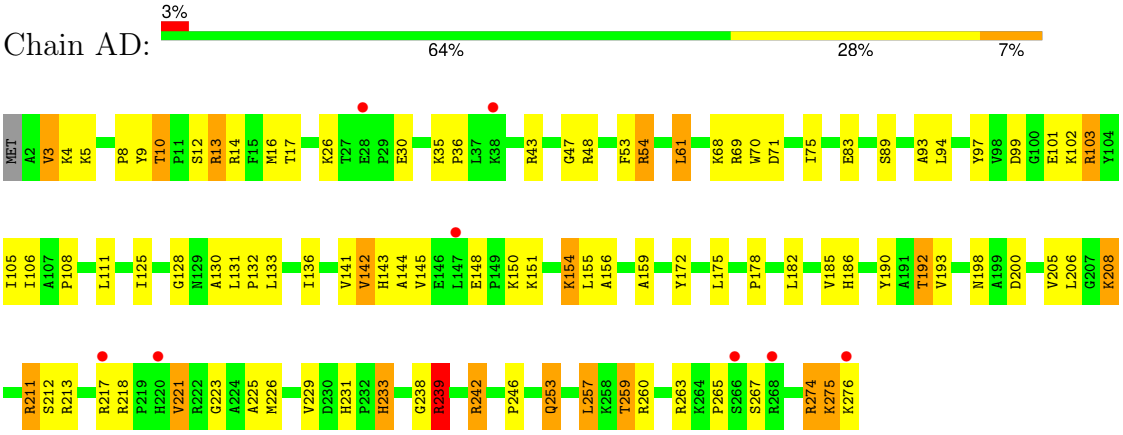
• Molecule 2: 5S ribosomal RNA

Chain BB:



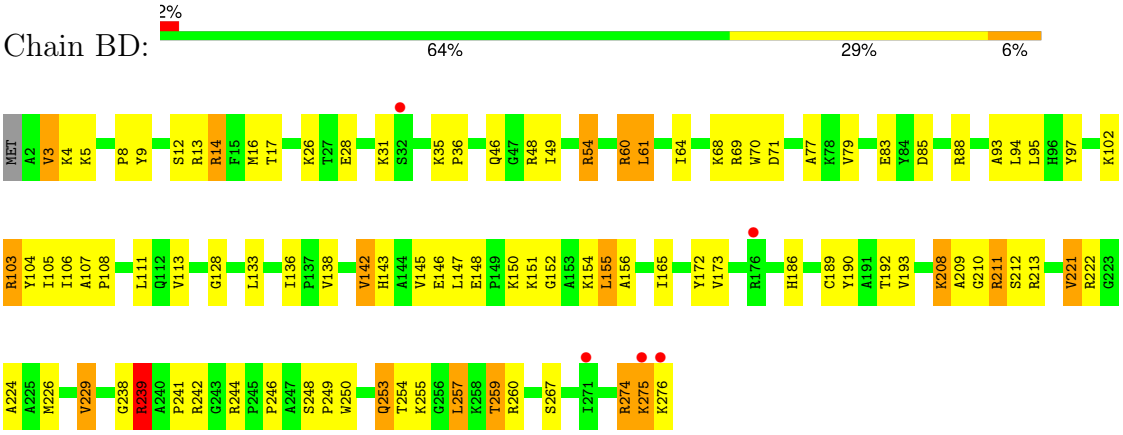

• Molecule 3: 50S ribosomal protein L2

Chain AD:



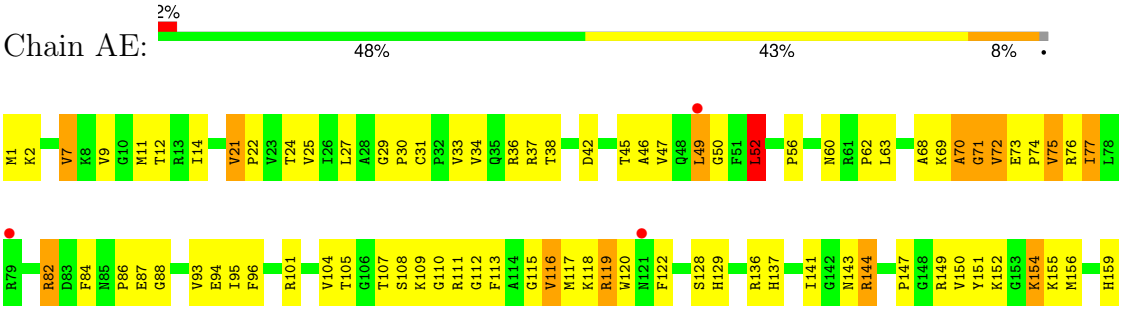

• Molecule 3: 50S ribosomal protein L2

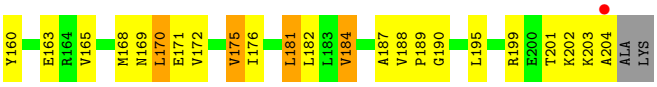
Chain BD:




• Molecule 4: 50S ribosomal protein L3

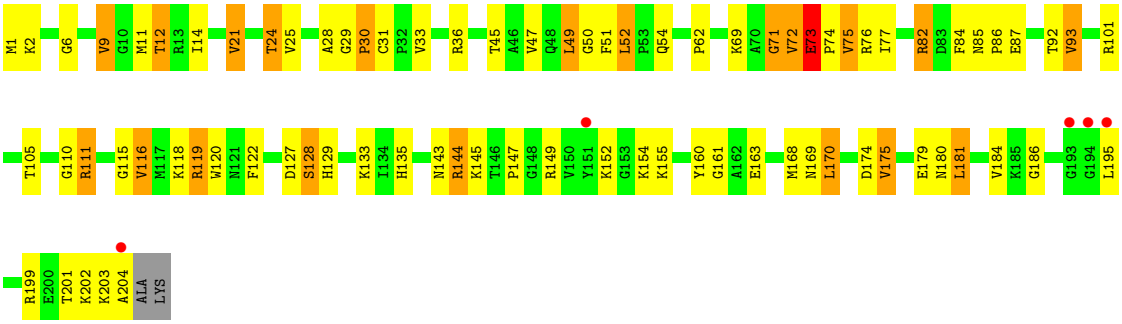
Chain AE:





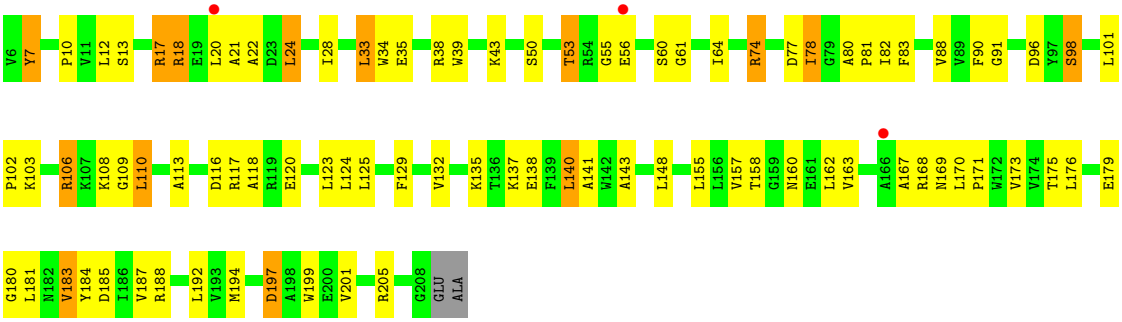
• Molecule 4: 50S ribosomal protein L3

Chain BE:

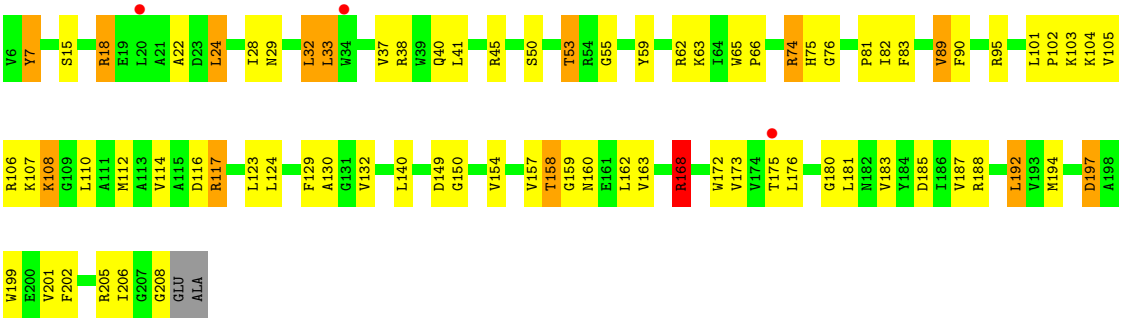
• Molecule 5: 50S ribosomal protein L4

Chain AF:

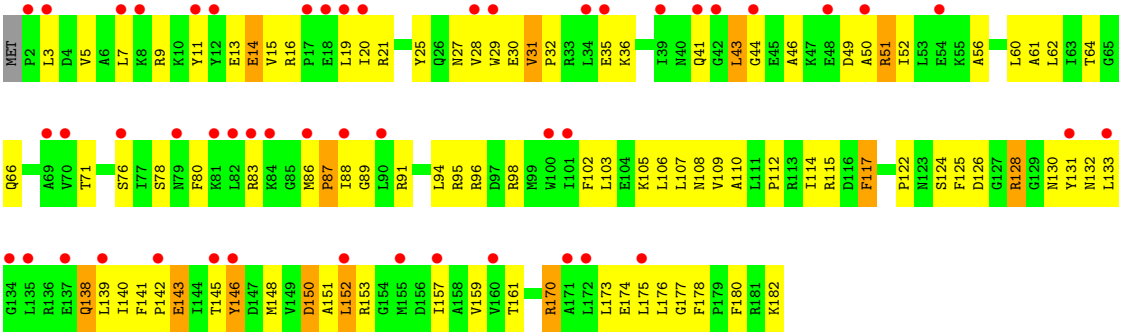
• Molecule 5: 50S ribosomal protein L4

Chain BF:

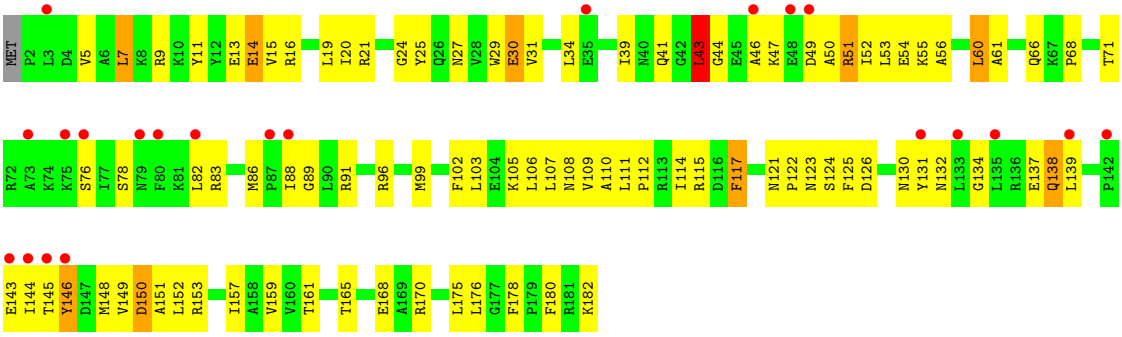
• Molecule 6: 50S ribosomal protein L5

Chain AG:



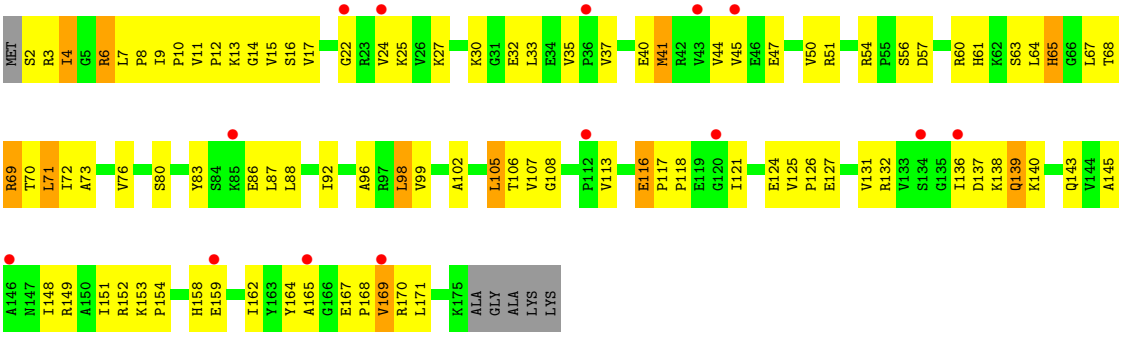
• Molecule 6: 50S ribosomal protein L5

Chain BG:

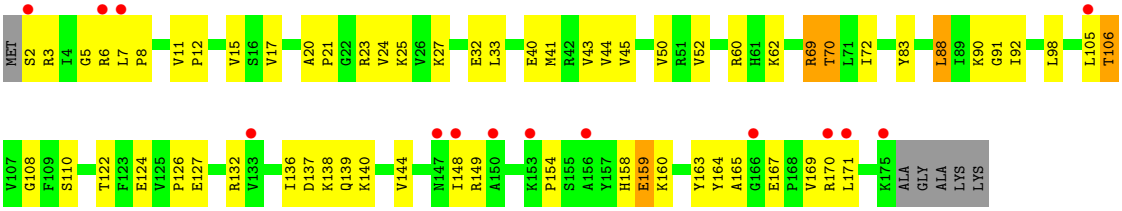
• Molecule 7: 50S ribosomal protein L6

Chain AH:

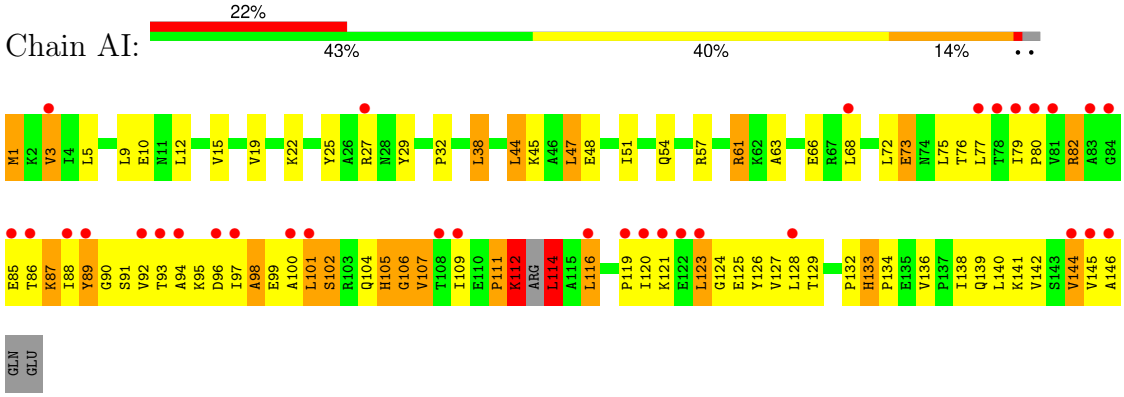
• Molecule 7: 50S ribosomal protein L6

Chain BH:

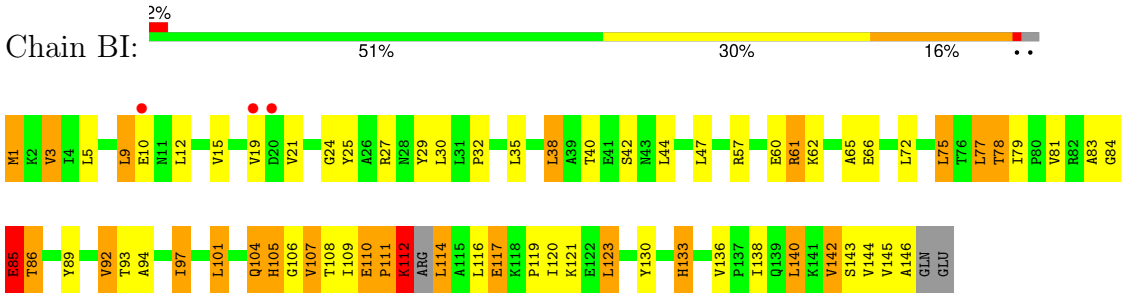
• Molecule 8: 50S ribosomal protein L9

Chain AI:



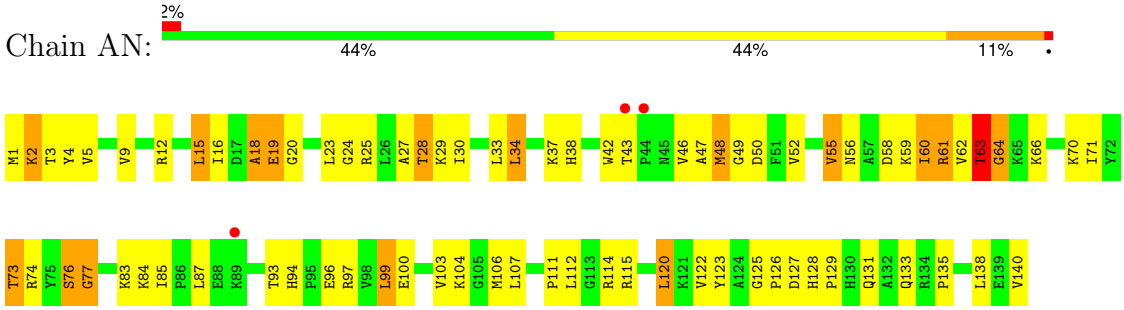

• Molecule 8: 50S ribosomal protein L9

Chain BI:



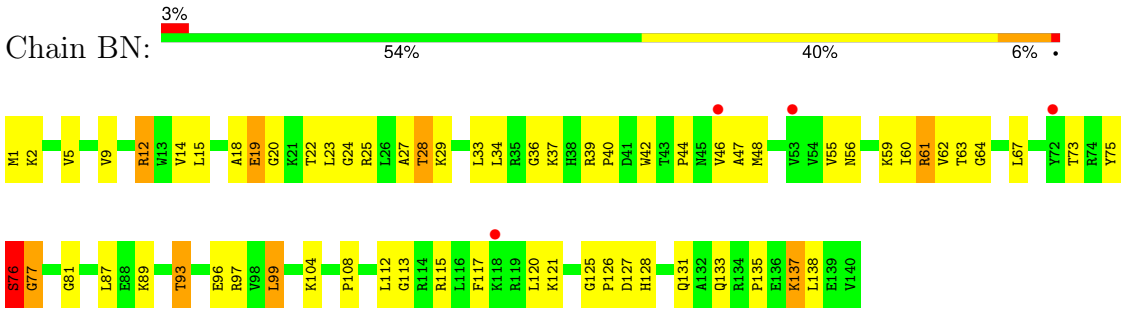

• Molecule 9: 50S ribosomal protein L13

Chain AN:



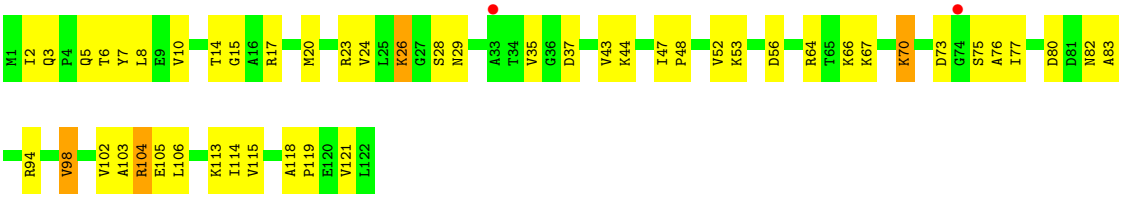

• Molecule 9: 50S ribosomal protein L13

Chain BN:



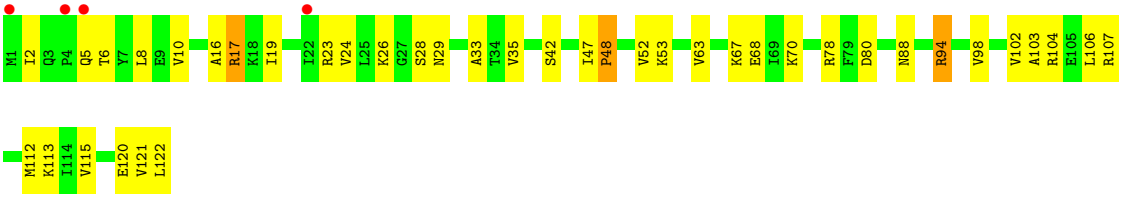

• Molecule 10: 50S ribosomal protein L14

Chain AO:



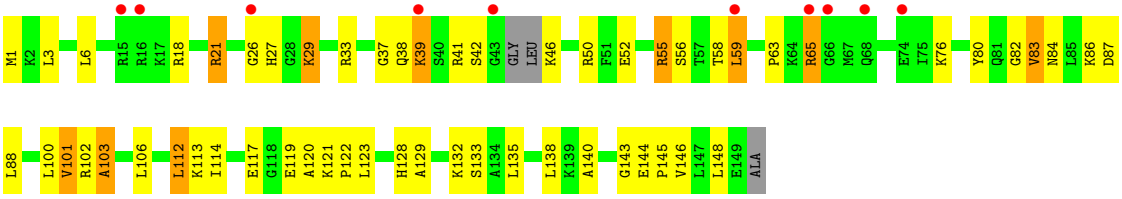
• Molecule 10: 50S ribosomal protein L14

Chain BO:

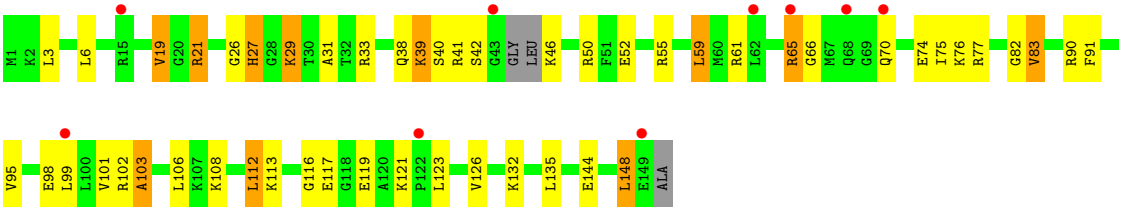
• Molecule 11: 50S ribosomal protein L15

Chain AP:

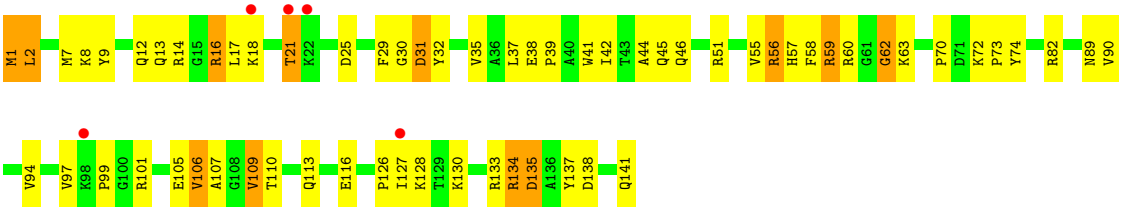
• Molecule 11: 50S ribosomal protein L15

Chain BP:

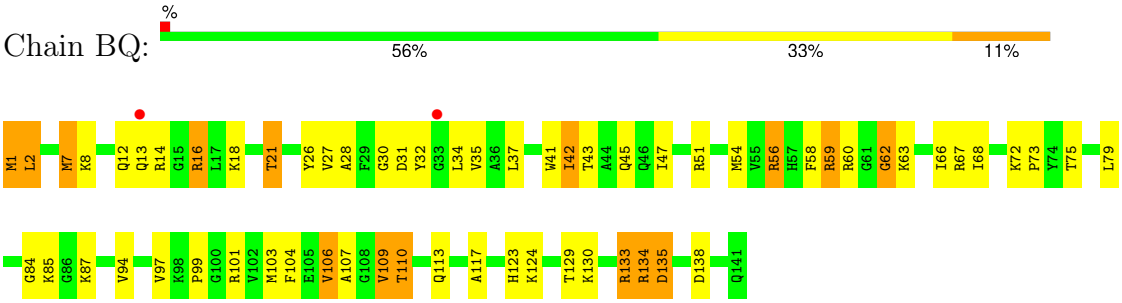
• Molecule 12: 50S ribosomal protein L16

Chain AQ:

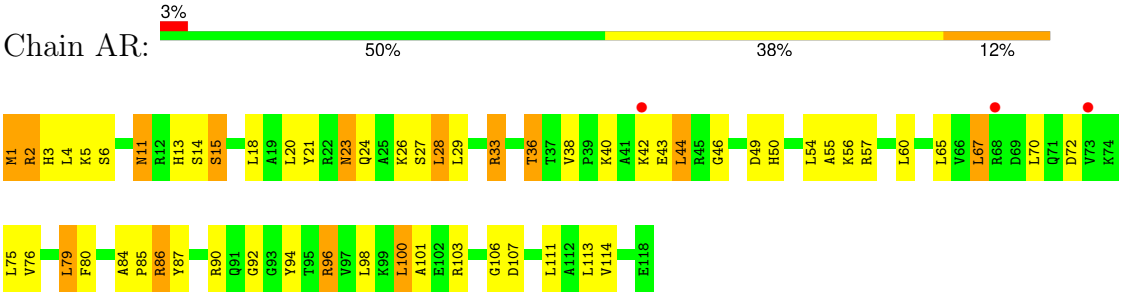
• Molecule 12: 50S ribosomal protein L16

Chain BQ:



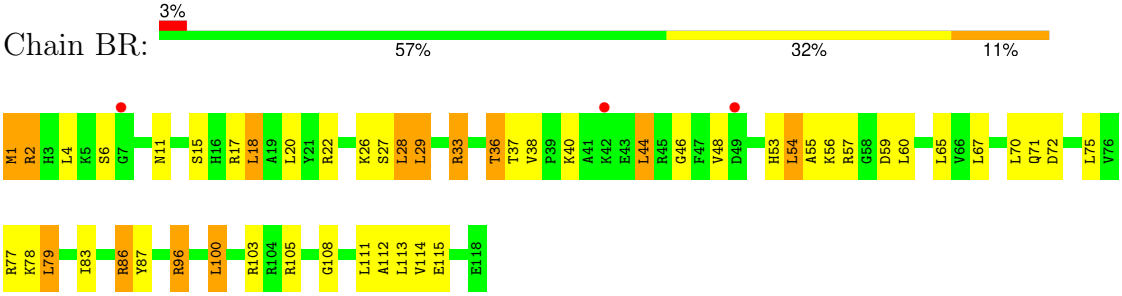

• Molecule 13: 50S ribosomal protein L17

Chain AR:



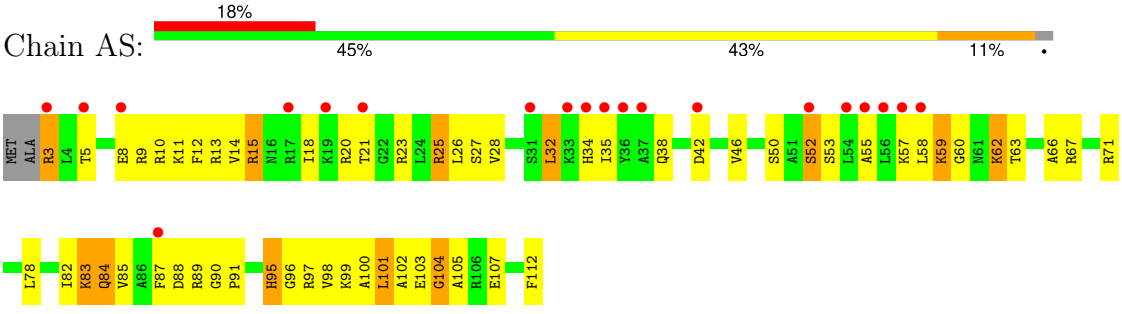

• Molecule 13: 50S ribosomal protein L17

Chain BR:



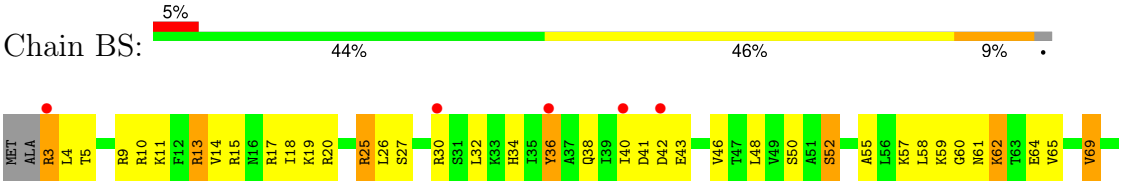

• Molecule 14: 50S ribosomal protein L18

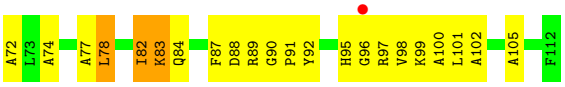
Chain AS:




• Molecule 14: 50S ribosomal protein L18

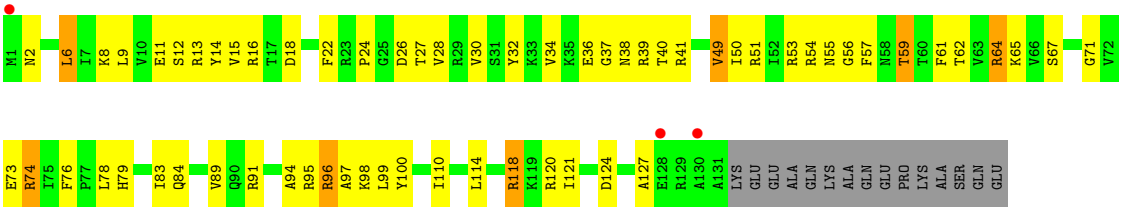
Chain BS:





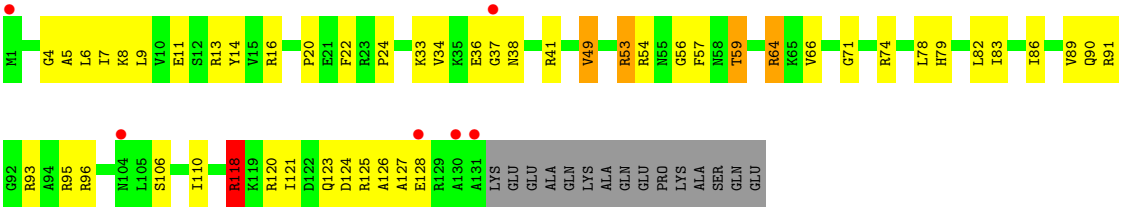

• Molecule 15: 50S ribosomal protein L19

Chain AT:


• Molecule 15: 50S ribosomal protein L19

Chain BT:


• Molecule 16: 50S ribosomal protein L20

Chain AU:



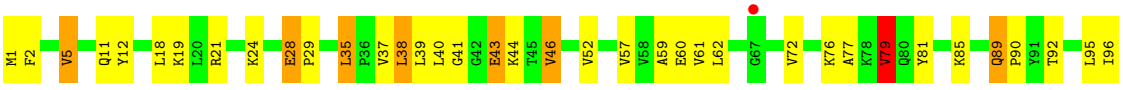
• Molecule 16: 50S ribosomal protein L20

Chain BU:



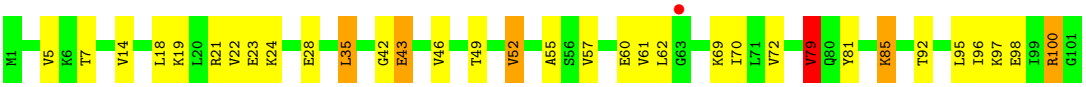
• Molecule 17: 50S ribosomal protein L21

Chain AV:

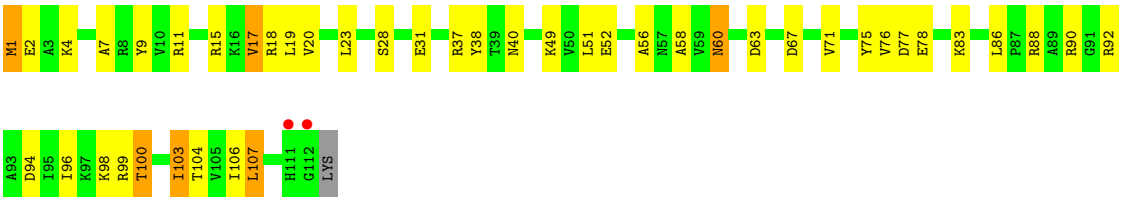

• Molecule 17: 50S ribosomal protein L21

Chain BV:

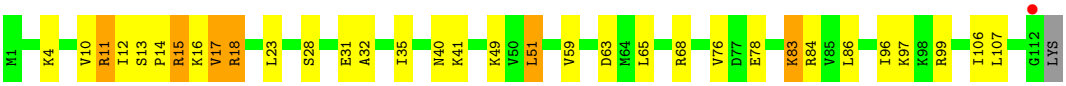

• Molecule 18: 50S ribosomal protein L22

Chain AW:

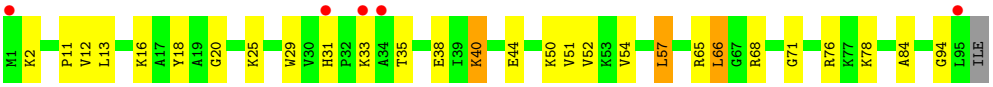

• Molecule 18: 50S ribosomal protein L22

Chain BW:

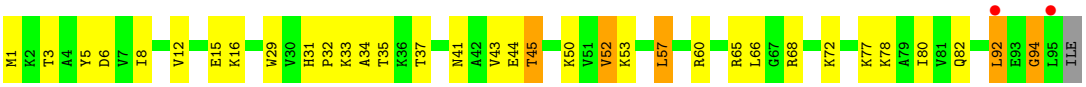

• Molecule 19: 50S ribosomal protein L23

Chain AX:


• Molecule 19: 50S ribosomal protein L23

Chain BX:

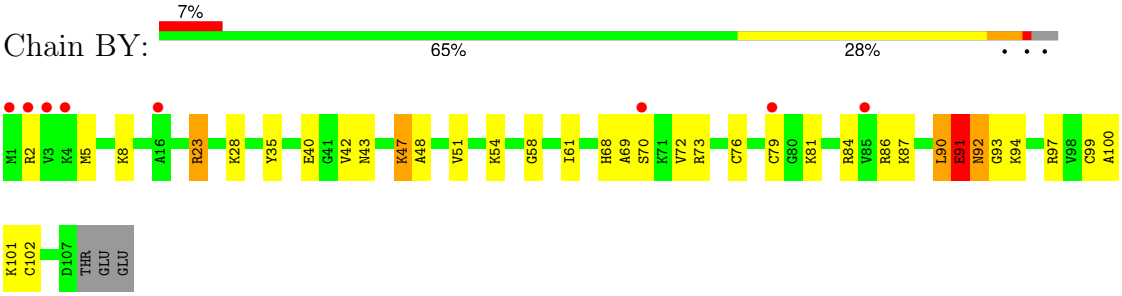

• Molecule 20: 50S ribosomal protein L24

Chain AY:



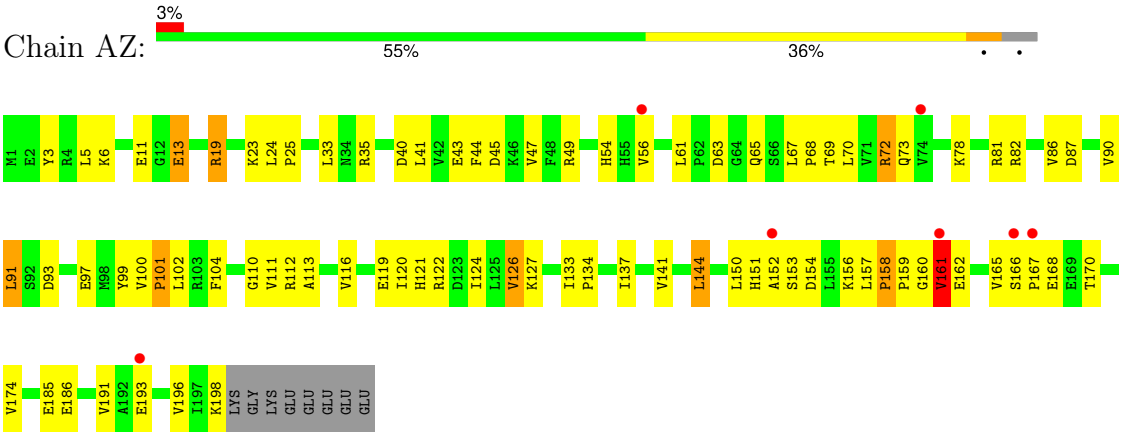
• Molecule 20: 50S ribosomal protein L24

Chain BY:



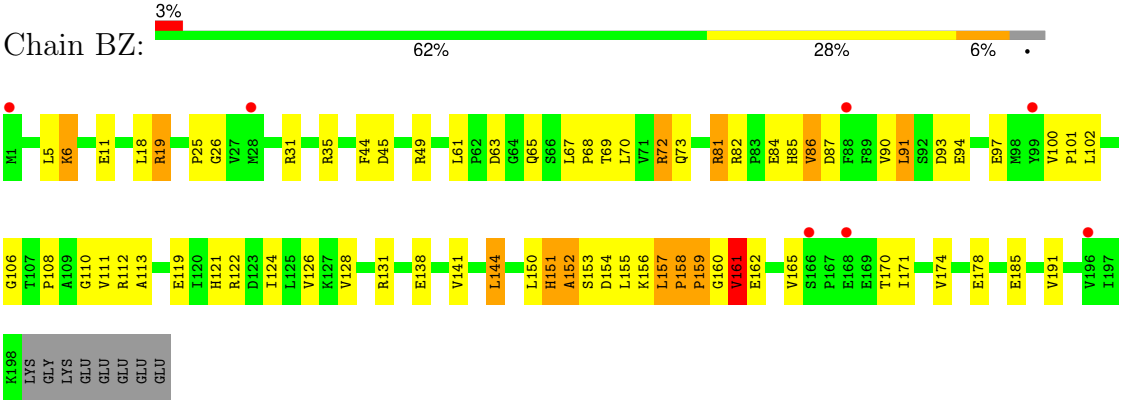

• Molecule 21: 50S ribosomal protein L25

Chain AZ:



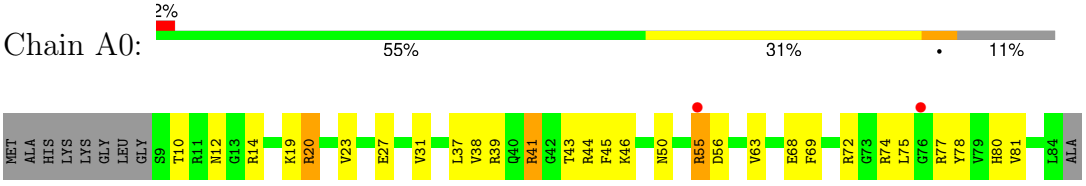

• Molecule 21: 50S ribosomal protein L25

Chain BZ:



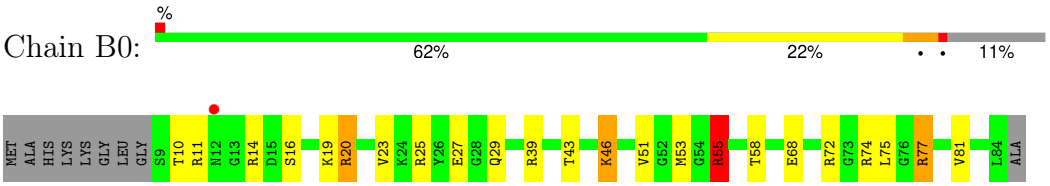

• Molecule 22: 50S ribosomal protein L27

Chain A0:



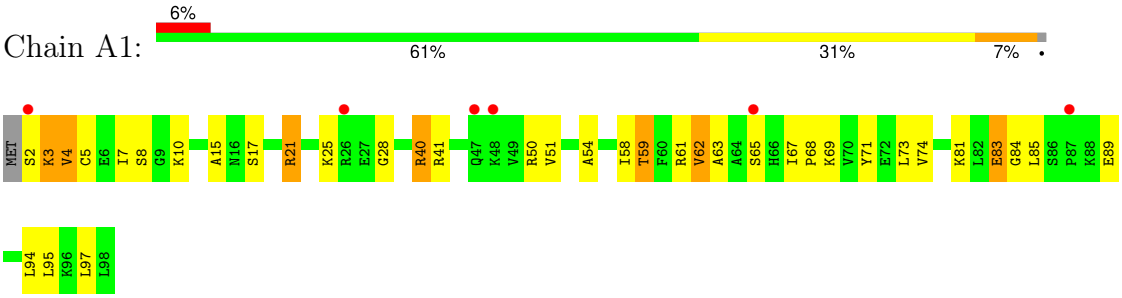

• Molecule 22: 50S ribosomal protein L27

Chain B0:



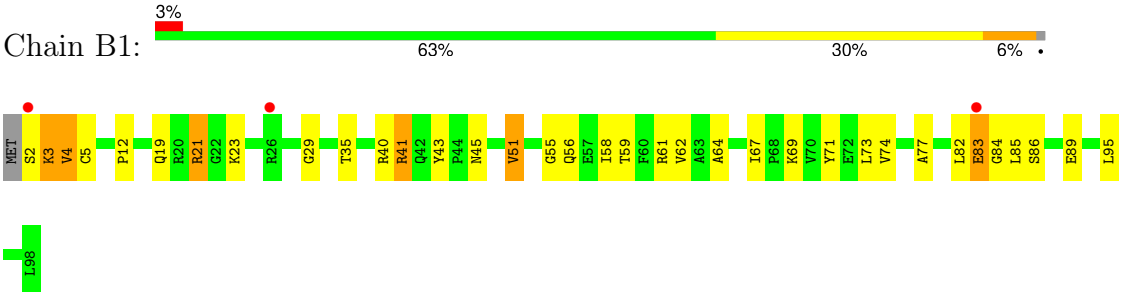

• Molecule 23: 50S ribosomal protein L28

Chain A1:



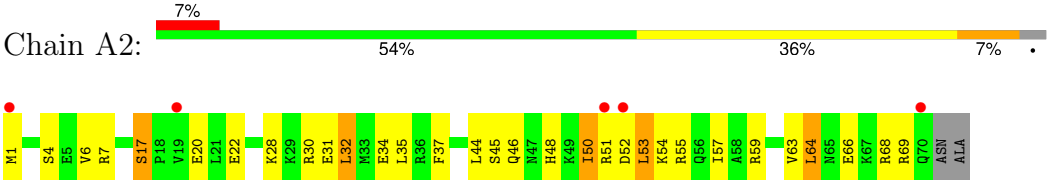

• Molecule 23: 50S ribosomal protein L28

Chain B1:



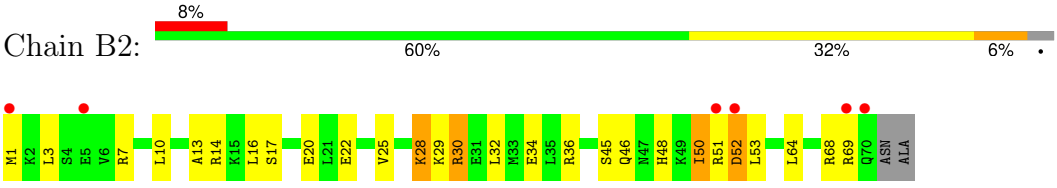

• Molecule 24: 50S ribosomal protein L29

Chain A2:



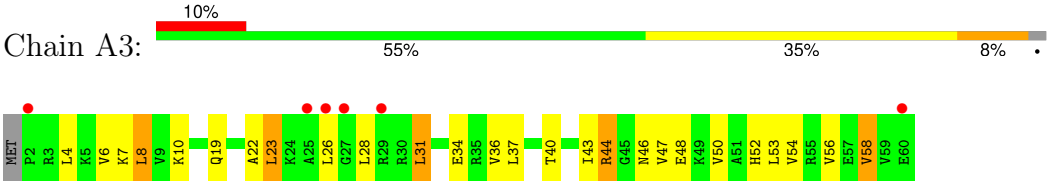

• Molecule 24: 50S ribosomal protein L29

Chain B2:



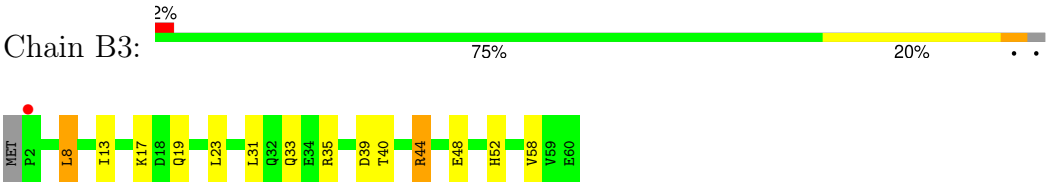

• Molecule 25: 50S ribosomal protein L30

Chain A3:



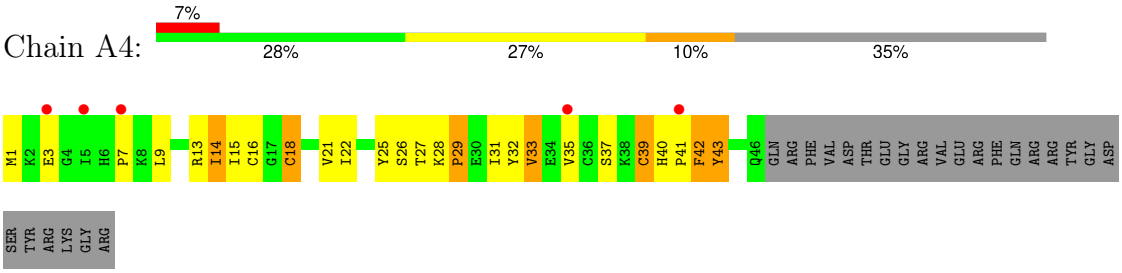

• Molecule 25: 50S ribosomal protein L30

Chain B3:



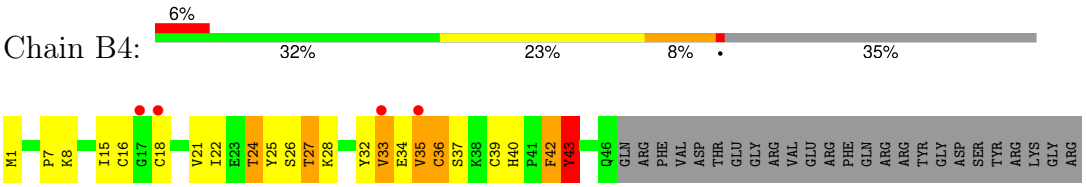

• Molecule 26: 50S ribosomal protein L31

Chain A4:



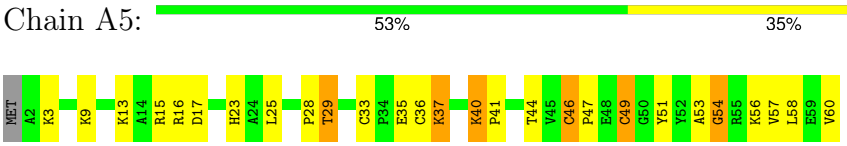

• Molecule 26: 50S ribosomal protein L31

Chain B4:



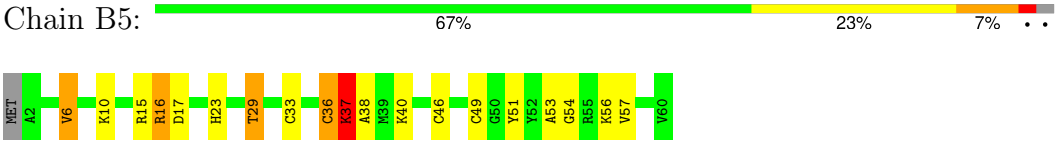

• Molecule 27: 50S ribosomal protein L32

Chain A5:



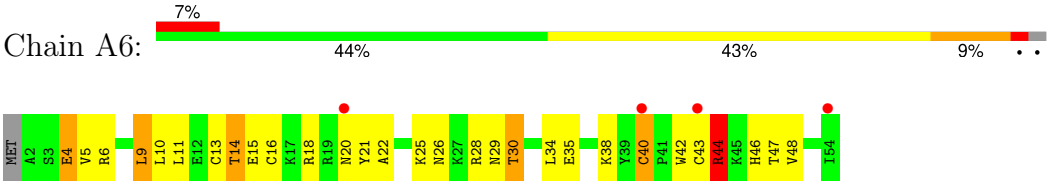

• Molecule 27: 50S ribosomal protein L32

Chain B5:



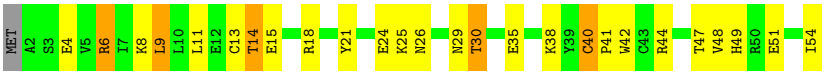

• Molecule 28: 50S ribosomal protein L33

Chain A6:



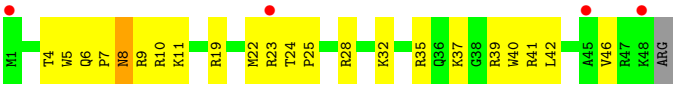

• Molecule 28: 50S ribosomal protein L33

Chain B6:



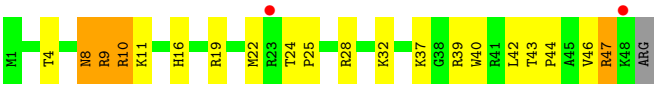

• Molecule 29: 50S ribosomal protein L34

Chain A7:

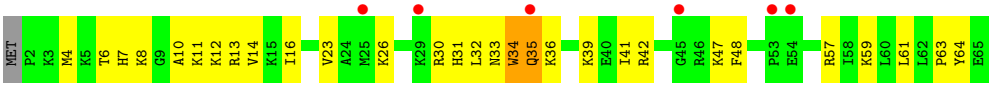

• Molecule 29: 50S ribosomal protein L34

Chain B7:


• Molecule 30: 50S ribosomal protein L35

Chain A8:

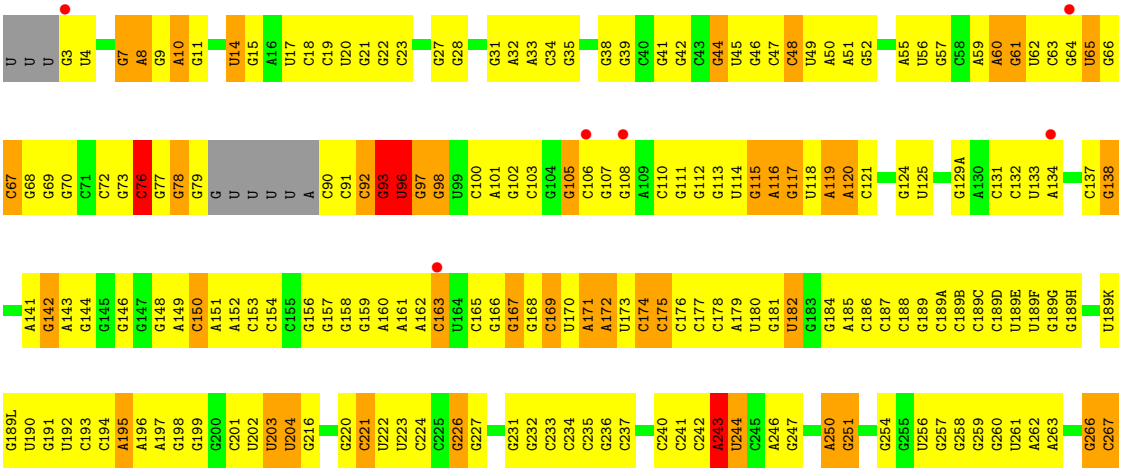

• Molecule 30: 50S ribosomal protein L35

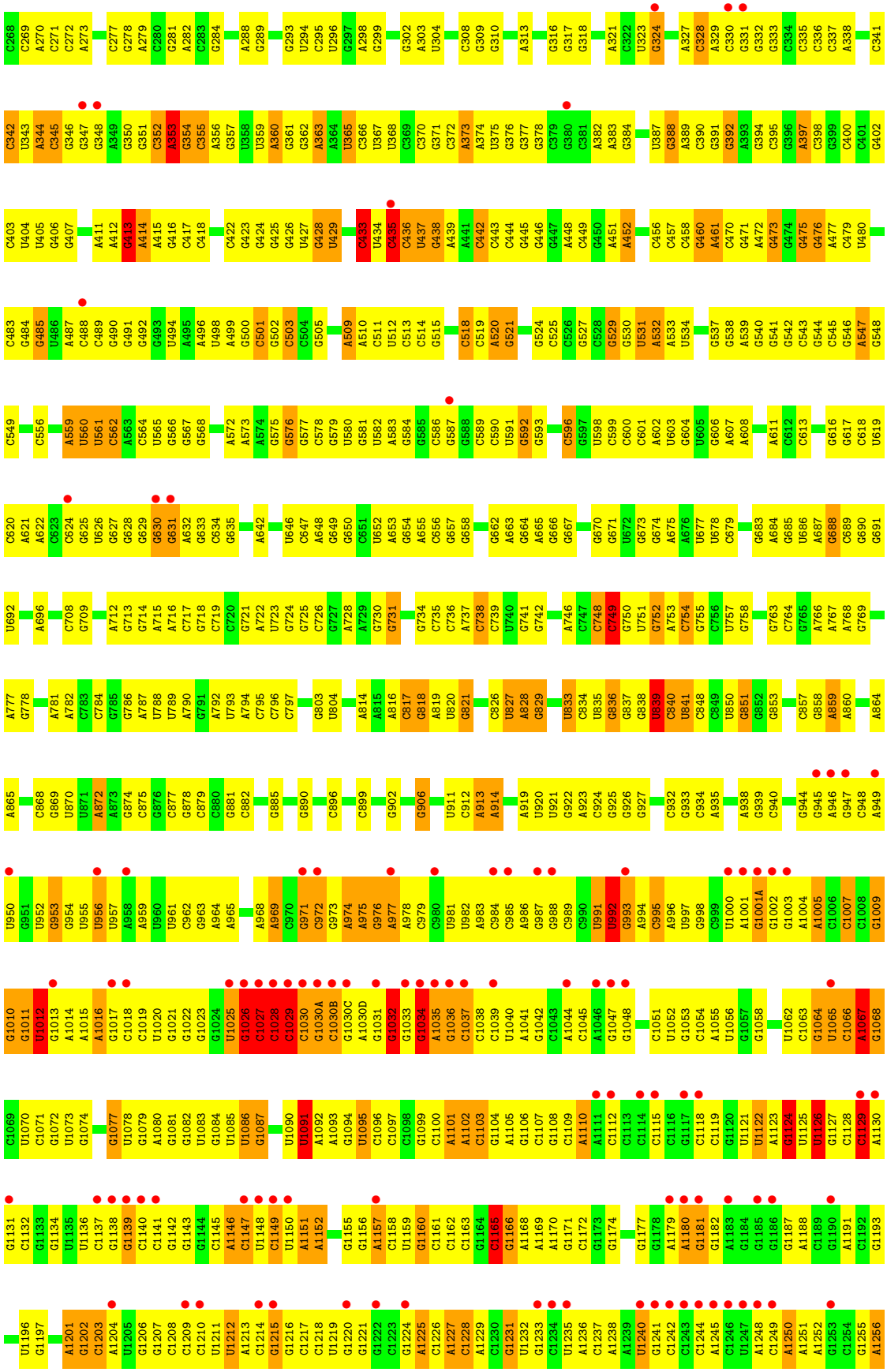
Chain B8:

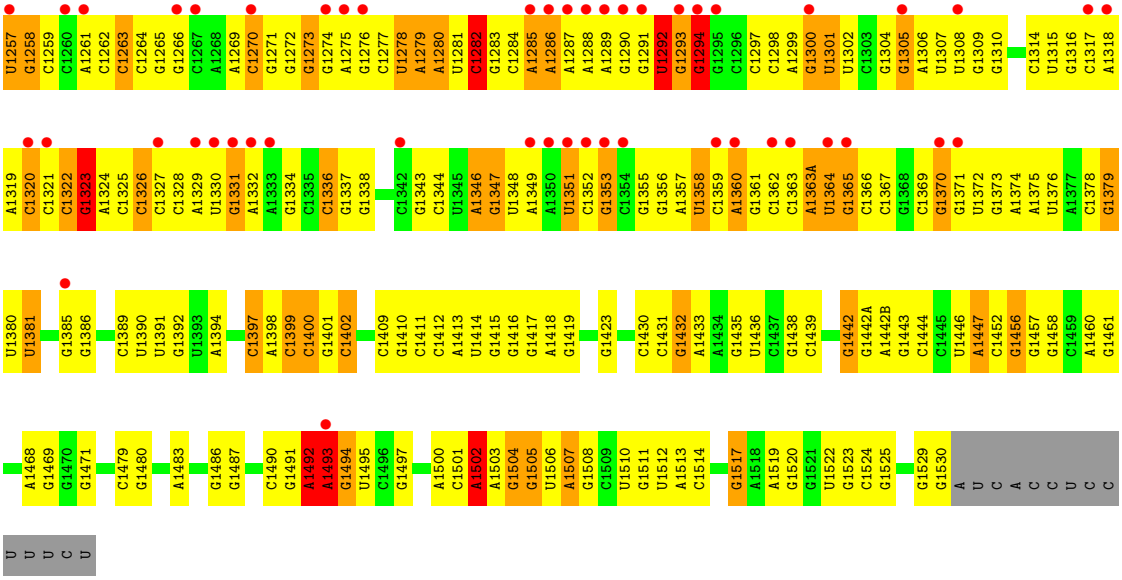


• Molecule 31: 16S ribosomal RNA

Chain CA:

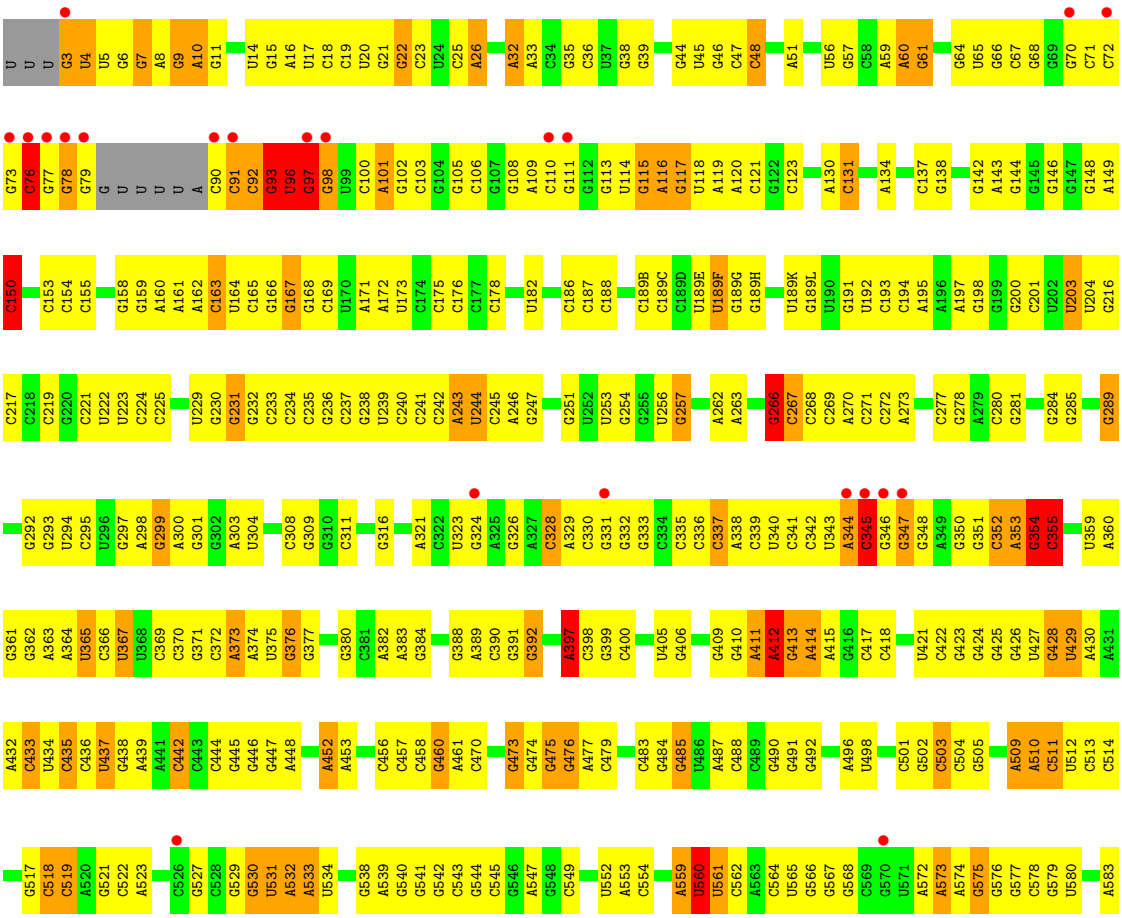



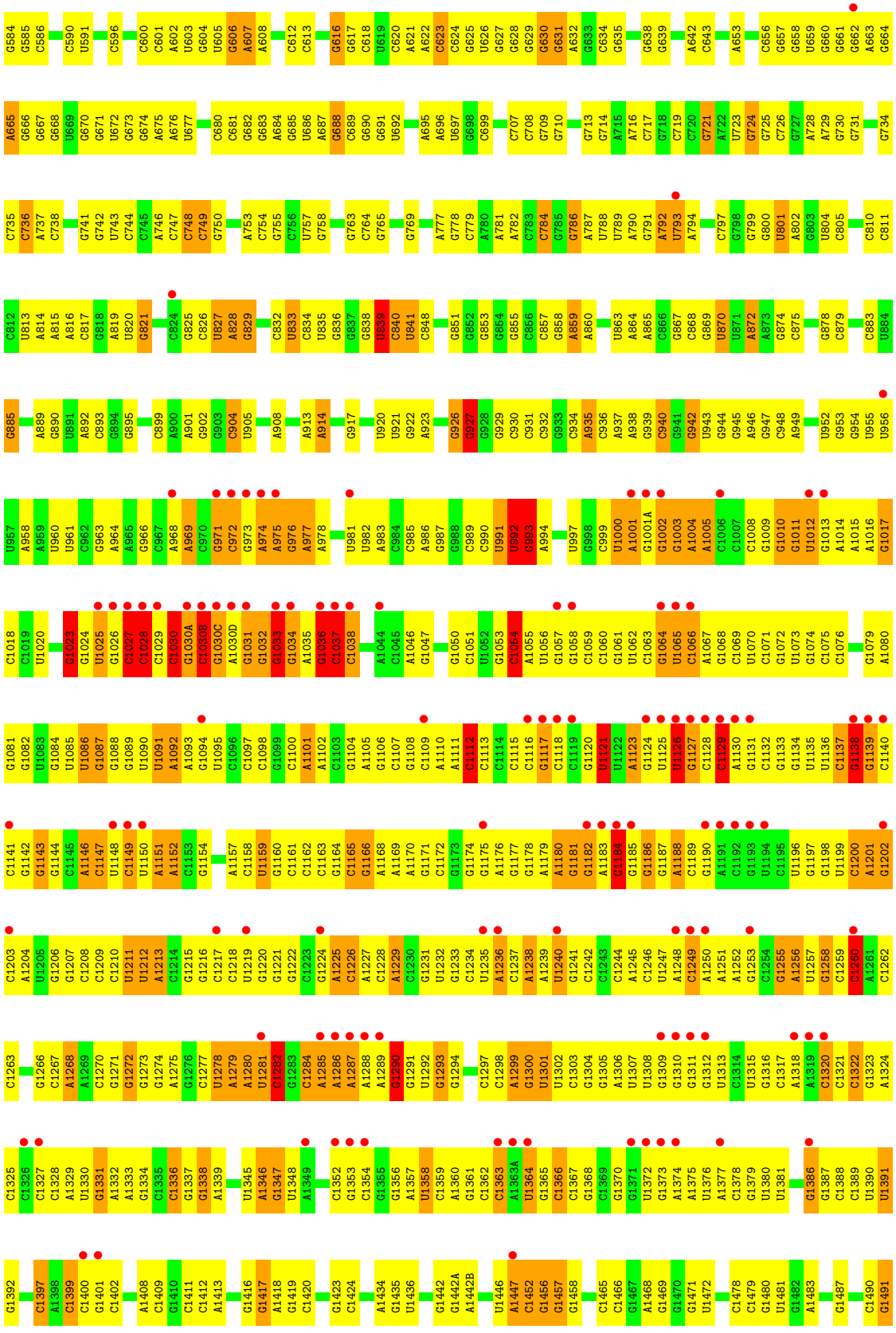


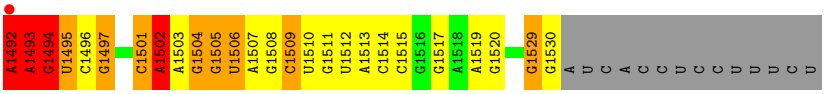


• Molecule 31: 16S ribosomal RNA

Chain DA:

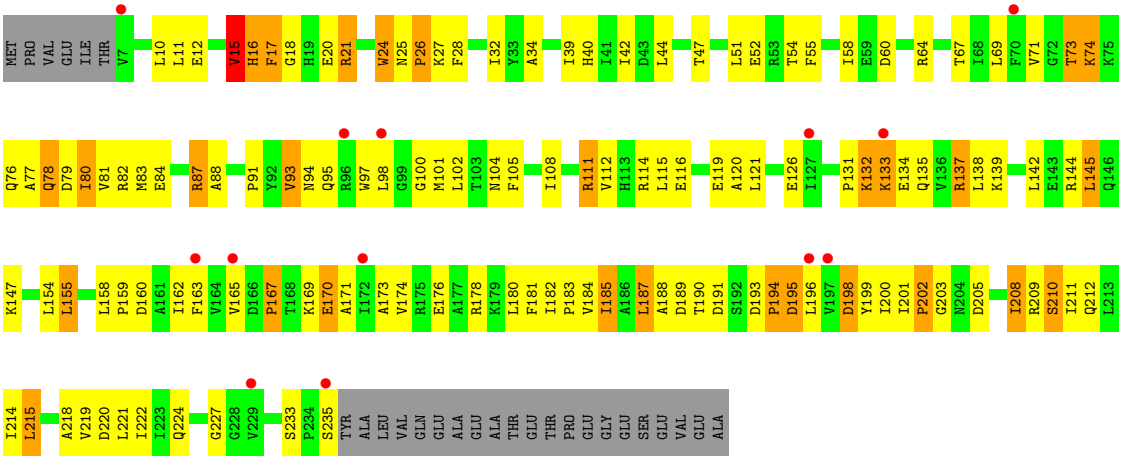







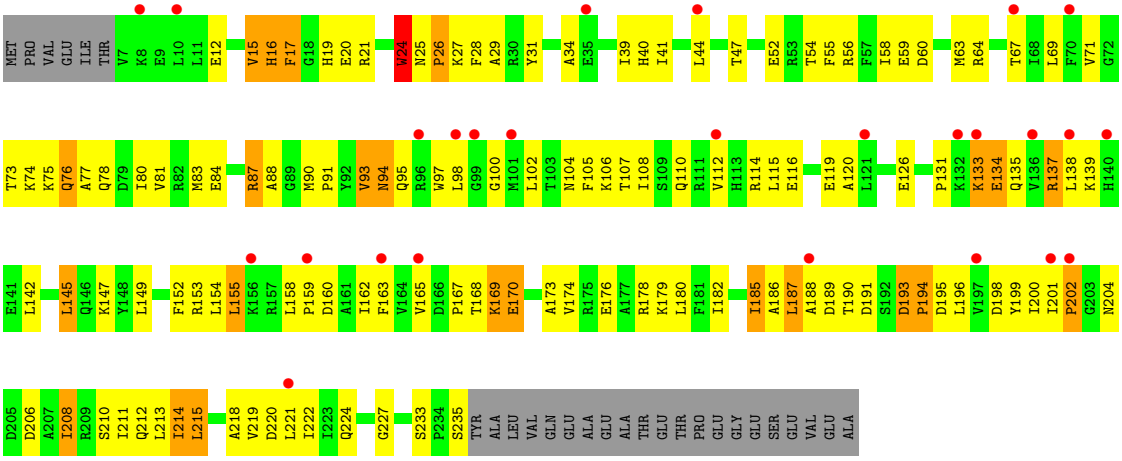

• Molecule 32: 30S ribosomal protein S2

Chain CB:

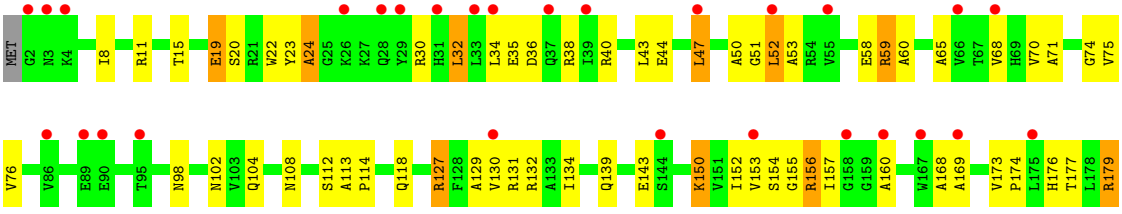

• Molecule 32: 30S ribosomal protein S2

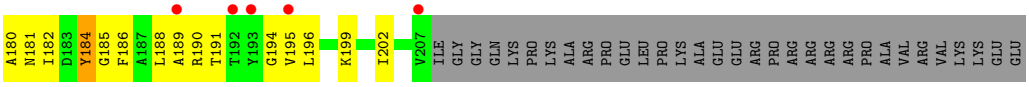
Chain DB:


• Molecule 33: 30S ribosomal protein S3

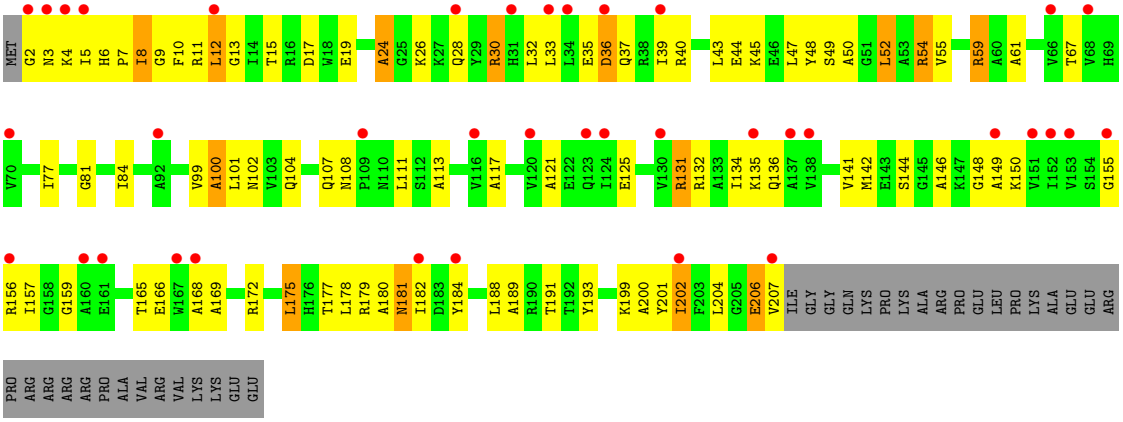
Chain CC:



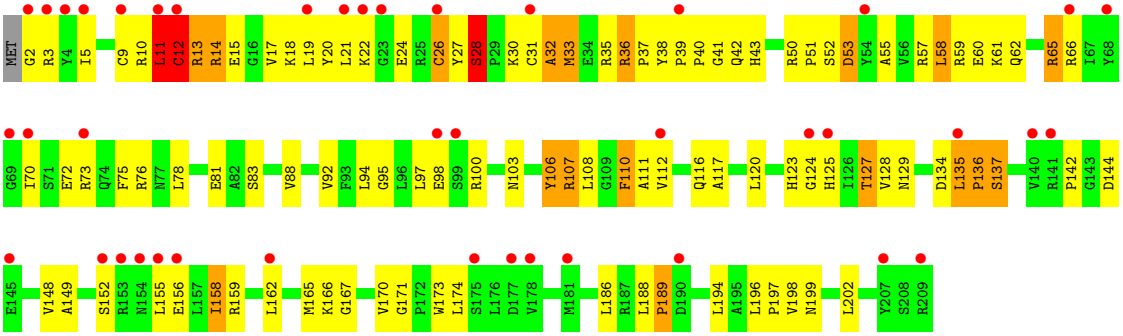
• Molecule 33: 30S ribosomal protein S3

Chain DC:

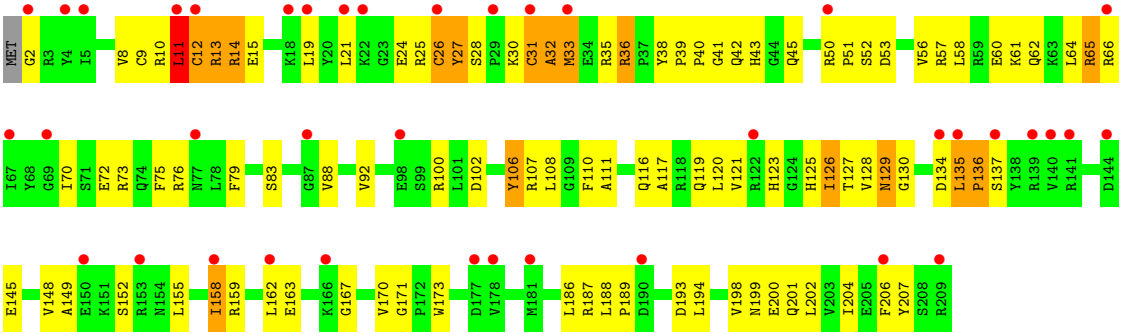
• Molecule 34: 30S ribosomal protein S4

Chain CD:

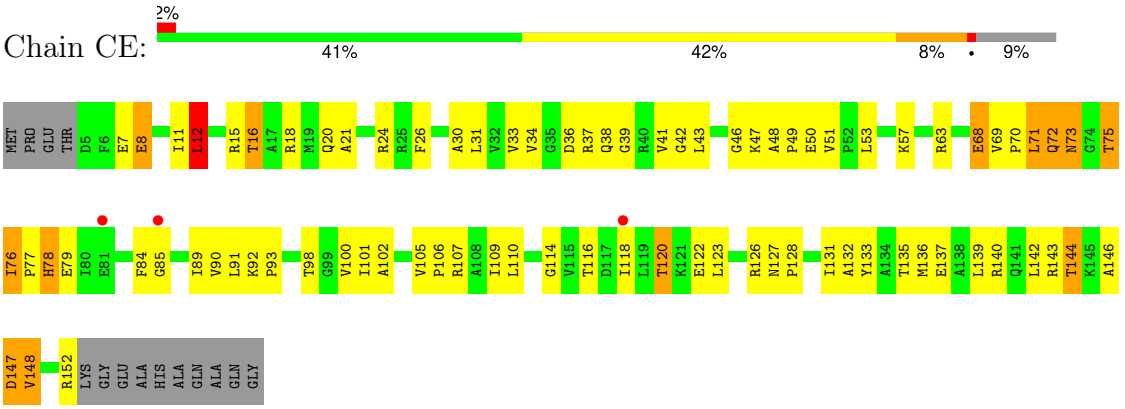
• Molecule 34: 30S ribosomal protein S4

Chain DD:

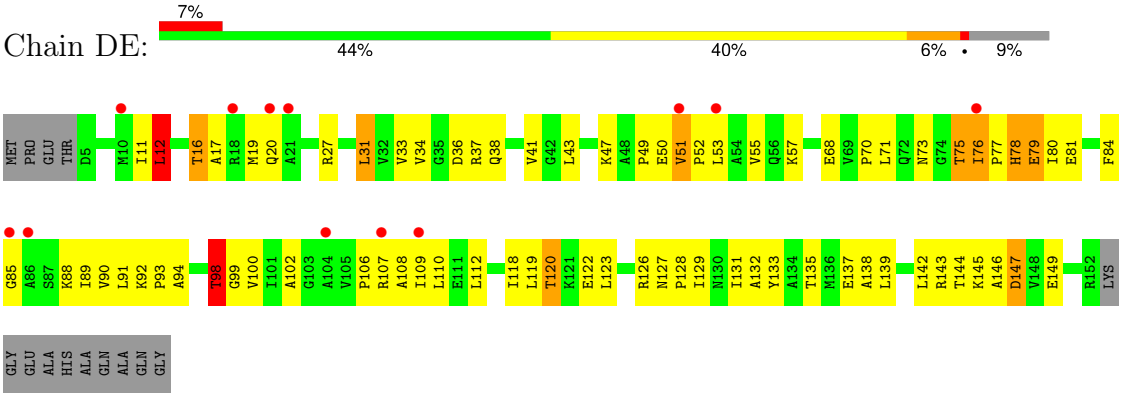
• Molecule 35: 30S ribosomal protein S5

Chain CE:



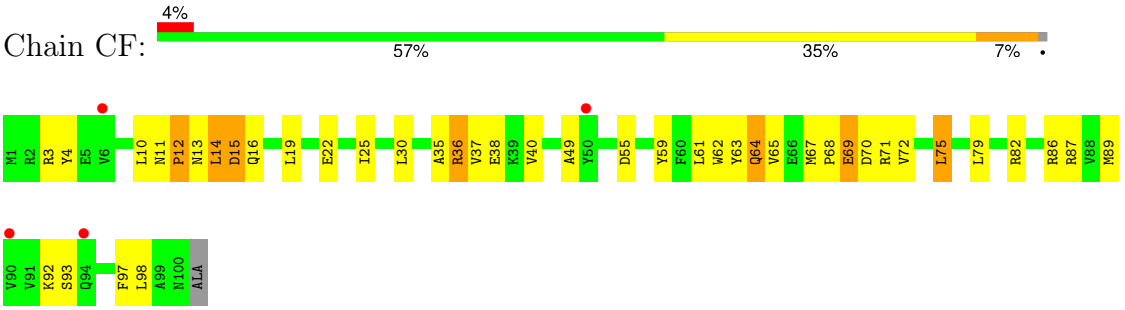

• Molecule 35: 30S ribosomal protein S5

Chain DE:



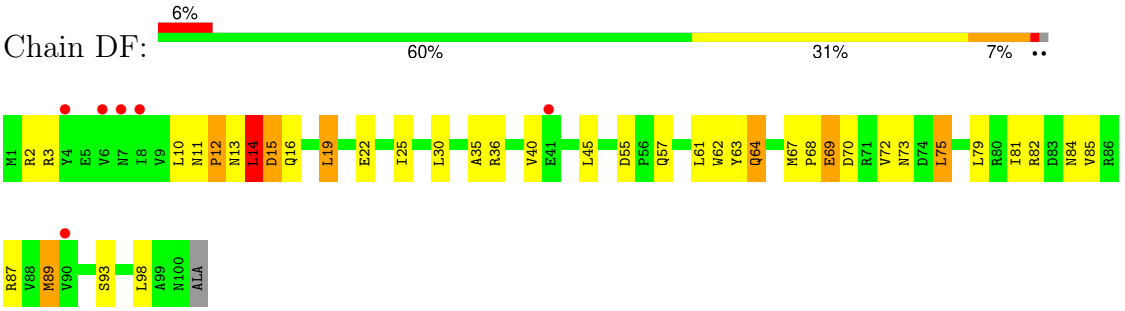

• Molecule 36: 30S ribosomal protein S6

Chain CF:



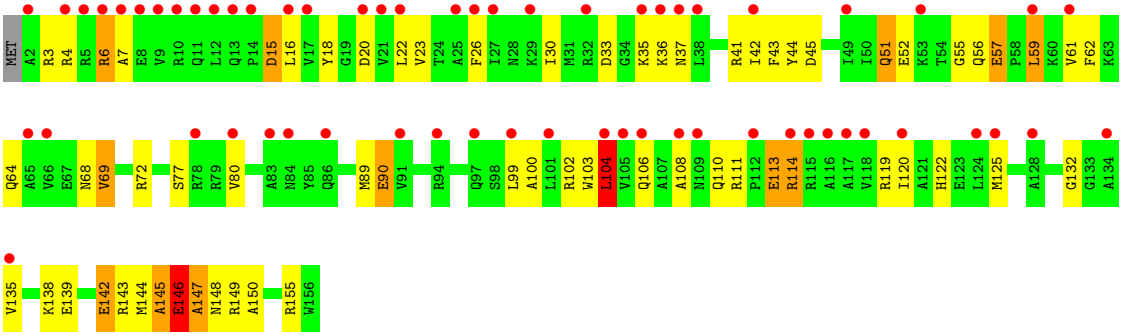

• Molecule 36: 30S ribosomal protein S6

Chain DF:

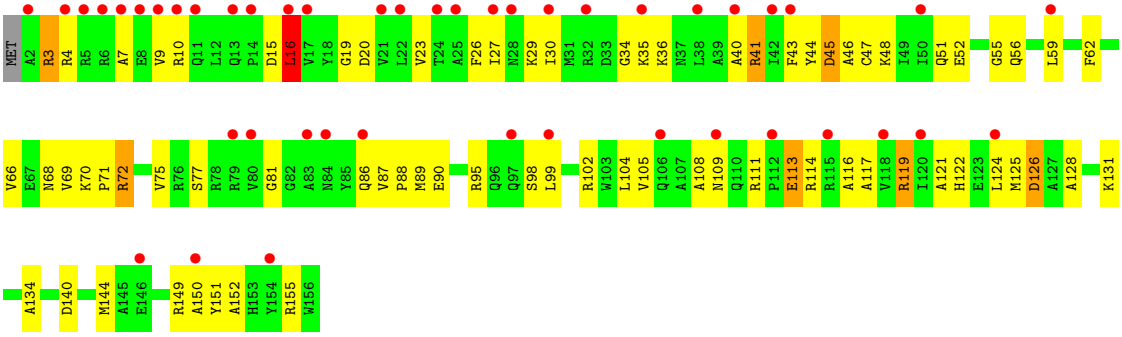



• Molecule 37: 30S ribosomal protein S7

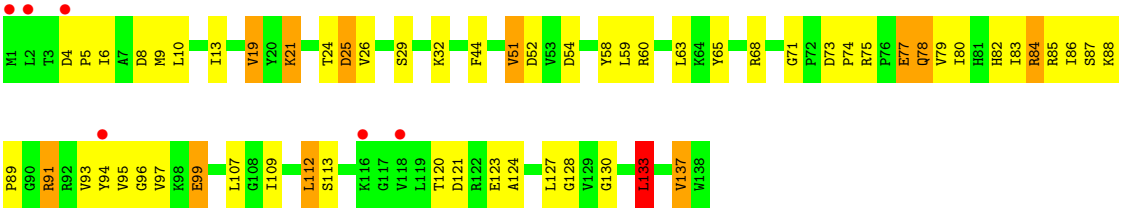
Chain CG:



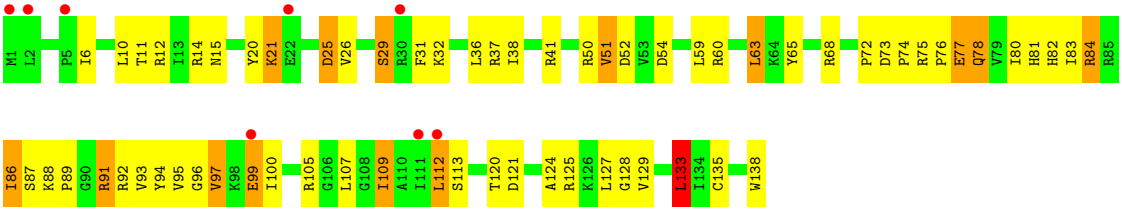

• Molecule 37: 30S ribosomal protein S7

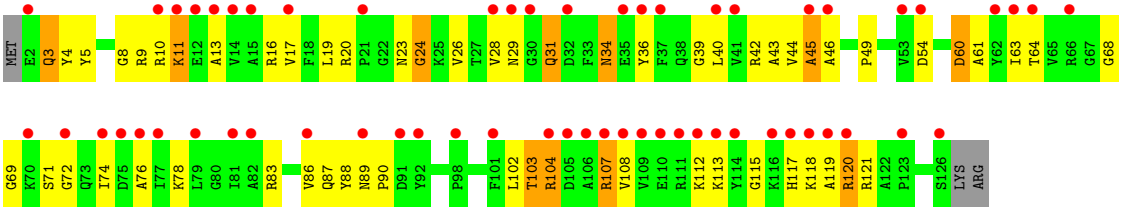

• Molecule 38: 30S ribosomal protein S8


• Molecule 38: 30S ribosomal protein S8

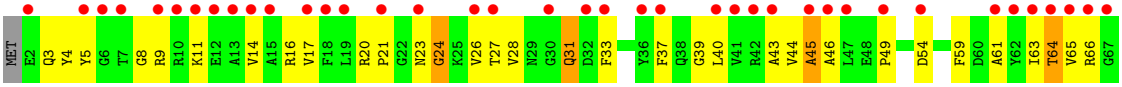

• Molecule 39: 30S ribosomal protein S9

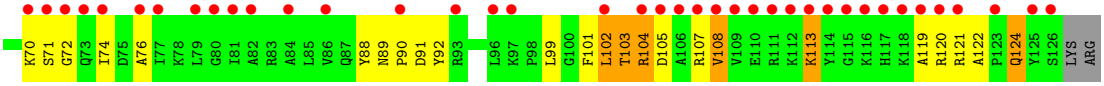




• Molecule 39: 30S ribosomal protein S9

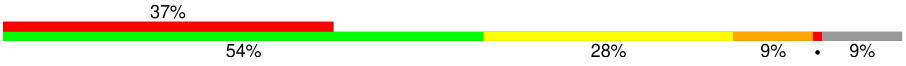
Chain DI:

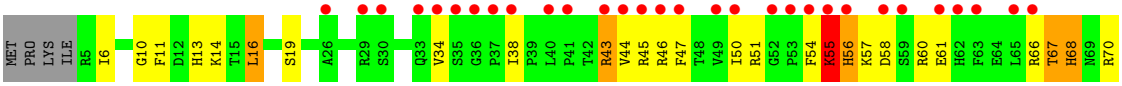



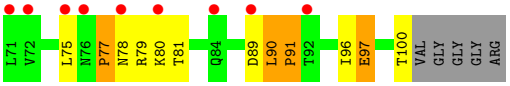


• Molecule 40: 30S ribosomal protein S10

Chain CJ:

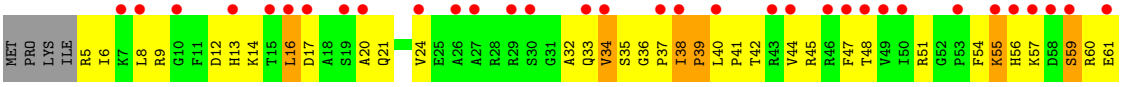




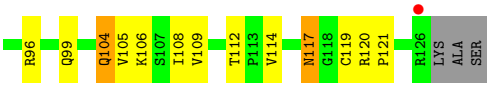
• Molecule 40: 30S ribosomal protein S10

Chain DJ:

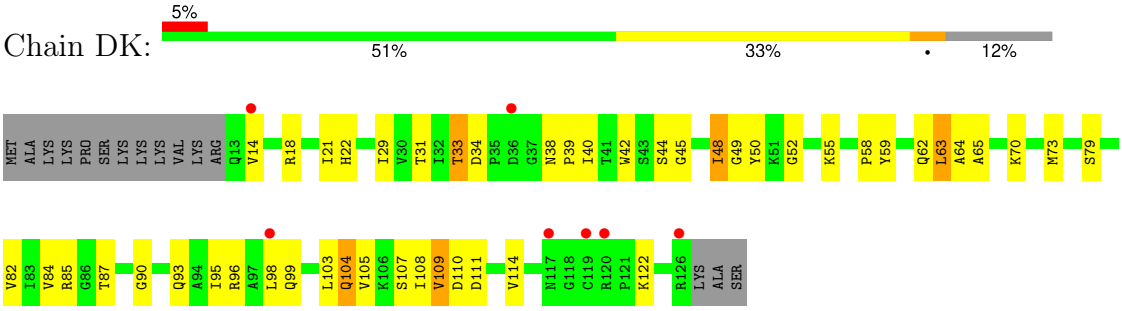
• Molecule 41: 30S ribosomal protein S11

Chain CK:

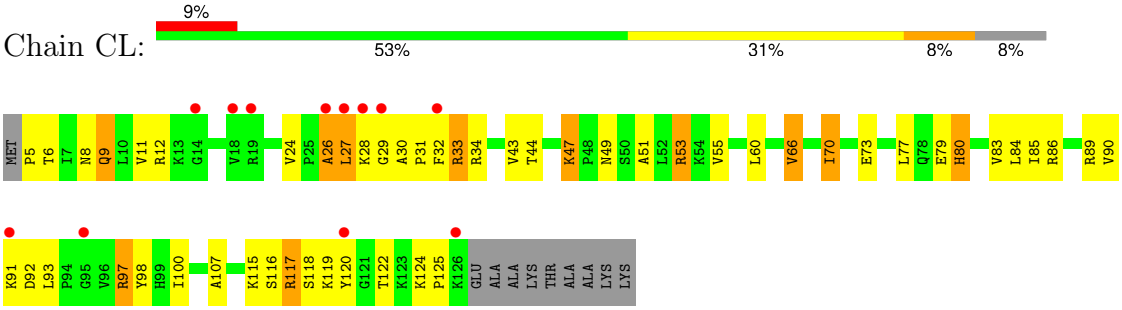
• Molecule 41: 30S ribosomal protein S11

Chain DK:



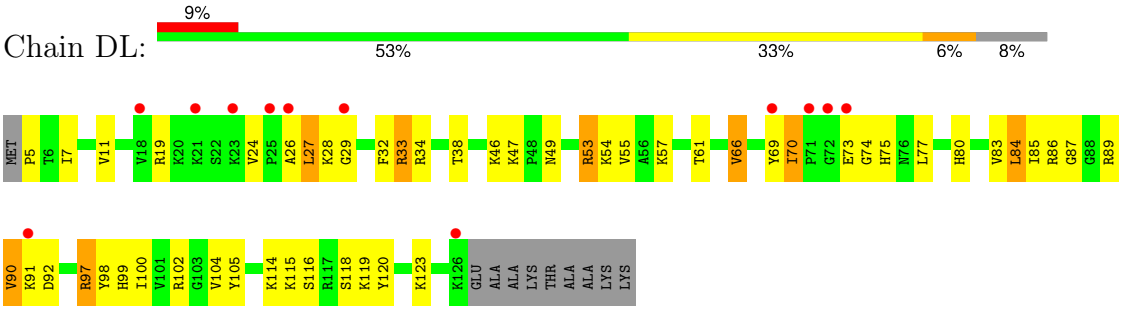

• Molecule 42: 30S ribosomal protein S12

Chain CL:



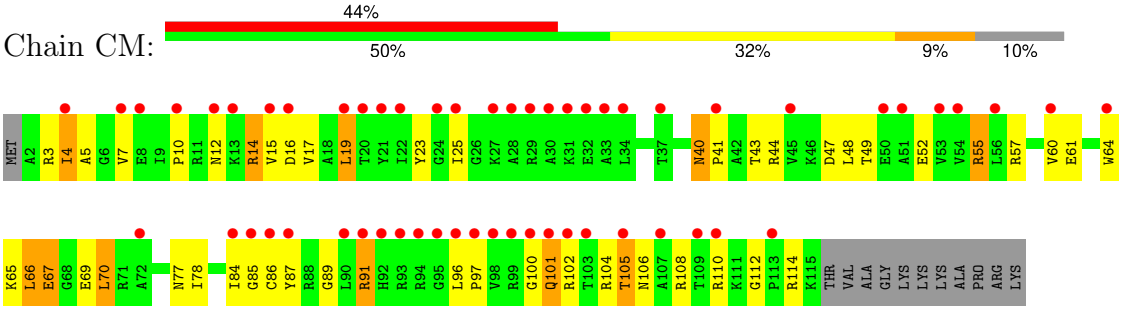

• Molecule 42: 30S ribosomal protein S12

Chain DL:



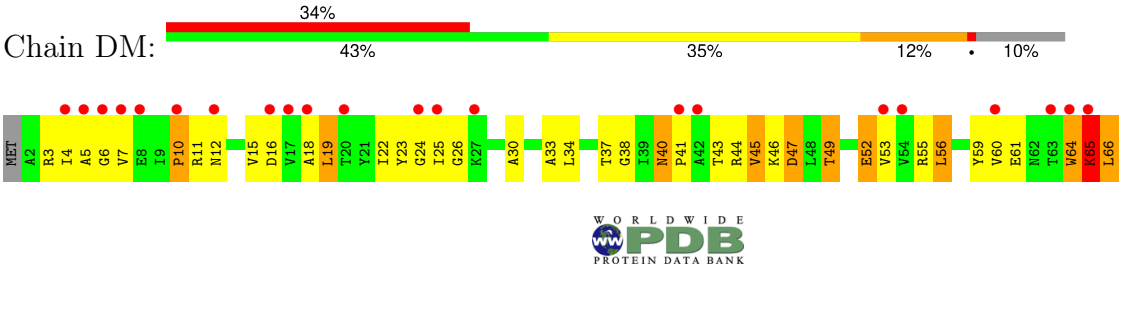

• Molecule 43: 30S ribosomal protein S13

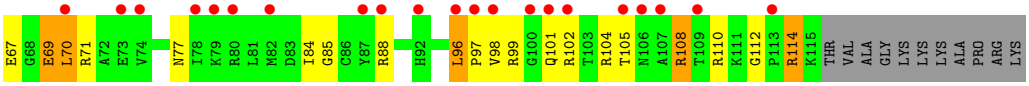
Chain CM:



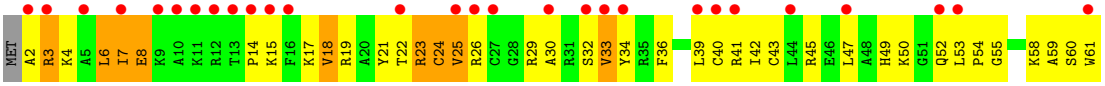

• Molecule 43: 30S ribosomal protein S13

Chain DM:

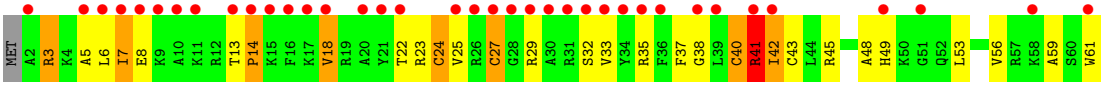




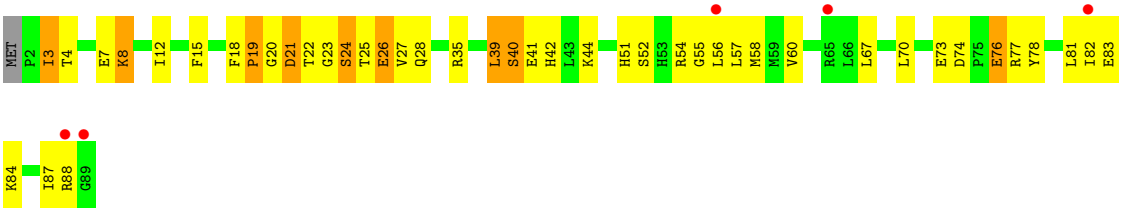

• Molecule 44: 30S ribosomal protein S14

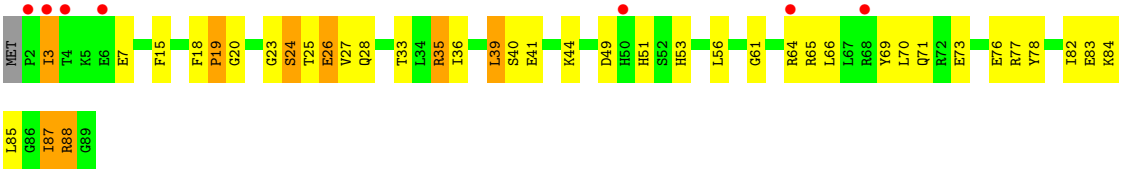

• Molecule 44: 30S ribosomal protein S14


• Molecule 45: 30S ribosomal protein S15

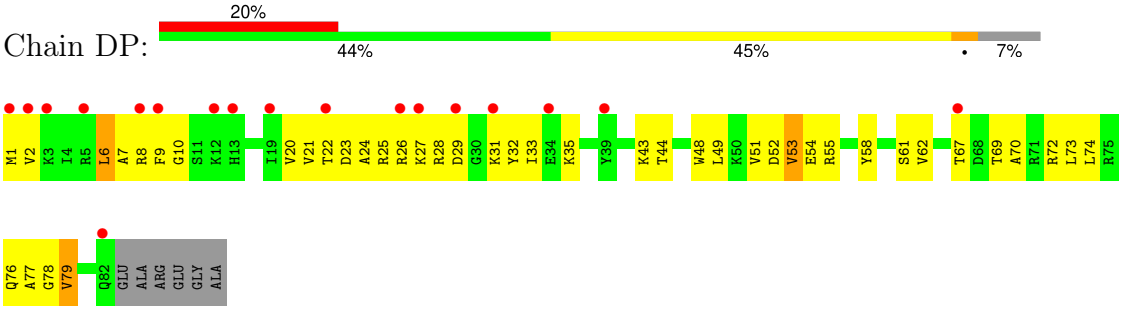

• Molecule 45: 30S ribosomal protein S15


• Molecule 46: 30S ribosomal protein S16

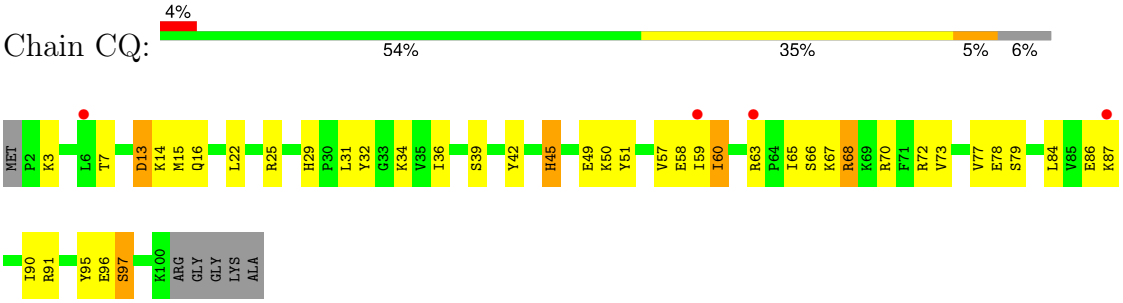

• Molecule 46: 30S ribosomal protein S16

Chain DP:



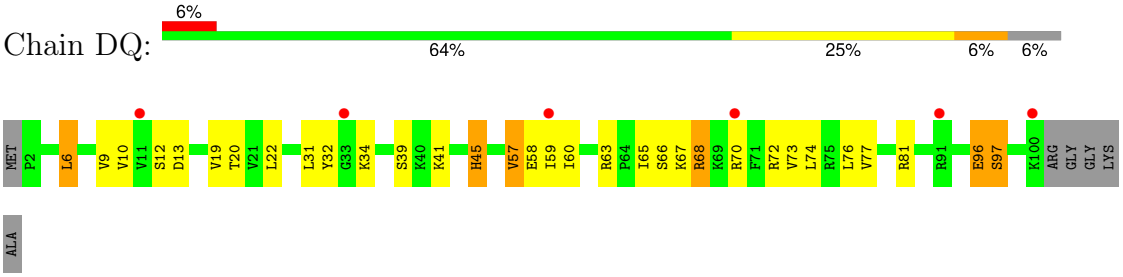

• Molecule 47: 30S ribosomal protein S17

Chain CQ:



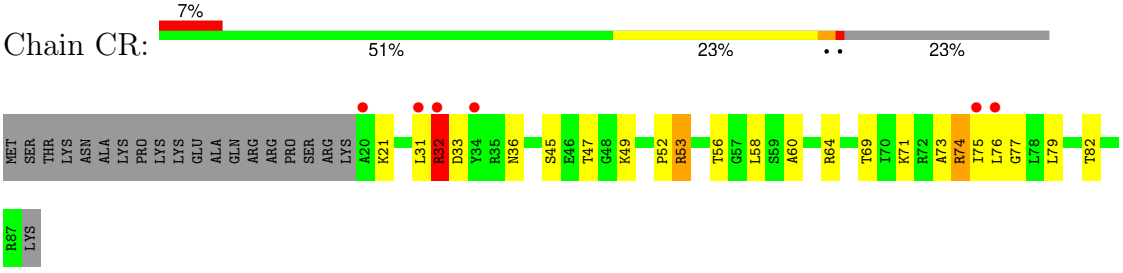

• Molecule 47: 30S ribosomal protein S17

Chain DQ:



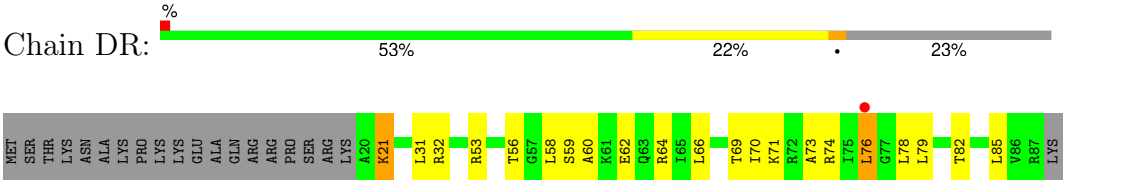

• Molecule 48: 30S ribosomal protein S18

Chain CR:



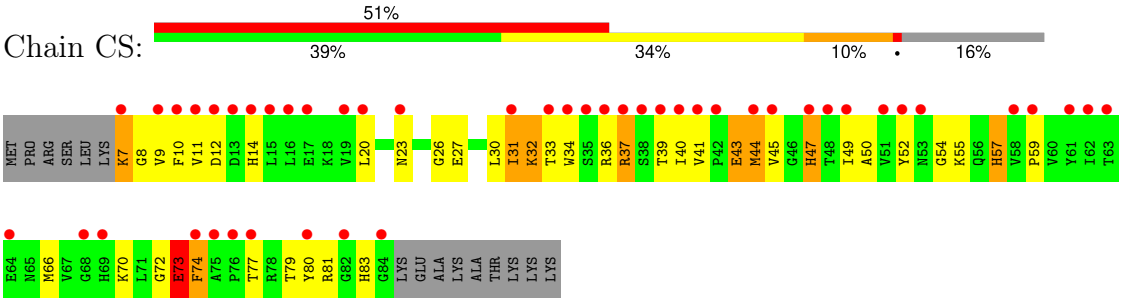

• Molecule 48: 30S ribosomal protein S18

Chain DR:



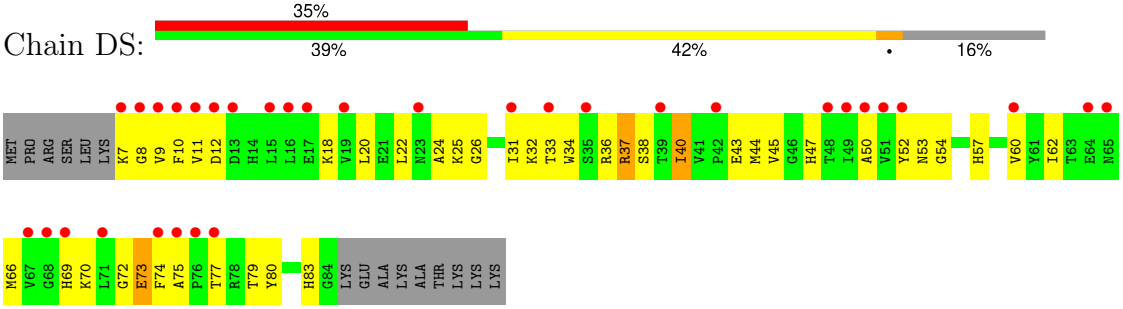

• Molecule 49: 30S ribosomal protein S19

Chain CS:



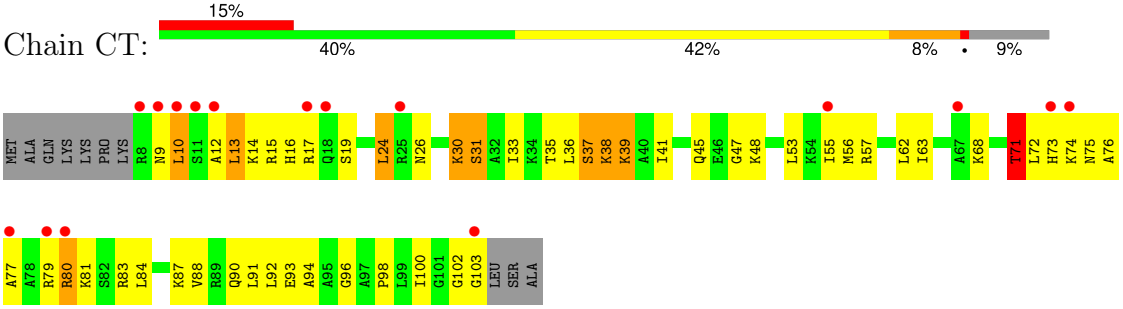

• Molecule 49: 30S ribosomal protein S19

Chain DS:



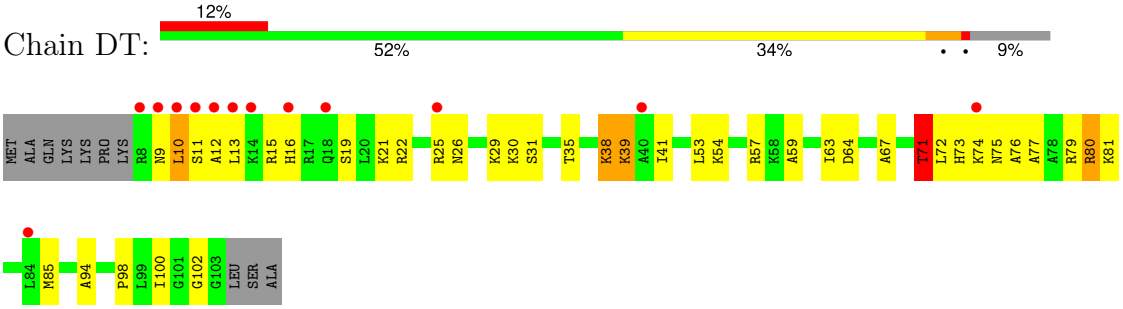

• Molecule 50: 30S ribosomal protein S20

Chain CT:



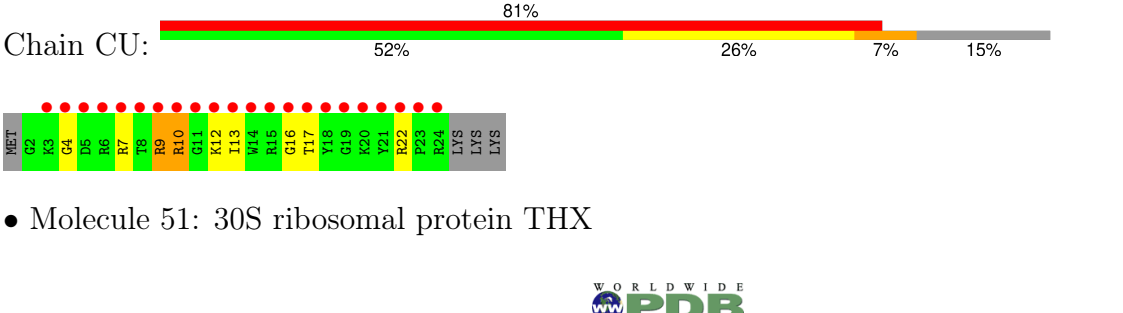

• Molecule 50: 30S ribosomal protein S20

Chain DT:



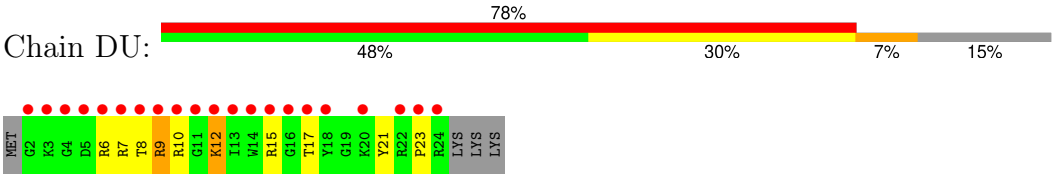

• Molecule 51: 30S ribosomal protein THX

Chain CU:




• Molecule 51: 30S ribosomal protein THX

Chain DU:


78%
48%
30%
7%
15%
MET
G2
K3
G4
D5
R6
R7
T8
R9
R10
G11
K12
I13
W14
R15
G16
T17
Y18
G19
K20
Y21
R22
P23
R24
LYS
LYS
LYS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 209.37Å 445.46Å 619.56Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.29 – 3.20<br>49.29 – 3.20 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 100.0 (49.29-3.20)<br>99.8 (49.29-3.20) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.13 (at 2.91Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.228 , 0.273<br>0.226 , 0.269 | Depositor<br>DCC |
| $R_{free}$ test set | 47287 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 75.4 | Xtriage |
| Anisotropy | 0.180 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 60.1 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 279316 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 80.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 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: MG, T8B

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | AA | 0.82 | 17/68203 (0.0%) | 1.30 | 624/106459 (0.6%) |
| 1 | BA | 1.20 | 70/68203 (0.1%) | 1.37 | 800/106459 (0.8%) |
| 2 | AB | 0.94 | 0/2879 | 1.25 | 21/4492 (0.5%) |
| 2 | BB | 0.88 | 0/2879 | 1.26 | 21/4492 (0.5%) |
| 3 | AD | 0.54 | 0/2186 | 0.75 | 2/2944 (0.1%) |
| 3 | BD | 0.67 | 0/2186 | 0.81 | 4/2944 (0.1%) |
| 4 | AE | 0.55 | 0/1588 | 0.76 | 0/2145 |
| 4 | BE | 0.72 | 0/1588 | 0.83 | 1/2145 (0.0%) |
| 5 | AF | 0.51 | 0/1609 | 0.70 | 0/2177 |
| 5 | BF | 0.73 | 0/1609 | 0.77 | 0/2177 |
| 6 | AG | 0.61 | 0/1393 | 0.66 | 0/1892 |
| 6 | BG | 0.46 | 0/1393 | 0.64 | 0/1892 |
| 7 | AH | 0.58 | 0/1343 | 0.68 | 1/1820 (0.1%) |
| 7 | BH | 0.59 | 0/1343 | 0.70 | 0/1820 |
| 8 | AI | 0.63 | 1/1061 (0.1%) | 0.78 | 0/1451 |
| 8 | BI | 0.50 | 0/1061 | 0.74 | 0/1451 |
| 9 | AN | 0.52 | 0/1139 | 0.72 | 0/1538 |
| 9 | BN | 0.74 | 0/1139 | 0.78 | 0/1538 |
| 10 | AO | 0.50 | 0/933 | 0.72 | 1/1257 (0.1%) |
| 10 | BO | 0.67 | 0/933 | 0.74 | 0/1257 |
| 11 | AP | 0.50 | 0/1135 | 0.75 | 1/1510 (0.1%) |
| 11 | BP | 0.64 | 0/1135 | 0.81 | 2/1510 (0.1%) |
| 12 | AQ | 0.53 | 0/1143 | 0.74 | 0/1527 |
| 12 | BQ | 0.64 | 0/1143 | 0.74 | 0/1527 |
| 13 | AR | 0.51 | 0/982 | 0.74 | 0/1312 |
| 13 | BR | 0.69 | 0/982 | 0.82 | 1/1312 (0.1%) |
| 14 | AS | 0.64 | 0/875 | 0.79 | 0/1168 |
| 14 | BS | 0.53 | 0/875 | 0.79 | 1/1168 (0.1%) |
| 15 | AT | 0.52 | 0/1077 | 0.73 | 0/1444 |
| 15 | BT | 0.61 | 0/1077 | 0.79 | 1/1444 (0.1%) |
| 16 | AU | 0.56 | 0/977 | 0.69 | 0/1301 |
| 16 | BU | 0.88 | 1/977 (0.1%) | 0.81 | 1/1301 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | AV | 0.58 | 0/782 | 0.67 | 0/1049 |
| 17 | BV | 0.70 | 0/782 | 0.77 | 0/1049 |
| 18 | AW | 0.56 | 0/891 | 0.75 | 0/1197 |
| 18 | BW | 0.82 | 0/891 | 0.80 | 0/1197 |
| 19 | AX | 0.55 | 0/756 | 0.77 | 1/1016 (0.1%) |
| 19 | BX | 0.66 | 0/756 | 0.76 | 1/1016 (0.1%) |
| 20 | AY | 0.50 | 0/798 | 0.77 | 0/1073 |
| 20 | BY | 0.61 | 0/798 | 0.80 | 1/1073 (0.1%) |
| 21 | AZ | 0.57 | 0/1555 | 0.68 | 0/2118 |
| 21 | BZ | 0.49 | 0/1555 | 0.71 | 0/2118 |
| 22 | A0 | 0.50 | 0/602 | 0.69 | 0/804 |
| 22 | B0 | 0.66 | 0/602 | 0.77 | 0/804 |
| 23 | A1 | 0.51 | 0/752 | 0.72 | 0/1003 |
| 23 | B1 | 0.62 | 0/752 | 0.76 | 0/1003 |
| 24 | A2 | 0.59 | 0/590 | 0.68 | 0/781 |
| 24 | B2 | 0.60 | 0/590 | 0.74 | 0/781 |
| 25 | A3 | 0.45 | 0/463 | 0.69 | 0/623 |
| 25 | B3 | 0.65 | 0/463 | 0.74 | 0/623 |
| 26 | A4 | 0.65 | 0/358 | 0.74 | 0/487 |
| 26 | B4 | 0.56 | 0/358 | 0.74 | 1/487 (0.2%) |
| 27 | A5 | 0.67 | 1/469 (0.2%) | 0.83 | 2/634 (0.3%) |
| 27 | B5 | 0.79 | 0/469 | 0.88 | 0/634 |
| 28 | A6 | 0.59 | 0/456 | 0.70 | 0/609 |
| 28 | B6 | 0.68 | 0/456 | 0.74 | 0/609 |
| 29 | A7 | 0.57 | 0/426 | 0.75 | 0/561 |
| 29 | B7 | 0.78 | 0/426 | 0.84 | 0/561 |
| 30 | A8 | 0.50 | 0/516 | 0.73 | 0/679 |
| 30 | B8 | 0.70 | 0/516 | 0.82 | 0/679 |
| 31 | CA | 0.80 | 10/36054 (0.0%) | 1.18 | 176/56272 (0.3%) |
| 31 | DA | 0.77 | 7/36054 (0.0%) | 1.19 | 211/56272 (0.4%) |
| 32 | CB | 0.51 | 0/1811 | 0.69 | 0/2452 |
| 32 | DB | 0.56 | 0/1811 | 0.69 | 0/2452 |
| 33 | CC | 0.56 | 0/1474 | 0.65 | 0/2003 |
| 33 | DC | 0.58 | 0/1474 | 0.65 | 0/2003 |
| 34 | CD | 0.53 | 0/1550 | 0.72 | 3/2106 (0.1%) |
| 34 | DD | 0.84 | 2/1550 (0.1%) | 0.78 | 4/2106 (0.2%) |
| 35 | CE | 0.49 | 0/1121 | 0.70 | 1/1517 (0.1%) |
| 35 | DE | 0.52 | 0/1121 | 0.72 | 1/1517 (0.1%) |
| 36 | CF | 0.49 | 0/794 | 0.64 | 0/1082 |
| 36 | DF | 0.49 | 0/794 | 0.67 | 1/1082 (0.1%) |
| 37 | CG | 0.57 | 0/1186 | 0.65 | 0/1603 |
| 37 | DG | 0.56 | 0/1186 | 0.62 | 0/1603 |
| 38 | CH | 0.44 | 0/1065 | 0.67 | 0/1445 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | DH | 0.44 | 0/1065 | 0.64 | 0/1445 |
| 39 | CI | 0.62 | 0/867 | 0.71 | 0/1180 |
| 39 | DI | 0.62 | 0/867 | 0.69 | 0/1180 |
| 40 | CJ | 0.60 | 0/672 | 0.74 | 1/919 (0.1%) |
| 40 | DJ | 0.60 | 0/672 | 0.70 | 1/919 (0.1%) |
| 41 | CK | 0.47 | 0/843 | 0.71 | 0/1144 |
| 41 | DK | 0.47 | 0/843 | 0.67 | 0/1144 |
| 42 | CL | 0.44 | 0/925 | 0.67 | 0/1251 |
| 42 | DL | 0.46 | 0/925 | 0.69 | 0/1251 |
| 43 | CM | 0.67 | 0/811 | 0.72 | 0/1103 |
| 43 | DM | 0.63 | 0/811 | 0.73 | 1/1103 (0.1%) |
| 44 | CN | 0.60 | 0/487 | 0.68 | 0/649 |
| 44 | DN | 0.59 | 0/487 | 0.74 | 0/649 |
| 45 | CO | 0.49 | 0/735 | 0.64 | 0/981 |
| 45 | DO | 0.47 | 0/735 | 0.61 | 0/981 |
| 46 | CP | 0.51 | 0/667 | 0.70 | 0/905 |
| 46 | DP | 0.43 | 0/667 | 0.65 | 0/905 |
| 47 | CQ | 0.46 | 0/836 | 0.68 | 0/1117 |
| 47 | DQ | 0.47 | 0/836 | 0.66 | 0/1117 |
| 48 | CR | 0.43 | 0/519 | 0.64 | 0/699 |
| 48 | DR | 0.50 | 0/519 | 0.67 | 0/699 |
| 49 | CS | 0.69 | 0/558 | 0.88 | 1/759 (0.1%) |
| 49 | DS | 0.76 | 1/558 (0.2%) | 0.87 | 3/759 (0.4%) |
| 50 | CT | 0.47 | 0/710 | 0.72 | 0/940 |
| 50 | DT | 0.42 | 0/710 | 0.68 | 0/940 |
| 51 | CU | 0.64 | 0/203 | 0.67 | 0/266 |
| 51 | DU | 0.59 | 0/203 | 0.70 | 0/266 |
| All | All | 0.86 | 110/303650 (0.0%) | 1.16 | 1892/454928 (0.4%) |

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 |
|---|---|---|---|
| 26 | A4 | 0 | 1 |
| 34 | CD | 0 | 1 |
| 34 | DD | 0 | 1 |
| 42 | CL | 0 | 1 |
| 42 | DL | 0 | 1 |
| All | All | 0 | 5 |

The worst 5 of 110 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 34 | DD | 12 | CYS | CB-SG | 19.94 | 2.16 | 1.82 |
| 34 | DD | 26 | CYS | CB-SG | 15.79 | 2.09 | 1.82 |
| 31 | DA | 1492 | A | C6-N6 | -12.21 | 1.24 | 1.33 |
| 31 | CA | 1492 | A | C2-N3 | 12.12 | 1.44 | 1.33 |
| 31 | CA | 1493 | A | N9-C4 | -11.96 | 1.30 | 1.37 |

The worst 5 of 1892 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | DA | 1492 | A | C6-N1-C2 | -28.45 | 101.53 | 118.60 |
| 31 | DA | 1492 | A | C5-C6-N1 | 26.41 | 130.90 | 117.70 |
| 31 | CA | 1492 | A | C8-N9-C4 | -21.05 | 97.38 | 105.80 |
| 1 | BA | 1332 | G | C2-N3-C4 | -19.65 | 102.08 | 111.90 |
| 1 | BA | 1332 | G | N3-C4-C5 | 17.99 | 137.59 | 128.60 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 26 | A4 | 42 | PHE | Peptide |
| 34 | CD | 11 | LEU | Peptide |
| 42 | CL | 26 | ALA | Peptide |
| 34 | DD | 11 | LEU | Peptide |
| 42 | DL | 26 | ALA | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | AA | 60900 | 0 | 30712 | 1406 | 0 |
| 1 | BA | 60900 | 0 | 30712 | 1060 | 0 |
| 2 | AB | 2574 | 0 | 1306 | 87 | 0 |
| 2 | BB | 2574 | 0 | 1306 | 35 | 0 |
| 3 | AD | 2136 | 0 | 2218 | 77 | 0 |
| 3 | BD | 2136 | 0 | 2218 | 81 | 0 |
| 4 | AE | 1555 | 0 | 1607 | 81 | 0 |
| 4 | BE | 1555 | 0 | 1607 | 54 | 0 |
| 5 | AF | 1576 | 0 | 1616 | 57 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | BF | 1576 | 0 | 1616 | 59 | 0 |
| 6 | AG | 1368 | 0 | 1324 | 70 | 0 |
| 6 | BG | 1368 | 0 | 1324 | 61 | 0 |
| 7 | AH | 1317 | 0 | 1376 | 66 | 0 |
| 7 | BH | 1317 | 0 | 1376 | 33 | 0 |
| 8 | AI | 1046 | 0 | 1067 | 55 | 2 |
| 8 | BI | 1046 | 0 | 1067 | 47 | 0 |
| 9 | AN | 1112 | 0 | 1180 | 60 | 0 |
| 9 | BN | 1112 | 0 | 1180 | 34 | 0 |
| 10 | AO | 923 | 0 | 981 | 28 | 0 |
| 10 | BO | 923 | 0 | 981 | 23 | 0 |
| 11 | AP | 1119 | 0 | 1186 | 38 | 0 |
| 11 | BP | 1119 | 0 | 1186 | 40 | 0 |
| 12 | AQ | 1122 | 0 | 1179 | 43 | 0 |
| 12 | BQ | 1122 | 0 | 1179 | 47 | 0 |
| 13 | AR | 968 | 0 | 1033 | 43 | 0 |
| 13 | BR | 968 | 0 | 1033 | 33 | 0 |
| 14 | AS | 865 | 0 | 905 | 62 | 0 |
| 14 | BS | 865 | 0 | 905 | 54 | 0 |
| 15 | AT | 1063 | 0 | 1103 | 48 | 0 |
| 15 | BT | 1063 | 0 | 1103 | 37 | 0 |
| 16 | AU | 959 | 0 | 1019 | 31 | 0 |
| 16 | BU | 959 | 0 | 1019 | 20 | 0 |
| 17 | AV | 771 | 0 | 830 | 22 | 0 |
| 17 | BV | 771 | 0 | 830 | 15 | 0 |
| 18 | AW | 881 | 0 | 935 | 25 | 0 |
| 18 | BW | 881 | 0 | 935 | 24 | 0 |
| 19 | AX | 742 | 0 | 799 | 22 | 0 |
| 19 | BX | 742 | 0 | 799 | 23 | 0 |
| 20 | AY | 785 | 0 | 832 | 36 | 0 |
| 20 | BY | 785 | 0 | 832 | 30 | 0 |
| 21 | AZ | 1522 | 0 | 1511 | 56 | 0 |
| 21 | BZ | 1522 | 0 | 1511 | 47 | 0 |
| 22 | A0 | 594 | 0 | 604 | 27 | 0 |
| 22 | B0 | 594 | 0 | 604 | 21 | 0 |
| 23 | A1 | 745 | 0 | 804 | 26 | 0 |
| 23 | B1 | 745 | 0 | 804 | 26 | 0 |
| 24 | A2 | 588 | 0 | 643 | 31 | 0 |
| 24 | B2 | 588 | 0 | 643 | 18 | 0 |
| 25 | A3 | 458 | 0 | 503 | 22 | 0 |
| 25 | B3 | 458 | 0 | 503 | 6 | 0 |
| 26 | A4 | 349 | 0 | 340 | 22 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 26 | B4 | 349 | 0 | 340 | 16 | 0 |
| 27 | A5 | 455 | 0 | 476 | 25 | 0 |
| 27 | B5 | 455 | 0 | 476 | 18 | 0 |
| 28 | A6 | 449 | 0 | 464 | 19 | 0 |
| 28 | B6 | 449 | 0 | 466 | 17 | 0 |
| 29 | A7 | 418 | 0 | 467 | 18 | 0 |
| 29 | B7 | 418 | 0 | 467 | 14 | 0 |
| 30 | A8 | 509 | 0 | 565 | 23 | 0 |
| 30 | B8 | 509 | 0 | 565 | 20 | 0 |
| 31 | CA | 32208 | 0 | 16256 | 921 | 2 |
| 31 | DA | 32208 | 0 | 16254 | 923 | 0 |
| 32 | CB | 1777 | 0 | 1747 | 100 | 0 |
| 32 | DB | 1777 | 0 | 1747 | 95 | 0 |
| 33 | CC | 1450 | 0 | 1314 | 45 | 0 |
| 33 | DC | 1450 | 0 | 1314 | 58 | 0 |
| 34 | CD | 1520 | 0 | 1407 | 73 | 0 |
| 34 | DD | 1520 | 0 | 1406 | 85 | 0 |
| 35 | CE | 1105 | 0 | 1130 | 48 | 0 |
| 35 | DE | 1105 | 0 | 1130 | 54 | 0 |
| 36 | CF | 781 | 0 | 741 | 25 | 0 |
| 36 | DF | 781 | 0 | 741 | 29 | 0 |
| 37 | CG | 1167 | 0 | 1108 | 39 | 0 |
| 37 | DG | 1167 | 0 | 1108 | 46 | 0 |
| 38 | CH | 1045 | 0 | 1033 | 45 | 0 |
| 38 | DH | 1045 | 0 | 1033 | 53 | 0 |
| 39 | CI | 852 | 0 | 742 | 43 | 0 |
| 39 | DI | 852 | 0 | 742 | 52 | 0 |
| 40 | CJ | 659 | 0 | 552 | 31 | 0 |
| 40 | DJ | 659 | 0 | 552 | 37 | 0 |
| 41 | CK | 828 | 0 | 822 | 24 | 0 |
| 41 | DK | 828 | 0 | 822 | 32 | 0 |
| 42 | CL | 909 | 0 | 927 | 43 | 0 |
| 42 | DL | 909 | 0 | 927 | 38 | 0 |
| 43 | CM | 801 | 0 | 743 | 33 | 0 |
| 43 | DM | 801 | 0 | 743 | 37 | 0 |
| 44 | CN | 478 | 0 | 498 | 33 | 0 |
| 44 | DN | 478 | 0 | 497 | 30 | 0 |
| 45 | CO | 724 | 0 | 749 | 32 | 0 |
| 45 | DO | 724 | 0 | 749 | 27 | 0 |
| 46 | CP | 651 | 0 | 638 | 33 | 0 |
| 46 | DP | 651 | 0 | 638 | 28 | 0 |
| 47 | CQ | 823 | 0 | 891 | 33 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 47 | DQ | 823 | 0 | 891 | 22 | 0 |
| 48 | CR | 514 | 0 | 530 | 19 | 0 |
| 48 | DR | 514 | 0 | 530 | 17 | 0 |
| 49 | CS | 544 | 0 | 457 | 21 | 0 |
| 49 | DS | 544 | 0 | 457 | 26 | 0 |
| 50 | CT | 708 | 0 | 764 | 37 | 0 |
| 50 | DT | 708 | 0 | 764 | 26 | 0 |
| 51 | CU | 199 | 0 | 208 | 8 | 0 |
| 51 | DU | 199 | 0 | 208 | 6 | 0 |
| 52 | AA | 44 | 0 | 20 | 31 | 0 |
| 52 | BA | 44 | 0 | 20 | 23 | 0 |
| 53 | AA | 2 | 0 | 0 | 0 | 0 |
| 53 | BA | 2 | 0 | 0 | 0 | 0 |
| All | All | 279316 | 0 | 185722 | 7170 | 2 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 7170 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 52:AA:3001:T8B:C13 | 31:DA:1492:A:H5" | 1.47 | 1.41 |
| 34:DD:26:CYS:SG | 34:DD:26:CYS:CB | 2.09 | 1.41 |
| 34:DD:12:CYS:SG | 34:DD:12:CYS:CB | 2.16 | 1.34 |
| 52:AA:3001:T8B:H13 | 52:AA:3001:T8B:C22 | 1.58 | 1.33 |
| 52:BA:3001:T8B:H13 | 52:BA:3001:T8B:C22 | 1.58 | 1.32 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:AI:89:TYR:O | 31:CA:357:G:O2'[2_654] | 2.11 | 0.09 |
| 8:AI:91:SER:OG | 31:CA:368:U:OP2[2_654] | 2.12 | 0.08 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | AD | 273/276 (99%) | 240 (88%) | 27 (10%) | 6 (2%) | 5 30 |
| 3 | BD | 273/276 (99%) | 246 (90%) | 23 (8%) | 4 (2%) | 8 38 |
| 4 | AE | 202/206 (98%) | 177 (88%) | 18 (9%) | 7 (4%) | 3 20 |
| 4 | BE | 202/206 (98%) | 174 (86%) | 21 (10%) | 7 (4%) | 3 20 |
| 5 | AF | 198/205 (97%) | 168 (85%) | 25 (13%) | 5 (2%) | 4 28 |
| 5 | BF | 198/205 (97%) | 170 (86%) | 21 (11%) | 7 (4%) | 3 20 |
| 6 | AG | 179/182 (98%) | 136 (76%) | 33 (18%) | 10 (6%) | 1 11 |
| 6 | BG | 179/182 (98%) | 135 (75%) | 30 (17%) | 14 (8%) | 1 5 |
| 7 | AH | 172/180 (96%) | 143 (83%) | 21 (12%) | 8 (5%) | 2 14 |
| 7 | BH | 172/180 (96%) | 144 (84%) | 22 (13%) | 6 (4%) | 3 20 |
| 8 | AI | 143/148 (97%) | 103 (72%) | 28 (20%) | 12 (8%) | 0 4 |
| 8 | BI | 143/148 (97%) | 109 (76%) | 24 (17%) | 10 (7%) | 1 6 |
| 9 | AN | 138/140 (99%) | 113 (82%) | 16 (12%) | 9 (6%) | 1 8 |
| 9 | BN | 138/140 (99%) | 119 (86%) | 13 (9%) | 6 (4%) | 2 16 |
| 10 | AO | 120/122 (98%) | 108 (90%) | 8 (7%) | 4 (3%) | 3 21 |
| 10 | BO | 120/122 (98%) | 109 (91%) | 7 (6%) | 4 (3%) | 3 21 |
| 11 | AP | 143/150 (95%) | 117 (82%) | 18 (13%) | 8 (6%) | 1 11 |
| 11 | BP | 143/150 (95%) | 126 (88%) | 12 (8%) | 5 (4%) | 3 20 |
| 12 | AQ | 139/141 (99%) | 126 (91%) | 9 (6%) | 4 (3%) | 3 24 |
| 12 | BQ | 139/141 (99%) | 126 (91%) | 9 (6%) | 4 (3%) | 3 24 |
| 13 | AR | 116/118 (98%) | 95 (82%) | 16 (14%) | 5 (4%) | 2 16 |
| 13 | BR | 116/118 (98%) | 108 (93%) | 7 (6%) | 1 (1%) | 14 49 |
| 14 | AS | 108/112 (96%) | 84 (78%) | 21 (19%) | 3 (3%) | 4 25 |
| 14 | BS | 108/112 (96%) | 93 (86%) | 12 (11%) | 3 (3%) | 4 25 |
| 15 | AT | 129/146 (88%) | 109 (84%) | 16 (12%) | 4 (3%) | 3 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 15 | BT | 129/146 (88%) | 116 (90%) | 12 (9%) | 1 (1%) | 16 51 |
| 16 | AU | 114/118 (97%) | 104 (91%) | 10 (9%) | 0 | 100 100 |
| 16 | BU | 114/118 (97%) | 111 (97%) | 3 (3%) | 0 | 100 100 |
| 17 | AV | 99/101 (98%) | 89 (90%) | 8 (8%) | 2 (2%) | 6 32 |
| 17 | BV | 99/101 (98%) | 89 (90%) | 9 (9%) | 1 (1%) | 13 47 |
| 18 | AW | 110/113 (97%) | 101 (92%) | 8 (7%) | 1 (1%) | 14 49 |
| 18 | BW | 110/113 (97%) | 104 (94%) | 6 (6%) | 0 | 100 100 |
| 19 | AX | 93/96 (97%) | 82 (88%) | 9 (10%) | 2 (2%) | 5 30 |
| 19 | BX | 93/96 (97%) | 82 (88%) | 9 (10%) | 2 (2%) | 5 30 |
| 20 | AY | 105/110 (96%) | 90 (86%) | 10 (10%) | 5 (5%) | 2 14 |
| 20 | BY | 105/110 (96%) | 88 (84%) | 13 (12%) | 4 (4%) | 2 18 |
| 21 | AZ | 196/206 (95%) | 153 (78%) | 32 (16%) | 11 (6%) | 1 11 |
| 21 | BZ | 196/206 (95%) | 158 (81%) | 31 (16%) | 7 (4%) | 3 20 |
| 22 | A0 | 74/85 (87%) | 67 (90%) | 6 (8%) | 1 (1%) | 9 40 |
| 22 | B0 | 74/85 (87%) | 67 (90%) | 6 (8%) | 1 (1%) | 9 40 |
| 23 | A1 | 95/98 (97%) | 88 (93%) | 5 (5%) | 2 (2%) | 5 31 |
| 23 | B1 | 95/98 (97%) | 86 (90%) | 6 (6%) | 3 (3%) | 3 22 |
| 24 | A2 | 68/72 (94%) | 59 (87%) | 8 (12%) | 1 (2%) | 8 38 |
| 24 | B2 | 68/72 (94%) | 63 (93%) | 5 (7%) | 0 | 100 100 |
| 25 | A3 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 100 |
| 25 | B3 | 57/60 (95%) | 54 (95%) | 2 (4%) | 1 (2%) | 7 35 |
| 26 | A4 | 44/71 (62%) | 30 (68%) | 10 (23%) | 4 (9%) | 0 3 |
| 26 | B4 | 44/71 (62%) | 30 (68%) | 10 (23%) | 4 (9%) | 0 3 |
| 27 | A5 | 57/60 (95%) | 50 (88%) | 6 (10%) | 1 (2%) | 7 35 |
| 27 | B5 | 57/60 (95%) | 49 (86%) | 6 (10%) | 2 (4%) | 3 20 |
| 28 | A6 | 51/54 (94%) | 46 (90%) | 4 (8%) | 1 (2%) | 6 32 |
| 28 | B6 | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 100 |
| 29 | A7 | 46/49 (94%) | 41 (89%) | 4 (9%) | 1 (2%) | 5 30 |
| 29 | B7 | 46/49 (94%) | 42 (91%) | 3 (6%) | 1 (2%) | 5 30 |
| 30 | A8 | 62/65 (95%) | 48 (77%) | 13 (21%) | 1 (2%) | 8 37 |
| 30 | B8 | 62/65 (95%) | 57 (92%) | 5 (8%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 32 | CB | 227/256 (89%) | 171 (75%) | 36 (16%) | 20 (9%) | 0 3 |
| 32 | DB | 227/256 (89%) | 173 (76%) | 39 (17%) | 15 (7%) | 1 7 |
| 33 | CC | 204/239 (85%) | 163 (80%) | 30 (15%) | 11 (5%) | 1 12 |
| 33 | DC | 204/239 (85%) | 144 (71%) | 42 (21%) | 18 (9%) | 0 3 |
| 34 | CD | 206/209 (99%) | 154 (75%) | 40 (19%) | 12 (6%) | 1 10 |
| 34 | DD | 206/209 (99%) | 152 (74%) | 47 (23%) | 7 (3%) | 3 21 |
| 35 | CE | 146/162 (90%) | 112 (77%) | 23 (16%) | 11 (8%) | 1 6 |
| 35 | DE | 146/162 (90%) | 116 (80%) | 25 (17%) | 5 (3%) | 3 21 |
| 36 | CF | 98/101 (97%) | 87 (89%) | 8 (8%) | 3 (3%) | 3 22 |
| 36 | DF | 98/101 (97%) | 85 (87%) | 9 (9%) | 4 (4%) | 2 17 |
| 37 | CG | 153/156 (98%) | 127 (83%) | 16 (10%) | 10 (6%) | 1 8 |
| 37 | DG | 153/156 (98%) | 129 (84%) | 18 (12%) | 6 (4%) | 2 18 |
| 38 | CH | 136/138 (99%) | 116 (85%) | 18 (13%) | 2 (2%) | 8 38 |
| 38 | DH | 136/138 (99%) | 118 (87%) | 13 (10%) | 5 (4%) | 2 19 |
| 39 | CI | 123/128 (96%) | 93 (76%) | 20 (16%) | 10 (8%) | 1 4 |
| 39 | DI | 123/128 (96%) | 94 (76%) | 21 (17%) | 8 (6%) | 1 8 |
| 40 | CJ | 94/105 (90%) | 66 (70%) | 19 (20%) | 9 (10%) | 0 3 |
| 40 | DJ | 94/105 (90%) | 74 (79%) | 14 (15%) | 6 (6%) | 1 8 |
| 41 | CK | 112/129 (87%) | 96 (86%) | 12 (11%) | 4 (4%) | 3 20 |
| 41 | DK | 112/129 (87%) | 90 (80%) | 19 (17%) | 3 (3%) | 4 26 |
| 42 | CL | 120/132 (91%) | 98 (82%) | 17 (14%) | 5 (4%) | 2 17 |
| 42 | DL | 120/132 (91%) | 100 (83%) | 15 (12%) | 5 (4%) | 2 17 |
| 43 | CM | 112/126 (89%) | 84 (75%) | 18 (16%) | 10 (9%) | 0 3 |
| 43 | DM | 112/126 (89%) | 80 (71%) | 20 (18%) | 12 (11%) | 0 2 |
| 44 | CN | 58/61 (95%) | 43 (74%) | 10 (17%) | 5 (9%) | 0 3 |
| 44 | DN | 58/61 (95%) | 48 (83%) | 7 (12%) | 3 (5%) | 1 12 |
| 45 | CO | 86/89 (97%) | 71 (83%) | 12 (14%) | 3 (4%) | 3 20 |
| 45 | DO | 86/89 (97%) | 68 (79%) | 16 (19%) | 2 (2%) | 5 29 |
| 46 | CP | 80/88 (91%) | 50 (62%) | 23 (29%) | 7 (9%) | 0 3 |
| 46 | DP | 80/88 (91%) | 52 (65%) | 25 (31%) | 3 (4%) | 2 18 |
| 47 | CQ | 97/105 (92%) | 84 (87%) | 8 (8%) | 5 (5%) | 1 12 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 47 | DQ | 97/105 (92%) | 81 (84%) | 13 (13%) | 3 (3%) | 3 22 |
| 48 | CR | 66/88 (75%) | 55 (83%) | 10 (15%) | 1 (2%) | 8 38 |
| 48 | DR | 66/88 (75%) | 60 (91%) | 6 (9%) | 0 | 100 100 |
| 49 | CS | 76/93 (82%) | 48 (63%) | 17 (22%) | 11 (14%) | 0 1 |
| 49 | DS | 76/93 (82%) | 54 (71%) | 17 (22%) | 5 (7%) | 1 7 |
| 50 | CT | 94/106 (89%) | 73 (78%) | 13 (14%) | 8 (8%) | 0 3 |
| 50 | DT | 94/106 (89%) | 72 (77%) | 15 (16%) | 7 (7%) | 1 6 |
| 51 | CU | 21/27 (78%) | 18 (86%) | 3 (14%) | 0 | 100 100 |
| 51 | DU | 21/27 (78%) | 16 (76%) | 3 (14%) | 2 (10%) | 0 3 |
| All | All | 11280/12044 (94%) | 9338 (83%) | 1460 (13%) | 482 (4%) | 2 16 |

5 of 482 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | AD | 239 | ARG |
| 3 | AD | 275 | LYS |
| 5 | AF | 60 | SER |
| 6 | AG | 14 | GLU |
| 6 | AG | 78 | SER |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | AD | 215/218 (99%) | 185 (86%) | 30 (14%) | 3 14 |
| 3 | BD | 215/218 (99%) | 189 (88%) | 26 (12%) | 4 19 |
| 4 | AE | 163/166 (98%) | 139 (85%) | 24 (15%) | 2 12 |
| 4 | BE | 163/166 (98%) | 134 (82%) | 29 (18%) | 1 7 |
| 5 | AF | 158/162 (98%) | 133 (84%) | 25 (16%) | 2 10 |
| 5 | BF | 158/162 (98%) | 138 (87%) | 20 (13%) | 3 17 |
| 6 | AG | 128/156 (82%) | 110 (86%) | 18 (14%) | 3 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 6 | BG | 128/156 (82%) | 114 (89%) | 14 (11%) | 5 23 |
| 7 | AH | 141/148 (95%) | 125 (89%) | 16 (11%) | 4 22 |
| 7 | BH | 141/148 (95%) | 124 (88%) | 17 (12%) | 4 19 |
| 8 | AI | 102/124 (82%) | 76 (74%) | 26 (26%) | 0 2 |
| 8 | BI | 102/124 (82%) | 76 (74%) | 26 (26%) | 0 2 |
| 9 | AN | 117/119 (98%) | 94 (80%) | 23 (20%) | 1 6 |
| 9 | BN | 117/119 (98%) | 91 (78%) | 26 (22%) | 1 4 |
| 10 | AO | 98/100 (98%) | 89 (91%) | 9 (9%) | 7 29 |
| 10 | BO | 98/100 (98%) | 89 (91%) | 9 (9%) | 7 29 |
| 11 | AP | 113/116 (97%) | 96 (85%) | 17 (15%) | 2 12 |
| 11 | BP | 113/116 (97%) | 97 (86%) | 16 (14%) | 2 13 |
| 12 | AQ | 111/111 (100%) | 94 (85%) | 17 (15%) | 2 11 |
| 12 | BQ | 111/111 (100%) | 94 (85%) | 17 (15%) | 2 11 |
| 13 | AR | 101/101 (100%) | 80 (79%) | 21 (21%) | 1 5 |
| 13 | BR | 101/101 (100%) | 79 (78%) | 22 (22%) | 1 4 |
| 14 | AS | 84/88 (96%) | 67 (80%) | 17 (20%) | 1 5 |
| 14 | BS | 84/88 (96%) | 72 (86%) | 12 (14%) | 2 13 |
| 15 | AT | 110/127 (87%) | 99 (90%) | 11 (10%) | 6 26 |
| 15 | BT | 110/127 (87%) | 100 (91%) | 10 (9%) | 7 29 |
| 16 | AU | 93/94 (99%) | 83 (89%) | 10 (11%) | 5 23 |
| 16 | BU | 93/94 (99%) | 77 (83%) | 16 (17%) | 1 8 |
| 17 | AV | 80/82 (98%) | 63 (79%) | 17 (21%) | 1 5 |
| 17 | BV | 80/82 (98%) | 63 (79%) | 17 (21%) | 1 5 |
| 18 | AW | 89/92 (97%) | 75 (84%) | 14 (16%) | 2 10 |
| 18 | BW | 89/92 (97%) | 78 (88%) | 11 (12%) | 4 18 |
| 19 | AX | 75/78 (96%) | 67 (89%) | 8 (11%) | 5 24 |
| 19 | BX | 75/78 (96%) | 66 (88%) | 9 (12%) | 4 19 |
| 20 | AY | 80/91 (88%) | 70 (88%) | 10 (12%) | 3 18 |
| 20 | BY | 80/91 (88%) | 72 (90%) | 8 (10%) | 6 26 |
| 21 | AZ | 159/179 (89%) | 139 (87%) | 20 (13%) | 3 18 |
| 21 | BZ | 159/179 (89%) | 137 (86%) | 22 (14%) | 3 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 22 | A0 | 59/67 (88%) | 52 (88%) | 7 (12%) | 4 19 |
| 22 | B0 | 59/67 (88%) | 52 (88%) | 7 (12%) | 4 19 |
| 23 | A1 | 78/83 (94%) | 68 (87%) | 10 (13%) | 3 17 |
| 23 | B1 | 78/83 (94%) | 70 (90%) | 8 (10%) | 6 25 |
| 24 | A2 | 65/67 (97%) | 56 (86%) | 9 (14%) | 3 14 |
| 24 | B2 | 65/67 (97%) | 57 (88%) | 8 (12%) | 4 19 |
| 25 | A3 | 49/52 (94%) | 43 (88%) | 6 (12%) | 4 19 |
| 25 | B3 | 49/52 (94%) | 43 (88%) | 6 (12%) | 4 19 |
| 26 | A4 | 39/63 (62%) | 32 (82%) | 7 (18%) | 1 7 |
| 26 | B4 | 39/63 (62%) | 30 (77%) | 9 (23%) | 0 3 |
| 27 | A5 | 50/52 (96%) | 43 (86%) | 7 (14%) | 3 14 |
| 27 | B5 | 50/52 (96%) | 43 (86%) | 7 (14%) | 3 14 |
| 28 | A6 | 50/52 (96%) | 40 (80%) | 10 (20%) | 1 5 |
| 28 | B6 | 50/52 (96%) | 41 (82%) | 9 (18%) | 1 7 |
| 29 | A7 | 41/42 (98%) | 35 (85%) | 6 (15%) | 2 13 |
| 29 | B7 | 41/42 (98%) | 32 (78%) | 9 (22%) | 1 4 |
| 30 | A8 | 52/55 (94%) | 45 (86%) | 7 (14%) | 3 15 |
| 30 | B8 | 52/55 (94%) | 47 (90%) | 5 (10%) | 7 28 |
| 32 | CB | 177/220 (80%) | 141 (80%) | 36 (20%) | 1 5 |
| 32 | DB | 177/220 (80%) | 142 (80%) | 35 (20%) | 1 6 |
| 33 | CC | 114/188 (61%) | 95 (83%) | 19 (17%) | 2 9 |
| 33 | DC | 114/188 (61%) | 96 (84%) | 18 (16%) | 2 10 |
| 34 | CD | 139/181 (77%) | 117 (84%) | 22 (16%) | 2 10 |
| 34 | DD | 139/181 (77%) | 120 (86%) | 19 (14%) | 3 14 |
| 35 | CE | 108/123 (88%) | 86 (80%) | 22 (20%) | 1 5 |
| 35 | DE | 108/123 (88%) | 88 (82%) | 20 (18%) | 1 7 |
| 36 | CF | 77/90 (86%) | 65 (84%) | 12 (16%) | 2 10 |
| 36 | DF | 77/90 (86%) | 65 (84%) | 12 (16%) | 2 10 |
| 37 | CG | 104/127 (82%) | 86 (83%) | 18 (17%) | 1 8 |
| 37 | DG | 104/127 (82%) | 88 (85%) | 16 (15%) | 2 11 |
| 38 | CH | 103/119 (87%) | 85 (82%) | 18 (18%) | 1 8 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 38 | DH | 103/119 (87%) | 84 (82%) | 19 (18%) | 1 7 |
| 39 | CI | 62/99 (63%) | 53 (86%) | 9 (14%) | 2 13 |
| 39 | DI | 62/99 (63%) | 54 (87%) | 8 (13%) | 3 17 |
| 40 | CJ | 52/92 (56%) | 42 (81%) | 10 (19%) | 1 6 |
| 40 | DJ | 52/92 (56%) | 41 (79%) | 11 (21%) | 1 5 |
| 41 | CK | 81/99 (82%) | 69 (85%) | 12 (15%) | 2 12 |
| 41 | DK | 81/99 (82%) | 71 (88%) | 10 (12%) | 4 19 |
| 42 | CL | 92/109 (84%) | 81 (88%) | 11 (12%) | 4 19 |
| 42 | DL | 92/109 (84%) | 83 (90%) | 9 (10%) | 6 27 |
| 43 | CM | 63/101 (62%) | 49 (78%) | 14 (22%) | 1 4 |
| 43 | DM | 63/101 (62%) | 49 (78%) | 14 (22%) | 1 4 |
| 44 | CN | 46/50 (92%) | 35 (76%) | 11 (24%) | 0 2 |
| 44 | DN | 46/50 (92%) | 33 (72%) | 13 (28%) | 0 1 |
| 45 | CO | 77/80 (96%) | 65 (84%) | 12 (16%) | 2 10 |
| 45 | DO | 77/80 (96%) | 66 (86%) | 11 (14%) | 2 13 |
| 46 | CP | 63/74 (85%) | 49 (78%) | 14 (22%) | 1 4 |
| 46 | DP | 63/74 (85%) | 53 (84%) | 10 (16%) | 2 10 |
| 47 | CQ | 94/97 (97%) | 90 (96%) | 4 (4%) | 25 57 |
| 47 | DQ | 94/97 (97%) | 84 (89%) | 10 (11%) | 5 24 |
| 48 | CR | 49/77 (64%) | 44 (90%) | 5 (10%) | 6 26 |
| 48 | DR | 49/77 (64%) | 46 (94%) | 3 (6%) | 15 47 |
| 49 | CS | 42/80 (52%) | 25 (60%) | 17 (40%) | 0 0 |
| 49 | DS | 42/80 (52%) | 36 (86%) | 6 (14%) | 2 13 |
| 50 | CT | 65/82 (79%) | 53 (82%) | 12 (18%) | 1 7 |
| 50 | DT | 65/82 (79%) | 57 (88%) | 8 (12%) | 4 19 |
| 51 | CU | 18/22 (82%) | 16 (89%) | 2 (11%) | 5 22 |
| 51 | DU | 18/22 (82%) | 14 (78%) | 4 (22%) | 1 4 |
| All | All | 8652/9990 (87%) | 7319 (85%) | 1333 (15%) | 2 11 |

5 of 1333 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | CH | 19 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | DD | 158 | ILE |
| 40 | CJ | 16 | LEU |
| 37 | CG | 146 | GLU |
| 47 | CQ | 60 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | BR | 13 | HIS |
| 40 | DJ | 13 | HIS |
| 35 | CE | 78 | HIS |
| 39 | DI | 124 | GLN |
| 45 | DO | 28 | GLN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | AA | 2819/2915 (96%) | 581 (20%) | 59 (2%) |
| 1 | BA | 2819/2915 (96%) | 586 (20%) | 60 (2%) |
| 2 | AB | 119/122 (97%) | 25 (21%) | 0 |
| 2 | BB | 119/122 (97%) | 21 (17%) | 0 |
| 31 | CA | 1496/1521 (98%) | 339 (22%) | 31 (2%) |
| 31 | DA | 1496/1521 (98%) | 341 (22%) | 27 (1%) |
| All | All | 8868/9116 (97%) | 1893 (21%) | 177 (1%) |

5 of 1893 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AA | 10 | G |
| 1 | AA | 14 | A |
| 1 | AA | 15 | G |
| 1 | AA | 34 | C |
| 1 | AA | 45 | C |

5 of 177 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BA | 2689 | U |
| 31 | CA | 1165 | C |
| 31 | CA | 60 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | CA | 428 | G |
| 31 | DA | 60 | A |

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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 | $\#\|Z\| > 2$ |
| 52 | T8B | BA | 3001 | 53 | 48,48,48 | 1.00 | 2 (4%) | 63,71,71 | 1.28 | 9 (14%) |
| 52 | T8B | AA | 3001 | 53 | 48,48,48 | 1.01 | 2 (4%) | 63,71,71 | 1.28 | 9 (14%) |

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 |
|---|---|---|---|---|---|---|---|
| 52 | T8B | BA | 3001 | 53 | - | 0/26/26/26 | 0/5/5/5 |
| 52 | T8B | AA | 3001 | 53 | - | 0/26/26/26 | 0/5/5/5 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | AA | 3001 | T8B | O11-C26 | 3.13 | 1.38 | 1.31 |
| 52 | BA | 3001 | T8B | O11-C26 | 3.12 | 1.38 | 1.31 |
| 52 | BA | 3001 | T8B | C25-C24 | 2.27 | 1.50 | 1.43 |
| 52 | AA | 3001 | T8B | C25-C24 | 2.25 | 1.50 | 1.43 |

The worst 5 of 18 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | BA | 3001 | T8B | C21-C23-C24 | -4.27 | 120.19 | 125.09 |
| 52 | AA | 3001 | T8B | C21-C23-C24 | -4.25 | 120.21 | 125.09 |
| 52 | BA | 3001 | T8B | O5-C14-O6 | 3.22 | 120.29 | 116.45 |
| 52 | AA | 3001 | T8B | O5-C14-O6 | 3.22 | 120.29 | 116.45 |
| 52 | BA | 3001 | T8B | O11-C26-C25 | 2.94 | 124.96 | 121.09 |

There are no chirality outliers.

There are no torsion outliers.

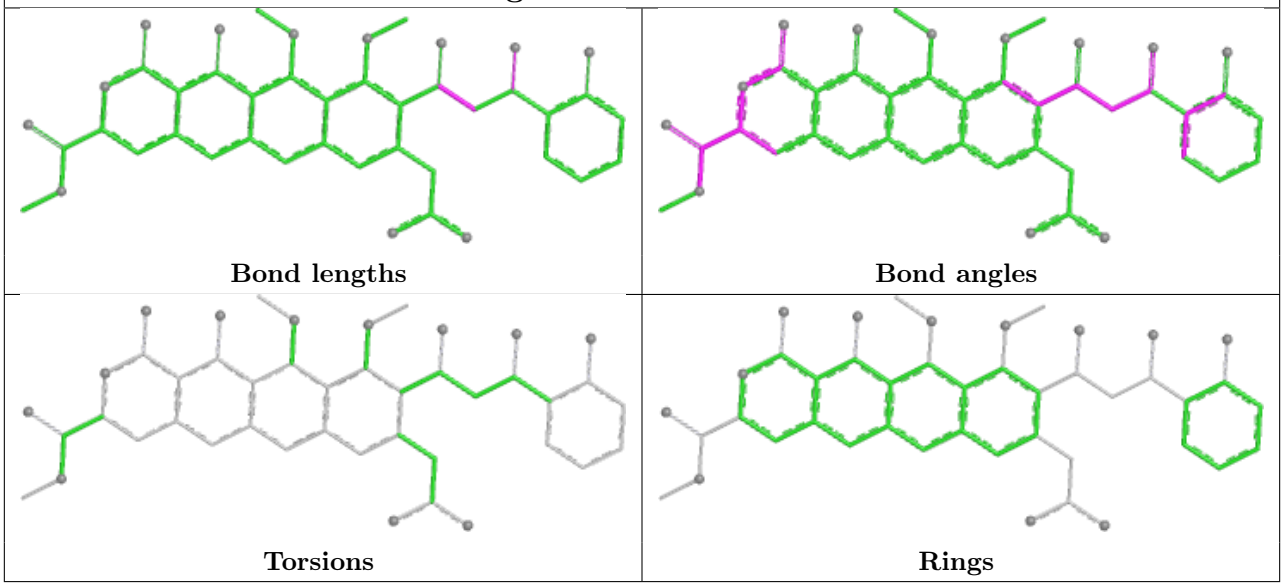
There are no ring outliers.

2 monomers are involved in 54 short contacts:

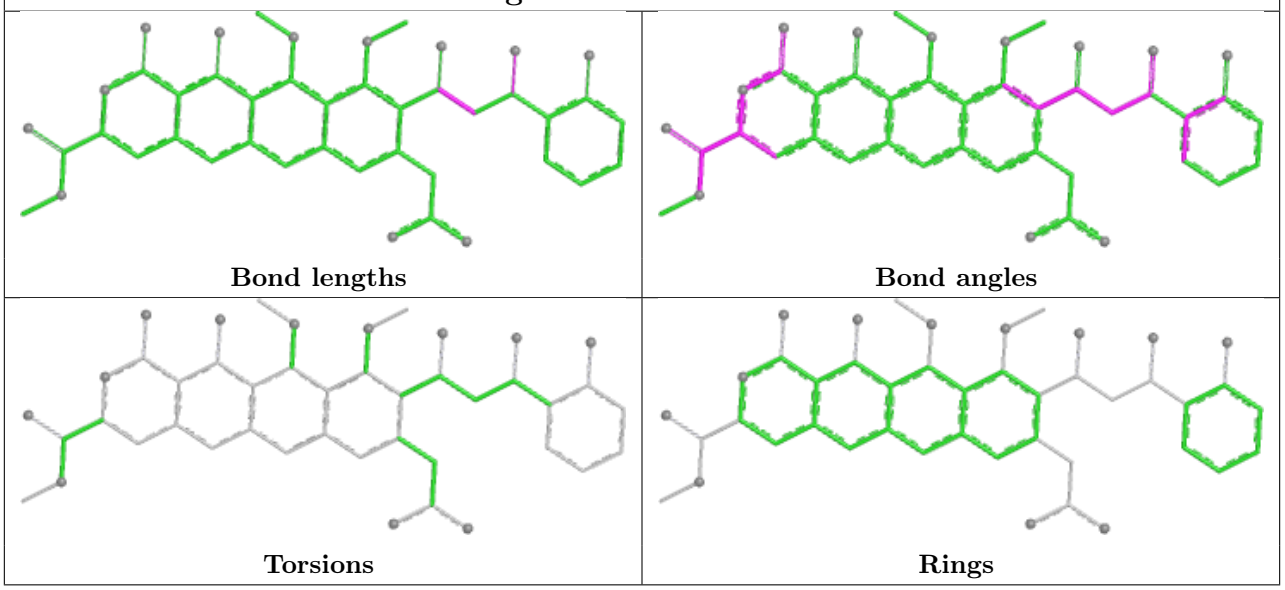
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 52 | BA | 3001 | T8B | 23 | 0 |
| 52 | AA | 3001 | T8B | 31 | 0 |

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

**Ligand T8B BA 3001**




**Ligand T8B AA 3001**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | AA | 2827/2915 (96%) | 0.03 | 112 (3%) 43 29 | 46, 70, 113, 128 | 0 |
| 1 | BA | 2827/2915 (96%) | -0.06 | 93 (3%) 49 34 | 27, 56, 110, 126 | 0 |
| 2 | AB | 120/122 (98%) | 0.77 | 11 (9%) 16 11 | 68, 95, 108, 111 | 0 |
| 2 | BB | 120/122 (98%) | 0.14 | 3 (2%) 58 42 | 46, 80, 95, 103 | 0 |
| 3 | AD | 275/276 (99%) | 0.20 | 8 (2%) 54 38 | 45, 67, 82, 103 | 0 |
| 3 | BD | 275/276 (99%) | 0.21 | 5 (1%) 67 52 | 36, 59, 78, 103 | 0 |
| 4 | AE | 204/206 (99%) | 0.08 | 4 (1%) 64 49 | 47, 72, 87, 98 | 0 |
| 4 | BE | 204/206 (99%) | 0.21 | 5 (2%) 58 42 | 33, 60, 81, 96 | 0 |
| 5 | AF | 203/205 (99%) | 0.12 | 3 (1%) 71 56 | 44, 77, 95, 112 | 0 |
| 5 | BF | 203/205 (99%) | 0.19 | 3 (1%) 71 56 | 26, 64, 90, 110 | 0 |
| 6 | AG | 181/182 (99%) | 1.51 | 50 (27%) 2 1 | 89, 106, 114, 116 | 0 |
| 6 | BG | 181/182 (99%) | 0.71 | 22 (12%) 10 7 | 81, 101, 110, 118 | 0 |
| 7 | AH | 174/180 (96%) | 0.84 | 14 (8%) 20 14 | 80, 93, 101, 108 | 0 |
| 7 | BH | 174/180 (96%) | 0.65 | 14 (8%) 20 14 | 63, 78, 91, 98 | 0 |
| 8 | AI | 145/148 (97%) | 1.31 | 33 (22%) 2 2 | 72, 104, 116, 123 | 0 |
| 8 | BI | 145/148 (97%) | 0.30 | 3 (2%) 63 47 | 68, 90, 98, 100 | 0 |
| 9 | AN | 140/140 (100%) | 0.19 | 3 (2%) 63 47 | 58, 73, 90, 94 | 0 |
| 9 | BN | 140/140 (100%) | 0.32 | 4 (2%) 54 38 | 38, 57, 82, 85 | 0 |
| 10 | AO | 122/122 (100%) | 0.15 | 2 (1%) 70 55 | 56, 73, 85, 91 | 0 |
| 10 | BO | 122/122 (100%) | 0.26 | 4 (3%) 49 34 | 43, 63, 82, 89 | 0 |
| 11 | AP | 147/150 (98%) | 0.51 | 10 (6%) 25 17 | 47, 81, 96, 105 | 0 |
| 11 | BP | 147/150 (98%) | 0.47 | 9 (6%) 28 19 | 28, 68, 91, 100 | 0 |
| 12 | AQ | 141/141 (100%) | 0.39 | 5 (3%) 47 33 | 60, 78, 91, 97 | 0 |
| 12 | BQ | 141/141 (100%) | 0.20 | 2 (1%) 73 58 | 44, 65, 78, 88 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | AR | 118/118 (100%) | 0.23 | 3 (2%) 58 42 | 47, 66, 78, 88 | 0 |
| 13 | BR | 118/118 (100%) | 0.17 | 3 (2%) 58 42 | 35, 53, 69, 86 | 0 |
| 14 | AS | 110/112 (98%) | 1.19 | 20 (18%) 4 3 | 74, 91, 102, 109 | 0 |
| 14 | BS | 110/112 (98%) | 0.54 | 6 (5%) 32 21 | 58, 79, 93, 100 | 0 |
| 15 | AT | 131/146 (89%) | 0.23 | 3 (2%) 61 44 | 66, 76, 99, 109 | 0 |
| 15 | BT | 131/146 (89%) | 0.39 | 6 (4%) 38 26 | 55, 68, 91, 102 | 0 |
| 16 | AU | 116/118 (98%) | 0.11 | 1 (0%) 81 68 | 53, 70, 84, 89 | 0 |
| 16 | BU | 116/118 (98%) | 0.05 | 1 (0%) 81 68 | 34, 50, 70, 84 | 0 |
| 17 | AV | 101/101 (100%) | 0.09 | 1 (0%) 79 66 | 48, 79, 93, 103 | 0 |
| 17 | BV | 101/101 (100%) | 0.05 | 1 (0%) 79 66 | 31, 61, 81, 95 | 0 |
| 18 | AW | 112/113 (99%) | 0.01 | 2 (1%) 67 52 | 50, 59, 80, 104 | 0 |
| 18 | BW | 112/113 (99%) | 0.07 | 1 (0%) 81 68 | 36, 45, 75, 106 | 0 |
| 19 | AX | 95/96 (98%) | 0.52 | 5 (5%) 33 22 | 54, 71, 89, 93 | 0 |
| 19 | BX | 95/96 (98%) | 0.33 | 2 (2%) 63 47 | 33, 59, 83, 91 | 0 |
| 20 | AY | 107/110 (97%) | 0.64 | 8 (7%) 22 15 | 71, 81, 94, 105 | 0 |
| 20 | BY | 107/110 (97%) | 0.61 | 8 (7%) 22 15 | 56, 71, 89, 103 | 0 |
| 21 | AZ | 198/206 (96%) | 0.55 | 7 (3%) 47 33 | 80, 92, 103, 108 | 0 |
| 21 | BZ | 198/206 (96%) | 0.35 | 7 (3%) 47 33 | 64, 82, 97, 103 | 0 |
| 22 | A0 | 76/85 (89%) | 0.32 | 2 (2%) 57 41 | 59, 74, 84, 89 | 0 |
| 22 | B0 | 76/85 (89%) | 0.20 | 1 (1%) 74 60 | 46, 60, 74, 82 | 0 |
| 23 | A1 | 97/98 (98%) | 0.55 | 6 (6%) 28 18 | 54, 71, 94, 99 | 0 |
| 23 | B1 | 97/98 (98%) | 0.31 | 3 (3%) 51 36 | 42, 65, 91, 95 | 0 |
| 24 | A2 | 70/72 (97%) | 0.48 | 5 (7%) 23 16 | 65, 81, 92, 101 | 0 |
| 24 | B2 | 70/72 (97%) | 0.48 | 6 (8%) 18 12 | 52, 70, 85, 102 | 0 |
| 25 | A3 | 59/60 (98%) | 0.62 | 6 (10%) 13 9 | 63, 74, 92, 101 | 0 |
| 25 | B3 | 59/60 (98%) | 0.36 | 1 (1%) 69 53 | 43, 56, 84, 94 | 0 |
| 26 | A4 | 46/71 (64%) | 1.02 | 5 (10%) 12 9 | 101, 109, 113, 119 | 0 |
| 26 | B4 | 46/71 (64%) | 0.78 | 4 (8%) 17 12 | 98, 107, 113, 118 | 0 |
| 27 | A5 | 59/60 (98%) | 0.10 | 0 100 100 | 46, 64, 78, 91 | 0 |
| 27 | B5 | 59/60 (98%) | 0.19 | 0 100 100 | 28, 52, 71, 89 | 0 |
| 28 | A6 | 53/54 (98%) | 0.37 | 4 (7%) 22 15 | 62, 76, 87, 89 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | B6 | 53/54 (98%) | 0.22 | 0 100 100 | 52, 66, 77, 85 | 0 |
| 29 | A7 | 48/49 (97%) | 0.27 | 4 (8%) 19 13 | 43, 54, 79, 99 | 0 |
| 29 | B7 | 48/49 (97%) | 0.17 | 2 (4%) 41 28 | 29, 44, 73, 89 | 0 |
| 30 | A8 | 64/65 (98%) | 0.67 | 6 (9%) 15 11 | 60, 68, 76, 85 | 0 |
| 30 | B8 | 64/65 (98%) | 0.44 | 2 (3%) 51 36 | 45, 56, 65, 79 | 0 |
| 31 | CA | 1498/1521 (98%) | 0.76 | 160 (10%) 12 9 | 59, 99, 120, 126 | 0 |
| 31 | DA | 1498/1521 (98%) | 0.72 | 136 (9%) 16 11 | 65, 99, 120, 128 | 0 |
| 32 | CB | 229/256 (89%) | 0.67 | 13 (5%) 30 20 | 93, 103, 111, 117 | 0 |
| 32 | DB | 229/256 (89%) | 0.96 | 26 (11%) 11 8 | 95, 105, 112, 115 | 0 |
| 33 | CC | 206/239 (86%) | 1.15 | 33 (16%) 6 4 | 92, 106, 112, 115 | 0 |
| 33 | DC | 206/239 (86%) | 1.20 | 38 (18%) 4 3 | 97, 108, 115, 120 | 0 |
| 34 | CD | 208/209 (99%) | 1.24 | 42 (20%) 3 3 | 85, 98, 108, 114 | 0 |
| 34 | DD | 208/209 (99%) | 1.15 | 39 (18%) 4 3 | 87, 97, 107, 123 | 0 |
| 35 | CE | 148/162 (91%) | 0.37 | 3 (2%) 64 49 | 74, 93, 103, 110 | 0 |
| 35 | DE | 148/162 (91%) | 0.63 | 12 (8%) 19 13 | 84, 96, 104, 110 | 0 |
| 36 | CF | 100/101 (99%) | 0.46 | 4 (4%) 43 29 | 80, 92, 101, 107 | 0 |
| 36 | DF | 100/101 (99%) | 0.58 | 6 (6%) 29 19 | 84, 93, 103, 110 | 0 |
| 37 | CG | 155/156 (99%) | 1.93 | 60 (38%) 1 1 | 99, 109, 115, 120 | 0 |
| 37 | DG | 155/156 (99%) | 1.58 | 45 (29%) 1 1 | 97, 109, 115, 119 | 0 |
| 38 | CH | 138/138 (100%) | 0.53 | 6 (4%) 40 27 | 82, 94, 101, 104 | 0 |
| 38 | DH | 138/138 (100%) | 0.76 | 8 (5%) 30 20 | 86, 96, 102, 106 | 0 |
| 39 | CI | 125/128 (97%) | 2.10 | 59 (47%) 0 1 | 97, 111, 117, 120 | 0 |
| 39 | DI | 125/128 (97%) | 2.58 | 78 (62%) 0 1 | 100, 112, 118, 120 | 0 |
| 40 | CJ | 96/105 (91%) | 1.89 | 39 (40%) 1 1 | 100, 109, 115, 117 | 0 |
| 40 | DJ | 96/105 (91%) | 2.03 | 45 (46%) 0 1 | 97, 110, 115, 119 | 0 |
| 41 | CK | 114/129 (88%) | 0.64 | 6 (5%) 33 22 | 72, 93, 101, 105 | 0 |
| 41 | DK | 114/129 (88%) | 0.49 | 7 (6%) 28 19 | 75, 95, 103, 107 | 0 |
| 42 | CL | 122/132 (92%) | 0.80 | 12 (9%) 14 10 | 72, 85, 96, 100 | 0 |
| 42 | DL | 122/132 (92%) | 0.81 | 12 (9%) 14 10 | 77, 87, 96, 105 | 0 |
| 43 | CM | 114/126 (90%) | 2.21 | 56 (49%) 0 1 | 102, 111, 118, 126 | 0 |
| 43 | DM | 114/126 (90%) | 1.89 | 43 (37%) 1 1 | 101, 109, 115, 117 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | CN | 60/61 (98%) | 2.08 | 28 (46%) 0 1 | 99, 108, 116, 118 | 0 |
| 44 | DN | 60/61 (98%) | 2.65 | 37 (61%) 0 1 | 103, 111, 116, 122 | 0 |
| 45 | CO | 88/89 (98%) | 0.48 | 5 (5%) 30 20 | 72, 91, 101, 107 | 0 |
| 45 | DO | 88/89 (98%) | 0.65 | 7 (7%) 20 14 | 81, 93, 103, 107 | 0 |
| 46 | CP | 82/88 (93%) | 1.06 | 11 (13%) 8 6 | 88, 96, 106, 112 | 0 |
| 46 | DP | 82/88 (93%) | 1.26 | 18 (21%) 3 2 | 86, 94, 103, 111 | 0 |
| 47 | CQ | 99/105 (94%) | 0.57 | 4 (4%) 43 29 | 78, 90, 98, 102 | 0 |
| 47 | DQ | 99/105 (94%) | 0.67 | 6 (6%) 28 19 | 79, 92, 100, 103 | 0 |
| 48 | CR | 68/88 (77%) | 0.65 | 6 (8%) 17 12 | 80, 91, 102, 103 | 0 |
| 48 | DR | 68/88 (77%) | 0.42 | 1 (1%) 71 56 | 85, 93, 104, 106 | 0 |
| 49 | CS | 78/93 (83%) | 2.39 | 47 (60%) 0 1 | 107, 111, 117, 123 | 0 |
| 49 | DS | 78/93 (83%) | 1.92 | 33 (42%) 1 1 | 91, 112, 117, 119 | 0 |
| 50 | CT | 96/106 (90%) | 0.91 | 16 (16%) 5 4 | 84, 93, 99, 102 | 0 |
| 50 | DT | 96/106 (90%) | 0.85 | 13 (13%) 8 6 | 82, 92, 100, 101 | 0 |
| 51 | CU | 23/27 (85%) | 4.80 | 22 (95%) 0 0 | 106, 112, 117, 119 | 0 |
| 51 | DU | 23/27 (85%) | 3.68 | 21 (91%) 0 0 | 104, 109, 112, 113 | 0 |
| All | All | 20372/21160 (96%) | 0.51 | 1827 (8%) 17 11 | 26, 84, 115, 128 | 0 |

The worst 5 of 1827 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 31 | CA | 1286 | A | 9.2 |
| 51 | CU | 14 | TRP | 8.8 |
| 49 | CS | 40 | ILE | 8.7 |
| 39 | DI | 126 | SER | 8.2 |
| 31 | CA | 1353 | G | 8.1 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

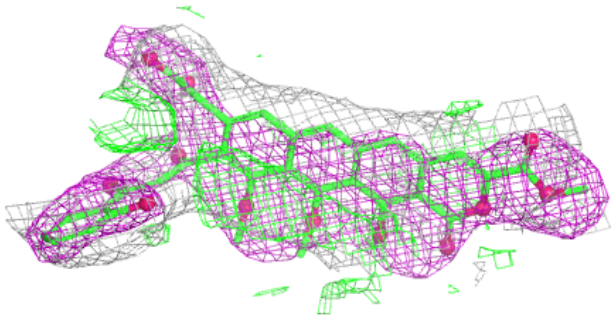
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

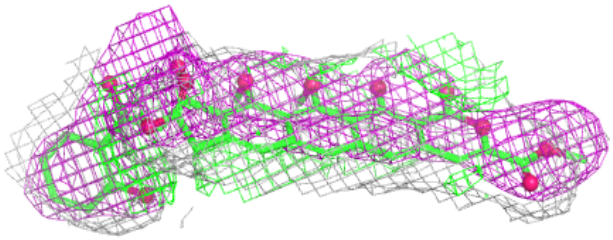
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 52 | T8B | AA | 3001 | 44/44 | 0.74 | 0.15 | 20,20,20,20 | 0 |
| 53 | MG | BA | 3002 | 1/1 | 0.77 | 0.13 | 30,30,30,30 | 0 |
| 52 | T8B | BA | 3001 | 44/44 | 0.79 | 0.13 | 20,20,20,20 | 0 |
| 53 | MG | AA | 3002 | 1/1 | 0.89 | 0.16 | 30,30,30,30 | 0 |
| 53 | MG | AA | 3003 | 1/1 | 0.97 | 0.15 | 30,30,30,30 | 0 |
| 53 | MG | BA | 3003 | 1/1 | 0.97 | 0.20 | 30,30,30,30 | 0 |

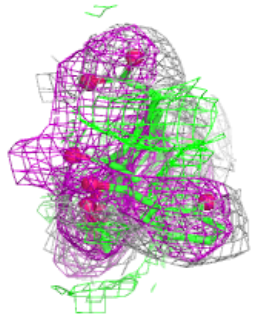
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around T8B AA 3001:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

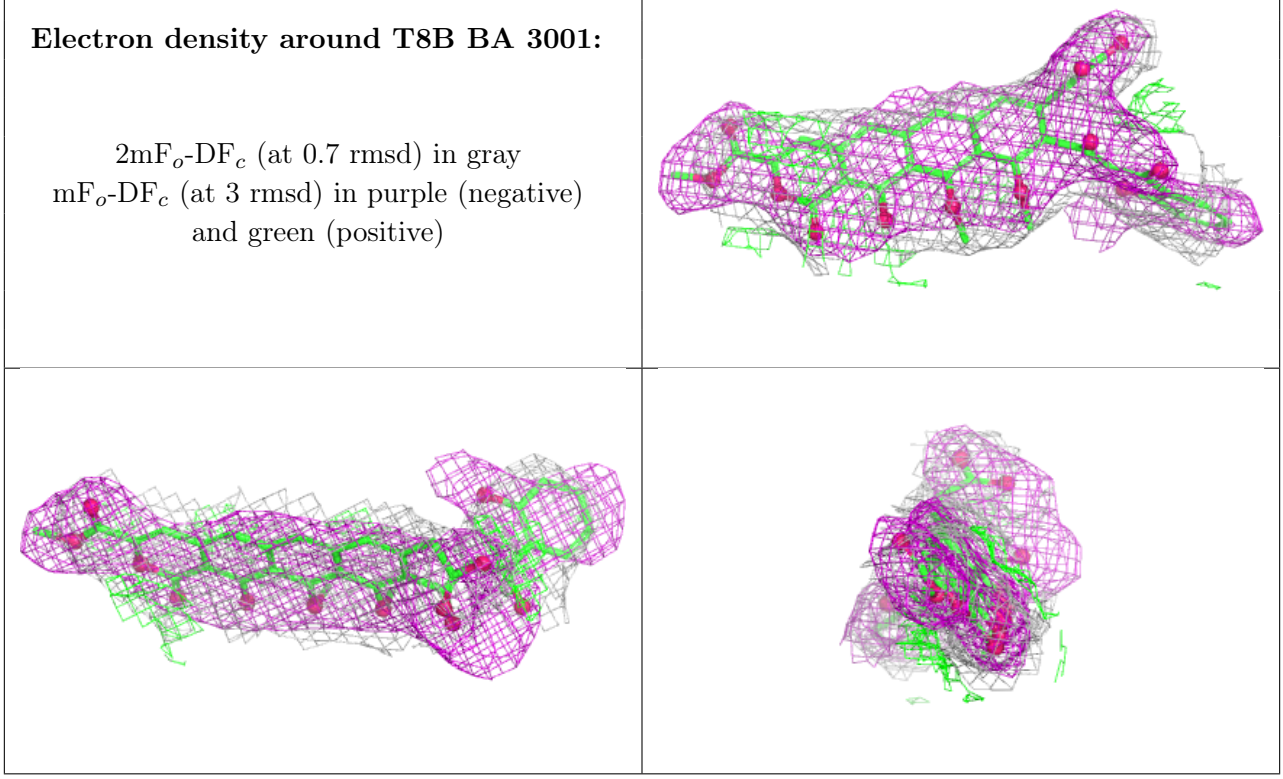






**Electron density around T8B BA 3001:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.5 Other polymers (i)

There are no such residues in this entry.