# wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:37 PM BST

| | | |
|---|---|---|
| PDB ID | : | 5ADY |
| EMDB ID: | : | EMD-3133 |
| Title | : | Cryo-EM structures of the 50S ribosome subunit bound with HflX |
| Authors | : | Zhang, Y.; Mandava, C.S.; Cao, W.; Li, X.; Zhang, D.; Li, N.; Zhang, Y.; Zhang, X.; Qin, Y.; Mi, K.; Lei, J.; Sanyal, S.; Gao, N. |
| Deposited on | : | 2015-08-25 |
| Resolution | : | 4.50 Å(reported) |
| Based on PDB ID | : | 3FIK |

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

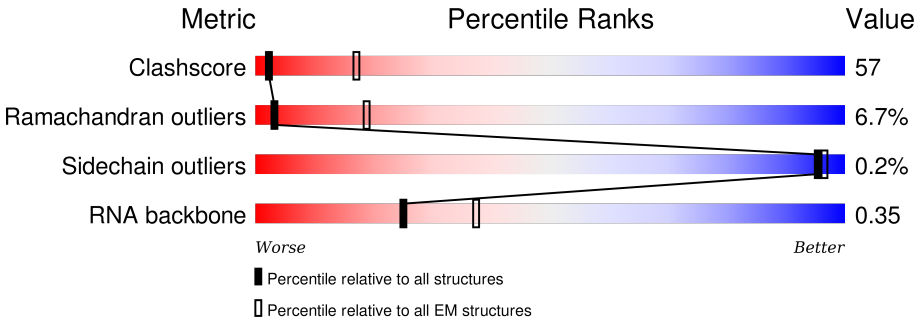
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk27241 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |
| RNA backbone | 3027 | 244 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0 | 57 | 25% 72% • • |
| 2 | 1 | 55 | 42% 51% 7% |
| 3 | 2 | 46 | 39% 54% 7% |
| 4 | 3 | 65 | 51% 48% • |
| 5 | 4 | 38 | 34% 58% 8% |
| 6 | 5 | 234 | 39% 56% • |
| 7 | 6 | 426 | 30% 65% • |
| 8 | 7 | 165 | 38% 55% 6% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | A | 120 | 62% 32% |
| 10 | B | 2903 | 60% 34% |
| 11 | C | 273 | 36% 59% 5% |
| 12 | D | 209 | 29% 64% 7% |
| 13 | E | 201 | 39% 56% |
| 14 | F | 179 | 30% 63% 7% |
| 15 | G | 177 | 33% 63% |
| 16 | H | 149 | 36% 54% 9% |
| 17 | I | 142 | 32% 65% |
| 18 | J | 142 | 27% 65% 7% |
| 19 | K | 123 | 24% 68% 7% |
| 20 | L | 144 | 37% 59% |
| 21 | M | 136 | 40% 57% |
| 22 | N | 127 | 41% 52% 5% |
| 23 | O | 117 | 26% 72% |
| 24 | P | 115 | 30% 65% |
| 25 | Q | 118 | 37% 56% 5% |
| 26 | R | 103 | 24% 69% 7% |
| 27 | S | 110 | 36% 59% 5% |
| 28 | T | 100 | 30% 61% 6% |
| 29 | U | 104 | 36% 58% 6% |
| 30 | V | 94 | 40% 60% |
| 31 | W | 85 | 33% 54% 6% 7% |
| 32 | X | 78 | 29% 64% 5% |
| 33 | Y | 63 | 30% 65% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | Z | 59 | 47% 47% |

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 |
|---|---|---|---|---|---|---|---|
| 35 | GNP | 6 | 527 | - | - | X | - |

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 97364 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 0 | 56 | 444 | 269 | 94 | 80 | 1 | 0 | 0 |

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 2 | 1 | 51 | 410 | 263 | 76 | 71 | 0 | 1 |

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | 2 | 46 | 377 | 228 | 90 | 57 | 2 | 0 | 0 |

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | 3 | 64 | 504 | 323 | 105 | 74 | 2 | 0 | 0 |

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | 4 | 38 | 302 | 185 | 65 | 48 | 4 | 0 | 0 |

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | 5 | 234 | 1733 | 1081 | 315 | 330 | 7 | 0 | 0 |

- Molecule 7 is a protein called GTPASE HFLX.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 6 | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3403 | 2129 | 624 | 641 | 9 | | |

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 7 | 164 | Total | C | N | O | S | 0 | 1 |
| | | | 1231 | 775 | 220 | 229 | 7 | | |

- Molecule 9 is a RNA chain called 5S RRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | A | 117 | Total | C | N | O | P | 0 | 0 |
| | | | 2504 | 1116 | 459 | 813 | 116 | | |

- Molecule 10 is a RNA chain called 23S RRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | B | 2903 | Total | C | N | O | P | 0 | 0 |
| | | | 62317 | 27801 | 11467 | 20147 | 2902 | | |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 264 | C | G | CONFLICT | GB 731469900 |
| B | 542 | C | U | CONFLICT | GB 731469900 |
| B | 846 | U | C | CONFLICT | GB 731469900 |
| B | 1211 | C | U | CONFLICT | GB 731469900 |
| B | 1220 | G | A | CONFLICT | GB 731469900 |
| B | 1229 | C | U | CONFLICT | GB 731469900 |
| B | 1723 | G | A | CONFLICT | GB 731469900 |
| B | 1725 | U | C | CONFLICT | GB 731469900 |
| B | 1726 | C | G | CONFLICT | GB 731469900 |
| B | 1727 | C | A | CONFLICT | GB 731469900 |
| B | 1730 | C | U | CONFLICT | GB 731469900 |
| B | 1733 | G | U | CONFLICT | GB 731469900 |
| B | 1734 | G | C | CONFLICT | GB 731469900 |
| B | 1735 | A | G | CONFLICT | GB 731469900 |
| B | 2794 | C | U | CONFLICT | GB 731469900 |
| B | 2796 | U | C | CONFLICT | GB 731469900 |
| B | 2799 | A | G | CONFLICT | GB 731469900 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 2802 | G | A | CONFLICT | GB 731469900 |

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | C | 272 | Total | C | N | O | S | 0 | 1 |
| | | | 2083 | 1288 | 424 | 364 | 7 | | |

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | D | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | E | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | F | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | |

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | I | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | |

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | J | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | K | 122 | Total | C | N | O | S | 0 | 1 |
| | | | 931 | 582 | 180 | 164 | 5 | | |

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | L | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | |

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | M | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | N | 121 | Total | C | N | O | S | 0 | 1 |
| | | | 961 | 593 | 197 | 166 | 5 | | |

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 23 | O | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | P | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 25 | Q | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | R | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | S | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | T | 94 | Total | C | N | O | S | 0 | 1 |
| | | | 739 | 466 | 140 | 131 | 2 | | |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 29 | U | 103 | Total | C | N | O | 0 | 1 |
| | | | 780 | 492 | 147 | 141 | | |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | V | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | W | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | X | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

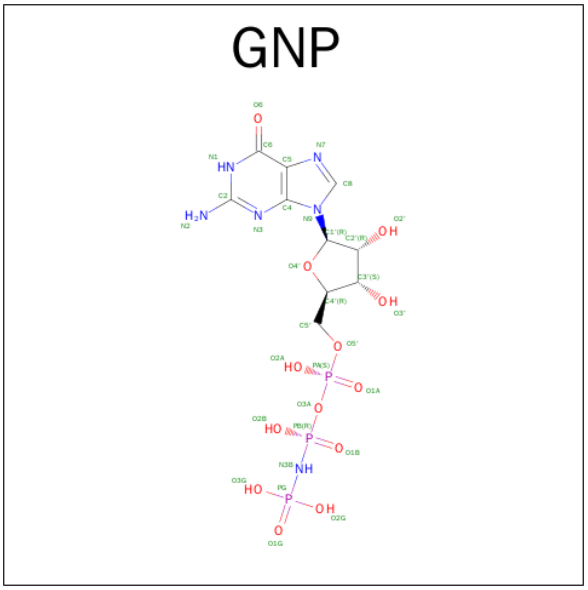
- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | Z | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 35 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 35 | 6 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 6 | 13 | 3 | |

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

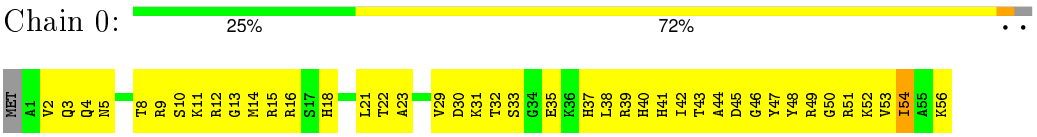
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 36 | 6 | 1 | 1 | 1 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

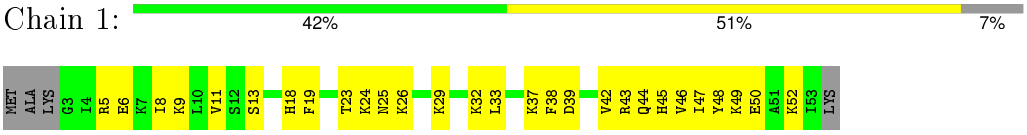
- Molecule 1: 50S RIBOSOMAL PROTEIN L32

Chain 0:



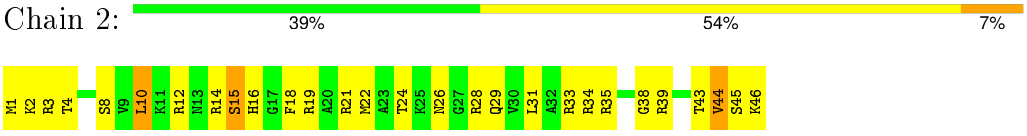

- Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1:



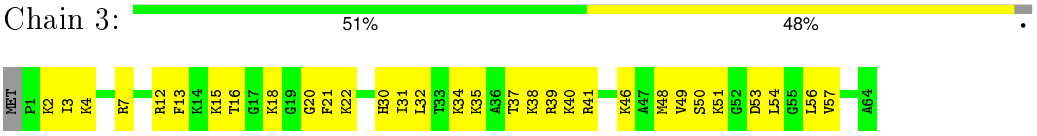

- Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:



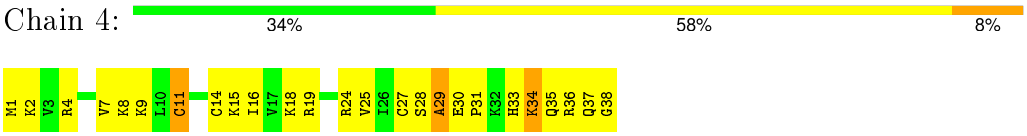

- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:



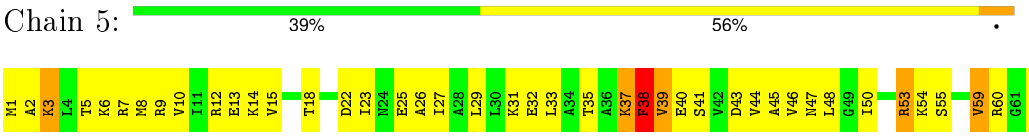

- Molecule 5: 50S RIBOSOMAL PROTEIN L36

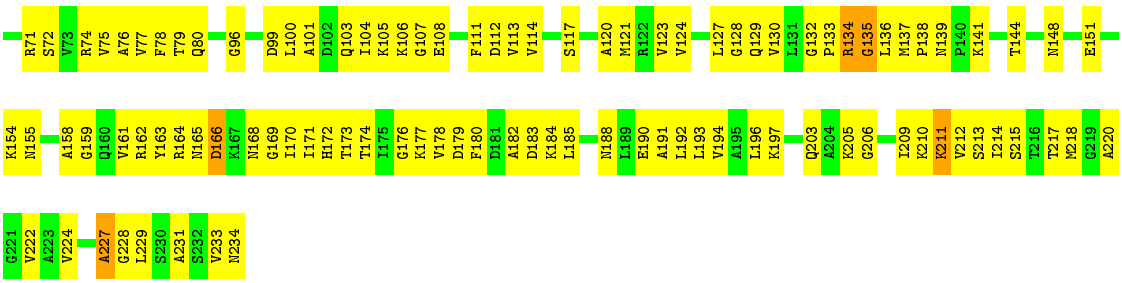
Chain 4:




- Molecule 6: 50S RIBOSOMAL PROTEIN L1

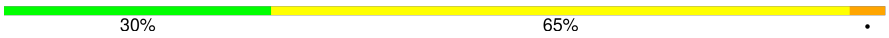
Chain 5:

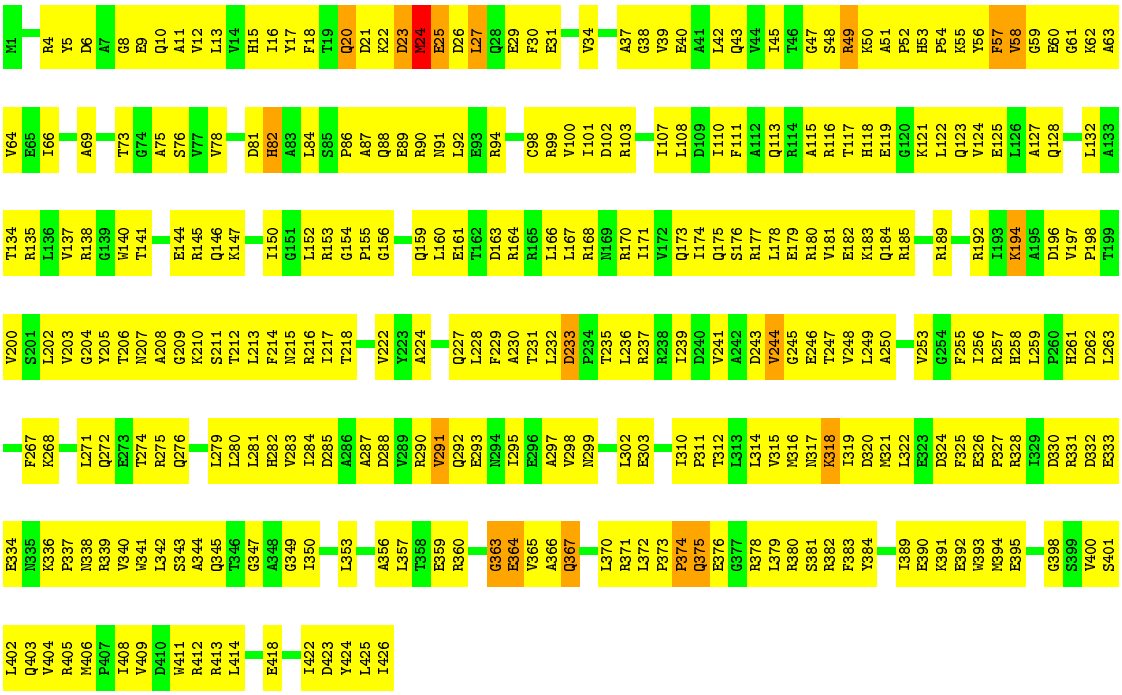





- Molecule 7: GTPASE HFLX

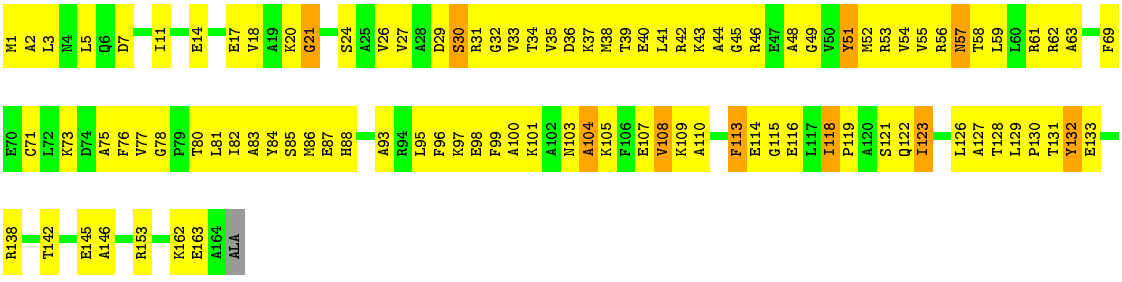
Chain 6:



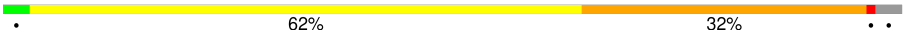

- Molecule 8: 50S RIBOSOMAL PROTEIN L10

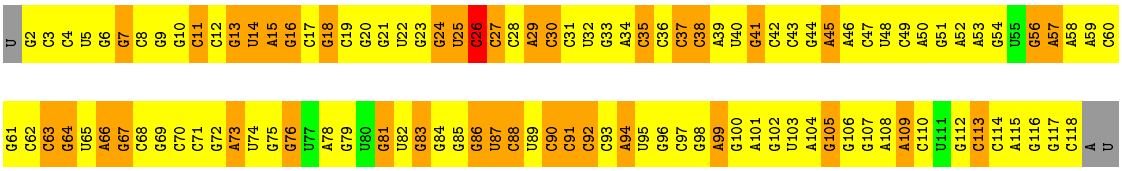
Chain 7:


- Molecule 9: 5S RRNA

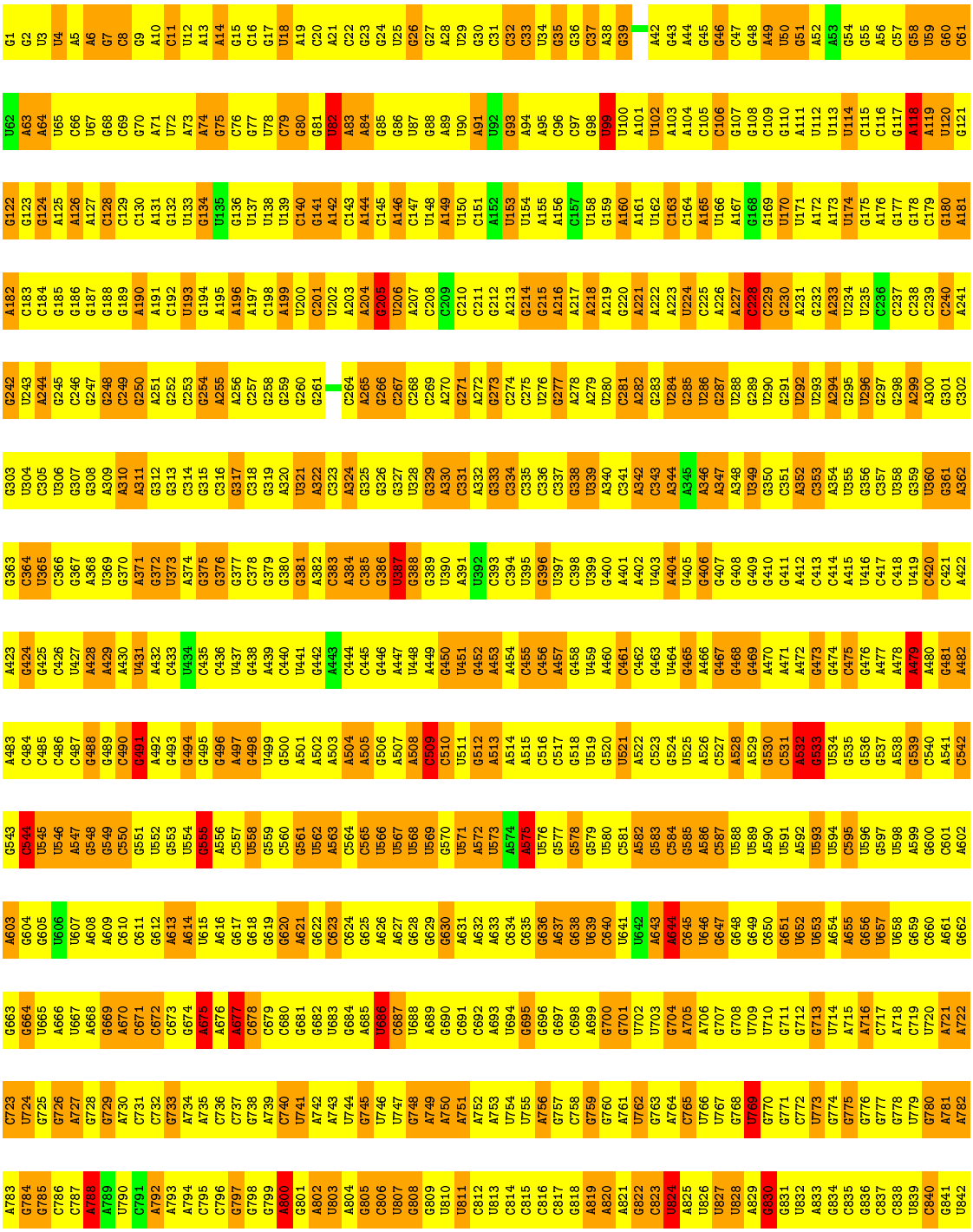
Chain A:

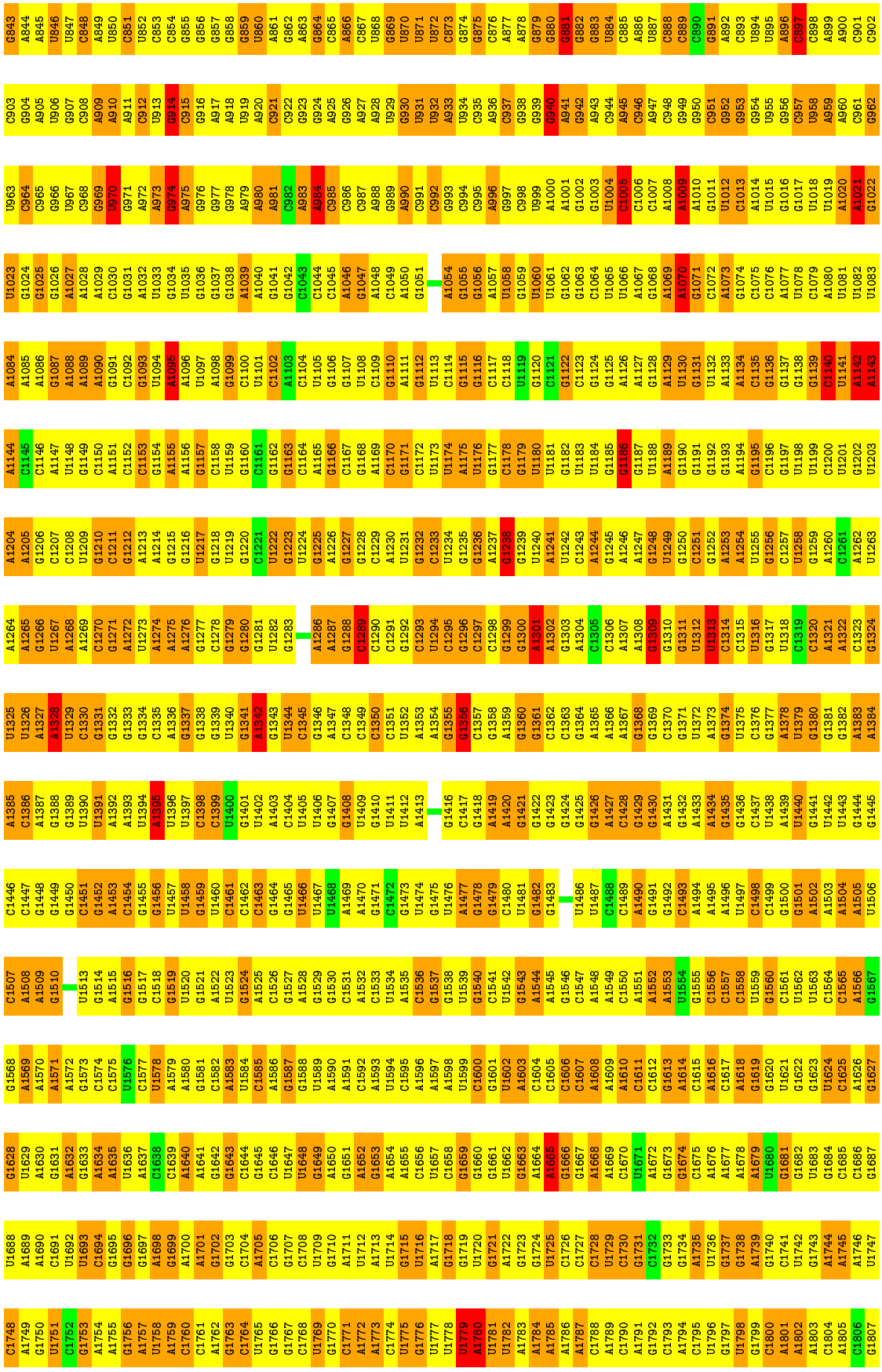


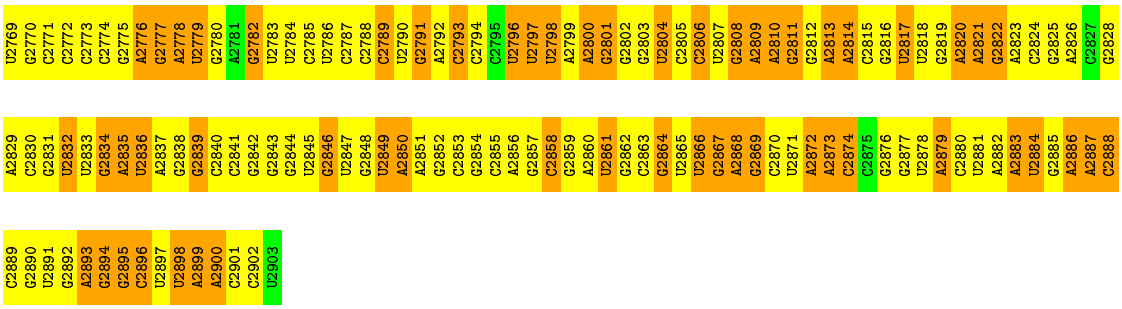



- Molecule 10: 23S RRNA

Chain B:

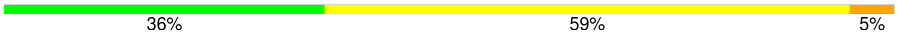



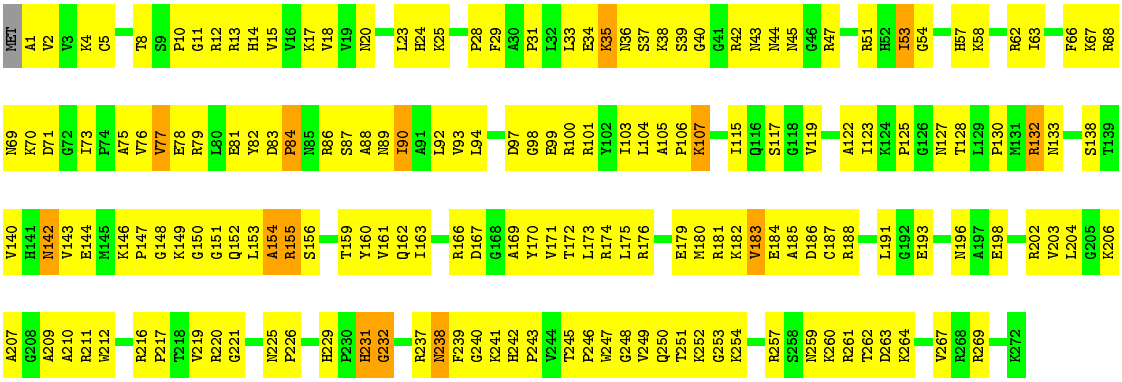





- Molecule 11: 50S RIBOSOMAL PROTEIN L2

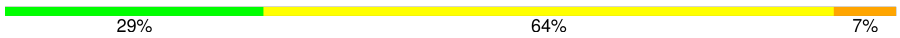
Chain C:




- Molecule 12: 50S RIBOSOMAL PROTEIN L3

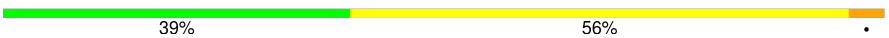
Chain D:

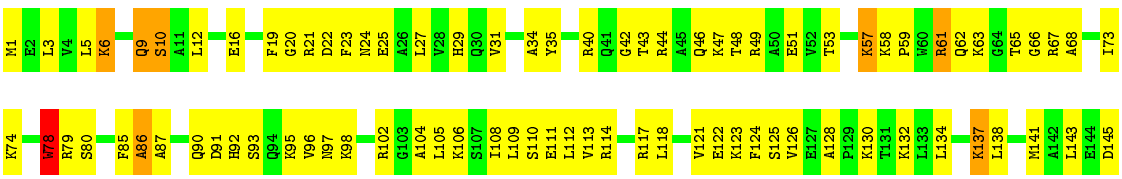




- Molecule 13: 50S RIBOSOMAL PROTEIN L4

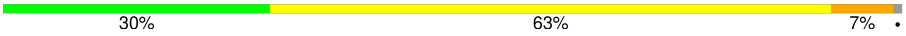
Chain E:

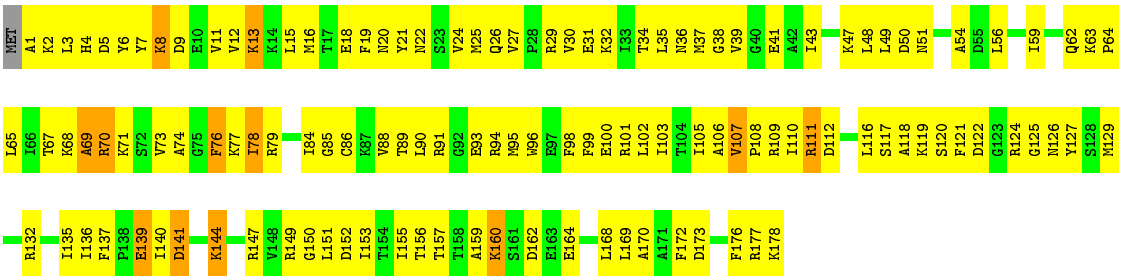



- Molecule 14: 50S RIBOSOMAL PROTEIN L5

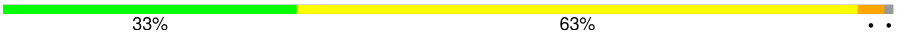
Chain F:




- Molecule 15: 50S RIBOSOMAL PROTEIN L6

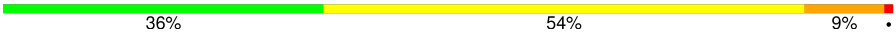
Chain G:





- Molecule 16: 50S RIBOSOMAL PROTEIN L9

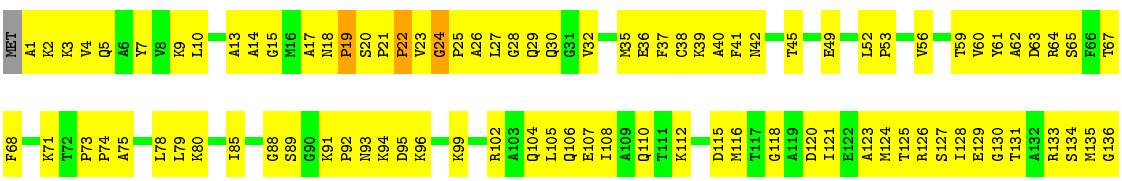
Chain H:





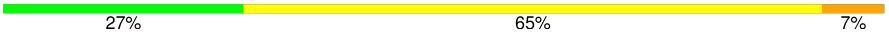
- Molecule 17: 50S RIBOSOMAL PROTEIN L11

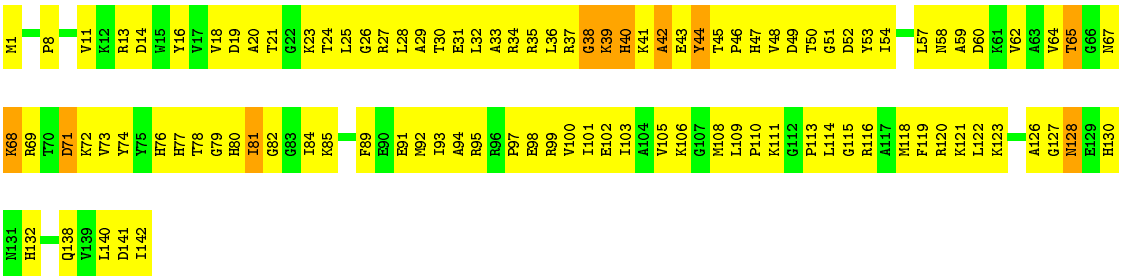
Chain I:


• Molecule 18: 50S RIBOSOMAL PROTEIN L13

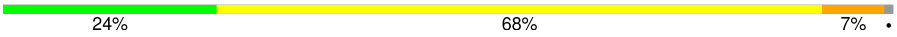
Chain J:

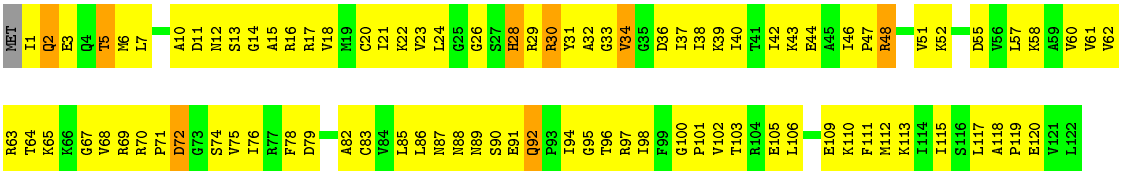



• Molecule 19: 50S RIBOSOMAL PROTEIN L14

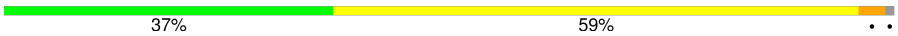
Chain K:

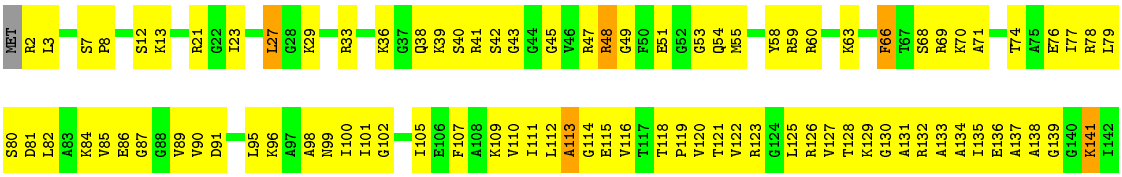



• Molecule 20: 50S RIBOSOMAL PROTEIN L15

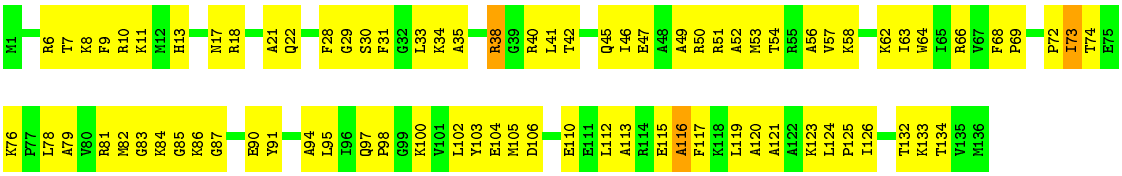
Chain L:



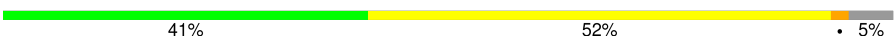

• Molecule 21: 50S RIBOSOMAL PROTEIN L16

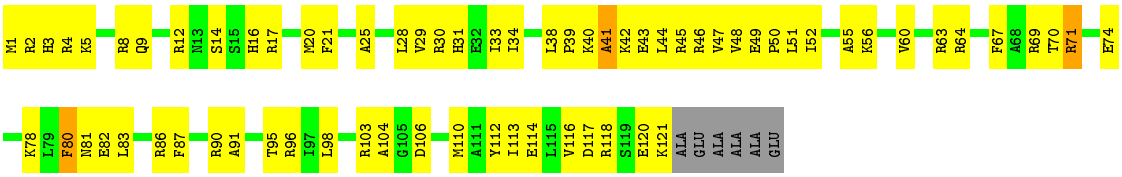
Chain M:


• Molecule 22: 50S RIBOSOMAL PROTEIN L17

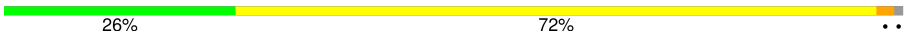
Chain N:






• Molecule 23: 50S RIBOSOMAL PROTEIN L18

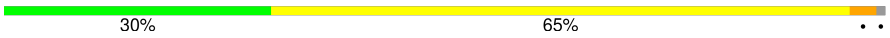
Chain O:

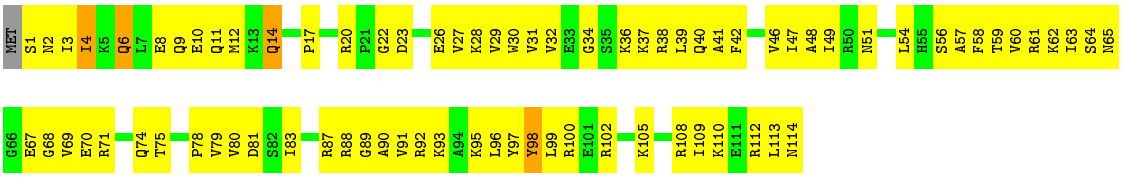




• Molecule 24: 50S RIBOSOMAL PROTEIN L19

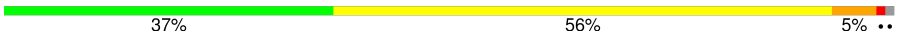
Chain P:

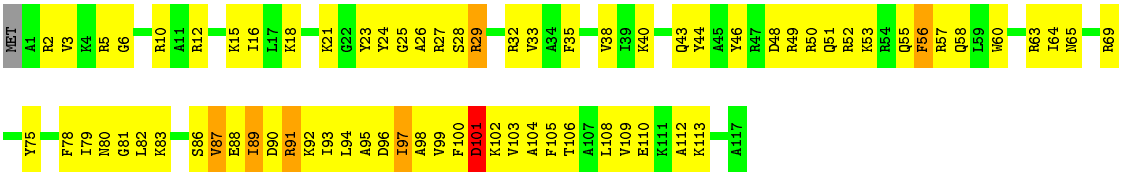



• Molecule 25: 50S RIBOSOMAL PROTEIN L20

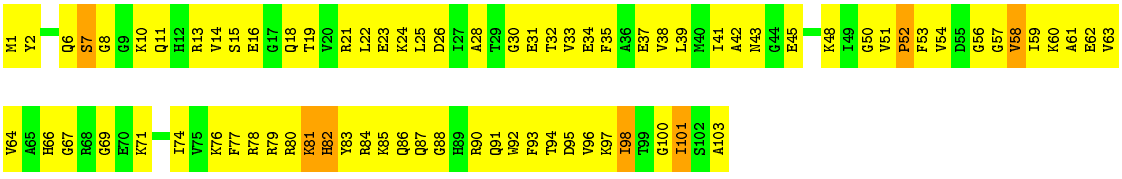
Chain Q:



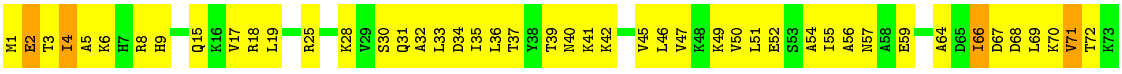

• Molecule 26: 50S RIBOSOMAL PROTEIN L21

Chain R:

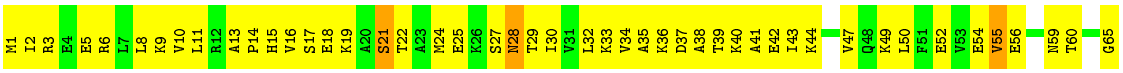

• Molecule 27: 50S RIBOSOMAL PROTEIN L22

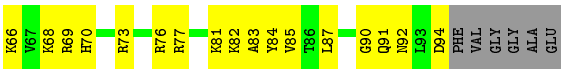
Chain S:


• Molecule 28: 50S RIBOSOMAL PROTEIN L23

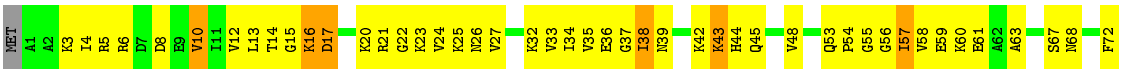
Chain T:


• Molecule 29: 50S RIBOSOMAL PROTEIN L24

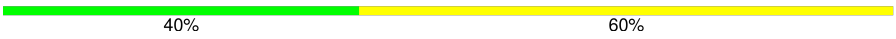
Chain U:

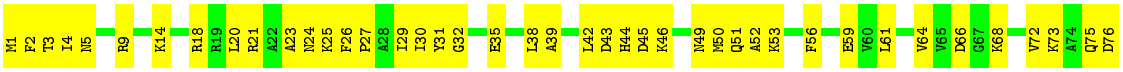



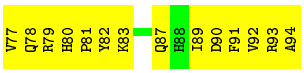


• Molecule 30: 50S RIBOSOMAL PROTEIN L25

Chain V:

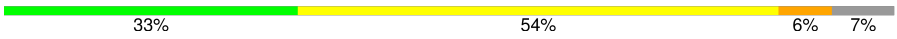


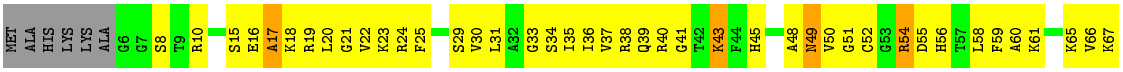




• Molecule 31: 50S RIBOSOMAL PROTEIN L27

Chain W:



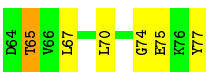





• Molecule 32: 50S RIBOSOMAL PROTEIN L28

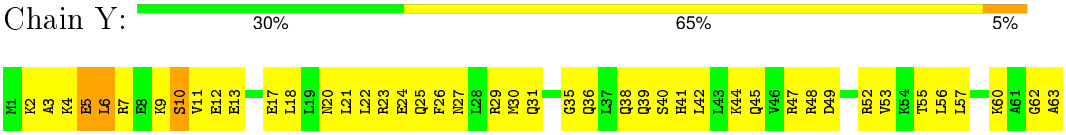
Chain X:





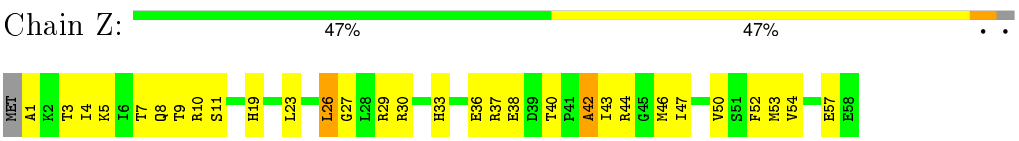
- Molecule 33: 50S RIBOSOMAL PROTEIN L29

Chain Y:




- Molecule 34: 50S RIBOSOMAL PROTEIN L30

Chain Z:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | OTHER | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 20 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 75000 | Depositor |
| Image detector | FEI EAGLE 4K X 4K CCD | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>2$ | RMSZ | #$\|Z\|>2$ |
| 1 | 0 | 0.65 | 0/450 | 0.77 | 0/599 |
| 10 | B | 1.18 | 47/69796 (0.1%) | 1.22 | 227/108888 (0.2%) |
| 11 | C | 0.63 | 0/2122 | 0.72 | 0/2854 |
| 12 | D | 0.66 | 0/1586 | 0.75 | 0/2134 |
| 13 | E | 0.58 | 0/1571 | 0.73 | 0/2113 |
| 14 | F | 0.46 | 0/1444 | 0.69 | 0/1937 |
| 15 | G | 0.57 | 0/1343 | 0.71 | 0/1816 |
| 16 | H | 0.46 | 0/1122 | 0.64 | 0/1515 |
| 17 | I | 0.41 | 0/1046 | 0.64 | 0/1410 |
| 18 | J | 0.64 | 0/1152 | 0.75 | 0/1551 |
| 19 | K | 0.60 | 0/940 | 0.75 | 0/1260 |
| 2 | 1 | 0.57 | 0/417 | 0.68 | 0/556 |
| 20 | L | 0.58 | 0/1054 | 0.79 | 1/1403 (0.1%) |
| 21 | M | 0.68 | 0/1093 | 0.71 | 0/1460 |
| 22 | N | 0.66 | 0/974 | 0.74 | 0/1303 |
| 23 | O | 0.54 | 0/902 | 0.70 | 0/1209 |
| 24 | P | 0.61 | 0/929 | 0.71 | 0/1242 |
| 25 | Q | 0.78 | 0/960 | 0.77 | 0/1278 |
| 26 | R | 0.64 | 0/829 | 0.71 | 0/1107 |
| 27 | S | 0.66 | 0/864 | 0.84 | 0/1156 |
| 28 | T | 0.61 | 0/745 | 0.77 | 0/996 |
| 29 | U | 0.53 | 0/788 | 0.72 | 0/1053 |
| 3 | 2 | 0.69 | 0/380 | 0.78 | 0/498 |
| 30 | V | 0.60 | 0/766 | 0.72 | 0/1025 |
| 31 | W | 0.64 | 0/603 | 0.80 | 0/797 |
| 32 | X | 0.62 | 0/635 | 0.71 | 0/848 |
| 33 | Y | 0.53 | 0/510 | 0.68 | 0/677 |
| 34 | Z | 0.60 | 0/453 | 0.77 | 1/605 (0.2%) |
| 4 | 3 | 0.64 | 0/513 | 0.76 | 0/676 |
| 5 | 4 | 0.65 | 0/303 | 0.77 | 0/397 |
| 6 | 5 | 0.35 | 0/1748 | 0.64 | 1/2355 (0.0%) |
| 7 | 6 | 0.55 | 0/3456 | 0.76 | 1/4675 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >2 | RMSZ | #\|Z\| >2 |
| 8 | 7 | 0.39 | 0/1245 | 0.63 | 0/1677 |
| 9 | A | 1.01 | 0/2800 | 1.16 | 6/4367 (0.1%) |
| All | All | 1.03 | 47/105539 (0.0%) | 1.10 | 237/157437 (0.2%) |

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 |
|---|---|---|---|
| 13 | E | 0 | 1 |
| 14 | F | 0 | 1 |
| 24 | P | 0 | 1 |
| 25 | Q | 0 | 1 |
| 6 | 5 | 0 | 1 |
| All | All | 0 | 5 |

The worst 5 of 47 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | B | 788 | A | N9-C4 | -8.84 | 1.32 | 1.37 |
| 10 | B | 118 | A | N9-C4 | -7.60 | 1.33 | 1.37 |
| 10 | B | 677 | A | N9-C4 | -6.86 | 1.33 | 1.37 |
| 10 | B | 1142 | A | N9-C4 | -6.60 | 1.33 | 1.37 |
| 10 | B | 1254 | A | N9-C4 | -6.54 | 1.33 | 1.37 |

The worst 5 of 237 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | B | 828 | U | C2-N1-C1' | 8.23 | 127.58 | 117.70 |
| 10 | B | 205 | G | C2-N3-C4 | -8.04 | 107.88 | 111.90 |
| 10 | B | 1816 | C | C2-N1-C1' | 8.01 | 127.61 | 118.80 |
| 10 | B | 544 | C | C2-N1-C1' | 7.58 | 127.14 | 118.80 |
| 10 | B | 1238 | G | N3-C4-C5 | 7.58 | 132.39 | 128.60 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 6 | 5 | 59 | VAL | Peptide |
| 13 | E | 59 | PRO | Peptide |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | F | 76 | PHE | Peptide |
| 24 | P | 14 | GLN | Peptide |
| 25 | Q | 101 | ASP | 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 | 0 | 444 | 0 | 461 | 53 | 0 |
| 2 | 1 | 410 | 0 | 440 | 42 | 0 |
| 3 | 2 | 377 | 0 | 418 | 42 | 0 |
| 4 | 3 | 504 | 0 | 574 | 60 | 0 |
| 5 | 4 | 302 | 0 | 343 | 35 | 0 |
| 6 | 5 | 1733 | 0 | 1823 | 197 | 0 |
| 7 | 6 | 3403 | 0 | 3433 | 387 | 0 |
| 8 | 7 | 1231 | 0 | 1282 | 124 | 0 |
| 9 | A | 2504 | 0 | 1271 | 249 | 0 |
| 10 | B | 62317 | 0 | 31345 | 6160 | 0 |
| 11 | C | 2083 | 0 | 2157 | 244 | 0 |
| 12 | D | 1565 | 0 | 1616 | 238 | 0 |
| 13 | E | 1552 | 0 | 1619 | 130 | 0 |
| 14 | F | 1420 | 0 | 1460 | 169 | 0 |
| 15 | G | 1323 | 0 | 1374 | 136 | 0 |
| 16 | H | 1111 | 0 | 1148 | 188 | 0 |
| 17 | I | 1032 | 0 | 1088 | 142 | 0 |
| 18 | J | 1129 | 0 | 1162 | 144 | 0 |
| 19 | K | 931 | 0 | 1003 | 116 | 0 |
| 20 | L | 1045 | 0 | 1117 | 121 | 0 |
| 21 | M | 1074 | 0 | 1157 | 105 | 0 |
| 22 | N | 961 | 0 | 1000 | 107 | 0 |
| 23 | O | 892 | 0 | 923 | 130 | 0 |
| 24 | P | 917 | 0 | 965 | 101 | 0 |
| 25 | Q | 947 | 0 | 1022 | 143 | 0 |
| 26 | R | 816 | 0 | 839 | 106 | 0 |
| 27 | S | 857 | 0 | 922 | 100 | 0 |
| 28 | T | 739 | 0 | 807 | 74 | 0 |
| 29 | U | 780 | 0 | 834 | 89 | 0 |
| 30 | V | 753 | 0 | 780 | 60 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 31 | W | 596 | 0 | 610 | 94 | 0 |
| 32 | X | 625 | 0 | 655 | 92 | 0 |
| 33 | Y | 509 | 0 | 543 | 52 | 0 |
| 34 | Z | 449 | 0 | 491 | 26 | 0 |
| 35 | 6 | 32 | 0 | 13 | 23 | 0 |
| 36 | 6 | 1 | 0 | 0 | 0 | 0 |
| All | All | 97364 | 0 | 66695 | 9059 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

The worst 5 of 9059 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) |
|---|---|---|---|
| 16:H:68:ARG:HG3 | 16:H:132:PHE:CD2 | 1.40 | 1.55 |
| 16:H:68:ARG:HG3 | 16:H:132:PHE:CE2 | 1.37 | 1.53 |
| 16:H:68:ARG:HD2 | 16:H:132:PHE:CE1 | 1.43 | 1.52 |
| 16:H:68:ARG:CG | 16:H:132:PHE:CZ | 2.00 | 1.43 |
| 7:6:24:MET:HE3 | 7:6:257:ARG:NH2 | 1.28 | 1.43 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | 0 | 54/57 (95%) | 45 (83%) | 5 (9%) | 4 (7%) | 1 21 |
| 2 | 1 | 49/55 (89%) | 45 (92%) | 4 (8%) | 0 | 100 100 |
| 3 | 2 | 44/46 (96%) | 35 (80%) | 6 (14%) | 3 (7%) | 1 24 |
| 4 | 3 | 62/65 (95%) | 58 (94%) | 4 (6%) | 0 | 100 100 |
| 5 | 4 | 36/38 (95%) | 26 (72%) | 5 (14%) | 5 (14%) | 0 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 6 | 5 | 232/234 (99%) | 190 (82%) | 27 (12%) | 15 (6%) | 1 | 26 |
| 7 | 6 | 424/426 (100%) | 364 (86%) | 39 (9%) | 21 (5%) | 3 | 31 |
| 8 | 7 | 162/165 (98%) | 128 (79%) | 23 (14%) | 11 (7%) | 1 | 24 |
| 11 | C | 270/273 (99%) | 219 (81%) | 34 (13%) | 17 (6%) | 2 | 26 |
| 12 | D | 207/209 (99%) | 166 (80%) | 20 (10%) | 21 (10%) | 1 | 13 |
| 13 | E | 199/201 (99%) | 160 (80%) | 21 (11%) | 18 (9%) | 1 | 16 |
| 14 | F | 176/179 (98%) | 131 (74%) | 30 (17%) | 15 (8%) | 1 | 17 |
| 15 | G | 174/177 (98%) | 142 (82%) | 21 (12%) | 11 (6%) | 2 | 26 |
| 16 | H | 147/149 (99%) | 97 (66%) | 29 (20%) | 21 (14%) | 0 | 6 |
| 17 | I | 139/142 (98%) | 122 (88%) | 13 (9%) | 4 (3%) | 6 | 45 |
| 18 | J | 140/142 (99%) | 109 (78%) | 19 (14%) | 12 (9%) | 1 | 17 |
| 19 | K | 120/123 (98%) | 96 (80%) | 14 (12%) | 10 (8%) | 1 | 18 |
| 20 | L | 141/144 (98%) | 113 (80%) | 20 (14%) | 8 (6%) | 2 | 28 |
| 21 | M | 134/136 (98%) | 113 (84%) | 13 (10%) | 8 (6%) | 2 | 27 |
| 22 | N | 119/127 (94%) | 96 (81%) | 18 (15%) | 5 (4%) | 3 | 35 |
| 23 | O | 114/117 (97%) | 105 (92%) | 6 (5%) | 3 (3%) | 7 | 47 |
| 24 | P | 112/115 (97%) | 89 (80%) | 18 (16%) | 5 (4%) | 3 | 33 |
| 25 | Q | 115/118 (98%) | 102 (89%) | 7 (6%) | 6 (5%) | 2 | 30 |
| 26 | R | 101/103 (98%) | 78 (77%) | 13 (13%) | 10 (10%) | 1 | 14 |
| 27 | S | 108/110 (98%) | 93 (86%) | 8 (7%) | 7 (6%) | 1 | 26 |
| 28 | T | 92/100 (92%) | 73 (79%) | 13 (14%) | 6 (6%) | 1 | 26 |
| 29 | U | 101/104 (97%) | 79 (78%) | 14 (14%) | 8 (8%) | 1 | 19 |
| 30 | V | 92/94 (98%) | 81 (88%) | 10 (11%) | 1 (1%) | 17 | 64 |
| 31 | W | 77/85 (91%) | 58 (75%) | 12 (16%) | 7 (9%) | 1 | 16 |
| 32 | X | 75/78 (96%) | 61 (81%) | 9 (12%) | 5 (7%) | 1 | 24 |
| 33 | Y | 61/63 (97%) | 49 (80%) | 6 (10%) | 6 (10%) | 1 | 14 |
| 34 | Z | 56/59 (95%) | 51 (91%) | 3 (5%) | 2 (4%) | 4 | 40 |
| All | All | 4133/4234 (98%) | 3374 (82%) | 484 (12%) | 275 (7%) | 3 | 24 |

5 of 275 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 4 | 11 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 4 | 34 | LYS |
| 6 | 5 | 38 | PHE |
| 6 | 5 | 39 | VAL |
| 6 | 5 | 135 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 0 | 47/48 (98%) | 47 (100%) | 0 | 100 100 |
| 2 | 1 | 45/49 (92%) | 45 (100%) | 0 | 100 100 |
| 3 | 2 | 38/38 (100%) | 38 (100%) | 0 | 100 100 |
| 4 | 3 | 51/52 (98%) | 51 (100%) | 0 | 100 100 |
| 5 | 4 | 34/34 (100%) | 34 (100%) | 0 | 100 100 |
| 6 | 5 | 181/181 (100%) | 179 (99%) | 2 (1%) | 80 90 |
| 7 | 6 | 364/364 (100%) | 363 (100%) | 1 (0%) | 94 96 |
| 8 | 7 | 123/123 (100%) | 123 (100%) | 0 | 100 100 |
| 11 | C | 216/218 (99%) | 216 (100%) | 0 | 100 100 |
| 12 | D | 164/164 (100%) | 163 (99%) | 1 (1%) | 90 95 |
| 13 | E | 165/165 (100%) | 164 (99%) | 1 (1%) | 90 95 |
| 14 | F | 149/150 (99%) | 149 (100%) | 0 | 100 100 |
| 15 | G | 137/138 (99%) | 137 (100%) | 0 | 100 100 |
| 16 | H | 114/114 (100%) | 113 (99%) | 1 (1%) | 84 92 |
| 17 | I | 109/110 (99%) | 109 (100%) | 0 | 100 100 |
| 18 | J | 116/116 (100%) | 116 (100%) | 0 | 100 100 |
| 19 | K | 102/104 (98%) | 102 (100%) | 0 | 100 100 |
| 20 | L | 102/103 (99%) | 102 (100%) | 0 | 100 100 |
| 21 | M | 109/109 (100%) | 109 (100%) | 0 | 100 100 |
| 22 | N | 100/103 (97%) | 100 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 23 | O | 86/87 (99%) | 86 (100%) | 0 | 100 100 |
| 24 | P | 99/100 (99%) | 99 (100%) | 0 | 100 100 |
| 25 | Q | 89/90 (99%) | 88 (99%) | 1 (1%) | 80 90 |
| 26 | R | 84/84 (100%) | 84 (100%) | 0 | 100 100 |
| 27 | S | 93/93 (100%) | 93 (100%) | 0 | 100 100 |
| 28 | T | 80/84 (95%) | 80 (100%) | 0 | 100 100 |
| 29 | U | 83/85 (98%) | 83 (100%) | 0 | 100 100 |
| 30 | V | 78/78 (100%) | 78 (100%) | 0 | 100 100 |
| 31 | W | 59/63 (94%) | 59 (100%) | 0 | 100 100 |
| 32 | X | 67/68 (98%) | 67 (100%) | 0 | 100 100 |
| 33 | Y | 55/55 (100%) | 55 (100%) | 0 | 100 100 |
| 34 | Z | 48/49 (98%) | 48 (100%) | 0 | 100 100 |
| All | All | 3387/3419 (99%) | 3380 (100%) | 7 (0%) | 95 97 |

5 of 7 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | D | 151 | THR |
| 25 | Q | 56 | PHE |
| 13 | E | 78 | TRP |
| 6 | 5 | 38 | PHE |
| 16 | H | 68 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | G | 115 | GLN |
| 21 | M | 17 | ASN |
| 32 | X | 15 | ASN |
| 16 | H | 33 | GLN |
| 18 | J | 40 | HIS |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 10 | B | 2902/2903 (99%) | 1015 (34%) | 56 (1%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 9 | A | 116/120 (96%) | 35 (30%) | 2 (1%) |
| All | All | 3018/3023 (99%) | 1050 (34%) | 58 (1%) |

5 of 1050 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | A | 7 | G |
| 9 | A | 11 | C |
| 9 | A | 13 | G |
| 9 | A | 14 | U |
| 9 | A | 15 | A |

5 of 58 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | B | 1267 | U |
| 10 | B | 1652 | A |
| 10 | B | 2688 | G |
| 10 | B | 1321 | A |
| 10 | B | 1395 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 35 | GNP | 6 | 527 | 36 | 29,34,34 | 2.14 | 9 (31%) | 29,54,54 | 2.81 | 10 (34%) |

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 |
|---|---|---|---|---|---|---|---|
| 35 | GNP | 6 | 527 | 36 | - | 0/13/38/38 | 0/3/3/3 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | 6 | 527 | GNP | PB-O3A | -7.21 | 1.50 | 1.59 |
| 35 | 6 | 527 | GNP | PB-O2B | -3.48 | 1.47 | 1.56 |
| 35 | 6 | 527 | GNP | C8-N7 | -2.45 | 1.29 | 1.34 |
| 35 | 6 | 527 | GNP | PG-O3G | -2.27 | 1.50 | 1.56 |
| 35 | 6 | 527 | GNP | PG-O2G | -2.20 | 1.50 | 1.56 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | 6 | 527 | GNP | C5-C6-N1 | -8.92 | 111.86 | 123.52 |
| 35 | 6 | 527 | GNP | PA-O3A-PB | -4.95 | 114.77 | 132.71 |
| 35 | 6 | 527 | GNP | O3G-PG-O1G | -3.22 | 105.11 | 113.58 |
| 35 | 6 | 527 | GNP | C2'-C1'-N9 | -3.05 | 105.29 | 113.47 |
| 35 | 6 | 527 | GNP | C2'-C3'-C4' | -2.81 | 96.89 | 102.64 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 35 | 6 | 527 | GNP | 23 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.