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

Feb 1, 2016 – 06:21 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 4KZZ |
| Title | : | Rabbit 40S ribosomal subunit in complex with mRNA, initiator tRNA and eIF1A |
| Authors | : | Lomakin, I.B.; Steitz, T.A. |
| Deposited on | : | 2013-05-30 |
| Resolution | : | 7.03 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

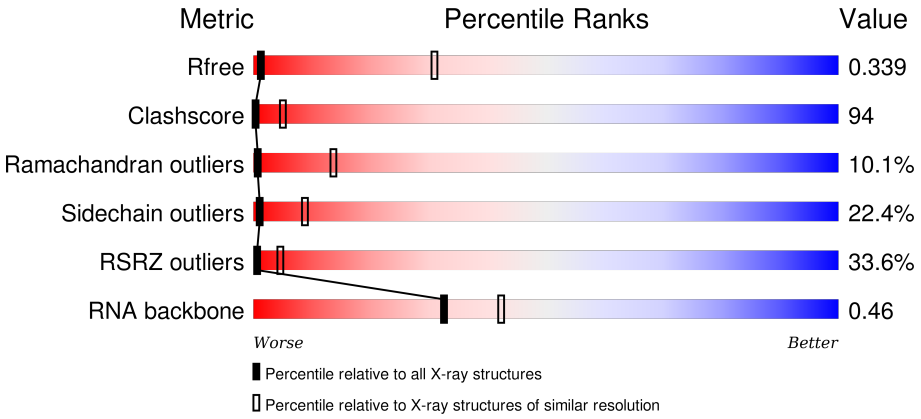
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 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 7.03 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)) |
|---|---|---|
| $R_{free}$ | 91344 | 1014 (9.50-3.66) |
| Clashscore | 102246 | 1063 (10.00-3.70) |
| Ramachandran outliers | 100387 | 1035 (9.50-3.66) |
| Sidechain outliers | 100360 | 1005 (9.50-3.66) |
| RSRZ outliers | 91569 | 1013 (9.50-3.66) |
| RNA backbone | 2183 | 1105 (10.00-2.80) |

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 on the lower 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% 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 | A | 295 | 15%, 9%, 39%, 19%, •, 29% |
| 2 | B | 264 | 30%, 14%, 45%, 20%, •, 19% |
| 3 | C | 278 | 40%, 14%, 46%, 18%, •, 19% |
| 4 | D | 243 | 68%, 21%, 45%, 23%, 5%, 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | E | 263 | 53% 23% 47% 25% |
| 6 | F | 204 | 75% 23% 48% 17% 6% 6% |
| 7 | G | 249 | 31% 22% 47% 23% 5% |
| 8 | H | 194 | 12% 16% 48% 23% 10% |
| 9 | I | 208 | 58% 30% 45% 15% 9% |
| 10 | J | 194 | 18% 14% 48% 22% 9% 6% |
| 11 | K | 165 | 19% 6% 28% 14% 12% 41% |
| 12 | L | 158 | 41% 28% 41% 23% 8% |
| 13 | M | 132 | 4% 23% 42% 22% 7% 6% |
| 14 | N | 151 | 18% 28% 47% 23% |
| 15 | O | 151 | 34% 16% 48% 23% 10% |
| 16 | P | 145 | 52% 12% 39% 26% 10% 12% |
| 17 | Q | 146 | 36% 18% 53% 20% 5% |
| 18 | R | 135 | 10% 19% 54% 10% 10% 7% |
| 19 | S | 152 | 19% 18% 43% 18% 10% 10% |
| 20 | T | 145 | 5% 21% 53% 19% 5% |
| 21 | U | 119 | 55% 15% 37% 26% 9% 13% |
| 22 | V | 83 | 17% 14% 43% 28% 13% |
| 23 | W | 130 | 37% 28% 58% 12% |
| 24 | X | 143 | 44% 26% 48% 20% 6% |
| 25 | Y | 133 | 8% 14% 49% 23% 9% 5% |
| 26 | Z | 125 | 11% 11% 30% 13% 6% 40% |
| 27 | a | 115 | 27% 63% 22% 7% 7% |
| 28 | b | 84 | 7% 65% 25% 10% |
| 29 | c | 69 | 54% 65% 20% 7% 7% |

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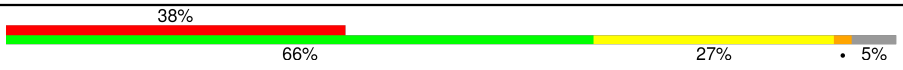
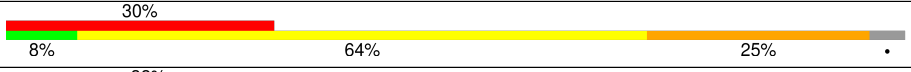
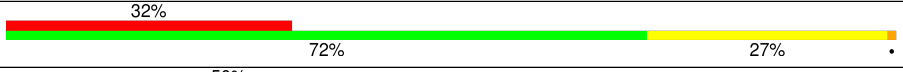
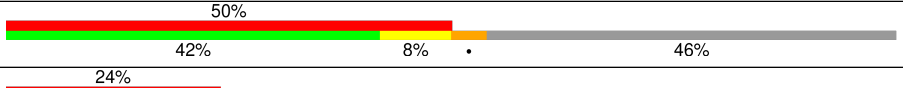
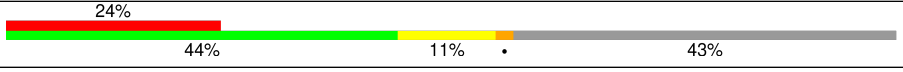
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 30 | d | 56 |   |
| 31 | e | 133 | |
| 32 | f | 156 | |
| 33 | g | 317 | |
| 34 | i | 1863 |   |
| 35 | j | 75 |   |
| 36 | k | 24 |   |
| 37 | n | 144 |   |

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 79048 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 protein called 40S Ribosomal Protein SA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1642 | 1045 | 289 | 300 | 8 | | | |

- Molecule 2 is a protein called 40S Ribosomal Protein S3A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1741 | 1107 | 309 | 310 | 15 | | | |

- Molecule 3 is a protein called 40S Ribosomal Protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1742 | 1127 | 300 | 306 | 9 | | | |

- Molecule 4 is a protein called 40S Ribosomal Protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 227 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1764 | 1124 | 317 | 315 | 8 | | | |

- Molecule 5 is a protein called 40S Ribosomal Protein S4X.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 263 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2083 | 1329 | 385 | 359 | 10 | | | |

- Molecule 6 is a protein called 40S Ribosomal Protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1509 | 943 | 286 | 273 | 7 | | | |

- Molecule 7 is a protein called 40S Ribosomal Protein S6.

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

- Molecule 8 is a protein called 40S Ribosomal Protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 190 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1530 | 975 | 281 | 273 | 1 | | | |

- Molecule 9 is a protein called 40S Ribosomal Protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1679 | 1054 | 329 | 291 | 5 | | | |

- Molecule 10 is a protein called 40S Ribosomal Protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 182 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1498 | 952 | 300 | 244 | 2 | | | |

- Molecule 11 is a protein called 40S Ribosomal Protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 827 | 539 | 148 | 134 | 6 | | | |

- Molecule 12 is a protein called 40S Ribosomal Protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 158 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1296 | 827 | 241 | 221 | 7 | | | |

- Molecule 13 is a protein called 40S Ribosomal Protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 594 | 169 | 179 | 8 | | | |

- Molecule 14 is a protein called 40S Ribosomal Protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | N | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1208 | 773 | 229 | 205 | 1 | | | |

- Molecule 15 is a protein called 40S Ribosomal Protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | O | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1016 | 621 | 199 | 190 | 6 | | | |

- Molecule 16 is a protein called 40S Ribosomal Protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | P | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1060 | 673 | 201 | 179 | 7 | | | |

- Molecule 17 is a protein called 40S Ribosomal Protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | Q | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1124 | 715 | 212 | 194 | 3 | | | |

- Molecule 18 is a protein called 40S Ribosomal Protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | R | 126 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1019 | 639 | 188 | 187 | 5 | | | |

- Molecule 19 is a protein called 40S Ribosomal Protein S18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | S | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1139 | 714 | 231 | 193 | 1 | | | |

- Molecule 20 is a protein called 40S Ribosomal Protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | T | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 701 | 213 | 195 | 3 | | | |

- Molecule 21 is a protein called 40S Ribosomal Protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | U | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 822 | 514 | 156 | 148 | 4 | | | |

- Molecule 22 is a protein called 40S Ribosomal Protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | V | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 619 | 378 | 117 | 119 | 5 | | | |

- Molecule 23 is a protein called 40S Ribosomal Protein S15A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | W | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1034 | 659 | 193 | 176 | 6 | | | |

- Molecule 24 is a protein called 40S Ribosomal Protein S23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | X | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1106 | 698 | 220 | 184 | 4 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| X | 1 | MET | ALA | SEE REMARK 999 | UNP G1SZ47 |

- Molecule 25 is a protein called 40S Ribosomal Protein S24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | Y | 126 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 645 | 198 | 173 | 5 | | | |

- Molecule 26 is a protein called 40S Ribosomal Protein S25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | Z | 75 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 598 | 382 | 111 | 104 | 1 | | | |

- Molecule 27 is a protein called 40S Ribosomal Protein S26.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | a | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 844 | 527 | 173 | 138 | 6 | | | |

- Molecule 28 is a protein called 40S Ribosomal Protein S27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | b | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 659 | 413 | 122 | 116 | 8 | | | |

- Molecule 29 is a protein called 40S Ribosomal Protein S28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | c | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 506 | 308 | 102 | 94 | 2 | | | |

- Molecule 30 is a protein called 40S Ribosomal Protein S29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | d | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 445 | 278 | 90 | 72 | 5 | | | |

- Molecule 31 is a protein called 40S Ribosomal Protein S30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | e | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 473 | 293 | 104 | 75 | 1 | | | |

- Molecule 32 is a protein called 40S Ribosomal Protein S27A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | f | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 367 | 109 | 98 | 7 | | | |

- Molecule 33 is a protein called 40S Ribosomal Protein RACK1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | g | 313 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2436 | 1535 | 424 | 465 | 12 | | | |

- Molecule 34 is a RNA chain called 18S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | i | 1797 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37514 | 16712 | 6634 | 12372 | 1796 | | | |

- Molecule 35 is a RNA chain called initiator Met-RNA-i.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | j | 75 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1607 | 717 | 298 | 517 | 75 | | | |

- Molecule 36 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | k | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 273 | 123 | 47 | 90 | 13 | | | |

- Molecule 37 is a protein called human initiation factor eIF1A.

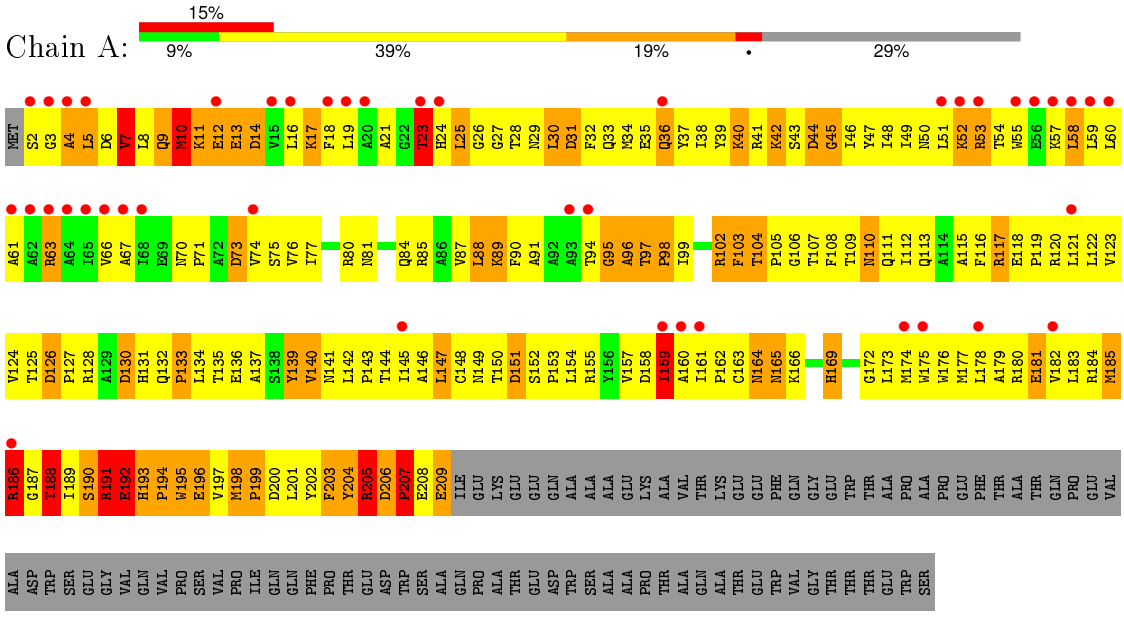
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | n | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 407 | 119 | 118 | 4 | | | |

# 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 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.

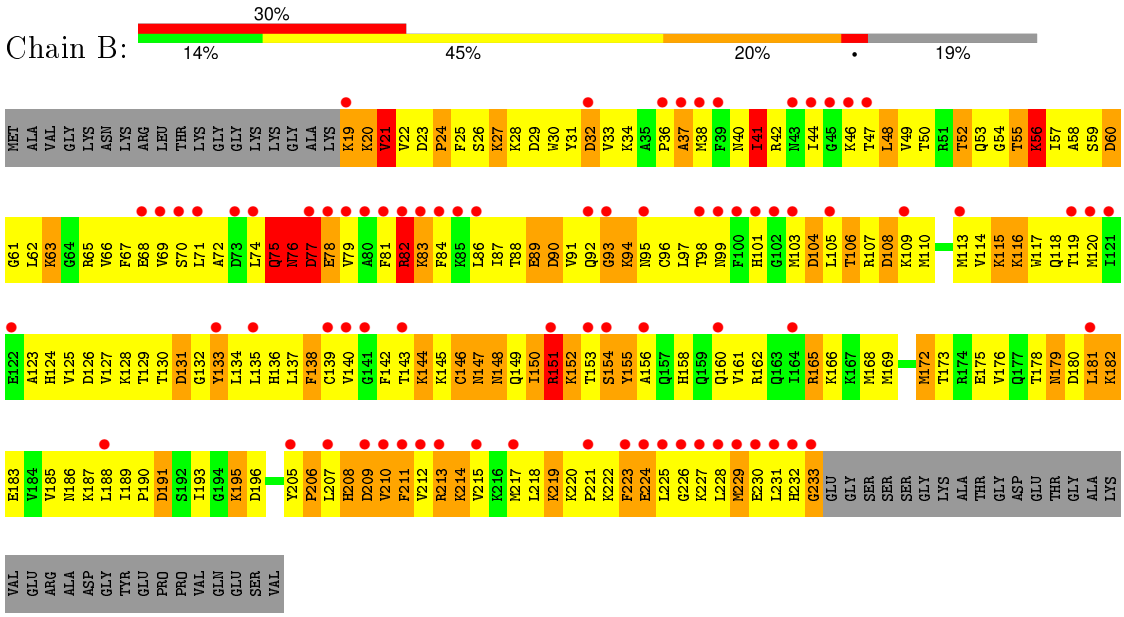
- Molecule 1: 40S Ribosomal Protein SA

Chain A:



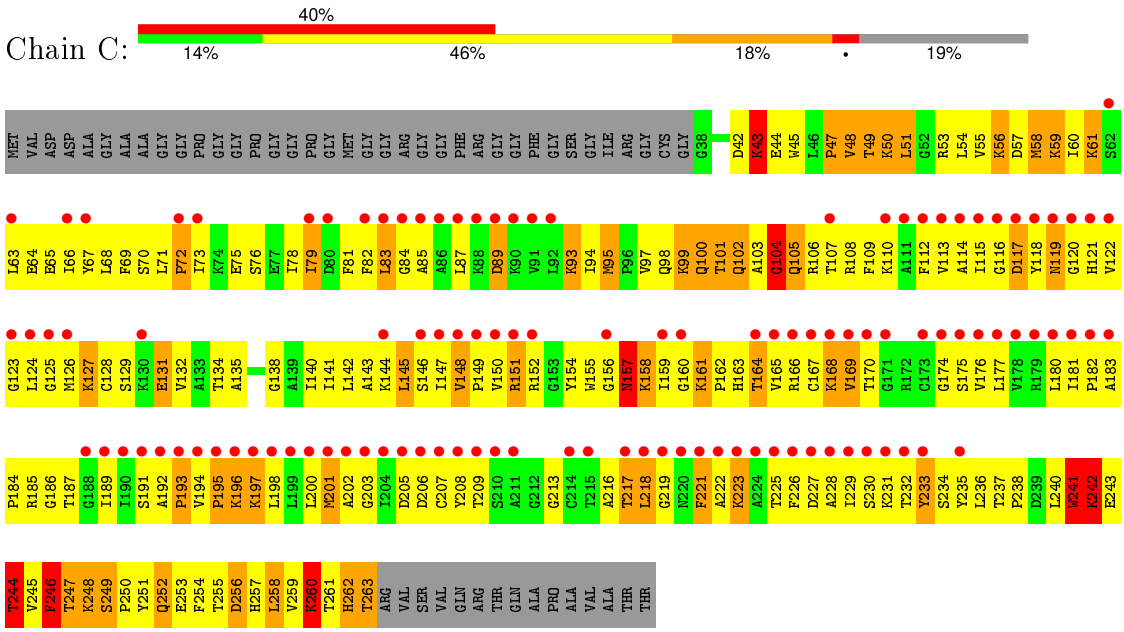

- Molecule 2: 40S Ribosomal Protein S3A

Chain B:



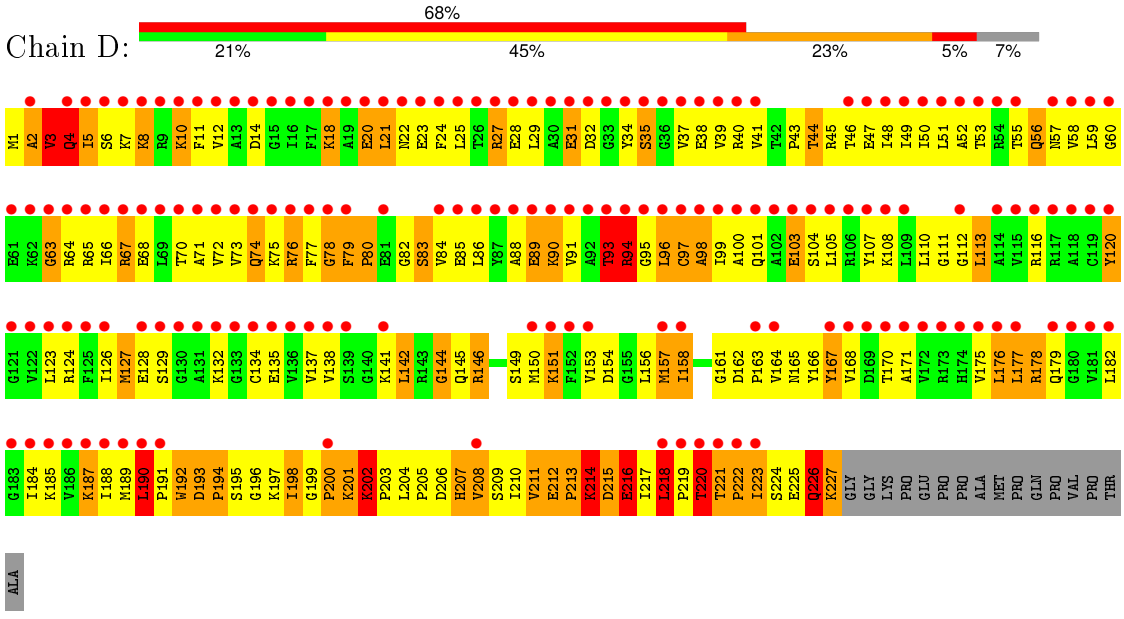
- Molecule 3: 40S Ribosomal Protein S2

Chain C:



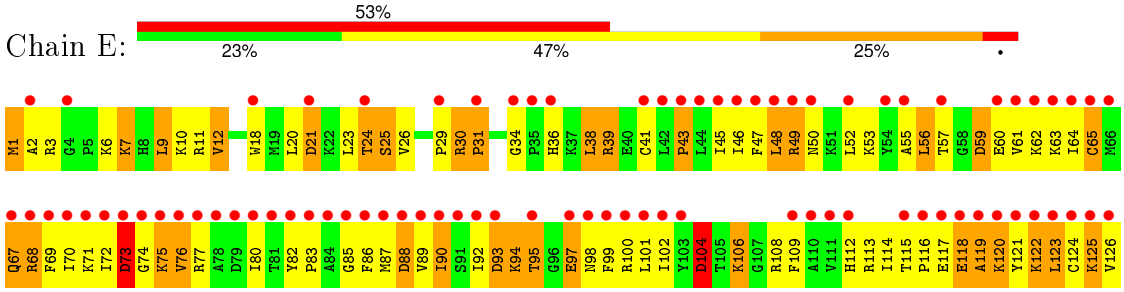

- Molecule 4: 40S Ribosomal Protein S3

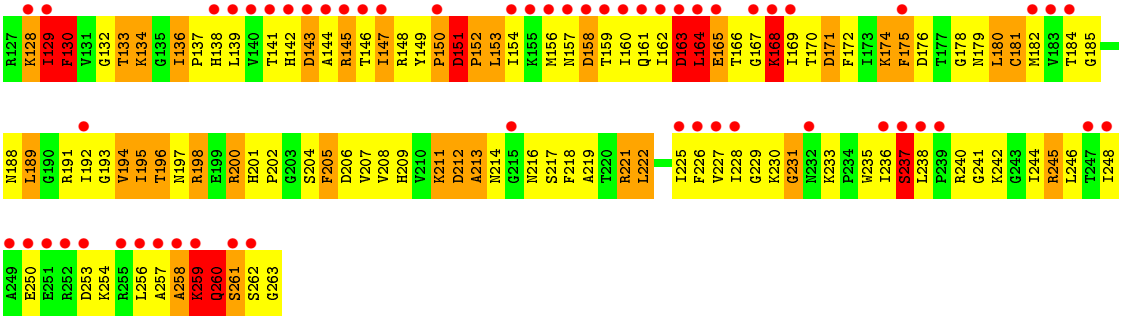
Chain D:




- Molecule 5: 40S Ribosomal Protein S4X

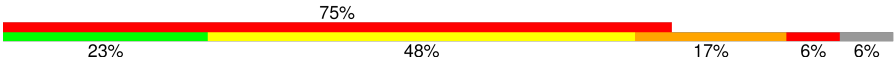
Chain E:

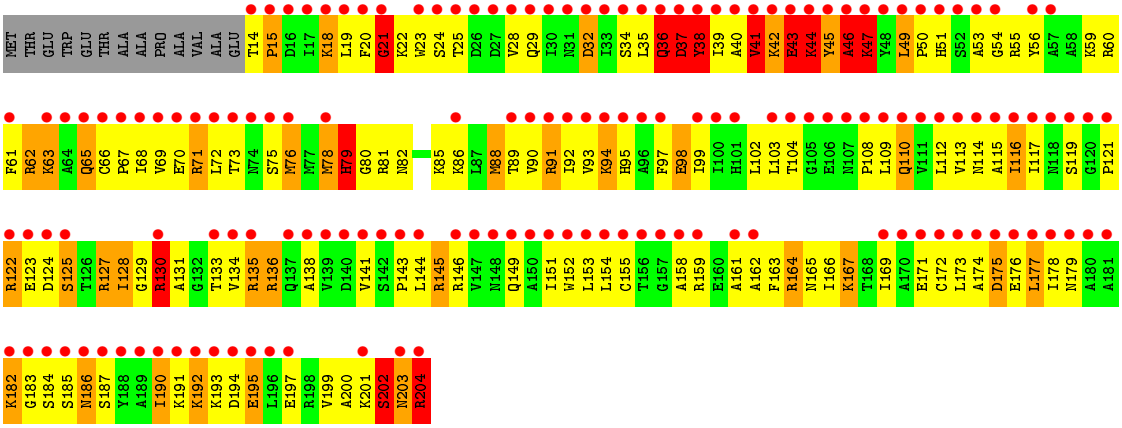





• Molecule 6: 40S Ribosomal Protein S5

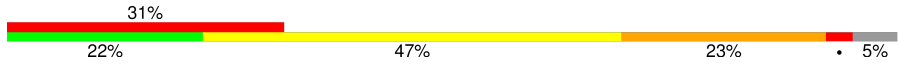
Chain F:

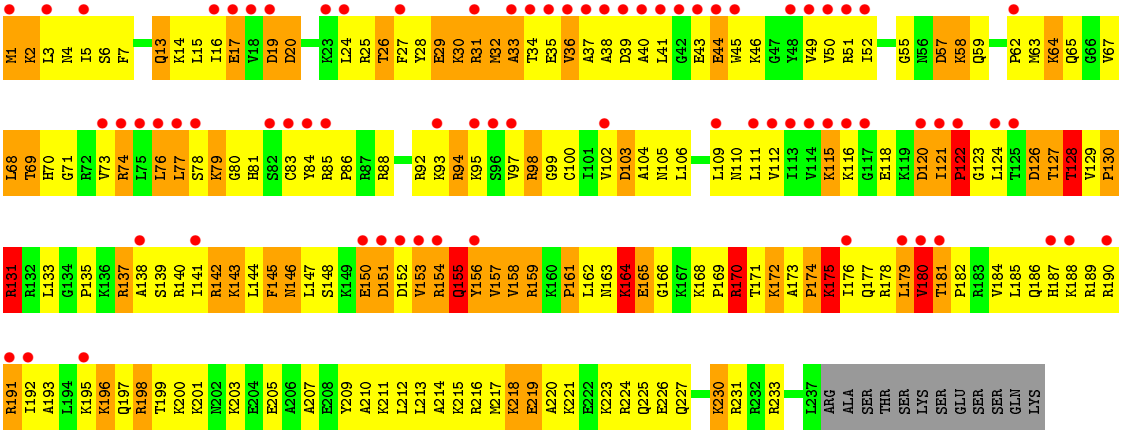



• Molecule 7: 40S Ribosomal Protein S6

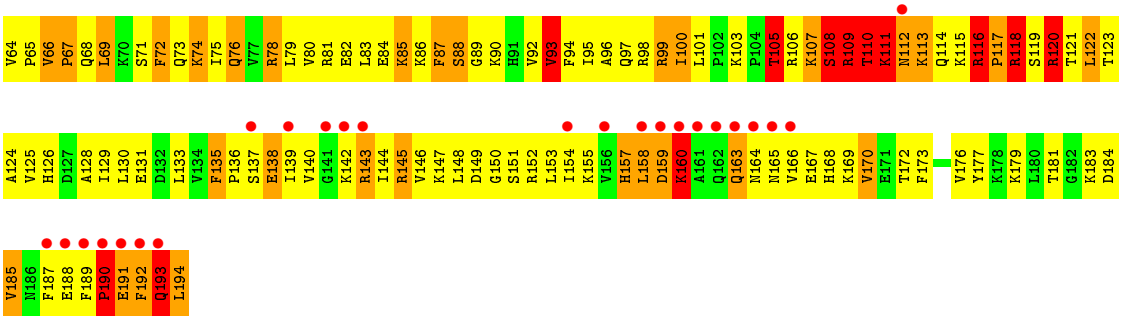
Chain G:




• Molecule 8: 40S Ribosomal Protein S7

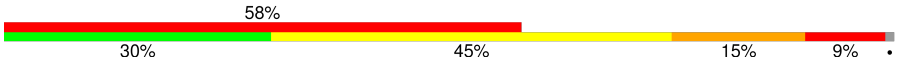
Chain H:

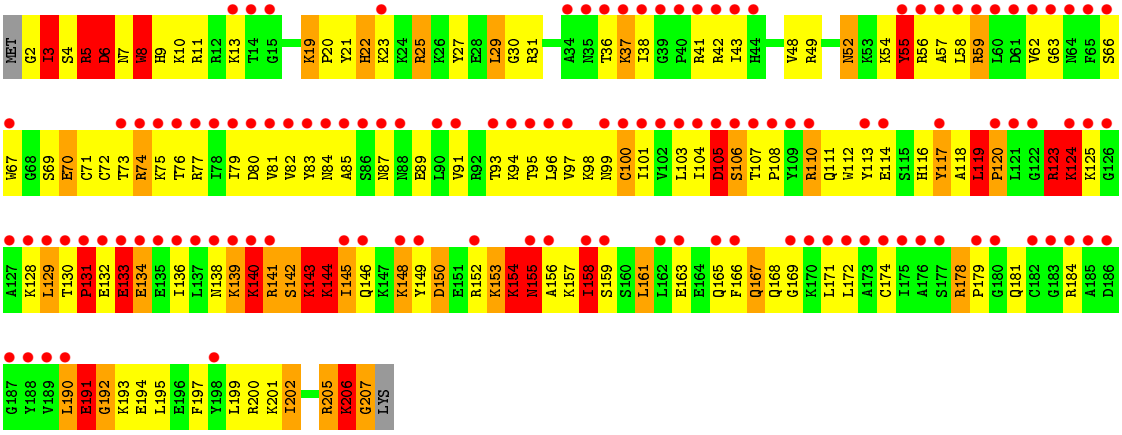




• Molecule 9: 40S Ribosomal Protein S8

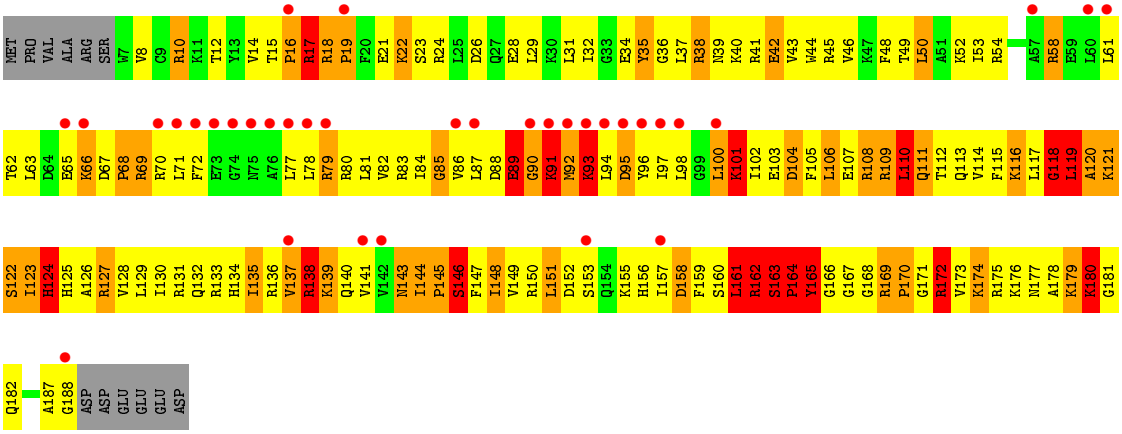
Chain I:



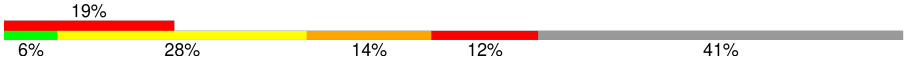
• Molecule 10: 40S Ribosomal Protein S9

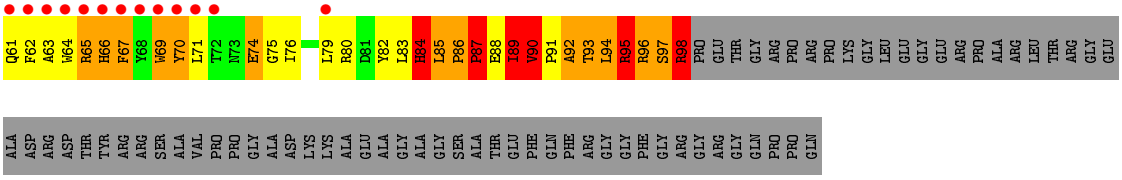
Chain J:



• Molecule 11: 40S Ribosomal Protein S10

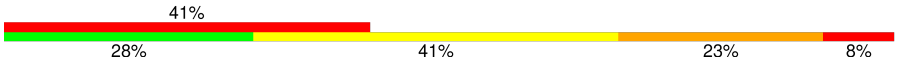
Chain K:

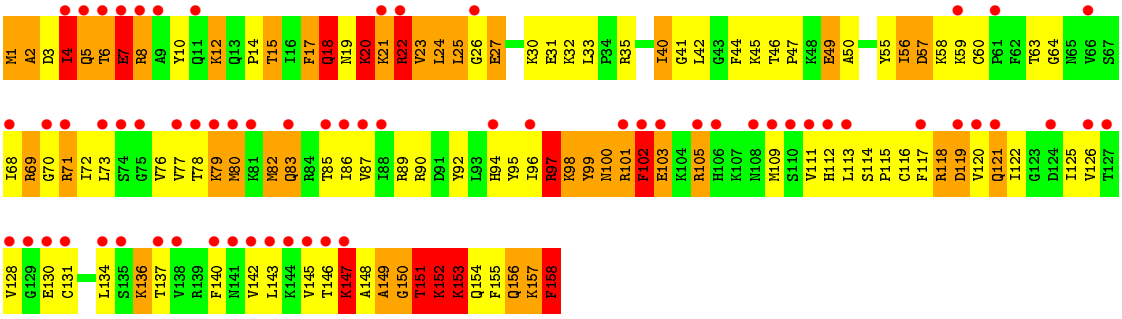




• Molecule 12: 40S Ribosomal Protein S11

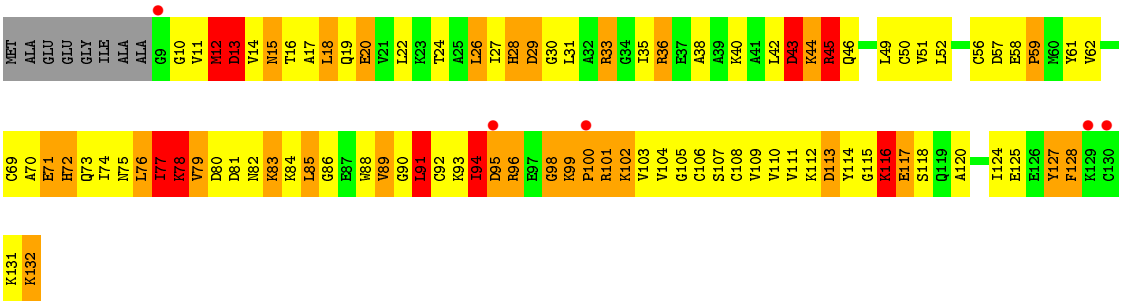
Chain L:



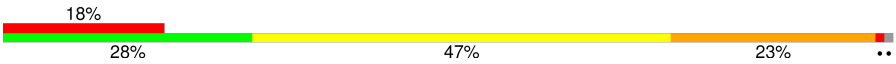
• Molecule 13: 40S Ribosomal Protein S12

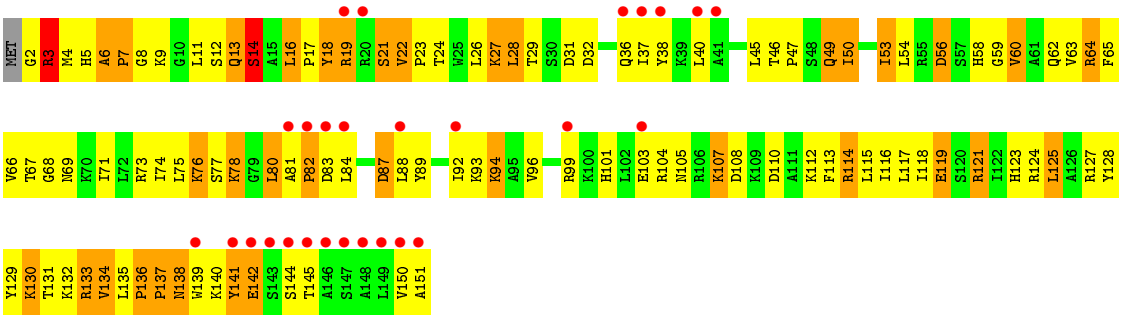
Chain M:



• Molecule 14: 40S Ribosomal Protein S13

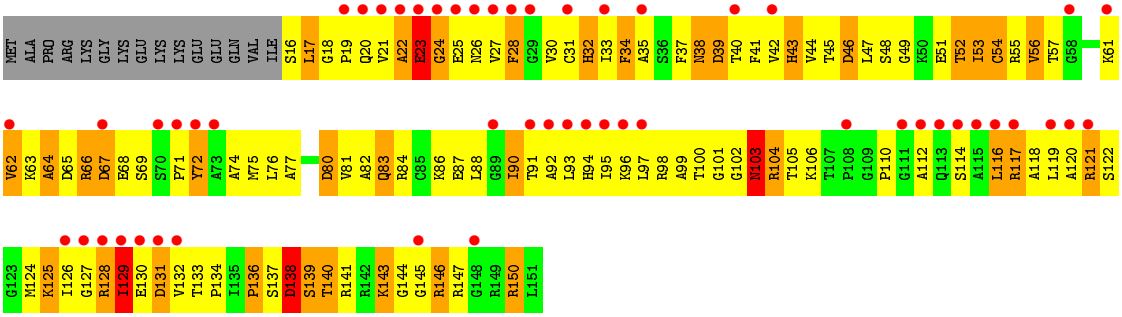
Chain N:



• Molecule 15: 40S Ribosomal Protein S14

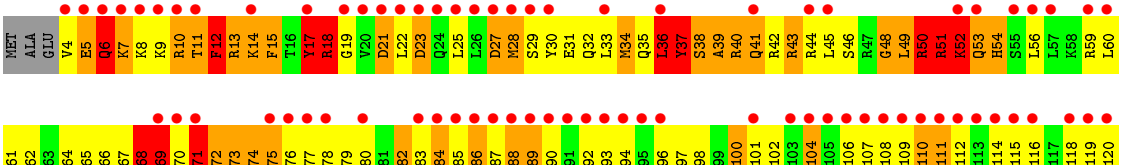
Chain O:

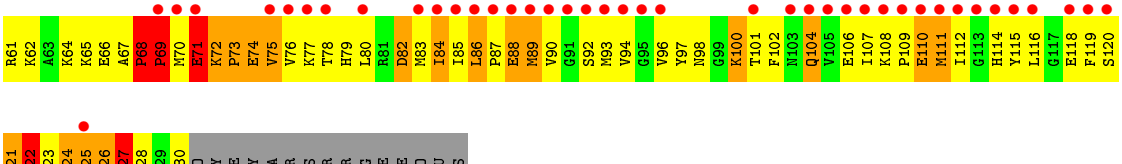


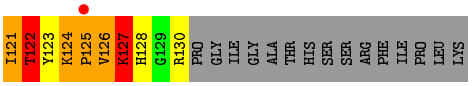


• Molecule 16: 40S Ribosomal Protein S15

Chain P:

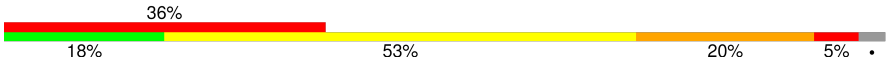


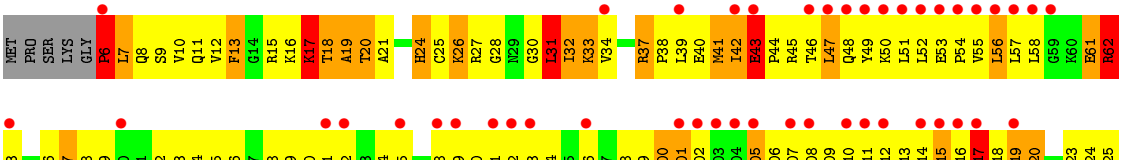


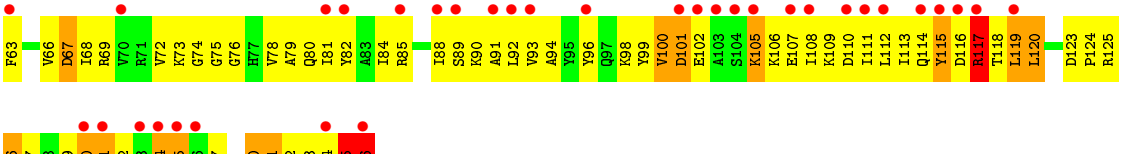


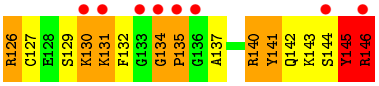
• Molecule 17: 40S Ribosomal Protein S16

Chain Q:



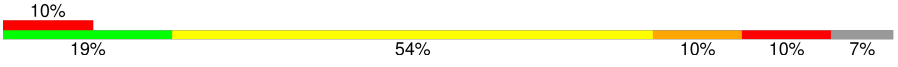



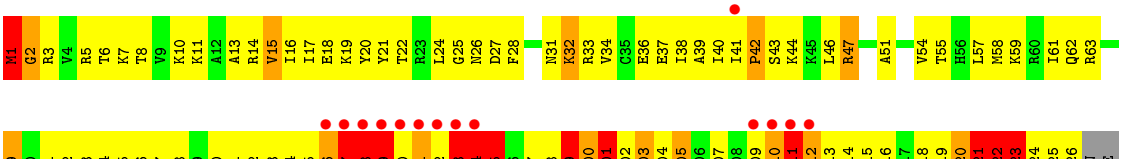


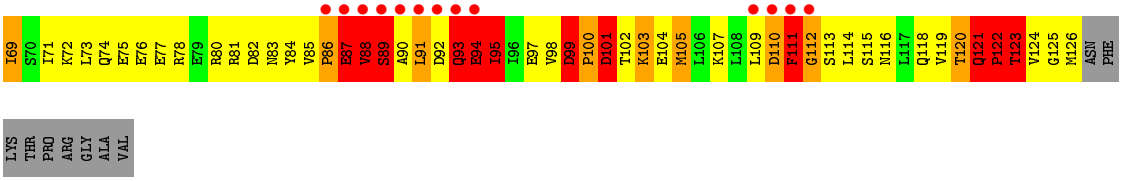


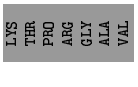
• Molecule 18: 40S Ribosomal Protein S17

Chain R:



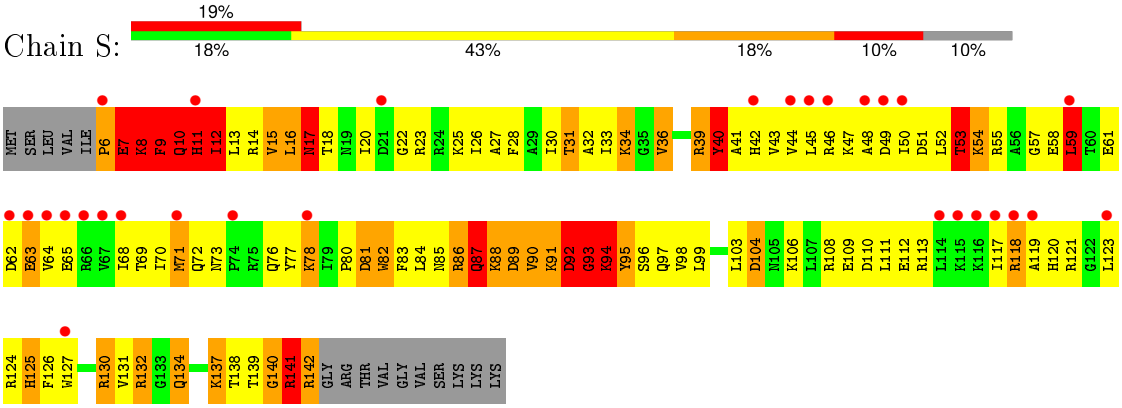







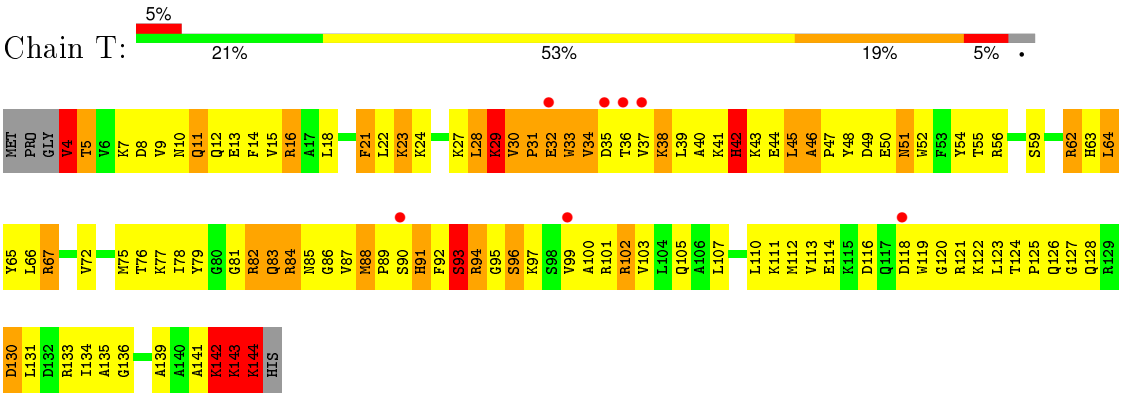
- Molecule 19: 40S Ribosomal Protein S18

Chain S:



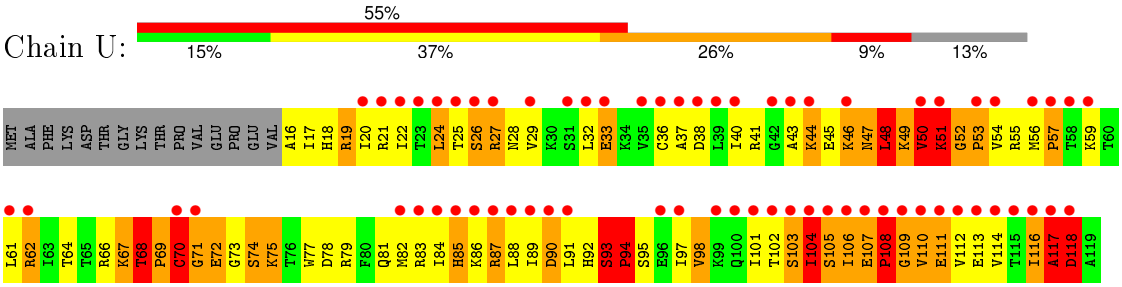

- Molecule 20: 40S Ribosomal Protein S19

Chain T:



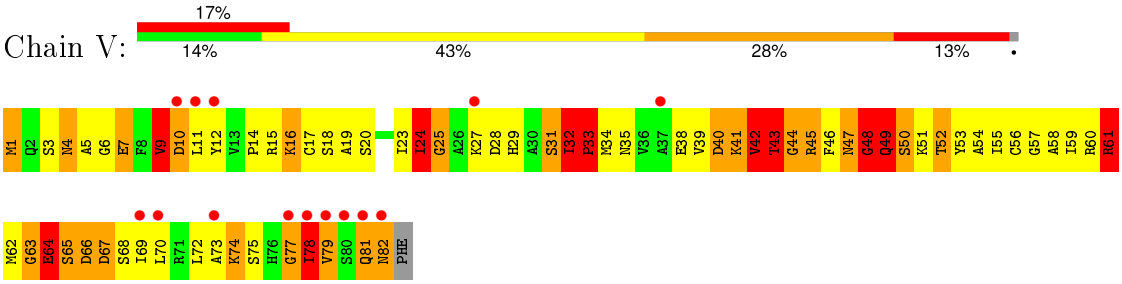

- Molecule 21: 40S Ribosomal Protein S20

Chain U:



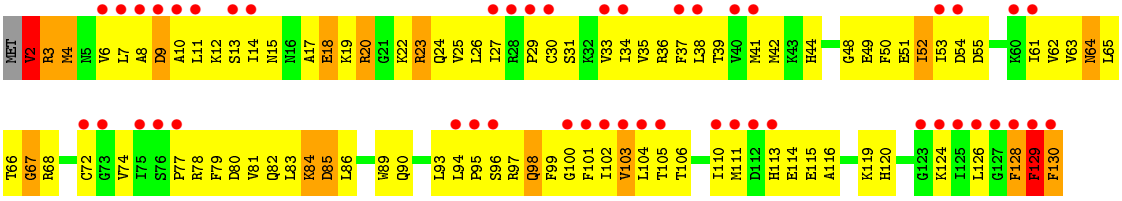

- Molecule 22: 40S Ribosomal Protein S21

Chain V:




- Molecule 23: 40S Ribosomal Protein S15A

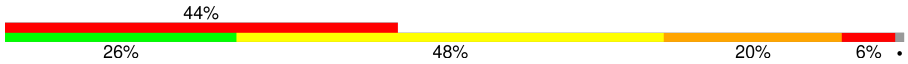
Chain W:

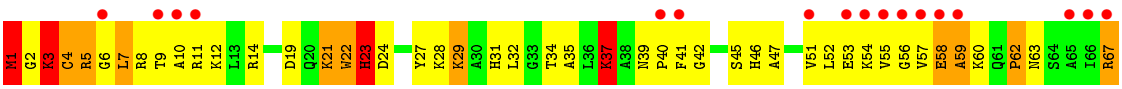


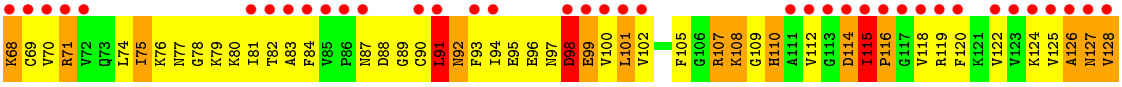


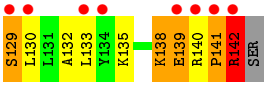
• Molecule 24: 40S Ribosomal Protein S23

Chain X:



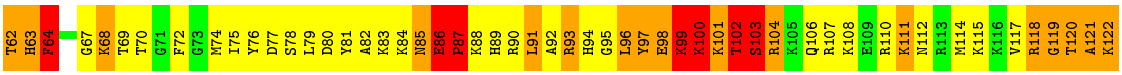







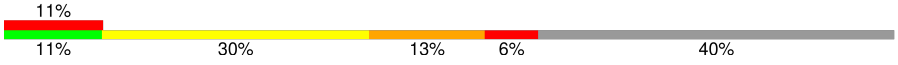
• Molecule 25: 40S Ribosomal Protein S24

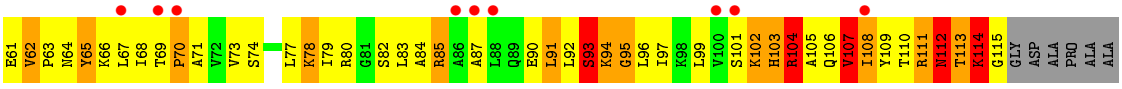
Chain Y:



• Molecule 26: 40S Ribosomal Protein S25

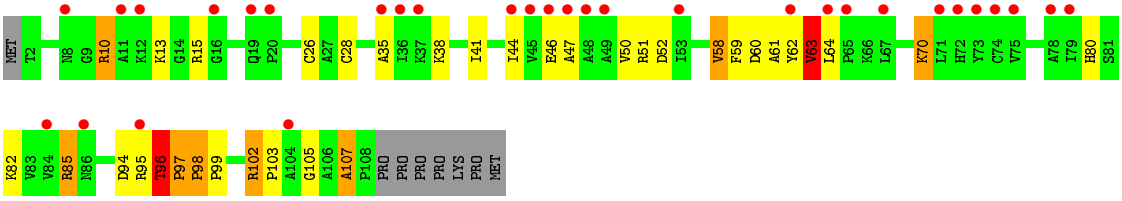
Chain Z:





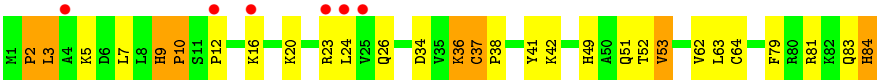
• Molecule 27: 40S Ribosomal Protein S26

Chain a:



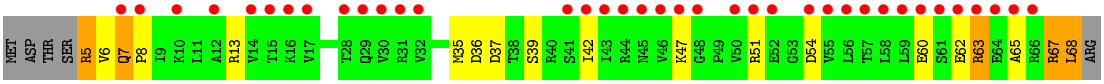
- Molecule 28: 40S Ribosomal Protein S27

Chain b:



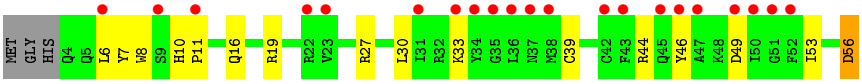
- Molecule 29: 40S Ribosomal Protein S28

Chain c:



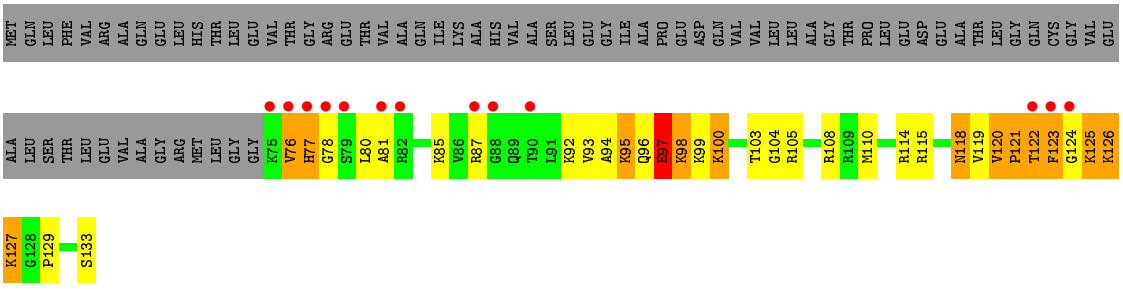
- Molecule 30: 40S Ribosomal Protein S29

Chain d:



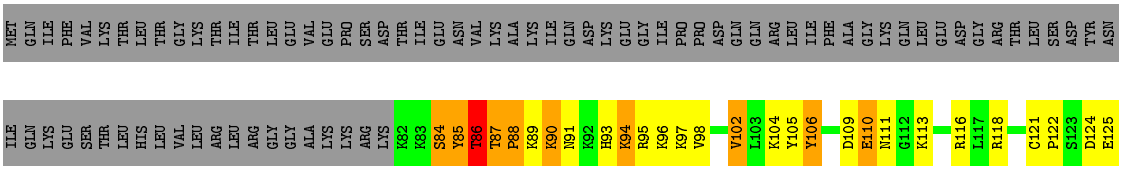
- Molecule 31: 40S Ribosomal Protein S30

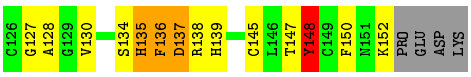
Chain e:



- Molecule 32: 40S Ribosomal Protein S27A

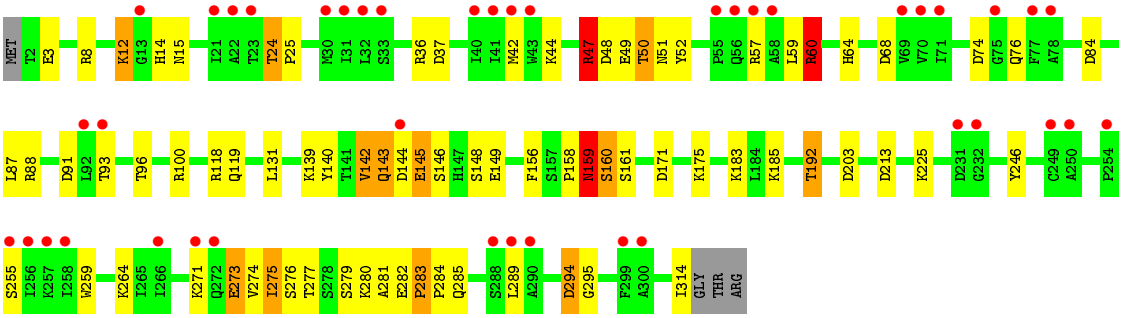
Chain f:





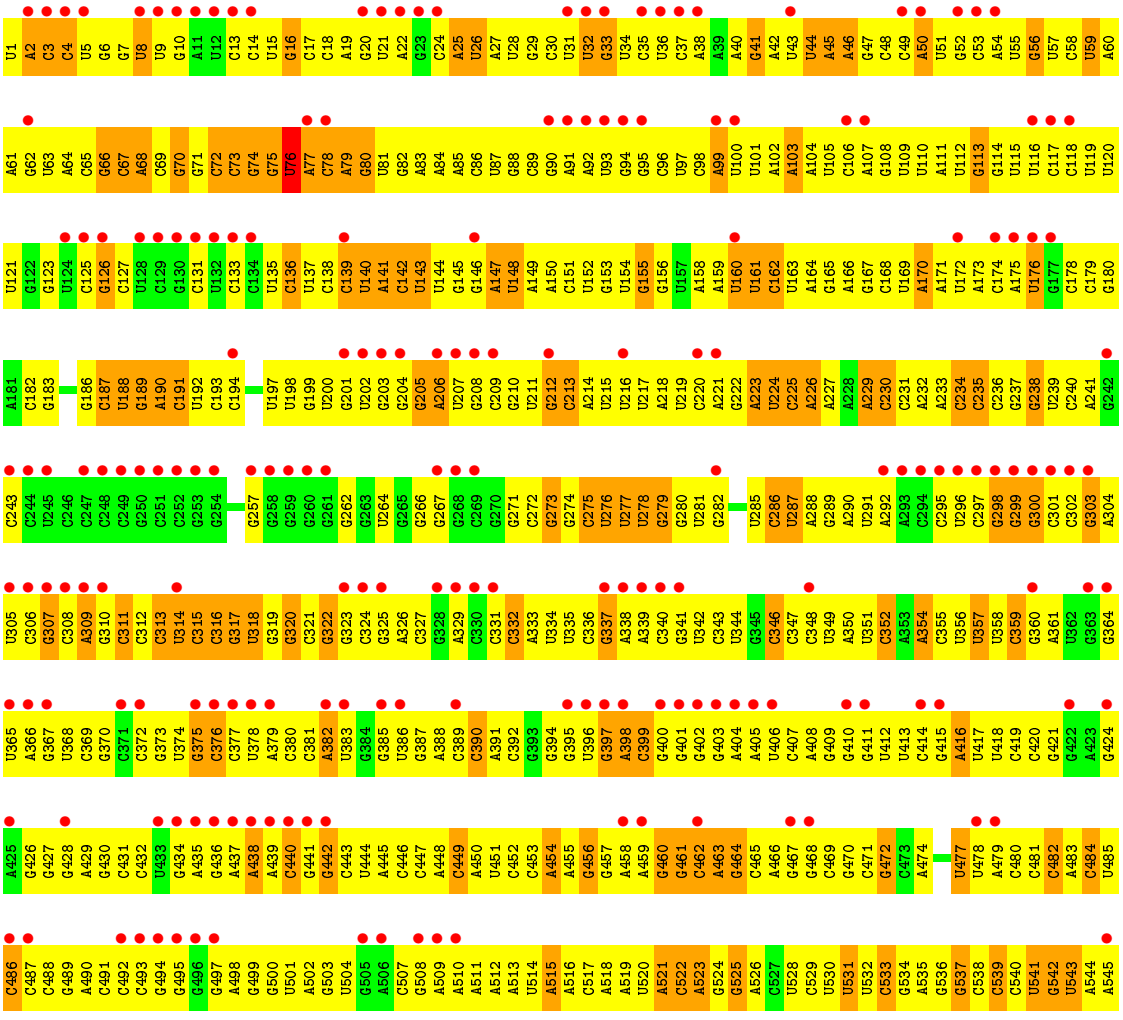

- Molecule 33: 40S Ribosomal Protein RACK1

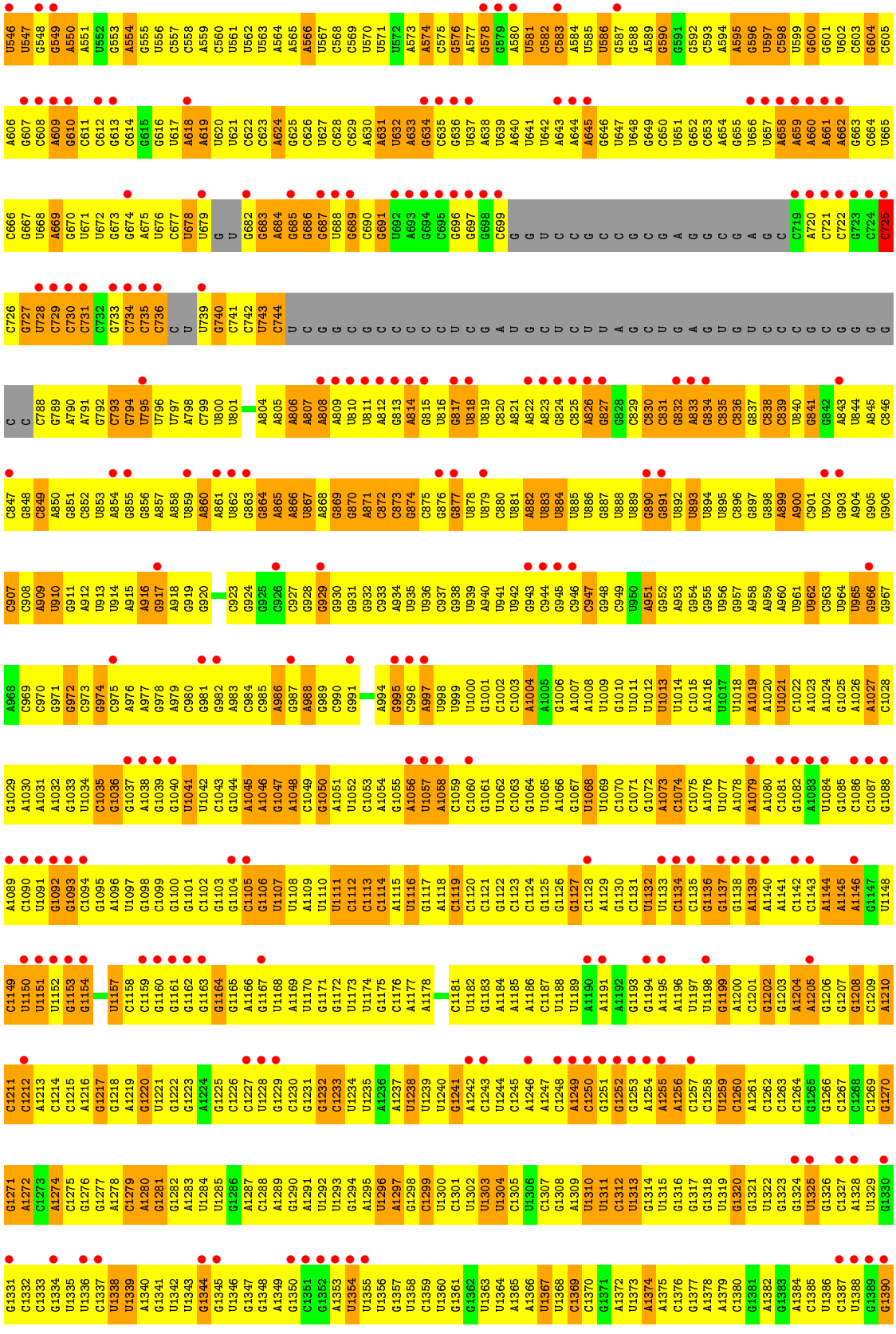
Chain g:

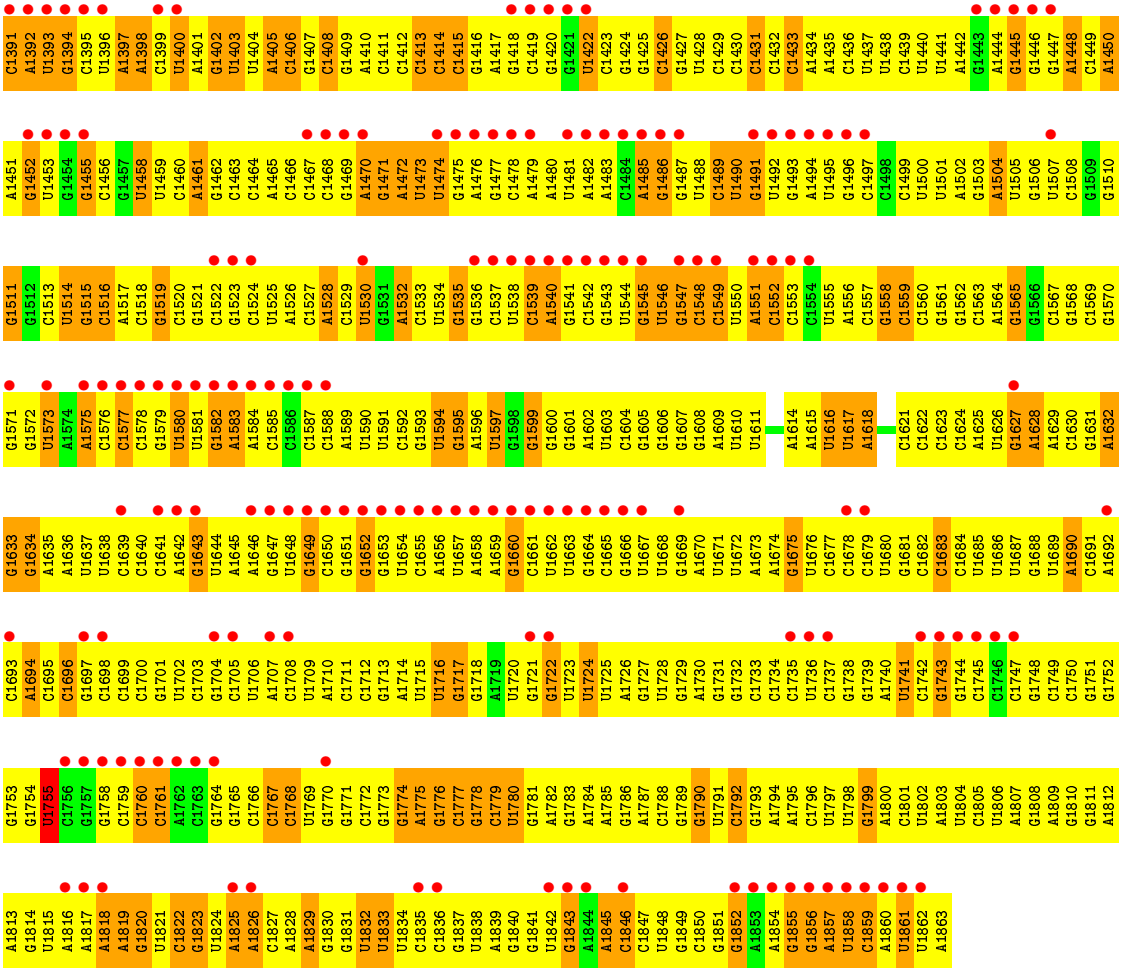



- Molecule 34: 18S Ribosomal RNA

Chain i:

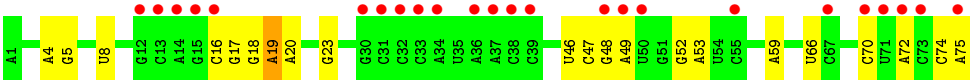






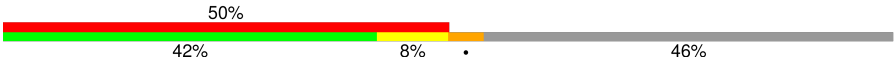
- Molecule 35: initiator Met-RNA-i

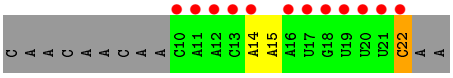
Chain j:



- Molecule 36: mRNA

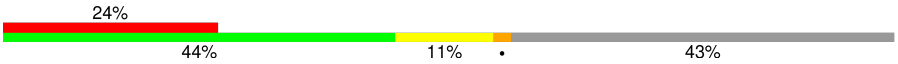
Chain k:

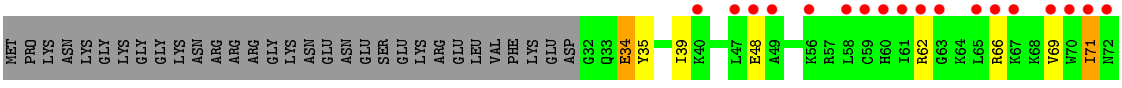


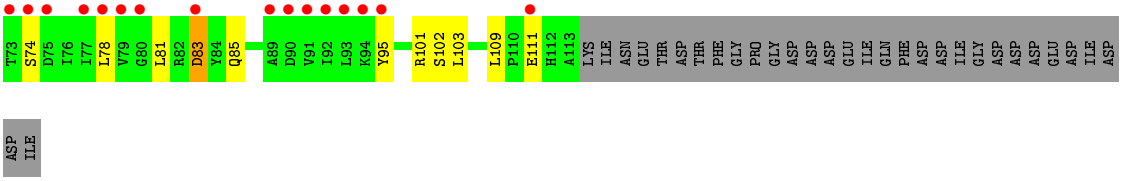



- Molecule 37: human initiation factor eIF1A

Chain n:




T73 S74 D75 I76 I77 L78 V79 G80 L81 R82 D83 Y84 Q85 A89 D90 V91 I92 L93 K94 Y95 R101 S102 L103 L109 P110 E111 H112 A113 LYS ILE ASN GLU THR ASP THR PHE GLY PRO GLY ASP ASP ASP GLU ILE GLN PHE ASP ASP ILE GLY ASP ASP ASP GLU ASP ILE ASP
ASP ILE

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 31 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 297.75Å 297.75Å 485.16Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 77.53 – 7.03<br>77.53 – 7.03 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.3 (77.53-7.03)<br>98.7 (77.53-7.03) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.98 (at 6.72Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.3_928) | Depositor |
| R, $R_{free}$ | 0.345 , 0.359<br>0.332 , 0.339 | Depositor<br>DCC |
| $R_{free}$ test set | 1942 reflections (5.02%) | DCC |
| Wilson B-factor (Å$^2$) | 566.4 | Xtriage |
| Anisotropy | 0.159 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.22 , 127.2 | EDS |
| Estimated twinning fraction | 0.055 for -h,-k,l | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.39$, $< L^2 > = 0.22$ | Xtriage |
| Outliers | 0 of 38850 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.86 | EDS |
| Total number of atoms | 79048 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 179.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.76 | 2/1679 (0.1%) | 1.06 | 17/2283 (0.7%) |
| 2 | B | 0.79 | 7/1769 (0.4%) | 1.08 | 22/2367 (0.9%) |
| 3 | C | 0.97 | 7/1778 (0.4%) | 1.19 | 18/2399 (0.8%) |
| 4 | D | 1.03 | 6/1792 (0.3%) | 1.30 | 22/2412 (0.9%) |
| 5 | E | 0.76 | 5/2125 (0.2%) | 0.98 | 23/2856 (0.8%) |
| 6 | F | 0.99 | 5/1531 (0.3%) | 1.21 | 17/2059 (0.8%) |
| 7 | G | 0.97 | 15/1946 (0.8%) | 1.23 | 25/2590 (1.0%) |
| 8 | H | 1.09 | 7/1553 (0.5%) | 2.19 | 29/2079 (1.4%) |
| 9 | I | 1.11 | 7/1708 (0.4%) | 1.51 | 33/2278 (1.4%) |
| 10 | J | 1.27 | 19/1522 (1.2%) | 1.51 | 42/2031 (2.1%) |
| 11 | K | 1.21 | 6/851 (0.7%) | 1.78 | 31/1147 (2.7%) |
| 12 | L | 1.10 | 6/1319 (0.5%) | 1.40 | 17/1761 (1.0%) |
| 13 | M | 1.00 | 3/960 (0.3%) | 1.23 | 7/1287 (0.5%) |
| 14 | N | 0.83 | 4/1232 (0.3%) | 1.01 | 12/1656 (0.7%) |
| 15 | O | 0.61 | 0/1029 | 1.05 | 12/1380 (0.9%) |
| 16 | P | 0.75 | 1/1079 (0.1%) | 1.43 | 32/1437 (2.2%) |
| 17 | Q | 0.71 | 3/1142 (0.3%) | 1.11 | 15/1528 (1.0%) |
| 18 | R | 1.23 | 10/1031 (1.0%) | 1.64 | 30/1383 (2.2%) |
| 19 | S | 1.21 | 10/1157 (0.9%) | 1.61 | 36/1548 (2.3%) |
| 20 | T | 0.95 | 3/1132 (0.3%) | 1.26 | 13/1517 (0.9%) |
| 21 | U | 0.96 | 1/832 (0.1%) | 1.59 | 29/1117 (2.6%) |
| 22 | V | 0.75 | 1/626 (0.2%) | 1.39 | 15/839 (1.8%) |
| 23 | W | 0.85 | 4/1051 (0.4%) | 0.86 | 9/1406 (0.6%) |
| 24 | X | 1.00 | 8/1124 (0.7%) | 1.24 | 21/1500 (1.4%) |
| 25 | Y | 0.93 | 3/1038 (0.3%) | 1.42 | 21/1380 (1.5%) |
| 26 | Z | 1.04 | 5/604 (0.8%) | 1.35 | 17/810 (2.1%) |
| 27 | a | 0.89 | 4/860 (0.5%) | 1.60 | 21/1156 (1.8%) |
| 28 | b | 1.02 | 2/673 (0.3%) | 1.36 | 12/902 (1.3%) |
| 29 | c | 0.80 | 1/508 (0.2%) | 1.18 | 8/680 (1.2%) |
| 30 | d | 0.90 | 2/455 (0.4%) | 0.79 | 3/603 (0.5%) |
| 31 | e | 1.47 | 5/478 (1.0%) | 1.43 | 11/628 (1.8%) |
| 32 | f | 1.10 | 4/593 (0.7%) | 1.49 | 16/786 (2.0%) |
| 33 | g | 0.91 | 1/2493 (0.0%) | 1.29 | 27/3394 (0.8%) |
| 34 | i | 2.41 | 1848/41879 (4.4%) | 2.21 | 2565/65157 (3.9%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 35 | j | 0.67 | 5/1798 (0.3%) | 0.82 | 0/2802 |
| 36 | k | 1.64 | 1/304 (0.3%) | 1.35 | 3/470 (0.6%) |
| 37 | n | 0.40 | 0/657 | 0.38 | 0/881 |
| All | All | 1.83 | 2021/84308 (2.4%) | 1.84 | 3231/122509 (2.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 11 |
| 2 | B | 0 | 4 |
| 3 | C | 1 | 5 |
| 4 | D | 0 | 5 |
| 5 | E | 1 | 2 |
| 6 | F | 0 | 3 |
| 7 | G | 0 | 1 |
| 8 | H | 0 | 10 |
| 9 | I | 0 | 8 |
| 10 | J | 1 | 11 |
| 11 | K | 0 | 11 |
| 12 | L | 0 | 7 |
| 13 | M | 0 | 1 |
| 14 | N | 0 | 4 |
| 15 | O | 0 | 1 |
| 16 | P | 0 | 10 |
| 17 | Q | 0 | 4 |
| 18 | R | 1 | 5 |
| 19 | S | 1 | 10 |
| 20 | T | 1 | 6 |
| 21 | U | 0 | 8 |
| 22 | V | 0 | 9 |
| 23 | W | 0 | 2 |
| 24 | X | 0 | 4 |
| 25 | Y | 1 | 6 |
| 26 | Z | 0 | 6 |
| 27 | a | 0 | 2 |
| 28 | b | 0 | 3 |
| 31 | e | 0 | 5 |
| 32 | f | 0 | 6 |
| 33 | g | 0 | 13 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 34 | i | 6 | 0 |
| All | All | 13 | 183 |

The worst 5 of 2021 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 36 | k | 22 | C | C1'-N1 | 28.08 | 1.90 | 1.48 |
| 34 | i | 1322 | U | C2'-C1' | -25.56 | 1.25 | 1.53 |
| 34 | i | 66 | G | C2'-C1' | -24.65 | 1.26 | 1.53 |
| 34 | i | 652 | G | C2'-C1' | -23.81 | 1.27 | 1.53 |
| 34 | i | 858 | A | C2'-C1' | -23.76 | 1.27 | 1.53 |

The worst 5 of 3231 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | H | 109 | ARG | NE-CZ-NH2 | -53.45 | 93.58 | 120.30 |
| 8 | H | 109 | ARG | NE-CZ-NH1 | 42.58 | 141.59 | 120.30 |
| 34 | i | 1774 | G | P-O3'-C3' | 38.31 | 165.68 | 119.70 |
| 34 | i | 1114 | C | O4'-C1'-N1 | 35.28 | 136.42 | 108.20 |
| 34 | i | 582 | C | O4'-C1'-N1 | 32.53 | 134.22 | 108.20 |

5 of 13 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 3 | C | 157 | ASN | CA |
| 5 | E | 171 | ASP | CA |
| 10 | J | 138 | ARG | CA |
| 18 | R | 3 | ARG | CA |
| 19 | S | 92 | ASP | CA |

5 of 183 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 146 | ALA | Mainchain |
| 1 | A | 23 | THR | Mainchain |
| 1 | A | 4 | ALA | Peptide |
| 1 | A | 63 | ARG | Sidechain |
| 1 | A | 97 | THR | Mainchain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1642 | 0 | 1638 | 603 | 0 |
| 2 | B | 1741 | 0 | 1808 | 523 | 0 |
| 3 | C | 1742 | 0 | 1829 | 582 | 0 |
| 4 | D | 1764 | 0 | 1855 | 595 | 0 |
| 5 | E | 2083 | 0 | 2189 | 523 | 0 |
| 6 | F | 1509 | 0 | 1556 | 476 | 0 |
| 7 | G | 1923 | 0 | 2086 | 499 | 3 |
| 8 | H | 1530 | 0 | 1624 | 476 | 0 |
| 9 | I | 1679 | 0 | 1762 | 431 | 3 |
| 10 | J | 1498 | 0 | 1598 | 537 | 0 |
| 11 | K | 827 | 0 | 853 | 351 | 18 |
| 12 | L | 1296 | 0 | 1370 | 397 | 0 |
| 13 | M | 950 | 0 | 969 | 245 | 0 |
| 14 | N | 1208 | 0 | 1294 | 261 | 0 |
| 15 | O | 1016 | 0 | 1037 | 293 | 0 |
| 16 | P | 1060 | 0 | 1120 | 483 | 0 |
| 17 | Q | 1124 | 0 | 1189 | 439 | 0 |
| 18 | R | 1019 | 0 | 1067 | 349 | 0 |
| 19 | S | 1139 | 0 | 1188 | 427 | 1 |
| 20 | T | 1112 | 0 | 1149 | 393 | 0 |
| 21 | U | 822 | 0 | 886 | 208 | 0 |
| 22 | V | 619 | 0 | 620 | 278 | 0 |
| 23 | W | 1034 | 0 | 1079 | 262 | 0 |
| 24 | X | 1106 | 0 | 1177 | 310 | 0 |
| 25 | Y | 1021 | 0 | 1083 | 490 | 0 |
| 26 | Z | 598 | 0 | 652 | 210 | 0 |
| 27 | a | 844 | 0 | 895 | 0 | 0 |
| 28 | b | 659 | 0 | 680 | 0 | 0 |
| 29 | c | 506 | 0 | 534 | 0 | 0 |
| 30 | d | 445 | 0 | 441 | 0 | 0 |
| 31 | e | 473 | 0 | 519 | 0 | 31 |
| 32 | f | 581 | 0 | 598 | 0 | 0 |
| 33 | g | 2436 | 0 | 2388 | 0 | 0 |
| 34 | i | 37514 | 0 | 18808 | 0 | 78 |
| 35 | j | 1607 | 0 | 811 | 0 | 0 |
| 36 | k | 273 | 0 | 139 | 0 | 0 |
| 37 | n | 648 | 0 | 642 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 79048 | 0 | 61133 | 9794 | 81 |

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 94.

The worst 5 of 9794 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:197:LYS:HA | 3:C:200:LEU:CD2 | 1.22 | 1.68 |
| 9:I:141:ARG:CB | 9:I:144:LYS:HB2 | 1.24 | 1.68 |
| 17:Q:135:PRO:HD3 | 17:Q:141:TYR:CE1 | 1.15 | 1.66 |
| 11:K:16:PHE:CE2 | 11:K:79:LEU:HB2 | 1.24 | 1.65 |
| 16:P:41:GLN:CG | 16:P:84:ILE:HG21 | 1.18 | 1.64 |

The worst 5 of 81 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) |
|---|---|---|---|
| 31:e:123:PHE:CD1 | 34:i:1759:C:C4'[3_564] | 0.62 | 1.58 |
| 31:e:123:PHE:CE1 | 34:i:1759:C:C5'[3_564] | 0.70 | 1.50 |
| 34:i:531:U:O2' | 34:i:1767:C:O4'[3_564] | 0.72 | 1.48 |
| 31:e:125:LYS:CE | 34:i:1761:C:OP1[3_564] | 0.73 | 1.47 |
| 11:K:97:SER:O | 34:i:76:U:OP1[3_564] | 0.95 | 1.25 |

## 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 |
|---|---|---|---|---|---|---|
| 1 | A | 206/295 (70%) | 156 (76%) | 23 (11%) | 27 (13%) | 0 7 |
| 2 | B | 213/264 (81%) | 174 (82%) | 24 (11%) | 15 (7%) | 1 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | C | 224/278 (81%) | 199 (89%) | 14 (6%) | 11 (5%) | 3 31 |
| 4 | D | 225/243 (93%) | 180 (80%) | 23 (10%) | 22 (10%) | 1 14 |
| 5 | E | 261/263 (99%) | 210 (80%) | 27 (10%) | 24 (9%) | 1 16 |
| 6 | F | 189/204 (93%) | 162 (86%) | 15 (8%) | 12 (6%) | 2 25 |
| 7 | G | 235/249 (94%) | 201 (86%) | 19 (8%) | 15 (6%) | 2 25 |
| 8 | H | 188/194 (97%) | 146 (78%) | 11 (6%) | 31 (16%) | 0 5 |
| 9 | I | 204/208 (98%) | 169 (83%) | 13 (6%) | 22 (11%) | 0 11 |
| 10 | J | 180/194 (93%) | 138 (77%) | 18 (10%) | 24 (13%) | 0 7 |
| 11 | K | 96/165 (58%) | 67 (70%) | 11 (12%) | 18 (19%) | 0 3 |
| 12 | L | 156/158 (99%) | 132 (85%) | 10 (6%) | 14 (9%) | 1 17 |
| 13 | M | 122/132 (92%) | 85 (70%) | 16 (13%) | 21 (17%) | 0 4 |
| 14 | N | 148/151 (98%) | 123 (83%) | 19 (13%) | 6 (4%) | 3 35 |
| 15 | O | 134/151 (89%) | 101 (75%) | 14 (10%) | 19 (14%) | 0 6 |
| 16 | P | 125/145 (86%) | 92 (74%) | 16 (13%) | 17 (14%) | 0 6 |
| 17 | Q | 139/146 (95%) | 110 (79%) | 19 (14%) | 10 (7%) | 1 22 |
| 18 | R | 124/135 (92%) | 97 (78%) | 13 (10%) | 14 (11%) | 0 10 |
| 19 | S | 135/152 (89%) | 106 (78%) | 20 (15%) | 9 (7%) | 1 24 |
| 20 | T | 139/145 (96%) | 119 (86%) | 10 (7%) | 10 (7%) | 1 22 |
| 21 | U | 102/119 (86%) | 76 (74%) | 10 (10%) | 16 (16%) | 0 5 |
| 22 | V | 80/83 (96%) | 55 (69%) | 11 (14%) | 14 (18%) | 0 4 |
| 23 | W | 127/130 (98%) | 111 (87%) | 14 (11%) | 2 (2%) | 12 56 |
| 24 | X | 140/143 (98%) | 121 (86%) | 11 (8%) | 8 (6%) | 2 27 |
| 25 | Y | 124/133 (93%) | 91 (73%) | 15 (12%) | 18 (14%) | 0 6 |
| 26 | Z | 73/125 (58%) | 52 (71%) | 12 (16%) | 9 (12%) | 0 8 |
| 27 | a | 105/115 (91%) | 72 (69%) | 14 (13%) | 19 (18%) | 0 4 |
| 28 | b | 82/84 (98%) | 57 (70%) | 14 (17%) | 11 (13%) | 0 7 |
| 29 | c | 62/69 (90%) | 44 (71%) | 13 (21%) | 5 (8%) | 1 19 |
| 30 | d | 51/56 (91%) | 46 (90%) | 3 (6%) | 2 (4%) | 4 36 |
| 31 | e | 57/133 (43%) | 37 (65%) | 7 (12%) | 13 (23%) | 0 2 |
| 32 | f | 69/156 (44%) | 38 (55%) | 13 (19%) | 18 (26%) | 0 1 |
| 33 | g | 311/317 (98%) | 271 (87%) | 23 (7%) | 17 (6%) | 2 29 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 37 | n | 80/144 (56%) | 61 (76%) | 15 (19%) | 4 (5%) | 3 31 |
| All | All | 4906/5679 (86%) | 3899 (80%) | 510 (10%) | 497 (10%) | 1 14 |

5 of 497 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 9 | GLN |
| 1 | A | 31 | ASP |
| 1 | A | 45 | GLY |
| 1 | A | 103 | PHE |
| 1 | A | 164 | ASN |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 |
|---|---|---|---|---|---|
| 1 | A | 174/244 (71%) | 139 (80%) | 35 (20%) | 1 11 |
| 2 | B | 196/231 (85%) | 155 (79%) | 41 (21%) | 1 10 |
| 3 | C | 187/215 (87%) | 147 (79%) | 40 (21%) | 1 9 |
| 4 | D | 190/202 (94%) | 144 (76%) | 46 (24%) | 1 6 |
| 5 | E | 225/225 (100%) | 173 (77%) | 52 (23%) | 1 7 |
| 6 | F | 161/170 (95%) | 116 (72%) | 45 (28%) | 0 4 |
| 7 | G | 207/218 (95%) | 157 (76%) | 50 (24%) | 1 6 |
| 8 | H | 170/174 (98%) | 124 (73%) | 46 (27%) | 0 4 |
| 9 | I | 177/179 (99%) | 142 (80%) | 35 (20%) | 1 12 |
| 10 | J | 157/168 (94%) | 128 (82%) | 29 (18%) | 2 14 |
| 11 | K | 89/136 (65%) | 61 (68%) | 28 (32%) | 0 2 |
| 12 | L | 142/142 (100%) | 105 (74%) | 37 (26%) | 0 5 |
| 13 | M | 101/108 (94%) | 78 (77%) | 23 (23%) | 1 8 |
| 14 | N | 130/131 (99%) | 103 (79%) | 27 (21%) | 1 10 |
| 15 | O | 106/119 (89%) | 87 (82%) | 19 (18%) | 2 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 16 | P | 116/130 (89%) | 84 (72%) | 32 (28%) | 0 4 |
| 17 | Q | 117/121 (97%) | 89 (76%) | 28 (24%) | 1 7 |
| 18 | R | 114/121 (94%) | 90 (79%) | 24 (21%) | 1 9 |
| 19 | S | 119/132 (90%) | 95 (80%) | 24 (20%) | 1 11 |
| 20 | T | 113/116 (97%) | 87 (77%) | 26 (23%) | 1 7 |
| 21 | U | 94/107 (88%) | 74 (79%) | 20 (21%) | 1 9 |
| 22 | V | 67/68 (98%) | 50 (75%) | 17 (25%) | 1 6 |
| 23 | W | 112/113 (99%) | 98 (88%) | 14 (12%) | 6 30 |
| 24 | X | 114/115 (99%) | 91 (80%) | 23 (20%) | 1 11 |
| 25 | Y | 108/115 (94%) | 85 (79%) | 23 (21%) | 1 9 |
| 26 | Z | 66/103 (64%) | 53 (80%) | 13 (20%) | 1 12 |
| 27 | a | 91/99 (92%) | 76 (84%) | 15 (16%) | 3 19 |
| 28 | b | 76/76 (100%) | 63 (83%) | 13 (17%) | 2 17 |
| 29 | c | 57/62 (92%) | 46 (81%) | 11 (19%) | 2 13 |
| 30 | d | 47/49 (96%) | 35 (74%) | 12 (26%) | 1 6 |
| 31 | e | 49/106 (46%) | 26 (53%) | 23 (47%) | 0 0 |
| 32 | f | 64/140 (46%) | 43 (67%) | 21 (33%) | 0 2 |
| 33 | g | 272/275 (99%) | 224 (82%) | 48 (18%) | 2 16 |
| 37 | n | 66/123 (54%) | 48 (73%) | 18 (27%) | 0 4 |
| All | All | 4274/4833 (88%) | 3316 (78%) | 958 (22%) | 1 9 |

5 of 958 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | K | 53 | LYS |
| 15 | O | 28 | PHE |
| 32 | f | 118 | ARG |
| 11 | K | 98 | ARG |
| 13 | M | 18 | LEU |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | L | 19 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | P | 41 | GLN |
| 33 | g | 20 | GLN |
| 12 | L | 121 | GLN |
| 13 | M | 82 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 34 | i | 1720/1863 (92%) | 496 (28%) | 0 |
| 35 | j | 74/75 (98%) | 17 (22%) | 0 |
| 36 | k | 12/24 (50%) | 3 (25%) | 0 |
| All | All | 1806/1962 (92%) | 516 (28%) | 0 |

5 of 516 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | i | 2 | A |
| 34 | i | 3 | C |
| 34 | i | 4 | C |
| 34 | i | 8 | U |
| 34 | i | 16 | G |

There are no RNA pucker outliers to report.

## 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)

There are no ligands in this entry.

## 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.

# 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 | A | 208/295 (70%) | 0.85 | 43 (20%) 1 7 | 188, 273, 325, 347 | 0 |
| 2 | B | 215/264 (81%) | 1.54 | 78 (36%) 0 4 | 140, 249, 309, 321 | 0 |
| 3 | C | 226/278 (81%) | 2.95 | 112 (49%) 0 4 | 76, 163, 267, 285 | 0 |
| 4 | D | 227/243 (93%) | 5.03 | 166 (73%) 0 2 | 110, 175, 253, 280 | 0 |
| 5 | E | 263/263 (100%) | 2.81 | 139 (52%) 0 3 | 38, 138, 196, 225 | 0 |
| 6 | F | 191/204 (93%) | 5.32 | 154 (80%) 0 2 | 133, 175, 212, 224 | 0 |
| 7 | G | 237/249 (95%) | 1.52 | 76 (32%) 1 5 | 68, 198, 289, 311 | 0 |
| 8 | H | 190/194 (97%) | 0.13 | 24 (12%) 5 11 | 129, 278, 329, 340 | 0 |
| 9 | I | 206/208 (99%) | 3.92 | 121 (58%) 0 3 | 17, 164, 268, 289 | 0 |
| 10 | J | 182/194 (93%) | 0.78 | 35 (19%) 2 7 | 73, 158, 221, 259 | 0 |
| 11 | K | 98/165 (59%) | 1.98 | 31 (31%) 1 5 | 167, 238, 289, 308 | 0 |
| 12 | L | 158/158 (100%) | 1.80 | 65 (41%) 0 4 | 22, 90, 224, 255 | 0 |
| 13 | M | 124/132 (93%) | -0.13 | 5 (4%) 42 40 | 280, 347, 384, 417 | 0 |
| 14 | N | 150/151 (99%) | 0.81 | 27 (18%) 2 7 | 46, 118, 251, 261 | 0 |
| 15 | O | 136/151 (90%) | 2.14 | 52 (38%) 0 4 | 45, 205, 320, 353 | 0 |
| 16 | P | 127/145 (87%) | 3.44 | 75 (59%) 0 3 | 163, 254, 297, 310 | 0 |
| 17 | Q | 141/146 (96%) | 2.01 | 53 (37%) 0 4 | 108, 200, 225, 231 | 0 |
| 18 | R | 126/135 (93%) | 0.12 | 14 (11%) 7 12 | 130, 194, 302, 306 | 0 |
| 19 | S | 137/152 (90%) | 1.02 | 29 (21%) 1 6 | 151, 218, 239, 249 | 0 |
| 20 | T | 141/145 (97%) | 0.15 | 7 (4%) 32 32 | 161, 214, 230, 234 | 0 |
| 21 | U | 104/119 (87%) | 4.20 | 66 (63%) 0 3 | 116, 213, 258, 269 | 0 |
| 22 | V | 82/83 (98%) | 0.73 | 14 (17%) 2 8 | 175, 237, 316, 328 | 0 |
| 23 | W | 129/130 (99%) | 1.83 | 48 (37%) 0 4 | 75, 141, 196, 216 | 0 |
| 24 | X | 142/143 (99%) | 2.57 | 63 (44%) 0 4 | 22, 54, 84, 93 | 0 |

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*Continued from previous page...*

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 25 | Y | 126/133 (94%) | 0.32 | 10 (7%) 15 19 | 85, 153, 198, 218 | 0 |
| 26 | Z | 75/125 (60%) | 0.90 | 14 (18%) 2 7 | 197, 207, 217, 225 | 0 |
| 27 | a | 107/115 (93%) | 1.68 | 31 (28%) 1 5 | 55, 111, 285, 317 | 0 |
| 28 | b | 84/84 (100%) | 0.09 | 6 (7%) 19 22 | 156, 236, 276, 286 | 0 |
| 29 | c | 64/69 (92%) | 2.58 | 37 (57%) 0 3 | 125, 173, 216, 221 | 0 |
| 30 | d | 53/56 (94%) | 1.87 | 21 (39%) 0 4 | 136, 159, 235, 256 | 0 |
| 31 | e | 59/133 (44%) | 0.79 | 13 (22%) 1 6 | 63, 136, 177, 192 | 0 |
| 32 | f | 71/156 (45%) | -0.53 | 0 100 100 | 145, 320, 392, 408 | 0 |
| 33 | g | 313/317 (98%) | 0.45 | 42 (13%) 4 10 | 190, 248, 277, 291 | 0 |
| 34 | i | 1797/1863 (96%) | 1.63 | 562 (31%) 1 5 | 13, 142, 348, 527 | 0 |
| 35 | j | 75/75 (100%) | 1.47 | 24 (32%) 1 5 | 308, 379, 421, 436 | 0 |
| 36 | k | 13/24 (54%) | 4.04 | 12 (92%) 0 1 | 186, 317, 324, 325 | 0 |
| 37 | n | 82/144 (56%) | 1.83 | 34 (41%) 0 4 | 212, 216, 222, 224 | 0 |
| All | All | 6859/7641 (89%) | 1.78 | 2303 (33%) 0 4 | 13, 190, 328, 527 | 0 |

The worst 5 of 2303 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | i | 697 | G | 38.6 |
| 34 | i | 698 | G | 35.9 |
| 34 | i | 695 | C | 25.7 |
| 4 | D | 95 | GLY | 25.1 |
| 34 | i | 696 | G | 25.1 |

## 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 carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.