



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:04 am BST

PDB ID : 4V4Z
Title : 70S Thermus thermophilus ribosome functional complex with mRNA and E- and P-site tRNAs at 4.5Å.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 4.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

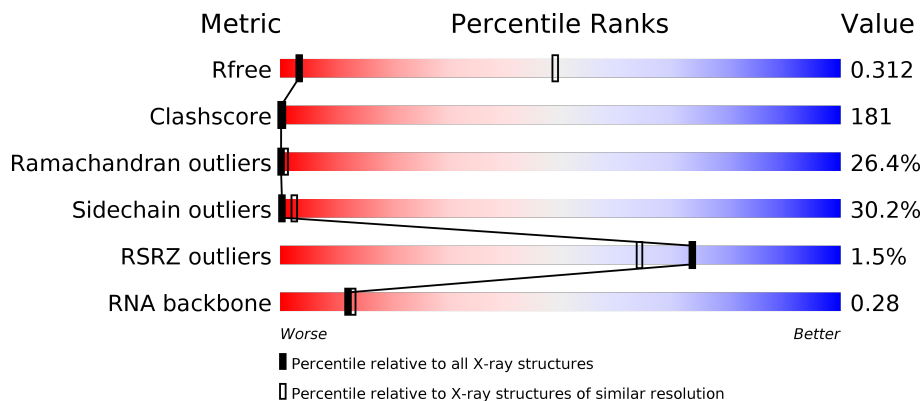
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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} | 130704 | 1056 (5.22-3.80) |
| Clashscore | 141614 | 1124 (5.22-3.80) |
| Ramachandran outliers | 138981 | 1070 (5.22-3.80) |
| Sidechain outliers | 138945 | 1051 (5.22-3.80) |
| RSRZ outliers | 127900 | 1101 (5.30-3.70) |
| RNA backbone | 3102 | 1063 (6.00-3.00) |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AA | 1522 | |
| 2 | AC | 76 | |
| 3 | AD | 76 | |
| 4 | A1 | 27 | |

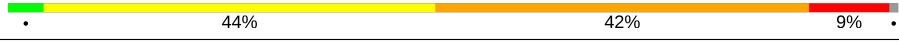

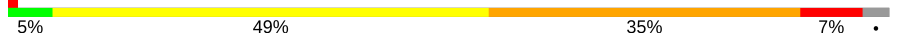
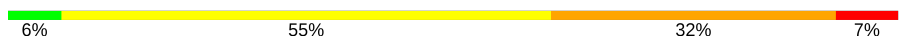








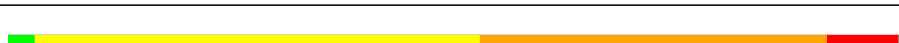
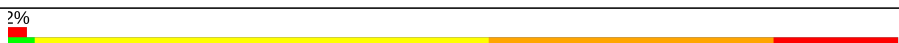
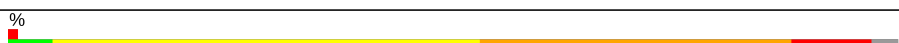

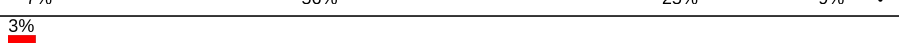
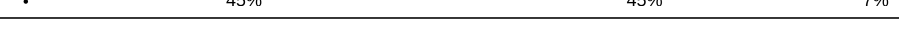
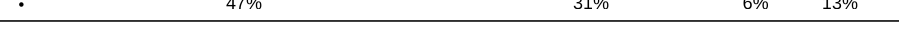

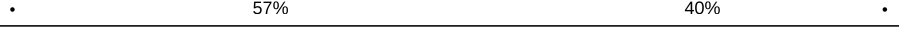
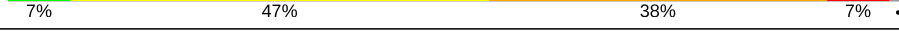


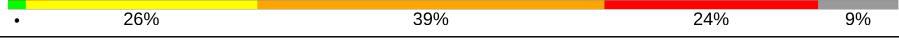
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5 | AE | 256 | |
| 6 | AF | 239 | |
| 7 | AG | 209 | |
| 8 | AH | 162 | |
| 9 | AI | 101 | |
| 10 | AJ | 156 | |
| 11 | AK | 138 | |
| 12 | AL | 128 | |
| 13 | AM | 105 | |
| 14 | AN | 129 | |
| 15 | AO | 132 | |
| 16 | AP | 126 | |
| 17 | AQ | 61 | |
| 18 | AR | 89 | |
| 19 | AS | 88 | |
| 20 | AT | 105 | |
| 21 | AU | 88 | |
| 22 | AV | 93 | |
| 23 | AW | 106 | |
| 24 | AX | 27 | |
| 25 | BA | 2916 | |
| 26 | BB | 123 | |
| 27 | BC | 229 | |
| 28 | BD | 276 | |
| 29 | BE | 206 | |


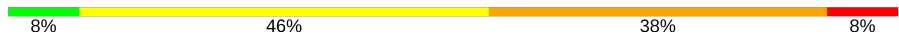
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 30 | BF | 210 |  |
| 31 | BG | 182 |  |
| 32 | BH | 180 |  |
| 33 | BK | 148 |  |
| 34 | BL | 147 |  |
| 35 | BM | 140 |  |
| 36 | BN | 122 |  |
| 37 | BO | 150 |  |
| 38 | BP | 141 |  |
| 39 | BQ | 118 |  |
| 40 | BR | 112 |  |
| 41 | BS | 146 |  |
| 42 | BT | 118 |  |
| 43 | BU | 101 |  |
| 44 | BV | 113 |  |
| 45 | BW | 96 |  |
| 46 | BX | 110 |  |
| 47 | BY | 206 |  |
| 48 | BZ | 85 |  |
| 49 | B1 | 67 |  |
| 50 | B2 | 60 |  |
| 51 | B3 | 71 |  |
| 52 | B4 | 60 |  |
| 53 | B5 | 54 |  |
| 54 | B6 | 49 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 55 | B7 | 65 |  46% 43% 9% |
| 56 | B8 | 37 |  8% 46% 38% 8% |

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 149640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | AA | 1515 | 32554 | 14490 | 6022 | 10527 | 1515 | 0 | 0 | 0 |

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 2 | AC | 76 | 1624 | 723 | 295 | 530 | 76 | 0 | 0 | 0 |

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 3 | AD | 76 | 1623 | 723 | 290 | 534 | 76 | 0 | 0 | 0 |

- Molecule 4 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 4 | A1 | 27 | 596 | 267 | 127 | 175 | 27 | 0 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 5 | AE | 234 | 1900 | 1213 | 341 | 341 | 5 | 0 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 6 | AF | 206 | 1612 | 1016 | 314 | 281 | 1 | 0 | 0 | 0 |

- Molecule 7 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 7 | AG | 208 | 1703 | 1066 | 339 | 291 | 7 | 0 | 0 | 0 |

- Molecule 8 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 8 | AH | 150 | 1146 | 724 | 217 | 201 | 4 | 0 | 0 | 0 |

- Molecule 9 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 9 | AI | 101 | 843 | 531 | 155 | 154 | 3 | 0 | 0 | 0 |

- Molecule 10 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 10 | AJ | 155 | 1257 | 781 | 252 | 218 | 6 | 0 | 0 | 0 |

- Molecule 11 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 11 | AK | 138 | 1116 | 705 | 215 | 193 | 3 | 0 | 0 | 0 |

- Molecule 12 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 12 | AL | 127 | 1010 | 639 | 197 | 174 | 0 | 0 | 0 |

- Molecule 13 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 13 | AM | 98 | 794 | 499 | 156 | 138 | 1 | 0 | 0 | 0 |

- Molecule 14 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 14 | AN | 119 | 885 | 549 | 168 | 165 | 3 | 0 | 0 | 0 |

- Molecule 15 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 15 | AO | 124 | 970 | 611 | 195 | 163 | 1 | 0 | 0 | 0 |

- Molecule 16 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 16 | AP | 125 | 997 | 617 | 207 | 171 | 2 | 0 | 0 | 0 |

- Molecule 17 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 17 | AQ | 60 | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |

- Molecule 18 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 18 | AR | 88 | 734 | 459 | 147 | 126 | 2 | 0 | 0 | 0 |

- Molecule 19 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 19 | AS | 83 | 700 | 443 | 139 | 117 | 1 | 0 | 0 | 0 |

- Molecule 20 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 20 | AT | 104 | 857 | 547 | 161 | 147 | 2 | 0 | 0 | 0 |

- Molecule 21 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 21 | AU | 73 | 597 | 380 | 118 | 99 | 0 | 0 | 0 |

- Molecule 22 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 22 | AV | 80 | 647 | 414 | 119 | 112 | 2 | 0 | 0 | 0 |

- Molecule 23 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 23 | AW | 99 | 763 | 470 | 162 | 129 | 2 | 0 | 0 | 0 |

- Molecule 24 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 24 | AX | 24 | 208 | 128 | 50 | 30 | 0 | 0 | 0 |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 25 | BA | 2889 | 62218 | 27691 | 11629 | 20009 | 2889 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-----------|
| BA | 493 | G | - | INSERTION | GB 48268 |

- Molecule 26 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 26 | BB | 123 | 2641 | 1175 | 488 | 855 | 123 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-----------|
| BB | -1 | A | - | INSERTION | GB 48271 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-----------|
| BB | 120 | U | - | INSERTION | GB 48271 |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 27 | BC | 228 | 1742 | 1102 | 318 | 319 | 3 | 0 | 0 | 0 |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 28 | BD | 272 | 2124 | 1339 | 424 | 358 | 3 | 0 | 0 | 0 |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 29 | BE | 206 | 1578 | 997 | 302 | 273 | 6 | 0 | 0 | 0 |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 30 | BF | 208 | 1625 | 1034 | 303 | 286 | 2 | 0 | 0 | 0 |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 31 | BG | 182 | 1482 | 947 | 269 | 261 | 5 | 0 | 0 | 0 |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 32 | BH | 174 | 1328 | 844 | 248 | 235 | 1 | 0 | 0 | 0 |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 33 | BK | 148 | 1155 | 737 | 205 | 212 | 1 | 0 | 0 | 0 |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 34 | BL | 138 | 1025 | 654 | 181 | 185 | 5 | 0 | 0 | 0 |

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 35 | BM | 139 | 1113 | 717 | 207 | 186 | 3 | 0 | 0 | 0 |

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 36 | BN | 122 | 932 | 587 | 171 | 170 | 4 | 0 | 0 | 0 |

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 37 | BO | 145 | 1106 | 688 | 226 | 190 | 2 | 0 | 0 | 0 |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 38 | BP | 136 | 1080 | 688 | 204 | 183 | 5 | 0 | 0 | 0 |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 39 | BQ | 117 | 960 | 599 | 202 | 159 | 0 | 0 | 0 |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 40 | BR | 110 | 877 | 553 | 175 | 149 | 0 | 0 | 0 |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 41 | BS | 117 | 976 | 614 | 197 | 164 | 1 | 0 | 0 | 0 |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 42 | BT | 117 | 964 | 610 | 202 | 151 | 1 | 0 | 0 | 0 |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 43 | BU | 101 | 779 | 501 | 142 | 135 | 1 | 0 | 0 | 0 |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 44 | BV | 110 | 876 | 552 | 171 | 151 | 2 | 0 | 0 | 0 |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 45 | BW | 94 | 742 | 483 | 133 | 126 | 0 | 0 | 0 |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 46 | BX | 110 | 844 | 539 | 158 | 141 | 6 | 0 | 0 | 0 |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 47 | BY | 180 | 1435 | 916 | 256 | 260 | 3 | 0 | 0 | 0 |

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 48 | BZ | 85 | 670 | 415 | 141 | 112 | 2 | 0 | 0 | 0 |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 49 | B1 | 67 | 567 | 350 | 116 | 99 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 50 | B2 | 59 | 469 | 298 | 90 | 81 | 0 | 0 | 0 |

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 51 | B3 | 71 | 581 | 364 | 108 | 104 | 5 | 0 | 0 | 0 |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 52 | B4 | 57 | 445 | 279 | 87 | 74 | 5 | 0 | 0 | 0 |

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 53 | B5 | 49 | 426 | 265 | 87 | 70 | 4 | 0 | 0 | 0 |

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 54 | B6 | 49 | 430 | 263 | 108 | 57 | 2 | 0 | 0 | 0 |

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 55 | B7 | 64 | 515 | 331 | 102 | 79 | 3 | 0 | 0 | 0 |

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 56 | B8 | 37 | 307 | 188 | 68 | 47 | 4 | 0 | 0 | 0 |

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C738 | C739 | C740 | C741 | C742 | C743 | C744 | C745 | C746 | C747 | C748 | C749 | C750 | C751 | C752 | C753 | C754 | C755 | C756 | C757 | C758 | C759 | C760 | C761 | C762 | C763 | C764 | C765 | C766 | C767 | C768 | C769 | C770 | C771 | C772 | C773 | C774 | C775 | C776 | C777 | C778 | C779 | C780 | C781 | C782 | C783 | C784 | C785 | C786 | C787 | C788 | C789 | C790 | C791 | C792 | C793 | C794 | C795 | C796 | C797 | | | |
| U1040 | A1041 | A1042 | G1043 | A1044 | A1045 | A1046 | G1047 | G1048 | U1049 | G1050 | A1051 | U1052 | G1053 | U1054 | A1055 | U1056 | G1057 | G1058 | C1059 | G1060 | G1061 | U1062 | C1063 | C1064 | U1065 | U1066 | C1067 | G1068 | A1069 | G1070 | C1071 | A1072 | G1073 | U1074 | C1075 | C1076 | G1077 | G1078 | G1079 | A1080 | G1081 | G1082 | U1083 | U1084 | U1085 | U1086 | G1087 | G1088 | G1089 | U1090 | U1091 | A1092 | G1093 | G1094 | U1095 | C1096 | C1097 | C1098 | C1099 | | | |
| C1100 | A1101 | A1102 | C1103 | A1104 | A1105 | A1106 | C1107 | G1108 | C1109 | A1110 | C1111 | A1112 | C1113 | C1114 | C1115 | G1116 | G1117 | C1118 | C1119 | G1120 | U1121 | U1122 | C1123 | G1124 | A1125 | U1126 | G1127 | A1128 | C1129 | A1130 | A1131 | C1132 | C1133 | G1134 | U1135 | U1136 | C1137 | G1138 | G1139 | C1140 | C1141 | G1142 | G1143 | G1144 | C1145 | U1146 | C1147 | G1148 | C1149 | U1150 | A1151 | A1152 | C1153 | G1154 | A1155 | G1156 | A1157 | C1158 | U1159 | | | |
| G1160 | C1161 | C1162 | C1163 | C1164 | C1165 | G1166 | A1167 | A1168 | A1169 | A1170 | G1171 | C1172 | G1173 | G1174 | G1175 | A1176 | G1177 | A1178 | A1179 | A1180 | G1181 | G1182 | A1183 | G1184 | A1185 | G1186 | A1187 | A1188 | C1189 | A1190 | A1191 | C1192 | C1193 | A1194 | C1195 | A1196 | G1197 | A1198 | U1199 | C1200 | A1201 | G1202 | C1203 | A1204 | U1205 | G1206 | C1208 | C1209 | C1210 | U1211 | U1212 | A1213 | C1214 | G1215 | G1216 | C1217 | A1218 | U1219 | C1220 | | | |
| G1221 | G1222 | C1223 | G1224 | A1225 | G1226 | A1227 | G1228 | A1229 | A1230 | G1231 | U1232 | G1233 | C1234 | U1235 | A1236 | C1237 | A1238 | A1239 | U1240 | G1241 | C1242 | C1243 | G1244 | A1245 | C1246 | U1247 | A1248 | C1249 | G1250 | A1251 | G1252 | C1253 | U1254 | A1255 | U1256 | G1257 | C1258 | A1259 | C1260 | A1261 | C1262 | G1263 | C1264 | G1265 | G1266 | A1268 | A1269 | C1270 | G1271 | A1272 | A1273 | G1274 | A1275 | G1276 | C1277 | U1278 | A1279 | A1280 | | | | |
| U1281 | C1282 | C1283 | C1284 | A1285 | A1286 | A1287 | A1288 | A1289 | A1290 | G1291 | U1292 | G1293 | G1294 | G1295 | C1296 | C1297 | C1298 | A1299 | G1300 | U1302 | C1303 | C1304 | G1305 | A1306 | U1307 | U1308 | C1309 | G1310 | G1311 | G1312 | U1313 | C1314 | C1315 | G1316 | C1317 | A1318 | A1319 | C1320 | C1321 | C1322 | G1323 | A1324 | C1325 | C1326 | C1328 | A1329 | U1330 | A1331 | A1332 | A1333 | G1334 | C1335 | C1336 | G1337 | A1338 | C1339 | A1340 | | | | | |
| U1341 | C1342 | C1343 | C1344 | U1345 | A1346 | C1347 | U1348 | A1349 | A1350 | U1351 | G1352 | C1353 | C1354 | C1355 | G1356 | U1357 | U1358 | C1359 | A1360 | C1361 | C1362 | C1362A | A1363 | U1364 | G1365 | C1366 | C1367 | C1368 | G1369 | G1370 | G1371 | U1372 | C1373 | A1374 | C1375 | U1376 | A1377 | C1378 | G1379 | U1380 | U1381 | C1382 | C1383 | C1384 | G1385 | G1386 | C1387 | C1388 | C1389 | U1390 | U1391 | G1392 | U1393 | U1394 | A1395 | C1396 | A1397 | C1399 | | | | |
| C1400 | G1401 | C1402 | C1403 | C1404 | G1405 | U1406 | U1407 | U1408 | A1409 | C1410 | G1411 | C1412 | G1413 | A1414 | G1415 | G1416 | G1417 | A1418 | U1419 | G1420 | C1421 | G1422 | G1423 | C1424 | U1425 | U1426 | U1427 | C1428 | A1429 | G1430 | G1431 | C1432 | U1433 | A1434 | U1435 | U1436 | A1437 | G1438 | C1439 | G1440 | G1441 | G1442 | G1443 | A1444 | G1447 | U1448 | A1449 | A1450 | C1451 | C1452 | G1453 | G1454 | A1455 | A1456 | G1457 | A1458 | A1459 | G1460 | G1461 | G1462 | A1463 | G1464 |
| C1465 | C1466 | G1467 | A1468 | G1469 | G1470 | G1471 | U1472 | A1473 | G1474 | G1475 | G1476 | G1477 | C1478 | C1479 | G1480 | U1481 | G1482 | A1483 | C1484 | U1485 | G1486 | G1487 | G1488 | G1489 | C1490 | U1491 | A1492 | A1493 | G1494 | U1495 | C1496 | G1497 | U1498 | A1499 | U1500 | G1501 | A1502 | G1503 | U1504 | G1505 | U1506 | A1507 | G1508 | U1509 | U1510 | U1511 | U1512 | A1513 | C1514 | C1515 | G1516 | G1517 | A1518 | A1519 | G1520 | G1521 | U1522 | G1523 | C1524 | | | |
| G1525 | G1526 | C1527 | U1528 | G1529 | G1530 | A1531 | U1532 | C1533 | A1534 | C1535 | G1536 | U1537 | C1538 | C1539 | U1540 | U1541 | U1542 | C | U | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

• Molecule 2: tRNA fMET (unmodified bases)

Chain AC:

49%

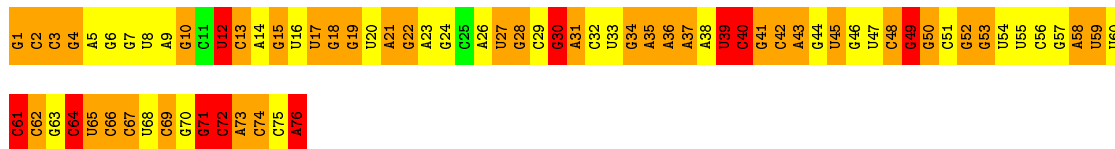
43%

8%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 | C9 | C10 | C11 | C12 | C13 | C14 | C15 | C16 | C17 | C18 | C19 | U20 | A21 | C22 | C23 | U24 | C25 | C26 | U27 | C28 | G29 | G30 | G31 | C32 | U33 | C34 | A35 | C36 | A37 | A38 | C39 | C40 | C41 | G42 | A43 | A44 | G45 | G46 | U47 | C48 | G49 | U50 | C51 | C52 | C53 | U54 | U55 | C56 | A57 | A58 | A59 | C60 |
| C61 | C62 | G63 | G64 | C65 | C66 | C67 | C68 | C69 | C70 | C71 | A72 | A73 | C74 | C75 | A76 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

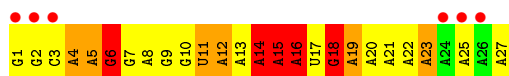
- Molecule 3: tRNA PHE (unmodified bases)

Chain AD:  37% 47% 13%



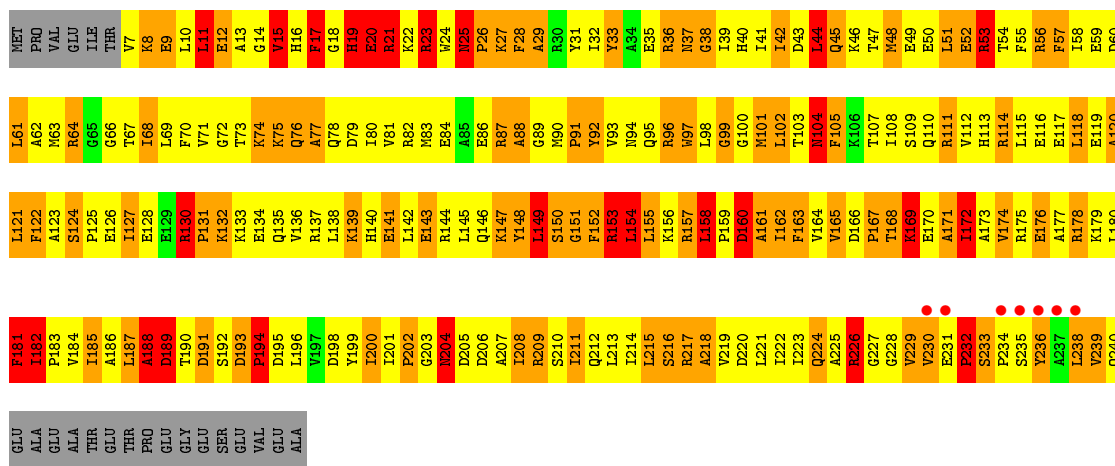
- Molecule 4: mRNA

Chain A1:  7% 52% 22% 19%



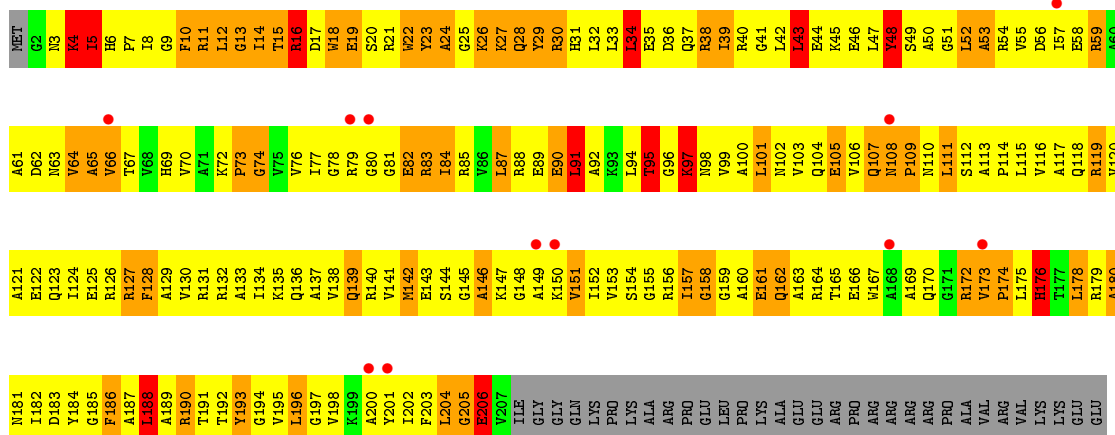
- Molecule 5: 30S ribosomal protein S2

Chain AE:  3% 45% 33% 11% 9%



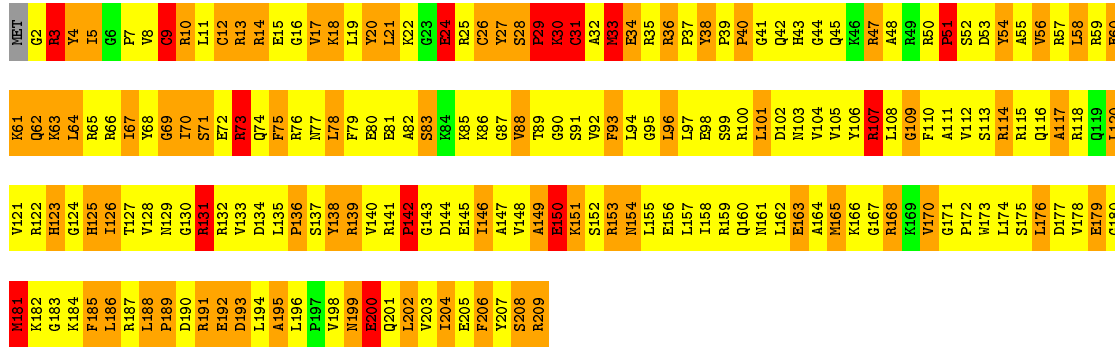
- Molecule 6: 30S ribosomal protein S3

Chain AF:  5% 51% 25% 5% 14%



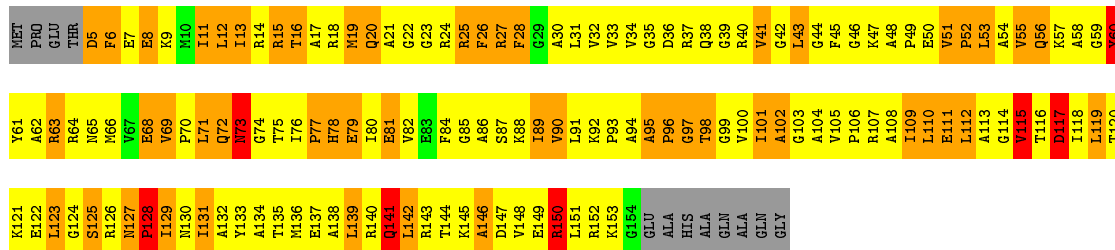
• Molecule 7: 30S ribosomal protein S4

Chain AG: 54% 34% 7%



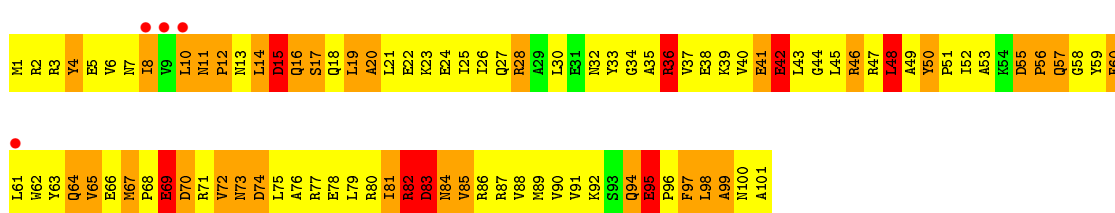
• Molecule 8: 30S ribosomal protein S5

Chain AH: 54% 31% 7%



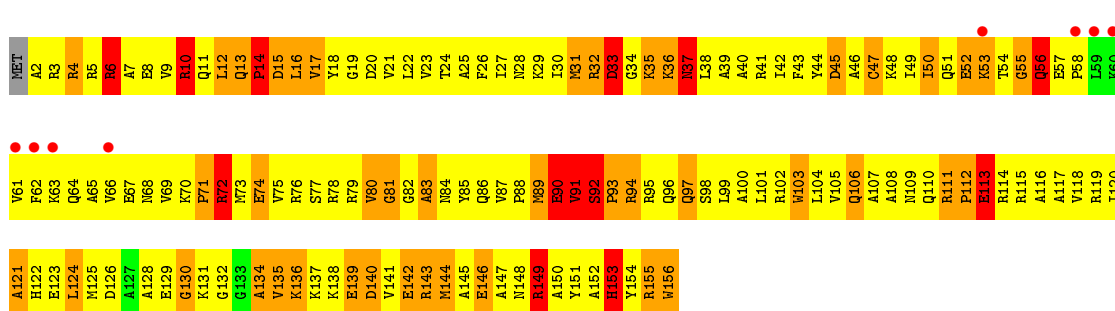
• Molecule 9: 30S ribosomal protein S6

Chain AI: 4% 5% 55% 32% 8%

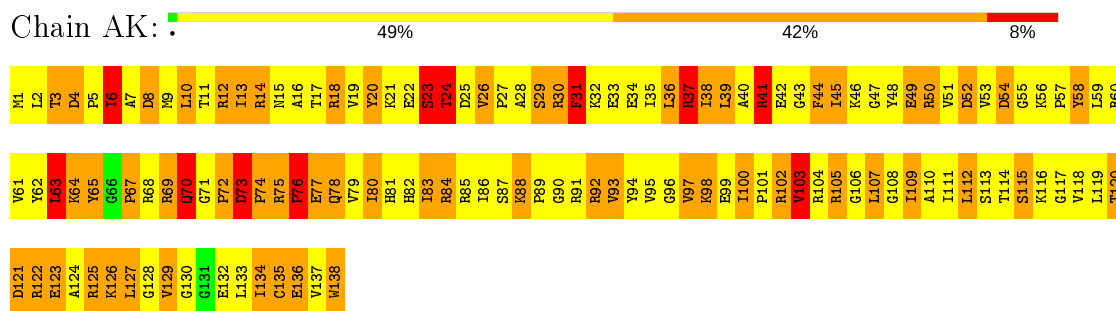


• Molecule 10: 30S ribosomal protein S7

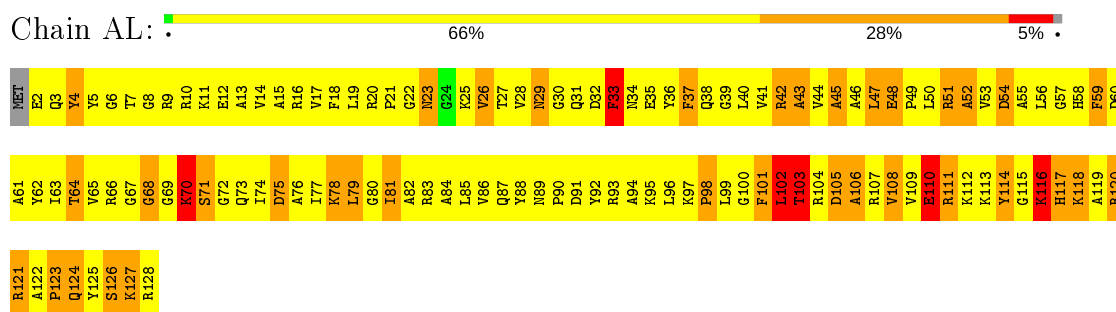
Chain AJ: 5% 61% 28% 8%



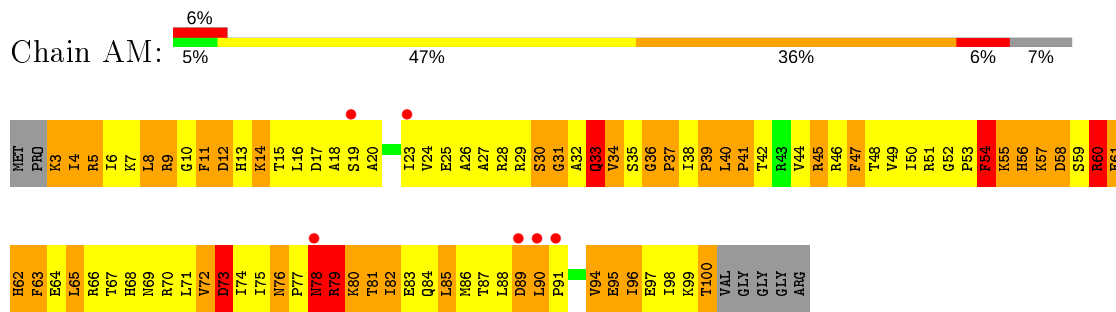
● Molecule 11: 30S ribosomal protein S8



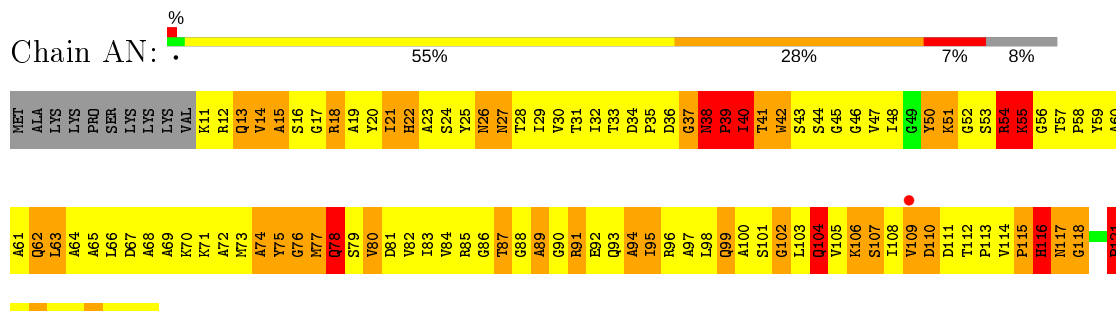
● Molecule 12: 30S ribosomal protein S9



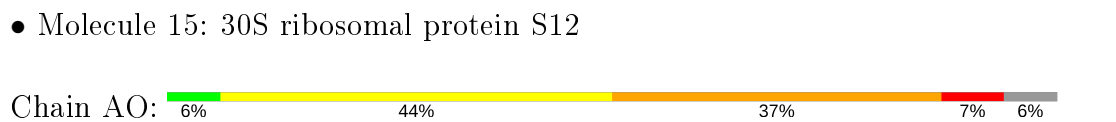
● Molecule 13: 30S ribosomal protein S10

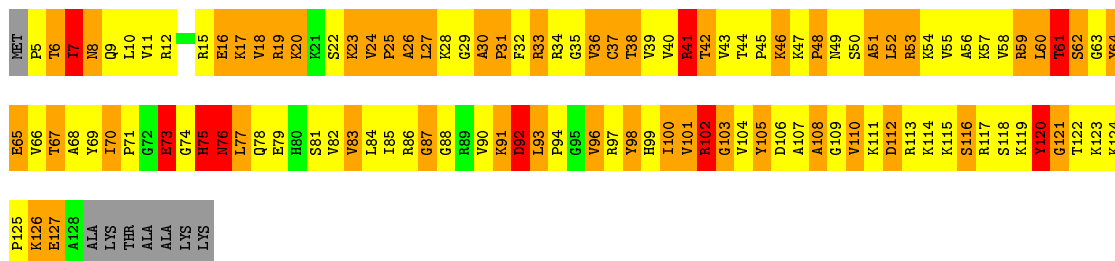


● Molecule 14: 30S ribosomal protein S11

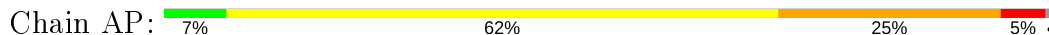


● Molecule 15: 30S ribosomal protein S12

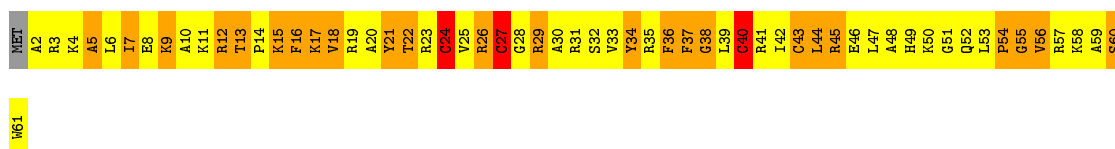




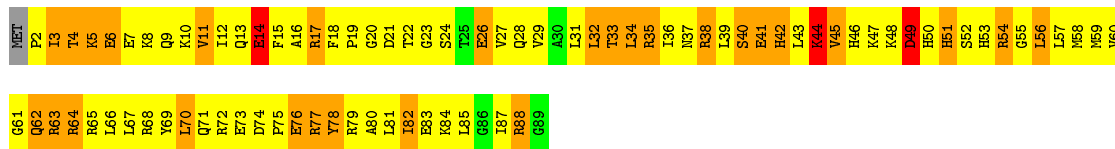
• Molecule 16: 30S ribosomal protein S13



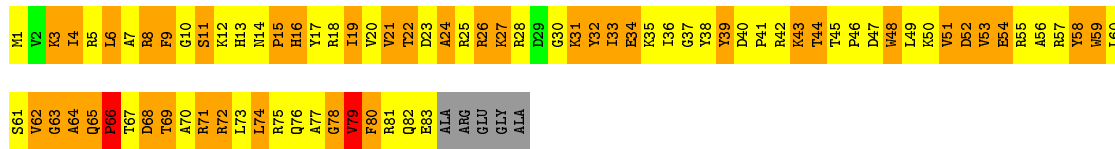
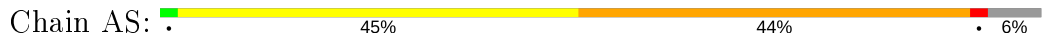
• Molecule 17: 30S ribosomal protein S14



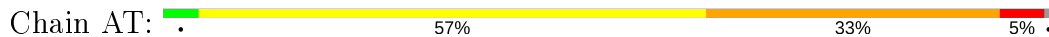
• Molecule 18: 30S ribosomal protein S15

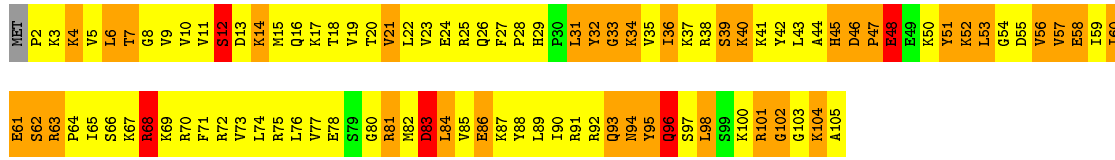


• Molecule 19: 30S ribosomal protein S16

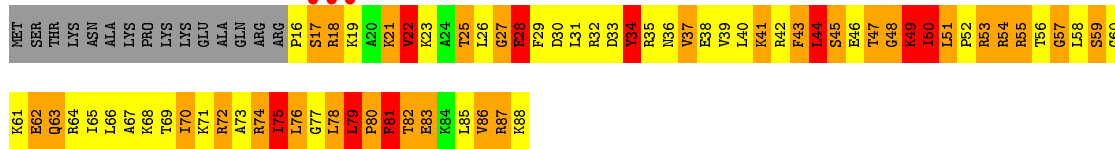


• Molecule 20: 30S ribosomal protein S17

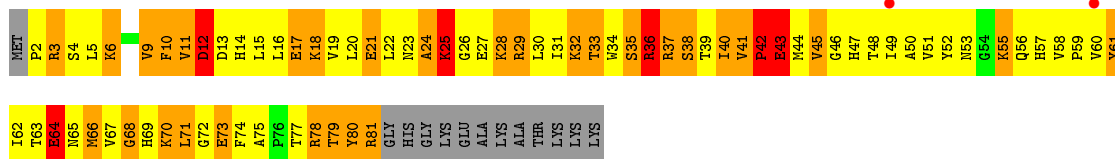




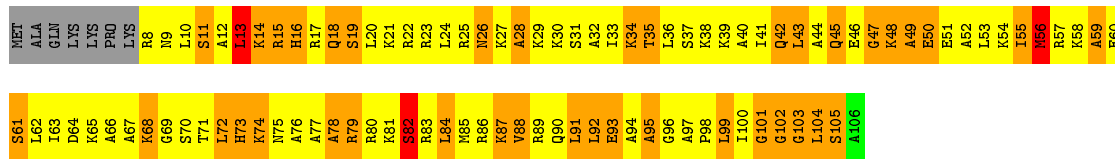
• Molecule 21: 30S ribosomal protein S18



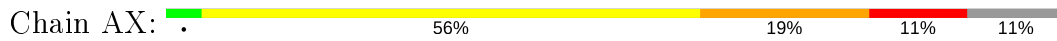
• Molecule 22: 30S ribosomal protein S19



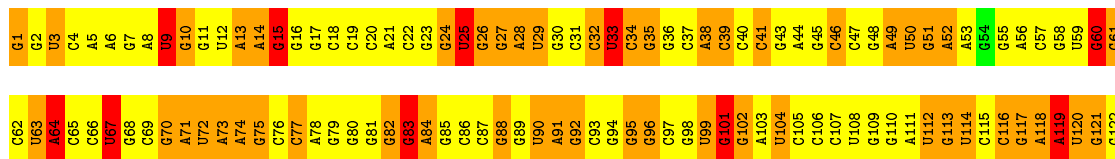
• Molecule 23: 30S ribosomal protein S20



• Molecule 24: 30S ribosomal protein Thx



• Molecule 25: 23S rRNA



| | | | | | | | | | | | | | | | | |
|--------|-------|-------|------|------|------|------|------|------|-------|------|------|-------|------|-------|------|-------|
| A1096 | G1036 | C974A | C914 | G853 | A793 | 6733 | 6673 | 6635 | 6577 | A515 | A454 | C337 | C277 | G252 | C182 | G123 |
| U1097 | G1037 | G975 | C915 | G854 | G794 | A734 | 6674 | 6636 | 6578 | C916 | C455 | G338 | A278 | C263 | U193 | G124 |
| A1098 | C1038 | G976 | G916 | G855 | G795 | A735 | 6675 | 6637 | 6579 | C917 | C456 | U339 | G279 | C264 | G194 | G125 |
| G1039 | G1039 | G977 | A917 | C856 | C796 | 6736 | 6676 | A637 | C580 | G918 | A457 | G340 | C280 | A255 | A195 | A126 |
| C1040 | C1040 | G978 | G918 | C857 | G797 | 6737 | 6677 | U639 | C581 | U919 | G458 | G341 | G281 | A256 | A196 | A127 |
| U1100 | G1041 | G979 | G919 | C858 | G798 | 6738 | 6678 | C640 | G582 | G920 | U459 | G342 | A282 | A257 | A197 | G128 |
| C1102 | G1042 | A980 | G920 | G859 | G799 | 6739 | 6679 | C641 | G583 | G921 | A460 | C343 | A283 | G258 | C198 | C129 |
| A1103 | C1043 | A981 | G921 | U860 | G800 | 6740 | 6680 | 6642 | G584 | G922 | C461 | C344 | A284 | G259 | A199 | C130 |
| G1044 | G1044 | G982 | U922 | A861 | A801 | 6741 | 6681 | A643 | G585 | G923 | C462 | A345 | G285 | G260 | U200 | G131 |
| U1105 | A1045 | C993 | C923 | G862 | G802 | 6742 | 6682 | A644 | A586 | U924 | G463 | A346 | C286 | G261 | C201 | G132 |
| A1106 | A1046 | A983 | U903 | A863 | U803 | 6743 | 6683 | C645 | G587 | U925 | U464 | A347 | C287 | A262 | U202 | C133 |
| G1047 | G1047 | C995 | C925 | G864 | A804 | 6744 | 6684 | A646 | U588 | A526 | G465 | G348 | C288 | C263 | C203 | C134 |
| U1108 | A1048 | C996 | G926 | G865 | G805 | 6745 | 6685 | U647 | C589 | C527 | A466 | G349 | A289 | C264 | A204 | G135 |
| C1109 | C1049 | G987 | G928 | A866 | C806 | 6746 | 6686 | 6648 | A590 | A528 | G467 | U350 | G290 | A265 | G205 | G136 |
| A1110 | A1050 | A988 | G929 | U867 | U807 | 6747 | 6687 | 6649 | C591 | A529 | G468 | G351 | C291 | G266 | U206 | G137 |
| G1111 | G1051 | G989 | U930 | G868 | G808 | 6748 | 6688 | C | G592 | G930 | G469 | A352 | C292 | C267 | A207 | G137A |
| C1112 | C1052 | A990 | G931 | G869 | G809 | 6749 | 6689 | G | C593 | C531 | A470 | G353 | U293 | C268 | C208 | G138 |
| U1113 | U1053 | C991 | G932 | A870 | U810 | 6750 | 6690 | U | U594 | A532 | A471 | G354 | G294 | U269 | C209 | G139 |
| G1114 | A1054 | G992 | A933 | U871 | U811 | 6751 | 6691 | A | C595 | G533 | A472 | G355 | G295 | A270 | C210 | A140 |
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|-------|-------|-------|-------|-------|-------|-------|-------|--------|--------|-------|--------|-------|-------|-------|-------|
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| G2151 | U2091 | A2031 | A1971 | G1842 | C1782 | U1706 | C1646 | A1587 | G1527 | G1466 | A1407 | G1347 | A1287 | A1227 | U1166 |
| G2152 | G2092 | G2032 | C1972 | C1843 | A1783 | G1707 | G1647 | A1588 | G1528 | C1467 | C1408 | G1348 | U1288 | U1228 | U1167 |
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| U2167 | C2107 | U2047 | G1987 | G1858 | U1798 | C1731 | C1662 | C1603 | A1543 | G1483 | G1423 | C1363 | A1303 | G1243 | G1183 |
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| G2184 | G2124 | C2064 | U1944 | A1884 | A1815 | A1755 | U1679 | G1620 | U1559 | G1500 | G1440 | G1380 | C1320 | G1260 | C1200 |
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| G2187 | C2127 | G2067 | C1947 | C1887 | U1818 | G1758 | A1682 | G1623 | A1562 | U1503 | G1443 | C1383 | U1323 | U1263 | G1203 |
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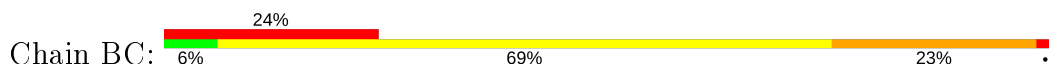
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
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| U2390 | G2391 | G2392 | G2393 | G2394 | G2395 | G2396 | G2397 | G2398 | G2399 | G2400 | G2401 | G2402 | G2403 | G2404 | G2405 | G2406 | G2407 | G2408 | G2409 | G2410 | G2411 | G2412 | G2413 | G2414 | G2415 | G2416 | G2417 | G2418 | G2419 | G2420 | G2421 | G2422 | G2423 | G2424 | G2425 | G2426 | G2427 | G2428 | G2429 | G2430 | G2431 | G2432 | G2433 | G2434 | G2435 | G2436 | G2437 | G2438 | G2439 | G2440 | G2441 | G2442 | G2443 | G2444 | G2445 | G2446 | G2447 | G2448 | G2449 | | | | | |
| A2450 | A2451 | A2452 | A2453 | A2454 | A2455 | A2456 | A2457 | A2458 | A2459 | A2460 | A2461 | A2462 | A2463 | A2464 | A2465 | A2466 | A2467 | A2468 | A2469 | A2470 | A2471 | A2472 | A2473 | A2474 | A2475 | A2476 | A2477 | A2478 | A2479 | A2480 | A2481 | A2482 | A2483 | A2484 | A2485 | A2486 | A2487 | A2488 | A2489 | A2490 | A2491 | A2492 | A2493 | A2494 | A2495 | A2496 | A2497 | A2498 | A2499 | A2500 | A2501 | A2502 | A2503 | A2504 | A2505 | A2506 | A2507 | A2508 | A2509 | | | | | |
| U2510 | U2511 | U2512 | U2513 | U2514 | U2515 | U2516 | U2517 | U2518 | U2519 | U2520 | U2521 | U2522 | U2523 | U2524 | U2525 | U2526 | U2527 | U2528 | U2529 | U2530 | U2531 | U2532 | U2533 | U2534 | U2535 | U2536 | U2537 | U2538 | U2539 | U2540 | U2541 | U2542 | U2543 | U2544 | U2545 | U2546 | U2547 | U2548 | U2549 | U2550 | U2551 | U2552 | U2553 | U2554 | U2555 | U2556 | U2557 | U2558 | U2559 | U2560 | U2561 | U2562 | U2563 | U2564 | U2565 | U2566 | U2567 | U2568 | U2569 | | | | | |
| G2570 | G2571 | A2572 | A2573 | A2574 | A2575 | G2576 | A2577 | A2578 | A2579 | U2580 | G2581 | G2582 | G2583 | U2584 | U2585 | G2586 | A2587 | A2588 | A2589 | A2590 | G2591 | G2592 | U2593 | G2594 | G2595 | U2596 | G2597 | A2598 | U2599 | G2600 | G2601 | G2602 | G2603 | U2604 | U2605 | G2606 | G2607 | G2608 | U2609 | G2610 | U2611 | G2612 | U2613 | A2614 | U2615 | G2616 | G2617 | G2618 | G2619 | G2620 | G2621 | G2622 | G2623 | G2624 | G2625 | G2626 | G2627 | G2628 | G2629 | | | | | |
| G2630 | G2631 | G2632 | G2633 | G2634 | G2635 | G2636 | G2637 | G2638 | G2639 | G2640 | G2641 | G2642 | G2643 | G2644 | G2645 | G2646 | G2647 | G2648 | G2649 | G2650 | G2651 | G2652 | U2653 | A2654 | G2655 | U2656 | G2657 | G2658 | A2659 | G2660 | G2661 | G2662 | G2663 | G2664 | A2665 | G2666 | G2667 | G2668 | G2669 | A2670 | G2671 | G2672 | G2673 | G2674 | G2675 | G2676 | G2677 | G2678 | G2679 | G2680 | G2681 | G2682 | G2683 | G2684 | G2685 | G2686 | G2687 | G2688 | G2689 | | | | | |
| G2690 | G2691 | G2692 | G2693 | G2694 | G2695 | G2696 | G2697 | G2698 | G2699 | G2700 | G2701 | G2702 | G2703 | G2704 | G2705 | A2706 | G2707 | G2708 | G2709 | G2710 | A2711 | G2712 | A2713 | A2714 | G2715 | G2716 | G2717 | G2718 | G2719 | G2720 | G2721 | G2722 | G2723 | G2724 | A2725 | G2726 | G2727 | G2728 | G2729 | G2730 | G2731 | G2732 | A2733 | A2734 | G2735 | G2736 | G2737 | G2738 | G2739 | G2740 | G2741 | G2742 | G2743 | G2744 | G2745 | G2746 | G2747 | G2748 | | | | | | |
| A2749 | A2750 | G2751 | G2752 | G2753 | G2754 | G2755 | G2756 | G2757 | G2758 | A2759 | G2760 | G2761 | G2762 | G2763 | G2764 | G2765 | G2766 | G2767 | G2768 | G2769 | G2770 | G2771 | G2772 | G2773 | G2774 | A2775 | G2776 | G2777 | G2778 | G2779 | G2780 | G2781 | G2782 | G2783 | G2784 | G2785 | G2786 | G2787 | G2788 | G2789 | A2790 | G2791 | G2792 | G2793 | G2794 | G2795 | G2796 | G2797 | G2798 | G2799 | A2800 | G2801 | G2802 | G2803 | G2804 | G2805 | G2806 | G2807 | G2808 | A2809 | G2810 | G2811 | | |
| G2812 | A2813 | G2814 | G2815 | G2816 | G2817 | G2818 | G2819 | G2820 | A2821 | G2822 | A2823 | G2824 | G2825 | A2826 | G2827 | G2828 | G2829 | G2830 | G2831 | G2832 | G2833 | G2834 | A2835 | G2836 | G2837 | G2838 | G2839 | G2840 | G2841 | G2842 | G2843 | G2844 | G2845 | G2846 | U2847 | G2848 | U2849 | A2850 | G2851 | G2852 | G2853 | G2854 | G2855 | G2856 | G2857 | G2858 | G2859 | A2860 | G2861 | G2862 | G2863 | G2864 | U2865 | G2866 | G2867 | G2868 | G2869 | G2870 | G2871 | | | | | |
| G2872 | A2873 | G2874 | G2875 | G2876 | G2877 | G2878 | G2879 | G2880 | G2881 | A2882 | G2883 | G2884 | G2885 | G2886 | U2887 | G2888 | G2889 | G2890 | G2891 | A2892 | G2893 | G2894 | U2895 | G2896 | U2897 | U2898 | G2899 | A2900 | G2901 | G2902 | C | C | C | G2903 | G2904 | G2905 | G2906 | G2907 | G2908 | G2909 | G2910 | G2911 | G2912 | G2913 | G2914 | G2915 | G2916 | G2917 | G2918 | G2919 | G2920 | G2921 | G2922 | G2923 | G2924 | G2925 | G2926 | G2927 | G2928 | G2929 | G2930 | | | |

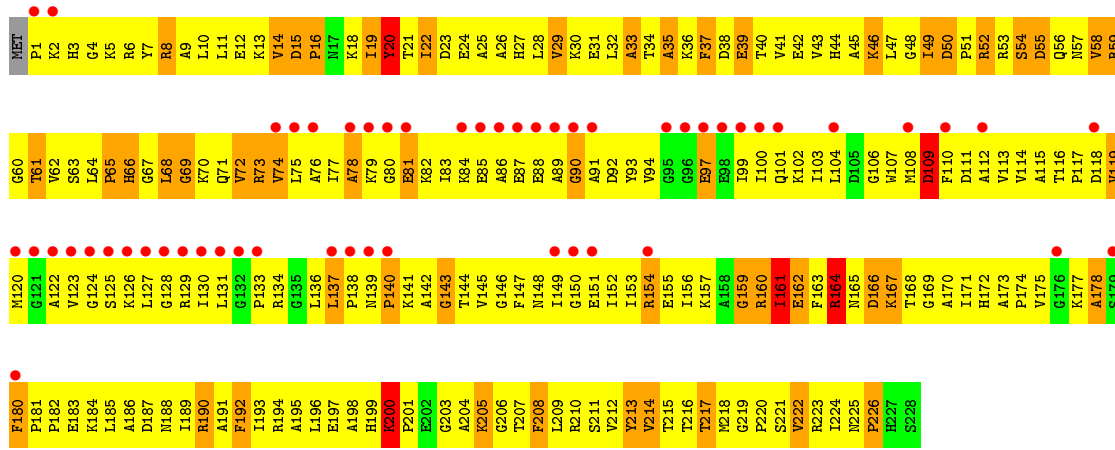
• Molecule 26: 5S rRNA



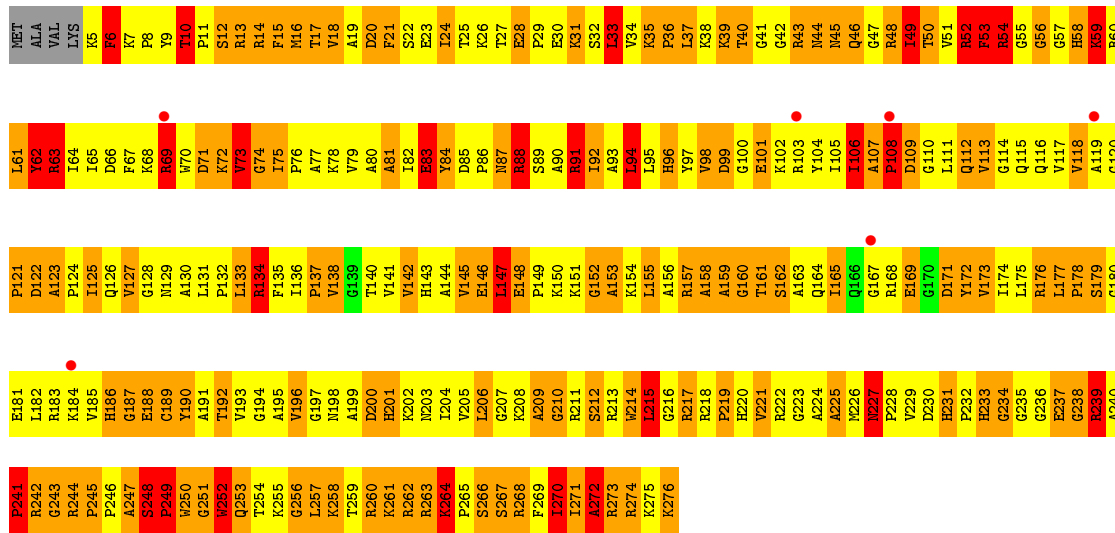
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A-1 | A0 | U1 | C2 | G3 | C4 | G5 | C6 | A66 | G67 | C68 | G69 | C70 | G71 | C72 | A73 | U74 | G75 | A76 | G77 | C78 | A79 | G80 | C81 | G82 | C83 | G84 | A85 | G86 | C87 | G88 | C89 | A90 | G91 | C92 | G93 | U94 | C94 | U95 | G96 | C97 | G98 | A99 | U100 | G101 | A101 | G102 | U103 | A104 | G105 | C106 | A107 | U108 | C109 | G110 | U111 | A112 | G113 | U114 | G115 | A116 | C117 |
|-----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

• Molecule 27: 50S RIBOSOMAL PROTEIN L1

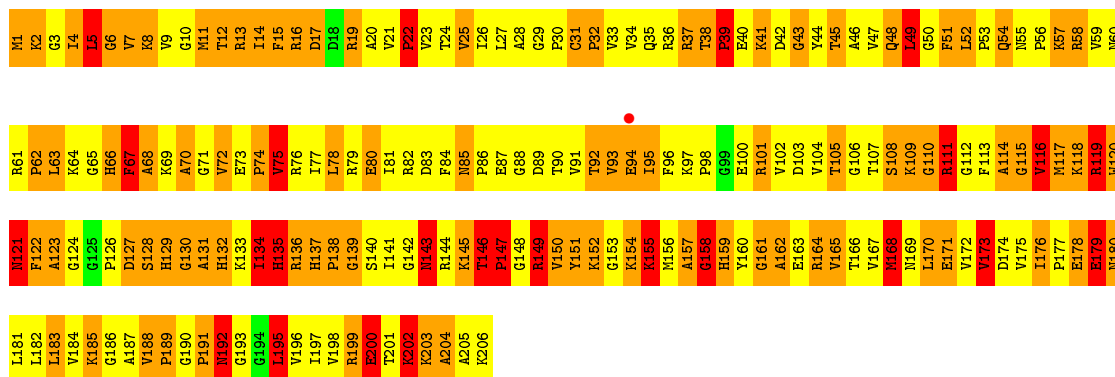
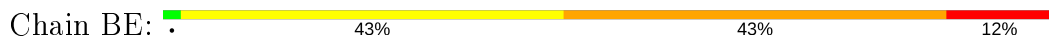




• Molecule 28: 50S RIBOSOMAL PROTEIN L2

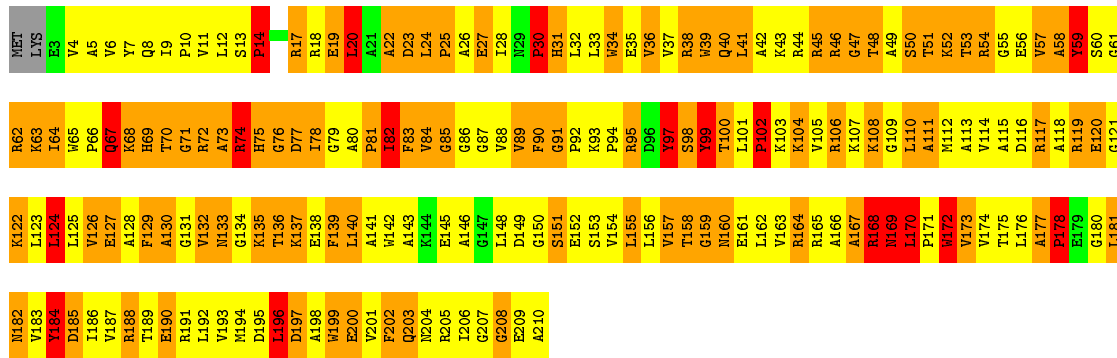


• Molecule 29: 50S RIBOSOMAL PROTEIN L3



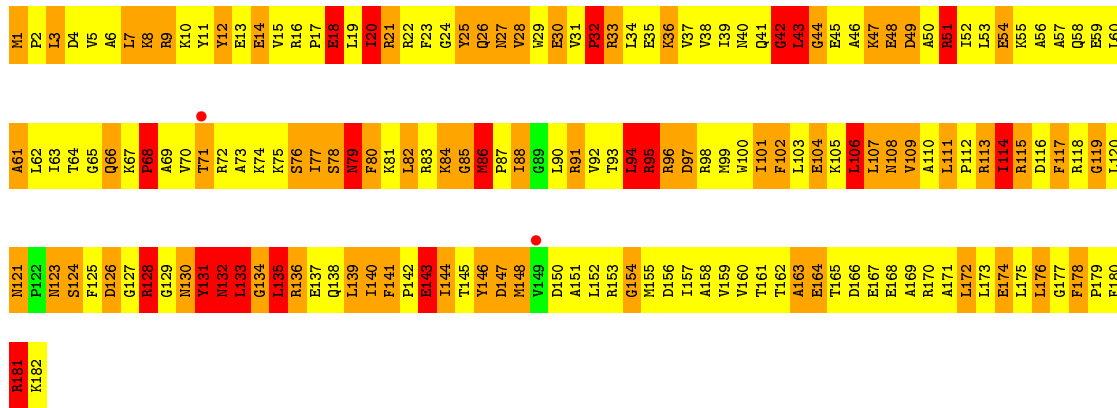
• Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain BF: 44% 42% 9%



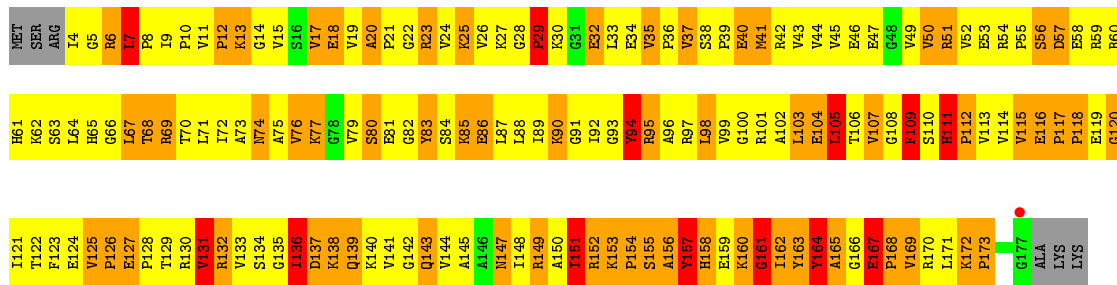
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain BG: 51% 36% 11%



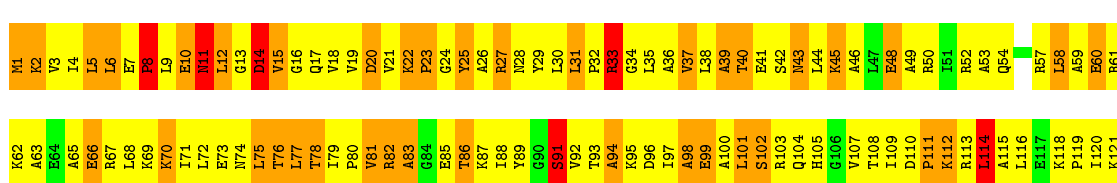
• Molecule 32: 50S RIBOSOMAL PROTEIN L6

Chain BH: 5% 49% 35% 7%



• Molecule 33: 50S RIBOSOMAL PROTEIN L9

Chain BK: 6% 55% 32% 7%



E122 L123 G124 E125 V126 Y127 L128 T129 Y130 K131 P132 H133 E135 V136 P137 I138 Q139 L140 K141 V142 S143 V144 V145 A146 Q147 E148

• Molecule 34: 50S RIBOSOMAL PROTEIN L11



MET K2 K3 V4 V5 V6 A6 V7 V8 V9 K10 L10 Q11 L12 P13 A14 G15 G16 A17 I18 I19 P19 A20 A21 F21 A22 A23 V23 V24 G24 A26 L27 G28 G29 H30 G31 G32 G33 I34 P35 E36 V37 V38 K39 A40 A41 F41 A42 A43 A44 A45 A46 A47 I47 A48 A49 K49 G49 D50 A51 A52 M12 V53 P54 V55 V56 E57 T58 T59 D119 Y60

A61 D62 R63 S64 F65 T66 F67 V68 V69 K70 K71 T71 P72 P73 A74 A75 Y76 L77 I78 I79 R79 K80 A81 A82 G83 L84 E85 K86 G87 A88 H89 K90 P91 G92 G93 R93 E94 K95 V96 G97 R98 R99 T100 W101 E102 Q103 V104 L105 E106 I107 A108 K109 Q110 M112 P113 D114 L115 M116 T117 T118 L120

E121 A122 A123 A124 F125 M126 L127 A128 G129 S130 A131 A132 S133 M134 G135 V136 E137 V138 V139 GLY ALA PRO GLU VAL LYS ASP ALA

• Molecule 35: 50S RIBOSOMAL PROTEIN L13



MET K2 T3 V4 V5 V6 K7 K8 V9 V10 P11 P12 R13 M14 V15 L16 I17 A18 E19 G20 G21 T22 L23 G24 G25 L26 L27 T28 R29 K30 I31 A32 T33 L34 R35 G36 K37 E38 R39 P40 D41 A42 T43 P44 M45 V46 A47 L48 P49 G49 D50 F51 V52 G53 R54 V55 M56 F57 D58 R59 L120

R61 V62 T63 G64 K65 K66 L67 E68 V69 K70 K71 I72 R73 T74 V75 S76 G77 V78 F79 G80 G81 L82 R83 G84 L85 P86 L87 T88 R89 N90 I91 K92 R93 T94 R94 P95 E96 G97 V98 L99 E100 H101 V103 K104 G105 M106 L107 P108 K109 G110 P111 L112 G113 R114 R115 L116 F117 K118 R119 L120

K121 V122 Y123 A124 G125 P126 K127 H128 P129 H130 Q131 Q132 Q133 R134 P135 E136 K137 L138 E139 V140

• Molecule 36: 50S RIBOSOMAL PROTEIN L14



M1 I2 Q3 P4 Q5 T6 V7 L8 E9 E10 V10 A11 D12 M13 T14 A15 A16 R17 K18 I19 M20 C21 L22 R23 A24 L25 K26 G27 S28 N29 A30 K31 R32 A33 T34 V35 G36 D37 V38 V39 G40 A41 S42 V43 K44 E45 A46 A47 P48 R49 G50 A51 V52 K53 E54 G55 D56 V57 V58 K59 A60

V61 V62 R63 T64 K65 K66 R67 E68 V69 K70 R71 P72 D73 G74 S75 I77 R78 F79 D80 D81 N82 G83 A84 V85 I86 L87 N88 R89 Q90 L91 E92 P93 R94 H95 T96 R97 V98 F99 G100 P101 A102 A103 R104 E105 L106 R107 E108 K109 G110 F111 M112 K113 I114 V115 S116 L117 A118 P119 E120

V121 L122

• Molecule 37: 50S RIBOSOMAL PROTEIN L15

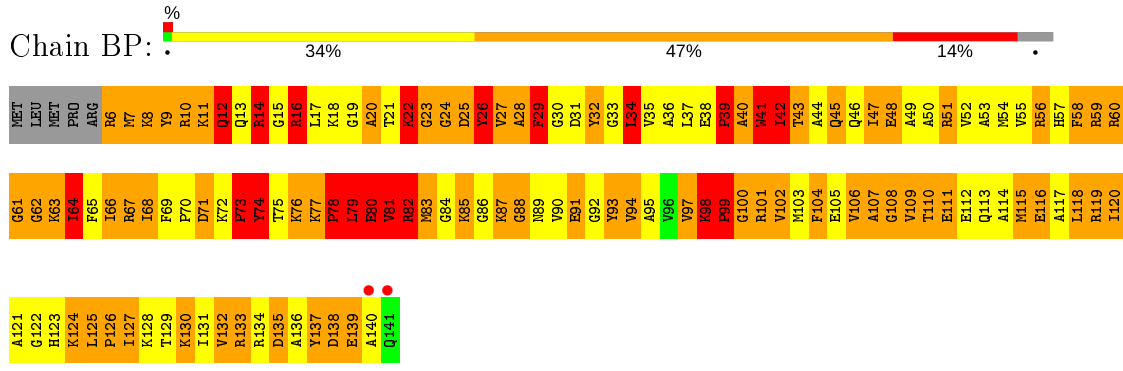


MET LYS LEU SER ASP L6 R7 R8 R9 P10 G11 A12 M13 K14 R15 R16 K17 R18 V19 G20 G21 G22 P23 G24 S25 G26 H27 G28 K29 T30 A31 T32 R33 G34 H35 K36 G37 Q38 K39 S40 R41 S42 G43 G44 L45 K46 D47 P48 R49 R50 F51 E52 G53 G54 R55 S56 T57 T58 L59 M60

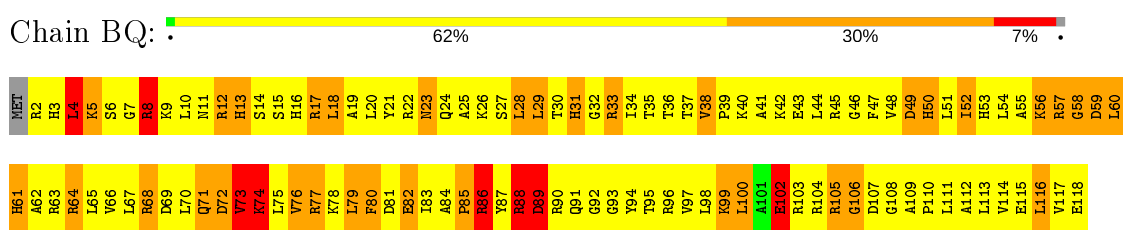
R61 L62 P63 R64 G65 G66 R67 K68 G69 V70 V71 F72 G73 E74 I75 R76 R77 F78 R79 Y80 Q81 G82 G83 V84 N85 K86 D87 L88 A89 R90 F91 E92 G93 E94 V95 T96 P97 E98 L99 L100 V101 R102 A103 G104 E105 L106 K107 K108 G109 Y110 R111 L112 K113 I114 L115 G116 E117 G118 E119 A120



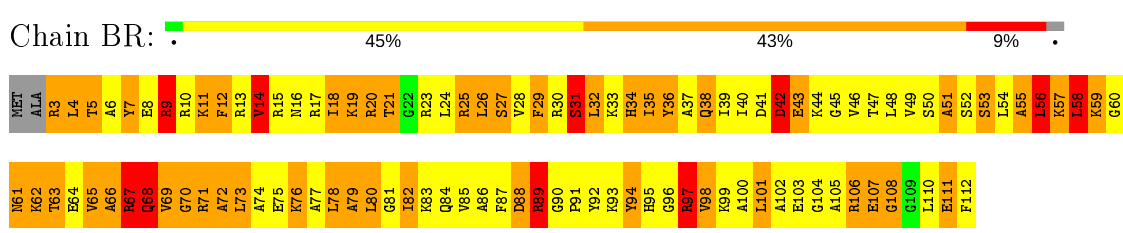
• Molecule 38: 50S RIBOSOMAL PROTEIN L16



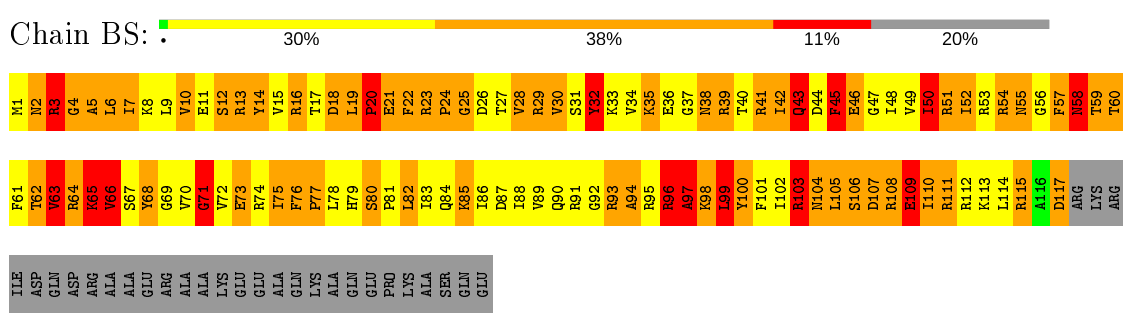
• Molecule 39: 50S RIBOSOMAL PROTEIN L17



• Molecule 40: 50S RIBOSOMAL PROTEIN L18

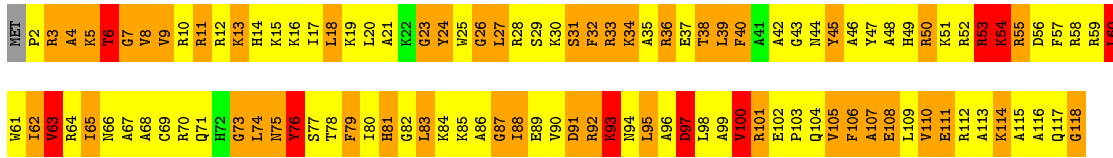


• Molecule 41: 50S RIBOSOMAL PROTEIN L19

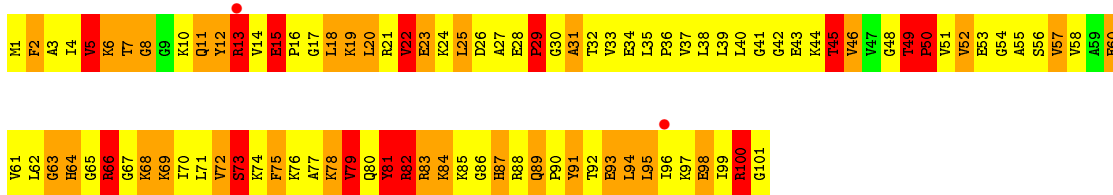


• Molecule 42: 50S RIBOSOMAL PROTEIN L20

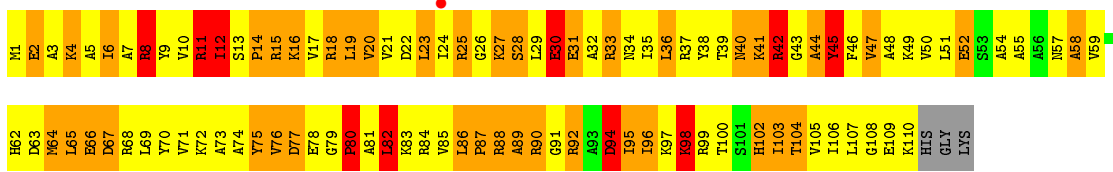




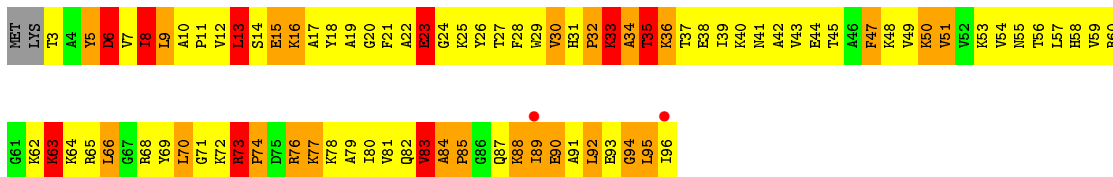
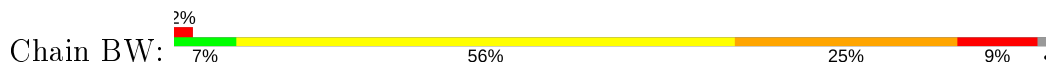
- Molecule 43: 50S RIBOSOMAL PROTEIN L21



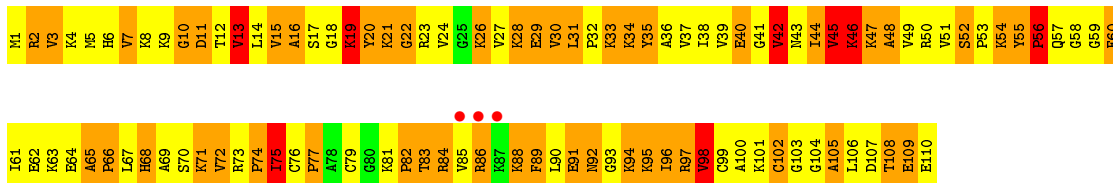
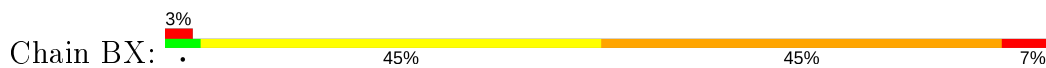
- Molecule 44: 50S RIBOSOMAL PROTEIN L22



- Molecule 45: 50S RIBOSOMAL PROTEIN L23

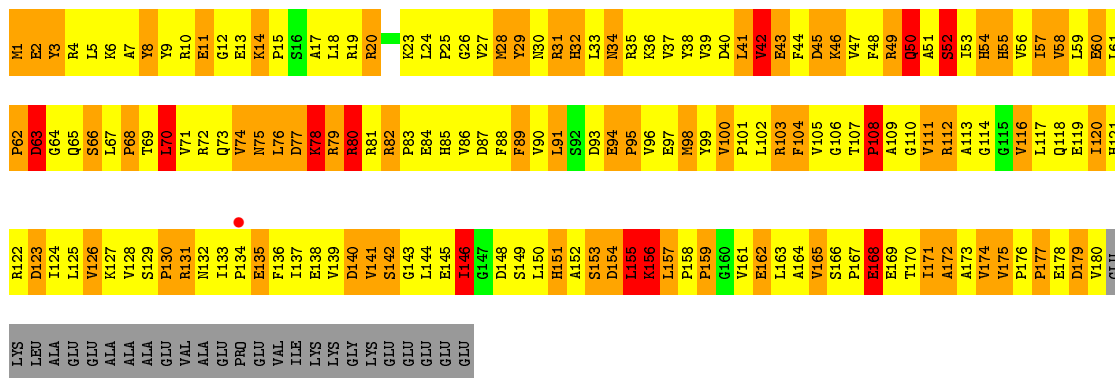


- Molecule 46: 50S RIBOSOMAL PROTEIN L24



- Molecule 47: 50S RIBOSOMAL PROTEIN L25





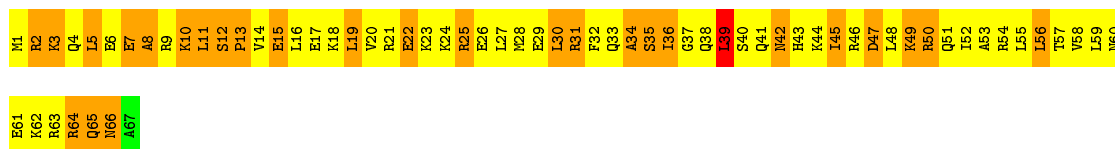
- Molecule 48: 50S RIBOSOMAL PROTEIN L27

Chain BZ: 64% 28% 6%



- Molecule 49: 50S RIBOSOMAL PROTEIN L29

Chain B1: 57% 40% 3%



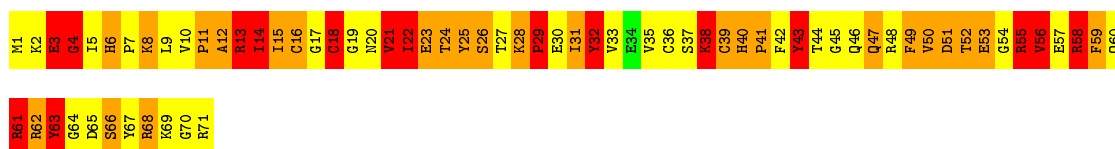
- Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain B2: 7% 47% 38% 7%



- Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain B3: 41% 35% 23%



- Molecule 52: 50S RIBOSOMAL PROTEIN L32

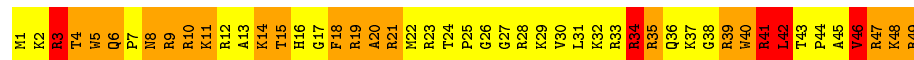
Chain B4: 27% 52% 15% 5%



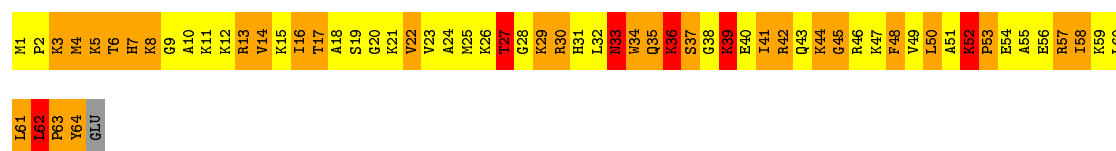
- Molecule 53: 50S RIBOSOMAL PROTEIN L33



- Molecule 54: 50S RIBOSOMAL PROTEIN L34



- Molecule 55: 50S RIBOSOMAL PROTEIN L35



- Molecule 56: 50S RIBOSOMAL PROTEIN L36



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | I 4 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 300.00 – 4.51 429.82 – 3.98 | Depositor EDS |
| % Data completeness (in resolution range) | 90.3 (300.00-4.51) 94.9 (429.82-3.98) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.00 (at 4.02Å) | Xtrriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.298 , 0.345 0.271 , 0.312 | Depositor DCC |
| R_{free} test set | 21439 reflections (4.85%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 198.7 | Xtrriage |
| Anisotropy | 0.113 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.09 , 116.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 149640 | wwPDB-VP |
| Average B, all atoms (Å ²) | 252.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | AA | 0.93 | 38/36438 (0.1%) | 1.05 | 172/56869 (0.3%) |
| 2 | AC | 0.93 | 2/1814 (0.1%) | 1.01 | 4/2825 (0.1%) |
| 3 | AD | 1.47 | 34/1813 (1.9%) | 1.27 | 21/2823 (0.7%) |
| 4 | A1 | 0.81 | 1/673 (0.1%) | 1.07 | 3/1048 (0.3%) |
| 5 | AE | 0.63 | 0/1935 | 1.01 | 4/2609 (0.2%) |
| 6 | AF | 0.53 | 0/1636 | 0.93 | 4/2205 (0.2%) |
| 7 | AG | 0.67 | 1/1733 (0.1%) | 1.10 | 7/2318 (0.3%) |
| 8 | AH | 0.70 | 0/1162 | 1.08 | 4/1564 (0.3%) |
| 9 | AI | 0.69 | 0/856 | 1.03 | 3/1154 (0.3%) |
| 10 | AJ | 0.54 | 0/1276 | 0.87 | 0/1709 |
| 11 | AK | 0.73 | 0/1136 | 1.08 | 3/1527 (0.2%) |
| 12 | AL | 0.51 | 0/1029 | 0.84 | 1/1379 (0.1%) |
| 13 | AM | 0.50 | 0/807 | 0.85 | 0/1085 |
| 14 | AN | 0.67 | 0/900 | 1.06 | 0/1213 |
| 15 | AO | 0.67 | 0/986 | 1.09 | 3/1320 (0.2%) |
| 16 | AP | 0.51 | 0/1008 | 0.91 | 2/1347 (0.1%) |
| 17 | AQ | 0.53 | 0/501 | 1.02 | 3/664 (0.5%) |
| 18 | AR | 0.67 | 0/745 | 0.98 | 0/992 |
| 19 | AS | 0.72 | 0/716 | 1.04 | 4/963 (0.4%) |
| 20 | AT | 0.67 | 0/870 | 1.05 | 2/1159 (0.2%) |
| 21 | AU | 0.65 | 0/603 | 1.12 | 3/799 (0.4%) |
| 22 | AV | 0.49 | 0/661 | 0.91 | 1/890 (0.1%) |
| 23 | AW | 0.66 | 0/765 | 1.05 | 1/1007 (0.1%) |
| 24 | AX | 0.47 | 0/212 | 0.82 | 0/277 |
| 25 | BA | 1.06 | 139/69685 (0.2%) | 1.19 | 514/108786 (0.5%) |
| 26 | BB | 0.80 | 2/2954 (0.1%) | 1.00 | 4/4606 (0.1%) |
| 27 | BC | 0.50 | 0/1775 | 0.89 | 2/2393 (0.1%) |
| 28 | BD | 0.88 | 2/2174 (0.1%) | 1.35 | 22/2927 (0.8%) |
| 29 | BE | 0.87 | 0/1611 | 1.36 | 19/2171 (0.9%) |
| 30 | BF | 0.74 | 0/1660 | 1.26 | 11/2247 (0.5%) |
| 31 | BG | 0.60 | 0/1507 | 1.07 | 5/2027 (0.2%) |
| 32 | BH | 0.64 | 0/1354 | 1.08 | 5/1831 (0.3%) |
| 33 | BK | 0.68 | 0/1170 | 1.10 | 8/1581 (0.5%) |
| 34 | BL | 0.50 | 0/1044 | 0.92 | 1/1415 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 35 | BM | 0.85 | 1/1140 (0.1%) | 1.19 | 7/1537 (0.5%) |
| 36 | BN | 1.07 | 4/942 (0.4%) | 1.42 | 7/1268 (0.6%) |
| 37 | BO | 0.75 | 0/1123 | 1.24 | 9/1493 (0.6%) |
| 38 | BP | 0.86 | 1/1100 (0.1%) | 1.23 | 9/1470 (0.6%) |
| 39 | BQ | 0.70 | 0/974 | 1.07 | 2/1302 (0.2%) |
| 40 | BR | 0.73 | 0/887 | 1.14 | 5/1180 (0.4%) |
| 41 | BS | 0.98 | 0/990 | 1.52 | 16/1325 (1.2%) |
| 42 | BT | 0.81 | 0/982 | 1.19 | 7/1306 (0.5%) |
| 43 | BU | 0.94 | 1/790 (0.1%) | 1.40 | 10/1057 (0.9%) |
| 44 | BV | 0.73 | 0/886 | 1.21 | 7/1189 (0.6%) |
| 45 | BW | 0.60 | 0/756 | 0.97 | 5/1015 (0.5%) |
| 46 | BX | 0.61 | 0/857 | 1.10 | 3/1142 (0.3%) |
| 47 | BY | 0.66 | 0/1467 | 1.11 | 5/1992 (0.3%) |
| 48 | BZ | 0.67 | 0/679 | 1.02 | 1/902 (0.1%) |
| 49 | B1 | 0.60 | 0/569 | 0.89 | 1/751 (0.1%) |
| 50 | B2 | 0.71 | 1/474 (0.2%) | 1.10 | 4/635 (0.6%) |
| 51 | B3 | 1.05 | 0/594 | 1.44 | 10/795 (1.3%) |
| 52 | B4 | 0.79 | 0/459 | 1.22 | 2/621 (0.3%) |
| 53 | B5 | 0.98 | 1/433 (0.2%) | 1.49 | 6/576 (1.0%) |
| 54 | B6 | 0.84 | 1/438 (0.2%) | 1.08 | 1/575 (0.2%) |
| 55 | B7 | 0.69 | 0/523 | 1.22 | 5/690 (0.7%) |
| 56 | B8 | 0.73 | 0/310 | 1.13 | 1/407 (0.2%) |
| All | All | 0.94 | 229/162582 (0.1%) | 1.13 | 959/242958 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 241 |
| 2 | AC | 0 | 9 |
| 3 | AD | 0 | 12 |
| 4 | A1 | 0 | 5 |
| 7 | AG | 0 | 1 |
| 8 | AH | 0 | 1 |
| 11 | AK | 0 | 2 |
| 14 | AN | 0 | 1 |
| 15 | AO | 0 | 1 |
| 20 | AT | 0 | 1 |
| 24 | AX | 0 | 1 |
| 25 | BA | 0 | 610 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 26 | BB | 0 | 20 |
| 28 | BD | 0 | 1 |
| 30 | BF | 0 | 1 |
| 32 | BH | 0 | 3 |
| 36 | BN | 0 | 2 |
| 38 | BP | 0 | 3 |
| 41 | BS | 0 | 2 |
| 42 | BT | 0 | 1 |
| 43 | BU | 0 | 2 |
| 44 | BV | 0 | 1 |
| 51 | B3 | 0 | 2 |
| 52 | B4 | 0 | 1 |
| 53 | B5 | 0 | 1 |
| 56 | B8 | 0 | 1 |
| All | All | 0 | 926 |

The worst 5 of 229 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 25 | BA | 1203 | G | O3'-P | -34.71 | 1.19 | 1.61 |
| 25 | BA | 1202 | C | O3'-P | 29.90 | 1.97 | 1.61 |
| 25 | BA | 2447 | G | O3'-P | -21.30 | 1.35 | 1.61 |
| 25 | BA | 2601 | C | O3'-P | 19.66 | 1.84 | 1.61 |
| 25 | BA | 2756 | U | O3'-P | 19.18 | 1.84 | 1.61 |

The worst 5 of 959 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 25 | BA | 412 | A | O5'-P-OP2 | -28.87 | 76.06 | 110.70 |
| 25 | BA | 1203 | G | P-O3'-C3' | 27.73 | 152.97 | 119.70 |
| 25 | BA | 2448 | A | C5'-C4'-O4' | -27.33 | 76.31 | 109.10 |
| 30 | BF | 20 | LEU | O-C-N | -25.54 | 81.83 | 122.70 |
| 1 | AA | 37 | U | N3-C4-O4 | -25.04 | 101.87 | 119.40 |

There are no chirality outliers.

5 of 926 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 12 | U | Sidechain |
| 1 | AA | 16 | A | Sidechain |
| 1 | AA | 21 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 24 | U | Sidechain |
| 1 | AA | 7 | G | Sidechain |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32554 | 0 | 16429 | 6699 | 0 |
| 2 | AC | 1624 | 0 | 826 | 331 | 0 |
| 3 | AD | 1623 | 0 | 809 | 304 | 0 |
| 4 | A1 | 596 | 0 | 296 | 65 | 0 |
| 5 | AE | 1900 | 0 | 1951 | 928 | 0 |
| 6 | AF | 1612 | 0 | 1677 | 661 | 0 |
| 7 | AG | 1703 | 0 | 1763 | 807 | 0 |
| 8 | AH | 1146 | 0 | 1207 | 482 | 0 |
| 9 | AI | 843 | 0 | 857 | 397 | 0 |
| 10 | AJ | 1257 | 0 | 1296 | 519 | 0 |
| 11 | AK | 1116 | 0 | 1177 | 666 | 0 |
| 12 | AL | 1010 | 0 | 1037 | 457 | 0 |
| 13 | AM | 794 | 0 | 840 | 327 | 0 |
| 14 | AN | 885 | 0 | 904 | 410 | 0 |
| 15 | AO | 970 | 0 | 1057 | 413 | 0 |
| 16 | AP | 997 | 0 | 1072 | 469 | 0 |
| 17 | AQ | 492 | 0 | 529 | 264 | 0 |
| 18 | AR | 734 | 0 | 771 | 353 | 0 |
| 19 | AS | 700 | 0 | 720 | 348 | 0 |
| 20 | AT | 857 | 0 | 930 | 385 | 0 |
| 21 | AU | 597 | 0 | 668 | 357 | 0 |
| 22 | AV | 647 | 0 | 673 | 241 | 0 |
| 23 | AW | 763 | 0 | 861 | 330 | 0 |
| 24 | AX | 208 | 0 | 221 | 87 | 0 |
| 25 | BA | 62218 | 0 | 31354 | 15682 | 0 |
| 26 | BB | 2641 | 0 | 1337 | 598 | 0 |
| 27 | BC | 1742 | 0 | 1796 | 761 | 0 |
| 28 | BD | 2124 | 0 | 2207 | 1434 | 0 |
| 29 | BE | 1578 | 0 | 1647 | 1120 | 0 |
| 30 | BF | 1625 | 0 | 1666 | 862 | 0 |
| 31 | BG | 1482 | 0 | 1546 | 838 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 32 | BH | 1328 | 0 | 1408 | 664 | 0 |
| 33 | BK | 1155 | 0 | 1244 | 574 | 0 |
| 34 | BL | 1025 | 0 | 1074 | 414 | 0 |
| 35 | BM | 1113 | 0 | 1183 | 722 | 0 |
| 36 | BN | 932 | 0 | 994 | 703 | 0 |
| 37 | BO | 1106 | 0 | 1183 | 801 | 0 |
| 38 | BP | 1080 | 0 | 1127 | 691 | 0 |
| 39 | BQ | 960 | 0 | 1021 | 505 | 0 |
| 40 | BR | 877 | 0 | 938 | 472 | 0 |
| 41 | BS | 976 | 0 | 1033 | 699 | 0 |
| 42 | BT | 964 | 0 | 1022 | 709 | 0 |
| 43 | BU | 779 | 0 | 852 | 626 | 0 |
| 44 | BV | 876 | 0 | 941 | 423 | 0 |
| 45 | BW | 742 | 0 | 800 | 336 | 0 |
| 46 | BX | 844 | 0 | 930 | 493 | 0 |
| 47 | BY | 1435 | 0 | 1463 | 683 | 0 |
| 48 | BZ | 670 | 0 | 700 | 365 | 0 |
| 49 | B1 | 567 | 0 | 621 | 303 | 0 |
| 50 | B2 | 469 | 0 | 518 | 302 | 0 |
| 51 | B3 | 581 | 0 | 577 | 375 | 0 |
| 52 | B4 | 445 | 0 | 459 | 271 | 0 |
| 53 | B5 | 426 | 0 | 452 | 306 | 0 |
| 54 | B6 | 430 | 0 | 480 | 275 | 0 |
| 55 | B7 | 515 | 0 | 587 | 415 | 0 |
| 56 | B8 | 307 | 0 | 335 | 126 | 0 |
| All | All | 149640 | 0 | 102066 | 45475 | 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 181.

The worst 5 of 45475 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) |
|-----------------|------------------|--------------------------|-------------------|
| 25:BA:1204:A:C2 | 30:BF:188:ARG:HA | 1.17 | 1.61 |
| 25:BA:2459:A:N3 | 25:BA:2460:U:H1' | 1.22 | 1.46 |
| 25:BA:1204:A:C2 | 30:BF:188:ARG:CA | 1.98 | 1.45 |
| 25:BA:2745:C:N4 | 25:BA:2756:U:C5 | 1.85 | 1.45 |
| 25:BA:1475:G:H1 | 25:BA:1477:A:N6 | 1.11 | 1.44 |

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 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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 5 | AE | 232/256 (91%) | 112 (48%) | 47 (20%) | 73 (32%) | 0 | 0 |
| 6 | AF | 204/239 (85%) | 115 (56%) | 43 (21%) | 46 (22%) | 0 | 1 |
| 7 | AG | 206/209 (99%) | 103 (50%) | 61 (30%) | 42 (20%) | 0 | 2 |
| 8 | AH | 148/162 (91%) | 92 (62%) | 34 (23%) | 22 (15%) | 0 | 4 |
| 9 | AI | 99/101 (98%) | 58 (59%) | 19 (19%) | 22 (22%) | 0 | 1 |
| 10 | AJ | 153/156 (98%) | 74 (48%) | 40 (26%) | 39 (26%) | 0 | 1 |
| 11 | AK | 136/138 (99%) | 71 (52%) | 32 (24%) | 33 (24%) | 0 | 1 |
| 12 | AL | 125/128 (98%) | 64 (51%) | 33 (26%) | 28 (22%) | 0 | 1 |
| 13 | AM | 96/105 (91%) | 55 (57%) | 14 (15%) | 27 (28%) | 0 | 0 |
| 14 | AN | 117/129 (91%) | 62 (53%) | 30 (26%) | 25 (21%) | 0 | 1 |
| 15 | AO | 122/132 (92%) | 62 (51%) | 22 (18%) | 38 (31%) | 0 | 0 |
| 16 | AP | 123/126 (98%) | 63 (51%) | 36 (29%) | 24 (20%) | 0 | 2 |
| 17 | AQ | 58/61 (95%) | 28 (48%) | 14 (24%) | 16 (28%) | 0 | 0 |
| 18 | AR | 86/89 (97%) | 40 (46%) | 33 (38%) | 13 (15%) | 0 | 4 |
| 19 | AS | 81/88 (92%) | 45 (56%) | 21 (26%) | 15 (18%) | 0 | 2 |
| 20 | AT | 102/105 (97%) | 63 (62%) | 22 (22%) | 17 (17%) | 0 | 3 |
| 21 | AU | 71/88 (81%) | 30 (42%) | 18 (25%) | 23 (32%) | 0 | 0 |
| 22 | AV | 78/93 (84%) | 32 (41%) | 18 (23%) | 28 (36%) | 0 | 0 |
| 23 | AW | 97/106 (92%) | 32 (33%) | 36 (37%) | 29 (30%) | 0 | 0 |
| 24 | AX | 22/27 (82%) | 9 (41%) | 8 (36%) | 5 (23%) | 0 | 1 |
| 27 | BC | 226/229 (99%) | 137 (61%) | 52 (23%) | 37 (16%) | 0 | 3 |
| 28 | BD | 270/276 (98%) | 129 (48%) | 49 (18%) | 92 (34%) | 0 | 0 |
| 29 | BE | 204/206 (99%) | 106 (52%) | 39 (19%) | 59 (29%) | 0 | 0 |
| 30 | BF | 206/210 (98%) | 100 (48%) | 47 (23%) | 59 (29%) | 0 | 0 |
| 31 | BG | 180/182 (99%) | 79 (44%) | 42 (23%) | 59 (33%) | 0 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|------------|-------------|---|
| 32 | BH | 172/180 (96%) | 89 (52%) | 41 (24%) | 42 (24%) | 0 | 1 |
| 33 | BK | 146/148 (99%) | 88 (60%) | 32 (22%) | 26 (18%) | 0 | 2 |
| 34 | BL | 136/147 (92%) | 66 (48%) | 32 (24%) | 38 (28%) | 0 | 0 |
| 35 | BM | 137/140 (98%) | 66 (48%) | 31 (23%) | 40 (29%) | 0 | 0 |
| 36 | BN | 120/122 (98%) | 63 (52%) | 21 (18%) | 36 (30%) | 0 | 0 |
| 37 | BO | 143/150 (95%) | 60 (42%) | 31 (22%) | 52 (36%) | 0 | 0 |
| 38 | BP | 134/141 (95%) | 51 (38%) | 35 (26%) | 48 (36%) | 0 | 0 |
| 39 | BQ | 115/118 (98%) | 64 (56%) | 33 (29%) | 18 (16%) | 0 | 4 |
| 40 | BR | 108/112 (96%) | 45 (42%) | 30 (28%) | 33 (31%) | 0 | 0 |
| 41 | BS | 115/146 (79%) | 53 (46%) | 26 (23%) | 36 (31%) | 0 | 0 |
| 42 | BT | 115/118 (98%) | 49 (43%) | 39 (34%) | 27 (24%) | 0 | 1 |
| 43 | BU | 99/101 (98%) | 51 (52%) | 22 (22%) | 26 (26%) | 0 | 1 |
| 44 | BV | 108/113 (96%) | 69 (64%) | 15 (14%) | 24 (22%) | 0 | 1 |
| 45 | BW | 92/96 (96%) | 59 (64%) | 14 (15%) | 19 (21%) | 0 | 2 |
| 46 | BX | 108/110 (98%) | 41 (38%) | 27 (25%) | 40 (37%) | 0 | 0 |
| 47 | BY | 178/206 (86%) | 93 (52%) | 48 (27%) | 37 (21%) | 0 | 2 |
| 48 | BZ | 83/85 (98%) | 50 (60%) | 14 (17%) | 19 (23%) | 0 | 1 |
| 49 | B1 | 65/67 (97%) | 27 (42%) | 26 (40%) | 12 (18%) | 0 | 2 |
| 50 | B2 | 57/60 (95%) | 32 (56%) | 16 (28%) | 9 (16%) | 0 | 3 |
| 51 | B3 | 69/71 (97%) | 26 (38%) | 19 (28%) | 24 (35%) | 0 | 0 |
| 52 | B4 | 55/60 (92%) | 16 (29%) | 12 (22%) | 27 (49%) | 0 | 0 |
| 53 | B5 | 47/54 (87%) | 13 (28%) | 7 (15%) | 27 (57%) | 0 | 0 |
| 54 | B6 | 47/49 (96%) | 16 (34%) | 16 (34%) | 15 (32%) | 0 | 0 |
| 55 | B7 | 62/65 (95%) | 29 (47%) | 11 (18%) | 22 (36%) | 0 | 0 |
| 56 | B8 | 35/37 (95%) | 20 (57%) | 4 (11%) | 11 (31%) | 0 | 0 |
| All | All | 5988/6337 (94%) | 2997 (50%) | 1412 (24%) | 1579 (26%) | 0 | 1 |

5 of 1579 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 13 | ALA |
| 5 | AE | 15 | VAL |
| 5 | AE | 17 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 19 | HIS |
| 5 | AE | 20 | GLU |

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 |
|-----|-------|----------------|-----------|----------|-------------|
| 5 | AE | 202/220 (92%) | 135 (67%) | 67 (33%) | 0 2 |
| 6 | AF | 160/188 (85%) | 123 (77%) | 37 (23%) | 1 5 |
| 7 | AG | 180/181 (99%) | 127 (71%) | 53 (29%) | 0 2 |
| 8 | AH | 115/123 (94%) | 75 (65%) | 40 (35%) | 0 1 |
| 9 | AI | 90/90 (100%) | 64 (71%) | 26 (29%) | 0 3 |
| 10 | AJ | 126/127 (99%) | 95 (75%) | 31 (25%) | 0 4 |
| 11 | AK | 119/119 (100%) | 76 (64%) | 43 (36%) | 0 1 |
| 12 | AL | 98/99 (99%) | 76 (78%) | 22 (22%) | 1 6 |
| 13 | AM | 88/92 (96%) | 65 (74%) | 23 (26%) | 0 4 |
| 14 | AN | 90/99 (91%) | 62 (69%) | 28 (31%) | 0 2 |
| 15 | AO | 104/109 (95%) | 77 (74%) | 27 (26%) | 0 4 |
| 16 | AP | 100/101 (99%) | 79 (79%) | 21 (21%) | 1 7 |
| 17 | AQ | 49/50 (98%) | 37 (76%) | 12 (24%) | 0 4 |
| 18 | AR | 79/80 (99%) | 56 (71%) | 23 (29%) | 0 3 |
| 19 | AS | 72/74 (97%) | 48 (67%) | 24 (33%) | 0 2 |
| 20 | AT | 96/97 (99%) | 71 (74%) | 25 (26%) | 0 4 |
| 21 | AU | 64/77 (83%) | 41 (64%) | 23 (36%) | 0 1 |
| 22 | AV | 71/80 (89%) | 57 (80%) | 14 (20%) | 1 9 |
| 23 | AW | 76/82 (93%) | 56 (74%) | 20 (26%) | 0 4 |
| 24 | AX | 19/22 (86%) | 13 (68%) | 6 (32%) | 0 2 |
| 27 | BC | 180/181 (99%) | 151 (84%) | 29 (16%) | 2 15 |
| 28 | BD | 215/218 (99%) | 151 (70%) | 64 (30%) | 0 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-------------|---|
| 29 | BE | 166/166 (100%) | 102 (61%) | 64 (39%) | 0 | 0 |
| 30 | BF | 164/166 (99%) | 104 (63%) | 60 (37%) | 0 | 1 |
| 31 | BG | 156/156 (100%) | 112 (72%) | 44 (28%) | 0 | 3 |
| 32 | BH | 143/148 (97%) | 97 (68%) | 46 (32%) | 0 | 2 |
| 33 | BK | 124/124 (100%) | 87 (70%) | 37 (30%) | 0 | 2 |
| 34 | BL | 105/111 (95%) | 85 (81%) | 20 (19%) | 1 | 9 |
| 35 | BM | 118/119 (99%) | 80 (68%) | 38 (32%) | 0 | 2 |
| 36 | BN | 100/100 (100%) | 65 (65%) | 35 (35%) | 0 | 1 |
| 37 | BO | 111/116 (96%) | 64 (58%) | 47 (42%) | 0 | 0 |
| 38 | BP | 106/111 (96%) | 55 (52%) | 51 (48%) | 0 | 0 |
| 39 | BQ | 100/101 (99%) | 69 (69%) | 31 (31%) | 0 | 2 |
| 40 | BR | 87/88 (99%) | 55 (63%) | 32 (37%) | 0 | 1 |
| 41 | BS | 105/127 (83%) | 69 (66%) | 36 (34%) | 0 | 1 |
| 42 | BT | 93/94 (99%) | 64 (69%) | 29 (31%) | 0 | 2 |
| 43 | BU | 82/82 (100%) | 59 (72%) | 23 (28%) | 0 | 3 |
| 44 | BV | 90/92 (98%) | 56 (62%) | 34 (38%) | 0 | 0 |
| 45 | BW | 76/78 (97%) | 55 (72%) | 21 (28%) | 0 | 3 |
| 46 | BX | 91/91 (100%) | 66 (72%) | 25 (28%) | 0 | 3 |
| 47 | BY | 159/179 (89%) | 110 (69%) | 49 (31%) | 0 | 2 |
| 48 | BZ | 67/67 (100%) | 52 (78%) | 15 (22%) | 1 | 6 |
| 49 | B1 | 62/62 (100%) | 46 (74%) | 16 (26%) | 0 | 4 |
| 50 | B2 | 51/52 (98%) | 34 (67%) | 17 (33%) | 0 | 2 |
| 51 | B3 | 63/63 (100%) | 42 (67%) | 21 (33%) | 0 | 2 |
| 52 | B4 | 50/52 (96%) | 30 (60%) | 20 (40%) | 0 | 0 |
| 53 | B5 | 48/52 (92%) | 32 (67%) | 16 (33%) | 0 | 2 |
| 54 | B6 | 42/42 (100%) | 30 (71%) | 12 (29%) | 0 | 3 |
| 55 | B7 | 54/55 (98%) | 40 (74%) | 14 (26%) | 0 | 4 |
| 56 | B8 | 34/34 (100%) | 25 (74%) | 9 (26%) | 0 | 4 |
| All | All | 5040/5237 (96%) | 3520 (70%) | 1520 (30%) | 0 | 2 |

5 of 1520 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | BE | 101 | ARG |
| 32 | BH | 103 | LEU |
| 49 | B1 | 45 | ILE |
| 29 | BE | 155 | LYS |
| 30 | BF | 175 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | AV | 23 | ASN |
| 29 | BE | 129 | HIS |
| 51 | B3 | 46 | GLN |
| 23 | AW | 45 | GLN |
| 28 | BD | 87 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1515/1522 (99%) | 479 (31%) | 151 (9%) |
| 2 | AC | 75/76 (98%) | 30 (40%) | 7 (9%) |
| 25 | BA | 2888/2916 (99%) | 1241 (42%) | 313 (10%) |
| 26 | BB | 122/123 (99%) | 46 (37%) | 5 (4%) |
| 3 | AD | 75/76 (98%) | 27 (36%) | 3 (4%) |
| 4 | A1 | 26/27 (96%) | 11 (42%) | 1 (3%) |
| All | All | 4701/4740 (99%) | 1834 (39%) | 480 (10%) |

5 of 1834 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 6 | G |
| 1 | AA | 8 | A |
| 1 | AA | 9 | G |
| 1 | AA | 13 | U |
| 1 | AA | 14 | U |

5 of 480 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | BA | 562 | U |
| 25 | BA | 974(A) | C |
| 25 | BA | 2610 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BA | 616 | A |
| 25 | BA | 783 | 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](#)

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 [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 25 | BA | 6 |
| 1 | AA | 2 |

The worst 5 of 8 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | BA | 1202:C | O3' | 1203:G | P | 1.97 |
| 1 | AA | 173:U | O3' | 174:C | P | 1.84 |
| 1 | BA | 2601:C | O3' | 2602:A | P | 1.84 |
| 1 | BA | 2756:U | O3' | 2757:A | P | 1.84 |
| 1 | BA | 2755:C | O3' | 2756:U | P | 1.75 |

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1515/1522 (99%) | -0.79 | 2 (0%) 95 94 | 188, 245, 349, 445 | 0 |
| 2 | AC | 76/76 (100%) | -0.94 | 0 100 100 | 213, 249, 283, 294 | 0 |
| 3 | AD | 76/76 (100%) | -0.82 | 0 100 100 | 301, 334, 358, 368 | 0 |
| 4 | A1 | 27/27 (100%) | 0.73 | 6 (22%) 0 1 | 225, 347, 415, 416 | 0 |
| 5 | AE | 234/256 (91%) | -0.27 | 7 (2%) 50 39 | 218, 248, 286, 307 | 0 |
| 6 | AF | 206/239 (86%) | 0.22 | 11 (5%) 26 23 | 246, 269, 288, 296 | 0 |
| 7 | AG | 208/209 (99%) | -0.80 | 0 100 100 | 202, 233, 251, 265 | 0 |
| 8 | AH | 150/162 (92%) | -0.56 | 0 100 100 | 202, 220, 245, 262 | 0 |
| 9 | AI | 101/101 (100%) | 0.31 | 4 (3%) 38 31 | 219, 237, 254, 271 | 0 |
| 10 | AJ | 155/156 (99%) | 0.13 | 8 (5%) 27 24 | 250, 273, 285, 301 | 0 |
| 11 | AK | 138/138 (100%) | -0.81 | 0 100 100 | 203, 222, 236, 246 | 0 |
| 12 | AL | 127/128 (99%) | -0.50 | 0 100 100 | 247, 317, 349, 353 | 0 |
| 13 | AM | 98/105 (93%) | 0.29 | 6 (6%) 21 17 | 256, 296, 311, 317 | 0 |
| 14 | AN | 119/129 (92%) | -0.24 | 1 (0%) 86 79 | 214, 234, 252, 279 | 0 |
| 15 | AO | 124/132 (93%) | -0.29 | 0 100 100 | 189, 217, 243, 263 | 0 |
| 16 | AP | 125/126 (99%) | -0.68 | 0 100 100 | 253, 281, 302, 306 | 0 |
| 17 | AQ | 60/61 (98%) | -0.43 | 0 100 100 | 243, 273, 286, 290 | 0 |
| 18 | AR | 88/89 (98%) | -1.04 | 0 100 100 | 199, 222, 244, 251 | 0 |
| 19 | AS | 83/88 (94%) | -0.89 | 0 100 100 | 192, 212, 232, 267 | 0 |
| 20 | AT | 104/105 (99%) | -1.08 | 0 100 100 | 192, 218, 252, 296 | 0 |
| 21 | AU | 73/88 (82%) | -0.47 | 3 (4%) 37 30 | 192, 228, 255, 277 | 0 |
| 22 | AV | 80/93 (86%) | 0.29 | 2 (2%) 57 48 | 251, 287, 306, 310 | 0 |
| 23 | AW | 99/106 (93%) | -0.93 | 0 100 100 | 200, 228, 250, 254 | 0 |
| 24 | AX | 24/27 (88%) | -1.06 | 0 100 100 | 268, 289, 303, 306 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 25 | BA | 2889/2916 (99%) | -0.78 | 0 100 100 | 168, 241, 340, 398 | 0 |
| 26 | BB | 123/123 (100%) | -0.58 | 0 100 100 | 236, 293, 329, 343 | 0 |
| 27 | BC | 228/229 (99%) | 0.98 | 54 (23%) 0 1 | 299, 326, 342, 347 | 0 |
| 28 | BD | 272/276 (98%) | -0.14 | 6 (2%) 62 52 | 184, 216, 235, 256 | 0 |
| 29 | BE | 206/206 (100%) | -0.61 | 1 (0%) 91 85 | 155, 205, 250, 276 | 0 |
| 30 | BF | 208/210 (99%) | -0.59 | 0 100 100 | 186, 255, 283, 288 | 0 |
| 31 | BG | 182/182 (100%) | -0.56 | 2 (1%) 80 72 | 247, 283, 306, 311 | 0 |
| 32 | BH | 174/180 (96%) | -0.41 | 1 (0%) 89 84 | 230, 260, 278, 284 | 0 |
| 33 | BK | 148/148 (100%) | -0.61 | 0 100 100 | 212, 241, 261, 265 | 0 |
| 34 | BL | 138/147 (93%) | 0.61 | 22 (15%) 1 2 | 305, 358, 399, 403 | 0 |
| 35 | BM | 139/140 (99%) | -0.60 | 2 (1%) 75 66 | 187, 217, 245, 270 | 0 |
| 36 | BN | 122/122 (100%) | -0.66 | 0 100 100 | 172, 201, 228, 240 | 0 |
| 37 | BO | 145/150 (96%) | -0.20 | 10 (6%) 16 13 | 189, 271, 304, 346 | 0 |
| 38 | BP | 136/141 (96%) | -0.41 | 2 (1%) 73 64 | 199, 234, 257, 266 | 0 |
| 39 | BQ | 117/118 (99%) | -0.77 | 0 100 100 | 195, 214, 246, 256 | 0 |
| 40 | BR | 110/112 (98%) | -0.93 | 0 100 100 | 232, 266, 293, 300 | 0 |
| 41 | BS | 117/146 (80%) | -0.60 | 0 100 100 | 182, 205, 238, 244 | 0 |
| 42 | BT | 117/118 (99%) | -0.61 | 0 100 100 | 191, 221, 241, 250 | 0 |
| 43 | BU | 101/101 (100%) | -0.15 | 2 (1%) 65 56 | 190, 244, 272, 277 | 0 |
| 44 | BV | 110/113 (97%) | -0.44 | 1 (0%) 84 77 | 203, 226, 250, 260 | 0 |
| 45 | BW | 94/96 (97%) | -0.50 | 2 (2%) 63 54 | 237, 253, 304, 309 | 0 |
| 46 | BX | 110/110 (100%) | -0.31 | 3 (2%) 54 45 | 244, 282, 303, 312 | 0 |
| 47 | BY | 180/206 (87%) | -0.11 | 1 (0%) 89 84 | 235, 267, 281, 287 | 0 |
| 48 | BZ | 85/85 (100%) | -0.99 | 0 100 100 | 236, 259, 272, 289 | 0 |
| 49 | B1 | 67/67 (100%) | -0.62 | 0 100 100 | 251, 264, 276, 281 | 0 |
| 50 | B2 | 59/60 (98%) | -0.57 | 0 100 100 | 208, 244, 261, 268 | 0 |
| 51 | B3 | 71/71 (100%) | -0.93 | 0 100 100 | 212, 239, 259, 276 | 0 |
| 52 | B4 | 57/60 (95%) | -0.61 | 0 100 100 | 200, 227, 276, 299 | 0 |
| 53 | B5 | 49/54 (90%) | -0.38 | 2 (4%) 37 30 | 211, 247, 269, 277 | 0 |
| 54 | B6 | 49/49 (100%) | -0.88 | 0 100 100 | 189, 228, 244, 250 | 0 |
| 55 | B7 | 64/65 (98%) | -0.81 | 0 100 100 | 201, 220, 235, 247 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 56 | B8 | 37/37 (100%) | -1.10 | 0 100 100 | 212, 230, 240, 244 | 0 |
| All | All | 10794/11077 (97%) | -0.55 | 161 (1%) 73 64 | 155, 245, 336, 445 | 0 |

The worst 5 of 161 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 37 | BO | 123 | LEU | 12.3 |
| 27 | BC | 126 | LYS | 9.8 |
| 4 | A1 | 1 | G | 9.3 |
| 27 | BC | 125 | SER | 9.2 |
| 27 | BC | 121 | GLY | 8.3 |

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.