



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 02:38 PM UTC

PDB ID : 4V4Y / pdb\_00004v4y  
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome with translocated and rotated Shine-Dalgarno Duplex.  
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.  
Deposited on : 2006-06-27  
Resolution : 5.50 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

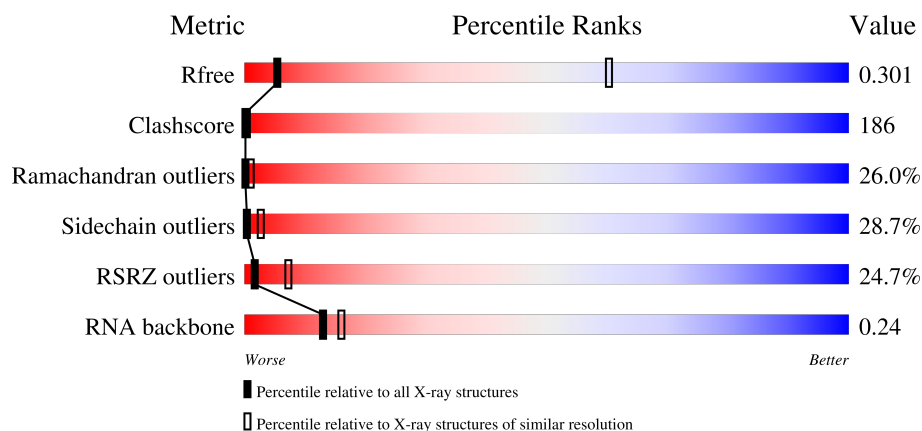
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 Å.

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



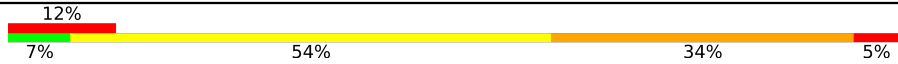
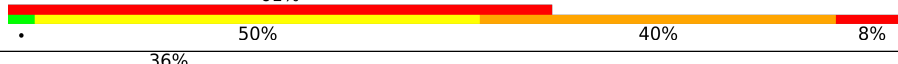
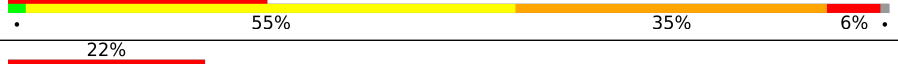
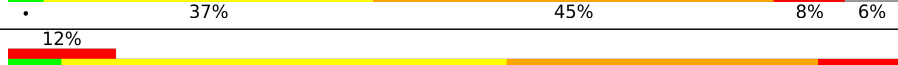
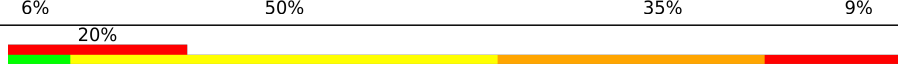
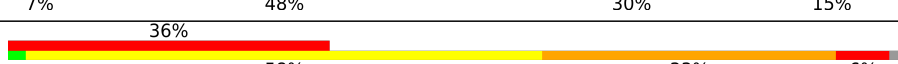
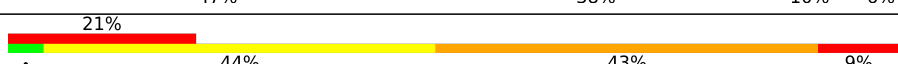
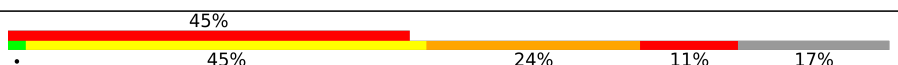
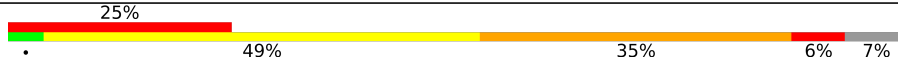
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1088 (7.00-4.00)                                      |
| Clashscore            | 190562                      | 1147 (7.00-4.00)                                      |
| Ramachandran outliers | 187476                      | 1012 (7.02-3.98)                                      |
| Sidechain outliers    | 187428                      | 1023 (7.04-3.96)                                      |
| RSRZ outliers         | 180081                      | 1081 (7.00-4.00)                                      |
| RNA backbone          | 3983                        | 1052 (7.80-3.10)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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   | <div> <div>13%</div> <div> <div>57%</div> <div>32%</div> <div>9%</div> </div> </div>               |
| 2   | A1    | 50     | <div> <div>76%</div> <div> <div>50%</div> <div>38%</div> <div>10%</div> </div> </div>              |
| 3   | AB    | 76     | <div> <div>71%</div> <div> <div>7%</div> <div>49%</div> <div>37%</div> <div>8%</div> </div> </div> |
| 3   | AC    | 76     | <div> <div>5%</div> <div> <div>59%</div> <div>34%</div> <div>7%</div> </div> </div>                |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | AD    | 76     |    |
| 4   | AE    | 256    |    |
| 5   | AF    | 239    |    |
| 6   | AG    | 209    |    |
| 7   | AH    | 162    |    |
| 8   | AI    | 101    |    |
| 9   | AJ    | 156    |    |
| 10  | AK    | 138    |    |
| 11  | AL    | 128    |    |
| 12  | AM    | 105    |    |
| 13  | AN    | 129    |    |
| 14  | AO    | 132    |   |
| 15  | AP    | 126    |  |
| 16  | AQ    | 61     |  |
| 17  | AR    | 89     |  |
| 18  | AS    | 88     |  |
| 19  | AT    | 105    |  |
| 20  | AU    | 88     |  |
| 21  | AV    | 93     |  |
| 22  | AW    | 106    |  |
| 23  | AX    | 27     |  |
| 24  | BA    | 2916   |  |
| 25  | BB    | 123    |  |
| 26  | BC    | 229    |  |
| 27  | BD    | 276    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BE    | 206    |                  |
| 29  | BF    | 210    |                  |
| 30  | BG    | 182    |                  |
| 31  | BH    | 180    |                  |
| 32  | BK    | 148    |                  |
| 33  | BL    | 147    |                  |
| 34  | BM    | 140    |                  |
| 35  | BN    | 122    |                  |
| 36  | BO    | 150    |                  |
| 37  | BP    | 141    |                  |
| 38  | BQ    | 118    |                  |
| 39  | BR    | 112    |                  |
| 40  | BS    | 146    |                  |
| 41  | BT    | 118    |                  |
| 42  | BU    | 101    |                  |
| 43  | BV    | 113    |                  |
| 44  | BW    | 96     |                  |
| 45  | BX    | 110    |                  |
| 46  | BY    | 206    |                  |
| 47  | BZ    | 85     |                  |
| 48  | B1    | 67     |                  |
| 49  | B2    | 60     |                  |
| 50  | B3    | 71     |                  |
| 51  | B4    | 60     |                  |
| 52  | B5    | 54     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | B6    | 49     |                  |
| 54  | B7    | 65     |                  |
| 55  | B8    | 37     |                  |

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 151691 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 ribosomal RNA.

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

- Molecule 2 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | A1    | 50       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1025  | 459 | 128 | 388 | 50 |         |         |       |

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

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

- Molecule 4 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AE    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | AF    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | AG    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AH    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AI    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AJ    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AK    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 11  | AL    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |  |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AM    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 794   | 499 | 156 | 138 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AN    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AO    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AP    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 16  | AQ    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AR    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | AS    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AT    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 20  | AU    | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | AV    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 647   | 414 | 119 | 112 | 2 |         |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | AW    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 23  | AX    | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 24  | BA    | 2889     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62218 | 27691 | 11629 | 20009 | 2889 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 25  | BB    | 123      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2641  | 1175 | 488 | 855 | 123 |         |         |       |

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 26 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | BC    | 228      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1742  | 1102 | 318 | 319 | 3 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27  | BD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2124  | 1339 | 424 | 358 | 3 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BE    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1578  | 997 | 302 | 273 | 6 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | BF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1034 | 303 | 286 | 2 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BG    | 182      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1482  | 947 | 269 | 261 | 5 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 844 | 248 | 235 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BK    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 737 | 205 | 212 | 1 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BL    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1025  | 654 | 181 | 185 | 5 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BM    | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1113  | 717 | 207 | 186 | 3 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 587 | 171 | 170 | 4 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BO    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1106  | 688 | 226 | 190 | 2 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BP    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1080  | 688 | 204 | 183 | 5 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 38  | BQ    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 39  | BR    | 110      | Total | C   | N   | O   |         |         |       |
|     |       |          | 877   | 553 | 175 | 149 | 0       | 0       | 0     |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BS    | 117      | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 976   | 614 | 197 | 164 | 1 | 0       | 0       | 0     |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BT    | 117      | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 964   | 610 | 202 | 151 | 1 | 0       | 0       | 0     |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BU    | 101      | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 779   | 501 | 142 | 135 | 1 | 0       | 0       | 0     |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BV    | 110      | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 876   | 552 | 171 | 151 | 2 | 0       | 0       | 0     |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44  | BW    | 94       | Total | C   | N   | O   |         |         |       |
|     |       |          | 742   | 483 | 133 | 126 | 0       | 0       | 0     |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BX    | 110      | Total | C   | N   | O   | S |         |         |       |
|     |       |          | 844   | 539 | 158 | 141 | 6 | 0       | 0       | 0     |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BY    | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1435  | 916 | 256 | 260 | 3 |         |         |       |

- Molecule 47 is a protein called Ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BZ    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 670   | 415 | 141 | 112 | 2 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 48  | B1    | 67       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 567   | 350 | 116 | 99 | 2 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49  | B2    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |   |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | B3    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | B4    | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 445   | 279 | 87 | 74 | 5 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B5    | 49       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 426   | 265 | 87 | 70 | 4 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53  | B6    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | B7    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 515   | 331 | 102 | 79 | 3 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L36.

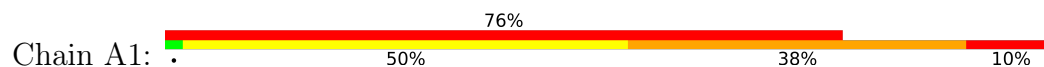
| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55  | B8    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |



|       |       |       |       |       |       |       |        |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|--------|------|------|------|------|------|
| G1464 | G1389 | A1340 | G1220 | U1159 | G1099 | C1039 | C984   | C924 | A864 | G798 | C738 | U678 |
| C1465 | C1400 | U1341 | G1221 | G1160 | C1100 | U1040 | C985   | G925 | A865 | G799 | C739 | C679 |
| C1466 | C1282 | C1342 | G1222 | C1161 | A1101 | A1041 | A986   | G926 | C866 | G800 | U740 | C680 |
| C1467 | C1283 | G1343 | C1223 | C1162 | A1102 | G1042 | G987   | G927 | G867 | U801 | G741 | C681 |
| A1468 | C1284 | C1344 | G1224 | C1163 | G1103 | A1043 | C988   | G928 | C868 | G803 | G742 | G682 |
| C1469 | C1285 | U1345 | A1225 | G1164 | G1104 | G1044 | C989   | G929 | G869 | G803 | U743 | G683 |
| G1470 | A1286 | A1346 | C1226 | C1165 | A1105 | C1045 | C990   | C930 | U870 | U804 | C744 | A684 |
| U1471 | U1287 | G1347 | A1227 | G1166 | A1106 | A1046 | U991   | C931 | U871 | C805 | C745 | G685 |
| U1472 | A1288 | U1348 | C1228 | A1167 | G1107 | G1047 | U992   | C932 | A872 | C806 | U746 | U686 |
| A1473 | A1289 | A1349 | U1229 | A1169 | G1108 | U1048 | A993   | G933 | A873 | C807 | C747 | A687 |
| G1474 | G1290 | A1350 | C1230 | A1170 | C1109 | U1049 | A994   | C934 | G874 | C808 | C748 | A688 |
| G1475 | G1291 | U1351 | G1231 | G1171 | A1110 | G1050 | A995   | A935 | C875 | G809 | C749 | C689 |
| G1476 | U1292 | C1352 | U1232 | C1172 | A1111 | C1051 | A996   | C936 | G876 | C810 | G750 | G690 |
| C1477 | G1293 | G1353 | G1233 | G1173 | C1112 | U1052 | U997   | A937 | C877 | C811 | U751 | G691 |
|       | G1294 | C1354 | C1234 | G1174 | C1113 | G1053 | C998   | A938 | C878 | C812 | G752 | U692 |
| C1478 | U1414 | G1355 | U1235 | G1175 | C1114 | C1054 | C998A  | G939 | C879 | U813 | A753 | G693 |
| C1479 | G1295 | G1356 | A1236 | A1176 | C1115 | A1055 | U999   | C940 | C880 | A814 | C754 | A694 |
| G1480 | C1296 | G1357 | G1237 | G1177 | C1116 | U1056 | A1000  | G941 | G881 | A815 | G755 | A695 |
| U1481 | C1297 | A1357 | C1238 | G1178 | C1117 | G1057 | G1001  | G942 | C882 | A816 | C756 | A696 |
| G1482 | C1298 | U1358 | A1238 | G1179 | C1118 | G1058 | G1002  | U943 | C883 | C817 | U757 | U697 |
| A1483 | A1299 | C1359 | A1239 | A1179 | C1119 | C1059 | G1003  | G944 | U884 | G818 | G758 | G698 |
| G1484 | G1300 | A1360 | U1240 | A1180 | C1119 | G1060 | A1004  | G945 | U885 | A819 | A759 | C699 |
| U1485 | U1301 | G1361 | G1241 | G1181 | G1120 | C1061 | A1005  | A946 | G886 | U820 | G760 | G700 |
| G1486 | C1302 | C1362 | C1242 | G1182 | U1121 | G1062 | C1006  | G947 | G887 | G821 | C761 | C701 |
| G1487 | G1303 | C1363 | C1243 | A1183 | U1122 | G1063 | C1007  | C948 | G888 | C822 | C762 | A702 |
| G1488 | G1304 | A1363 | C1244 | G1184 | G1123 | C1064 | C1008  | A949 | A889 | G823 | G763 | G703 |
| C1489 | G1305 | U1365 | A1245 | G1185 | G1124 | U1065 | G1009  | U950 | G890 | C824 | G764 | A704 |
| A1490 | A1306 | C1366 | C1246 | G1186 | U1125 | C1066 | G1010  | G951 | U891 | G825 | G765 | U705 |
| G1491 | U1307 | G1367 | U1247 | G1187 | C1126 | C1067 | G1011  | U952 | A892 | C826 | A766 | A706 |
| A1492 | G1308 | C1368 | A1248 | A1188 | G1127 | U1068 | G1012  | G953 | C893 | U827 | A767 | C707 |
| A1493 | U1309 | G1369 | C1249 | A1189 | C1128 | G1069 | G1013  | G954 | G894 | A828 | A768 | C708 |
| G1494 | G1310 | C1370 | A1250 | G1190 | C1129 | C1070 | A1014  | U955 | G895 | G829 | G769 | C709 |
| U1495 | C1311 | G1371 | A1251 | A1191 | A1130 | U1071 | A1015  | U956 | C896 | G830 | C770 | G710 |
| C1496 | G1312 | G1372 | C1252 | C1192 | G1131 | G1072 | A1016  | U957 | C897 | U831 | G771 | G711 |
| G1497 | U1313 | C1373 | G1253 | G1193 | C1132 | U1073 | G1017  | A958 | G898 | C832 | U772 | A712 |
| U1498 | C1314 | G1374 | C1254 | U1194 | G1133 | G1074 | C1018  | C959 | C899 | U833 | G773 | G713 |
| A1499 | U1315 | A1375 | G1255 | C1195 | G1134 | C1075 | C1019  | U960 | A900 | C834 | G774 | G714 |
| C1500 | G1316 | U1376 | A1256 | U1196 | U1135 | C1076 | U1020  | U961 | A891 | U835 | G775 | A715 |
| U1501 | C1317 | U1377 | U1257 | G1197 | U1136 | G1077 | G1021  | C962 | G902 | G836 | G776 | A716 |
| A1502 | A1318 | A1377 | G1258 | G1198 | C1137 | U1078 | G1022  | G963 | G903 | G837 | A777 | C717 |
| G1503 | C1319 | C1378 | C1259 | U1199 | G1138 | U1079 | G1023  | A964 | C904 | G838 | G778 | G718 |
| G1504 | U1320 | G1379 | C1260 | C1200 | C1139 | A1080 | G1024  | A965 | U905 | U841 | C779 | C719 |
| C1505 | C1321 | A1380 | A1261 | A1201 | G1140 | G1081 | U1025  | G966 | G906 | C942 | A780 | C720 |
| U1506 | G1322 | U1381 | C1262 | G1202 | G1141 | G1082 | C1026  | C967 | A907 | U843 | A781 | G721 |
| G1507 | C1323 | C1382 | G1263 | C1203 | G1142 | U1083 | C1027  | A968 | A908 | C948 | A782 | A722 |
| U1508 | A1324 | C1383 | C1264 | A1204 | G1143 | U1084 | C1028  | A969 | A909 | C949 | C783 | U723 |
| C1509 | C1325 | G1384 | G1265 | U1205 | C1144 | U1085 | C1028A | C970 | C910 | U850 | C784 | G724 |
| U1510 | C1326 | G1385 | G1266 | G1206 | G1145 | U1086 | C1028B | G971 | U911 | G851 | G785 | G725 |
| G1511 | C1327 | G1386 | C1267 | G1207 | A1146 | G1087 | G1029  | C972 | C912 | G852 | G786 | C726 |
| C1512 | C1328 | G1387 | A1268 | C1208 | C1147 | U1088 | C1030  | G973 | A913 | G853 | A787 | G727 |
| U1513 | A1329 | C1388 | A1269 | C1209 | U1148 | G1089 | G1031  | A974 | A914 | G854 | U788 | A728 |
| C1514 | U1330 | C1389 | C1270 | C1210 | C1149 | U1090 | A1032  | A975 | A915 | G855 | U789 | A729 |
| G1515 | G1331 | U1390 | G1271 | U1211 | U1150 | U1091 | C1032A | G976 | C916 | C956 | G790 | G730 |
| U1516 | A1332 | U1212 | G1272 | U1212 | A1151 | U1092 | G1032B | A977 | G917 | C957 | G791 | G731 |
| G1517 | C1333 | A1213 | C1273 | A1152 | C1153 | A1093 | G1033  | A978 | A918 | G858 | A792 | G732 |
| C1518 | G1334 | C1214 | G1274 | G1153 | C1154 | G1094 | G1034  | C979 | A919 | A859 | U793 | C733 |
| U1519 | C1335 | A1275 | A1275 | G1154 | G1155 | U1095 | A1035  | C980 | U920 | A860 | A794 | G734 |
| A1520 | C1336 | G1276 | G1276 | G1156 | G1156 | C1096 | G1036  | U921 | G921 | G861 | C795 | C735 |
| G1521 | G1337 | C1277 | U1277 | C1217 | U1157 | C1097 | C1037  | U982 | C922 | C962 | C796 | C736 |
| U1522 | G1338 | U1278 | C1278 | A1157 | C1097 | C1098 | C1038  | A983 | A923 | U863 | C797 | A737 |
| G1523 | A1339 | A1279 | A1279 | U1219 | C1158 |       |        |      |      |      |      |      |



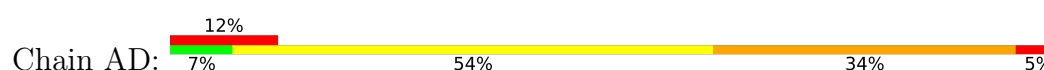
• Molecule 2: mRNA



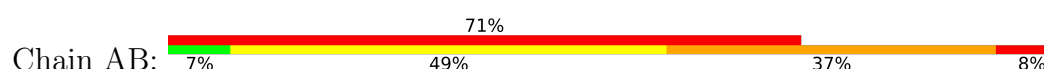
• Molecule 3: tRNA PHE (unmodified bases)



• Molecule 3: tRNA PHE (unmodified bases)

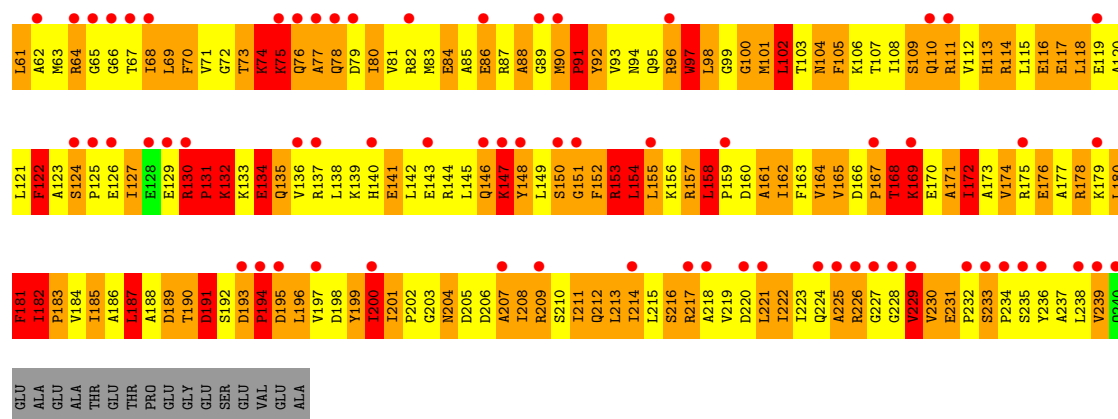


• Molecule 3: tRNA PHE (unmodified bases)

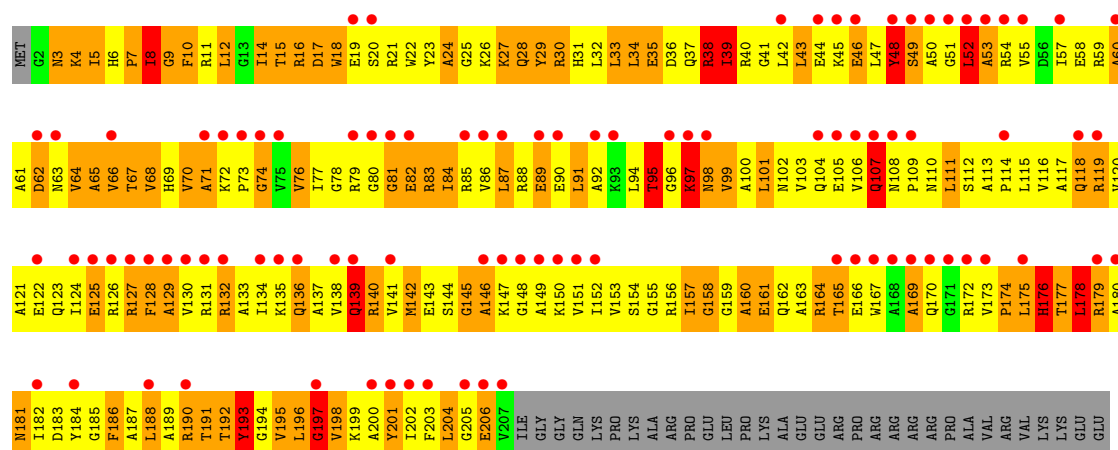


• Molecule 4: 30S ribosomal protein S2

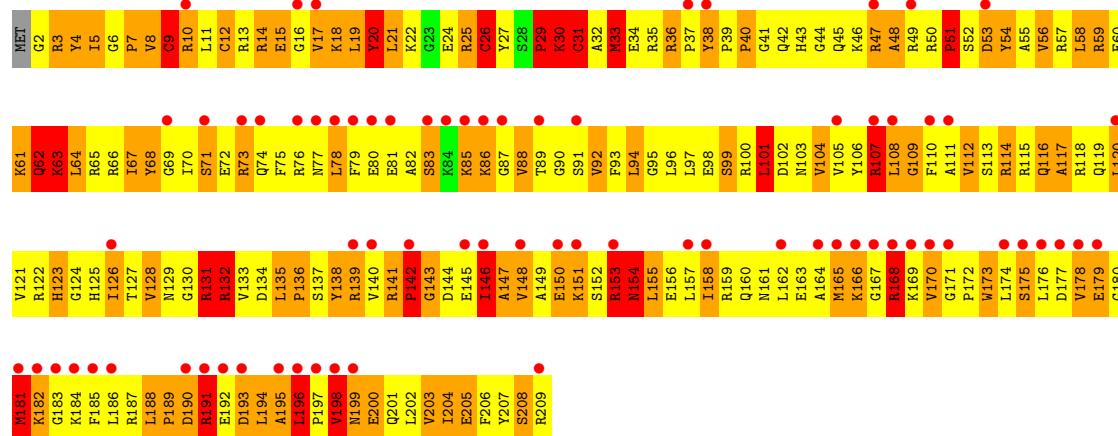




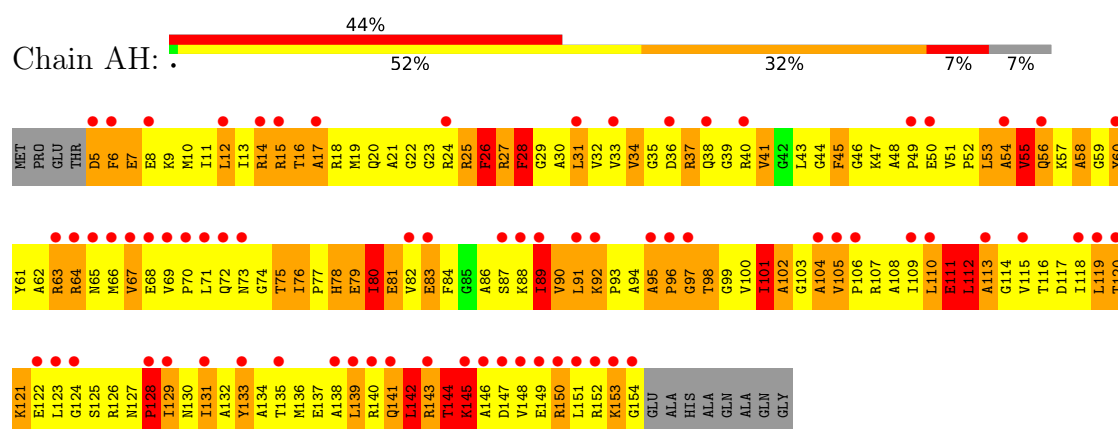
### • Molecule 5: 30S ribosomal protein S3



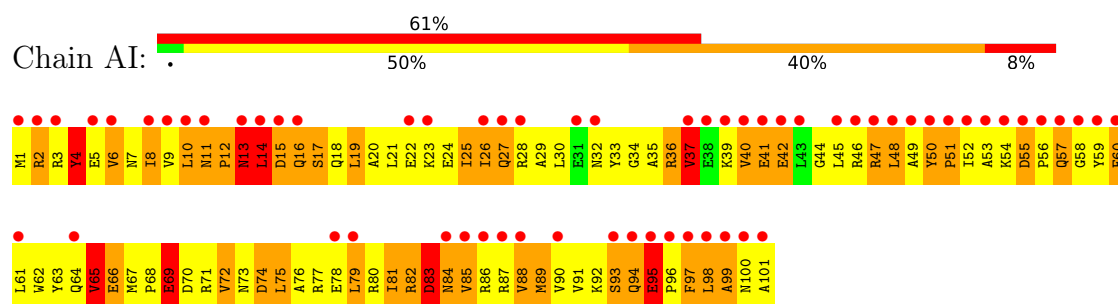
### • Molecule 6: 30S ribosomal protein S4



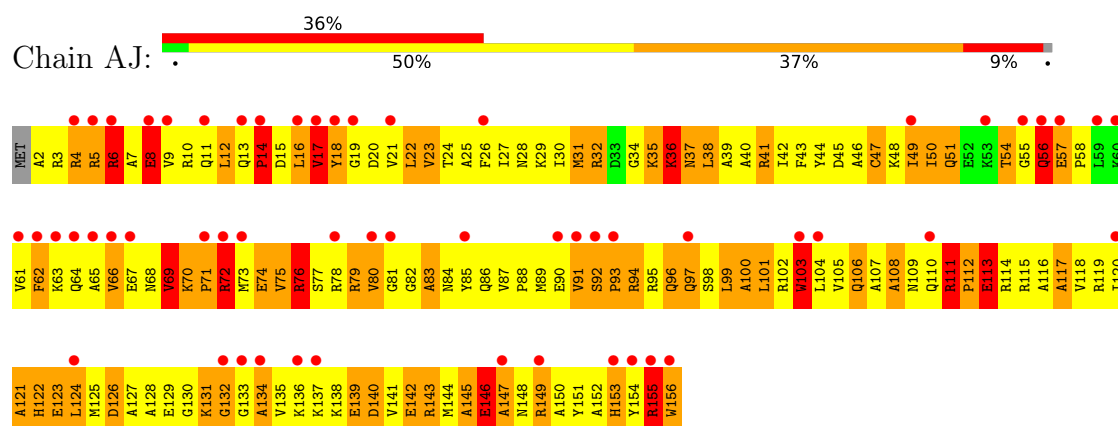
### • Molecule 7: 30S ribosomal protein S5



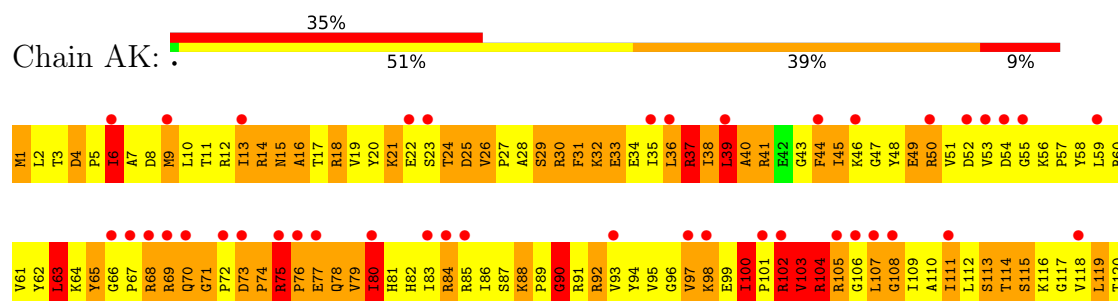
• Molecule 8: 30S ribosomal protein S6

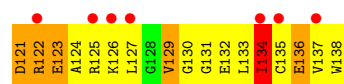


• Molecule 9: 30S ribosomal protein S7



• Molecule 10: 30S ribosomal protein S8

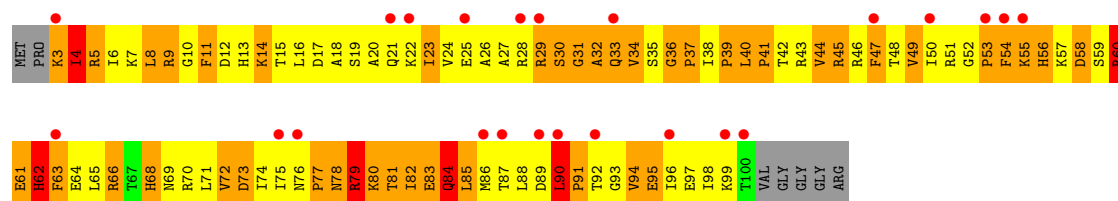




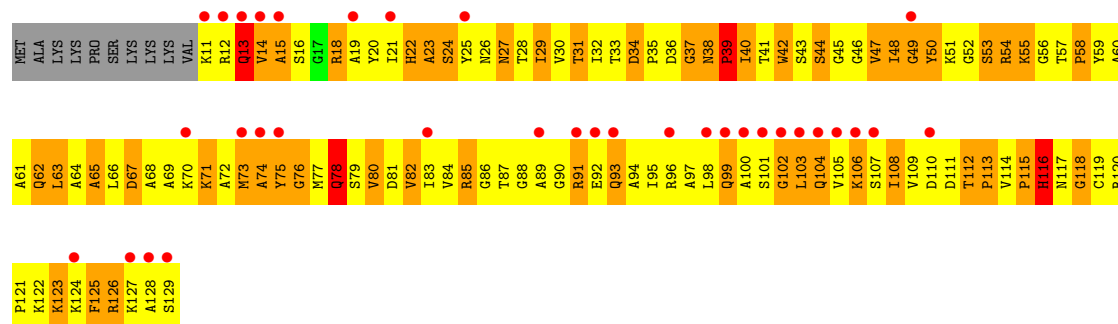
• Molecule 11: 30S ribosomal protein S9



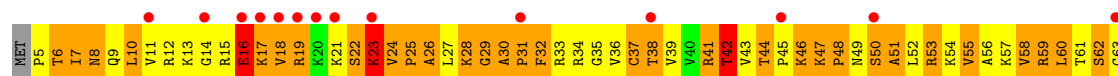
• Molecule 12: 30S ribosomal protein S10

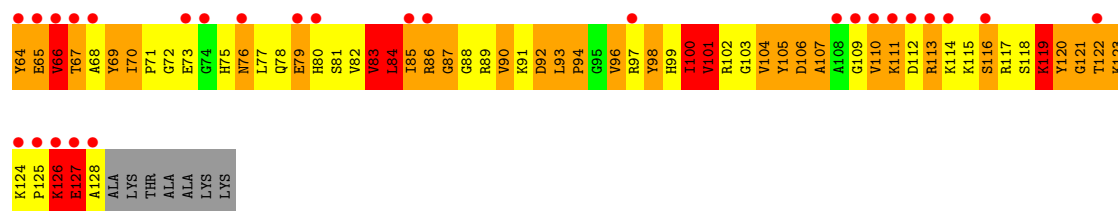


• Molecule 13: 30S ribosomal protein S11

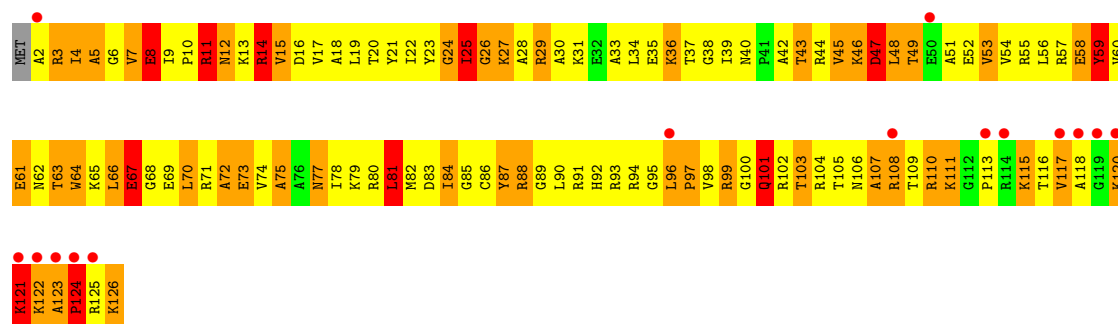


• Molecule 14: 30S ribosomal protein S12

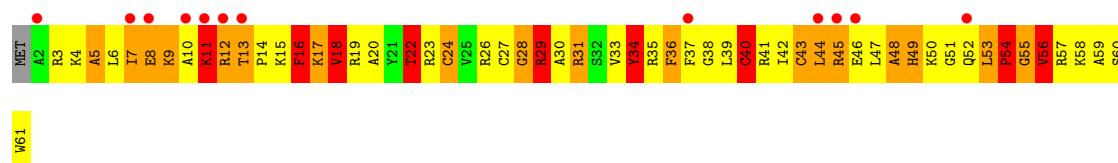




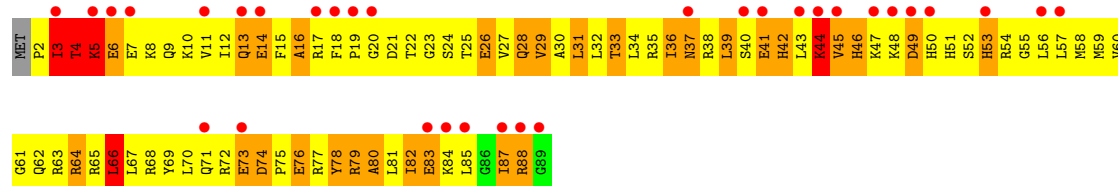
• Molecule 15: 30S ribosomal protein S13



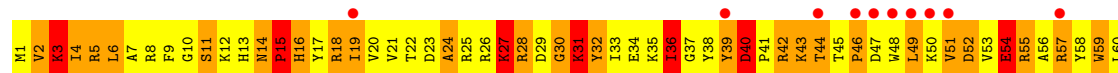
• Molecule 16: 30S ribosomal protein S14



• Molecule 17: 30S ribosomal protein S15



• Molecule 18: 30S ribosomal protein S16





|     |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | G2 | K3 | G4 | D5 | R6 | R7 | T8 | R9 | R10 | G11 | K12 | L13 | W14 | R15 | G16 | Y17 | Y18 | G19 | K20 | Y21 | R22 | P23 | R24 | K25 | LYS | LYS |
|-----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

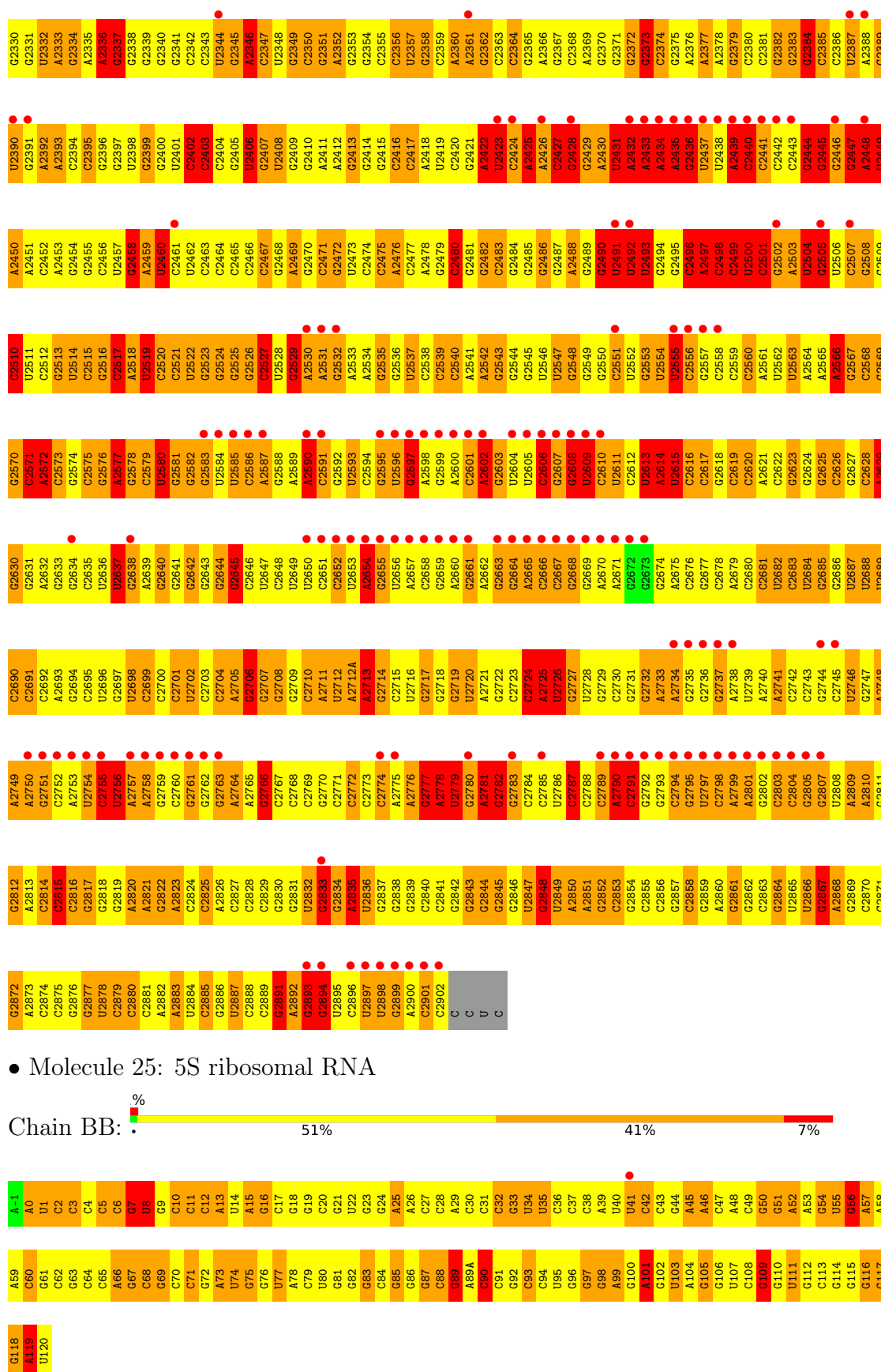
● Molecule 24: 23S ribosomal RNA

Chain BA: ● 19% 45% 39% 14%

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   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| G635 | G636 | A637 | G638 | U639 | C640 | C641 | G642 | A643 | A644 | C645 | A646 | G647 | G648 | G649 | C | G | C | A | A | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C | G | C 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| U1454 | A1395 | U1335 | A1214 | C1153 | U1094 | G1034 | C974A | C914 | G853 | A793 | G733 | C673 |
| G1455 | U1396 | A1336 | G1215 | G1154 | A1095 | U1035 | G975  | C915 | G854 | G794 | A734 | C674 |
| A1456 | U1397 | G1337 | G1216 | A1155 | A1096 | G1036 | C976  | G916 | G855 | A735 | A735 | A676 |
| A1457 | C1398 | G1338 | C1217 | A1156 | U1097 | G1037 | G977  | G917 | C856 | C796 | C736 | A677 |
| C1458 | C1399 | G1339 |       | A1157 | A1098 | C1038 | G978  | G918 | G857 | C797 | C737 | A678 |
| G1459 | G1400 | G1280 | A1220 | C1158 | G1099 | U1039 | G979  | G919 | U858 | G798 | G738 | C679 |
| A1460 | G1401 | G1281 | C1221 | U1159 | C1100 | C1040 | A980  | G920 | G859 | G799 | G739 | C680 |
| G1461 | C1402 | U1282 | C1222 | G1160 | U1101 | G1041 | A981  | G921 | U860 | A800 | U740 | C681 |
| C1462 | C1403 | G1283 | C1223 | C1161 | C1102 | G1042 | C982  | G922 | G861 | G801 | G741 | C682 |
| C1463 | C1404 | A1284 | G1224 | A1162 | A1103 | C1043 | A983  | C923 | G862 | A802 | G742 | C683 |
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| G1347 | A1287 | A1227 | A1227 | U1165 | G1106 | A1046 | C986  | A926 | C865 | G805 | G744 | A685 |
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| A1349 | C1289 | G1229 | G1229 | U1167 | G1108 | A1048 | A988  | G929 | C867 | U807 | U747 | C687 |
| A1469 | C1290 | C1230 | G1230 | G1168 | U1109 | C1049 | G989  | U930 | G868 | G808 | G748 | U688 |
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| A1354 | U1294 | U1234 | G1234 | G1173 | U1113 | C1053 | C993  | G934 | A872 | C812 | A752 | C692 |
| G1355 | C1295 | G1235 | G1235 | A1174 | G1114 | A1054 | C994  | C935 | G873 | U813 | C753 | C693 |
| G1356 | G1296 | A1236 | G1236 | G1175 | C1115 | G1055 | C995  | C936 | G874 | C814 | C754 | U694 |
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| A1360 | U1300 | U1240 | U1240 | C1179 | C1119 | G1059 | U999  | G940 | A878 | G818 | C758 | C698 |
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| C1375 | C1315 | U1255 | U1255 | A1194 | G1134 | G1074 | U1014 | G955 | C894 | U833 | U773 | G713 |
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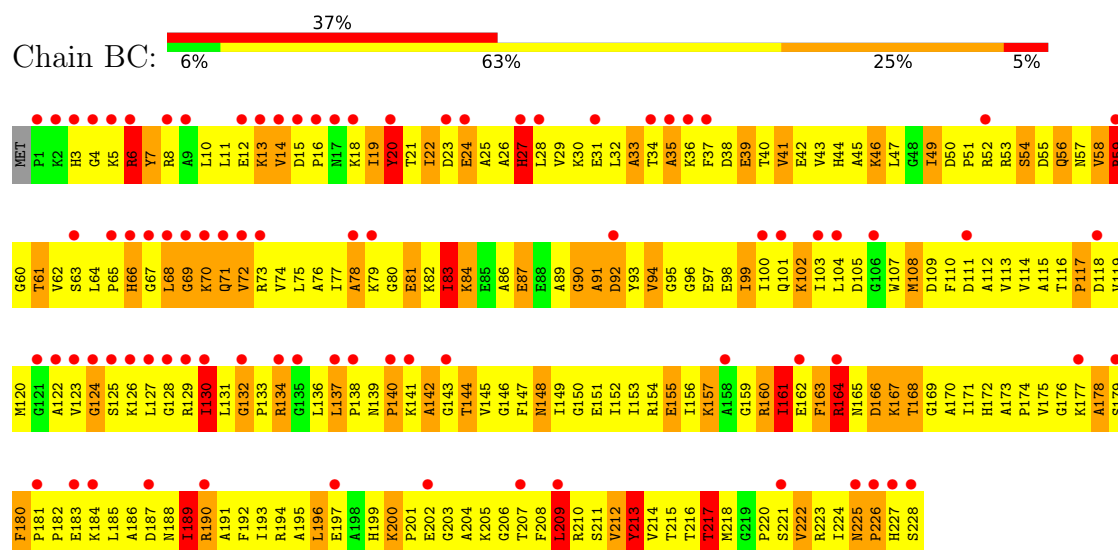
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| G1899 | A1900 | C1901 | C1902 | G1903 | G1904 | C1905 | G1906 | G1907 | C1908 | C1909 | G1910 | U1911 | A1912 | A1913 | C1914 | U1915 | A1916 | U1917 | U1918 | A1919 | C1920 | G1921 | G1922 | U1923 | G1924 | C1925 | U1926 | A1927 | A1928 | G1929 | G1930 | U1931 | A1932 | G1933 | C1934 | G1935 | A1936 | A1937 | A1938 | U1939 | U1940 | C1941 | C1942 | U1943 | G2004 | A1944 | G1945 | U1946 | C1947 | G1948 | G1949 | G1950 | U1951 | A1952 | A1953 | G1954 | U1955 | U1956  | C1957 | C1958 |       |       |       |       |
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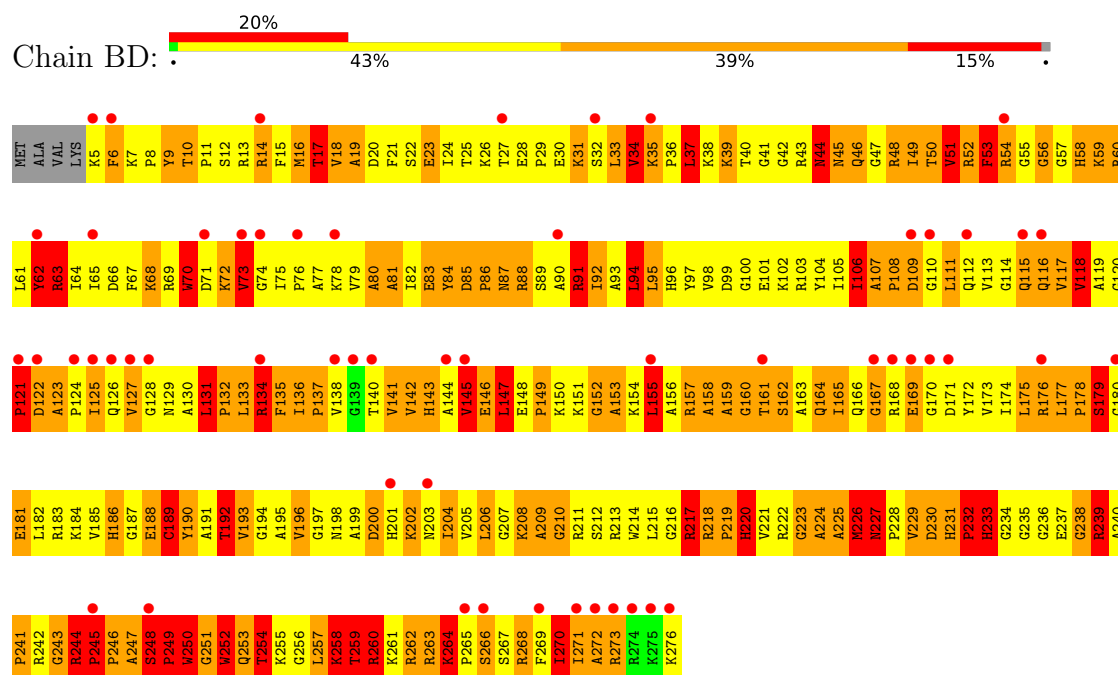
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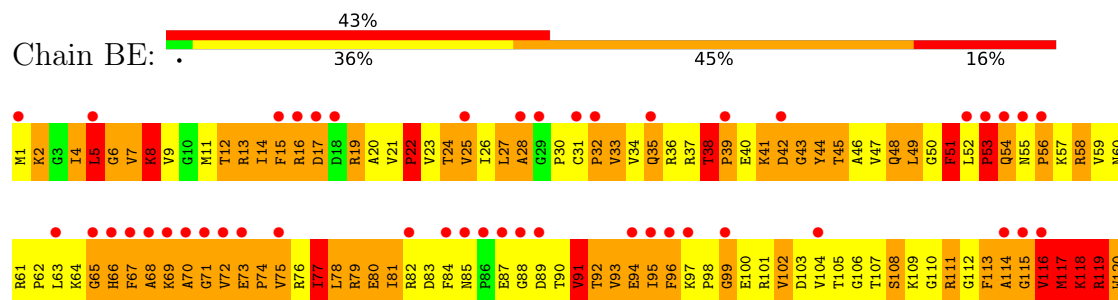
- Molecule 26: 50S ribosomal protein L1

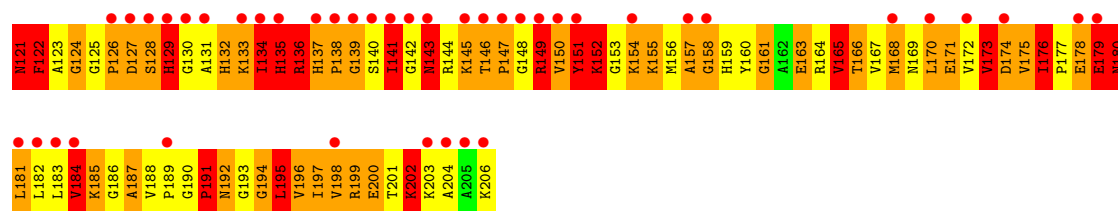


- Molecule 27: 50S ribosomal protein L2

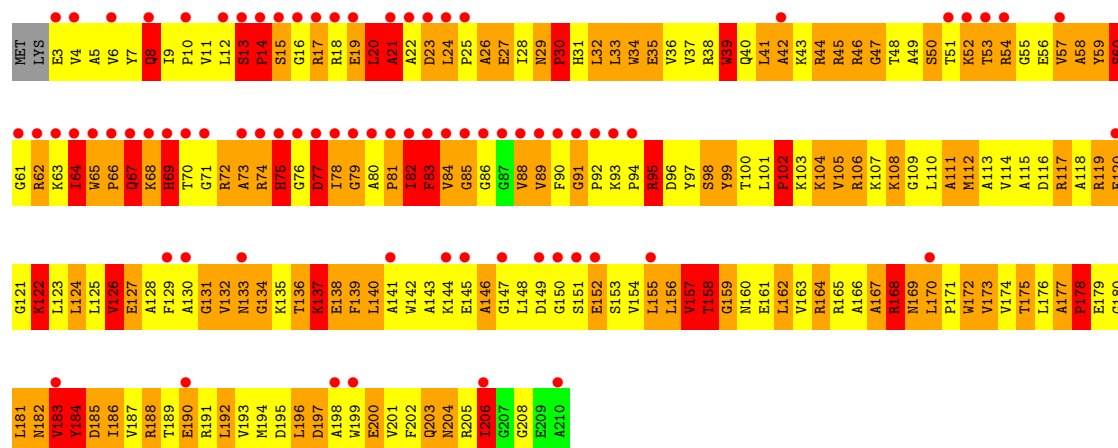


- Molecule 28: 50S ribosomal protein L3

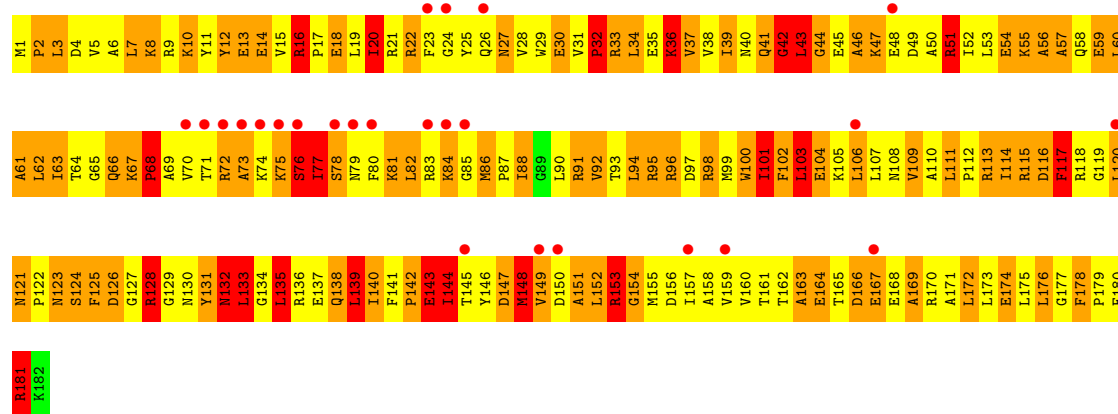




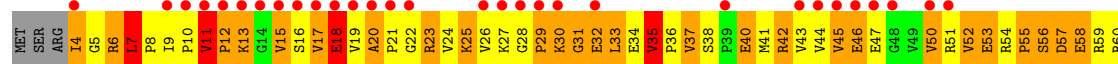
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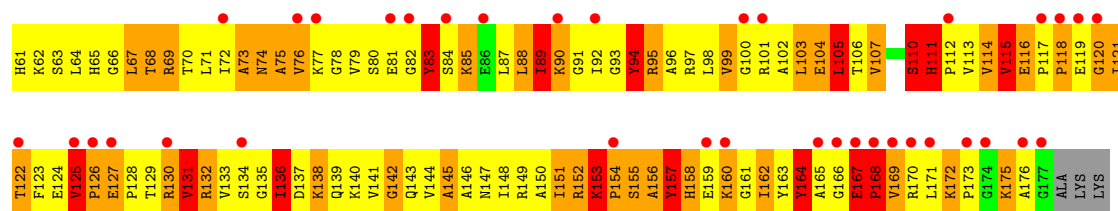


• Molecule 30: 50S ribosomal protein L5

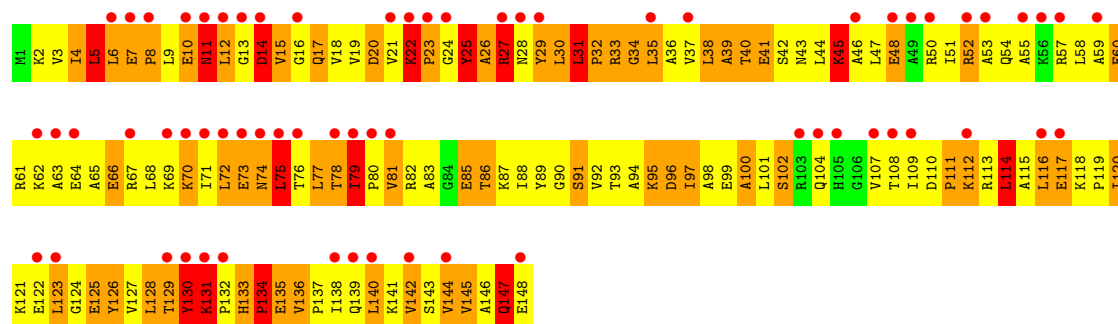


• Molecule 31: 50S ribosomal protein L6

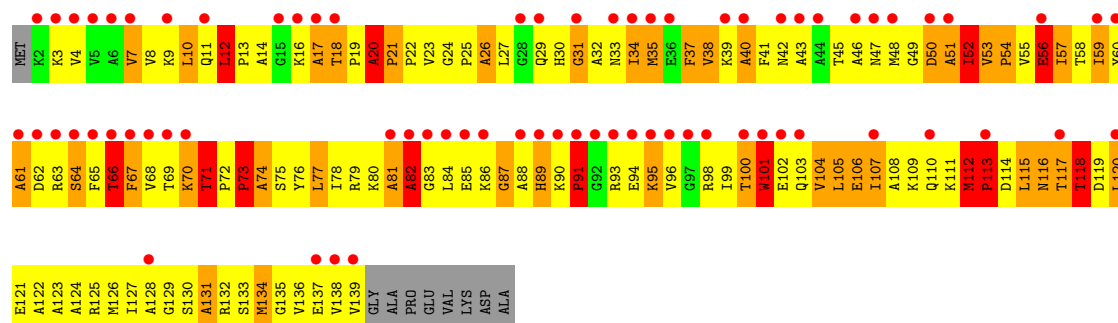




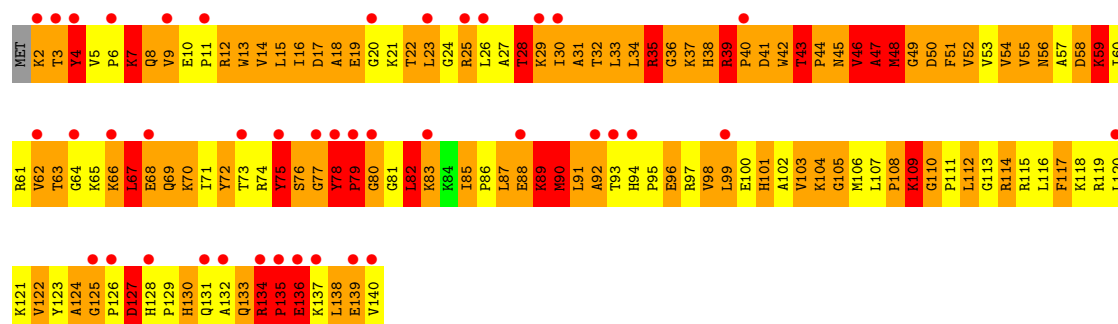
• Molecule 32: 50S ribosomal protein L9



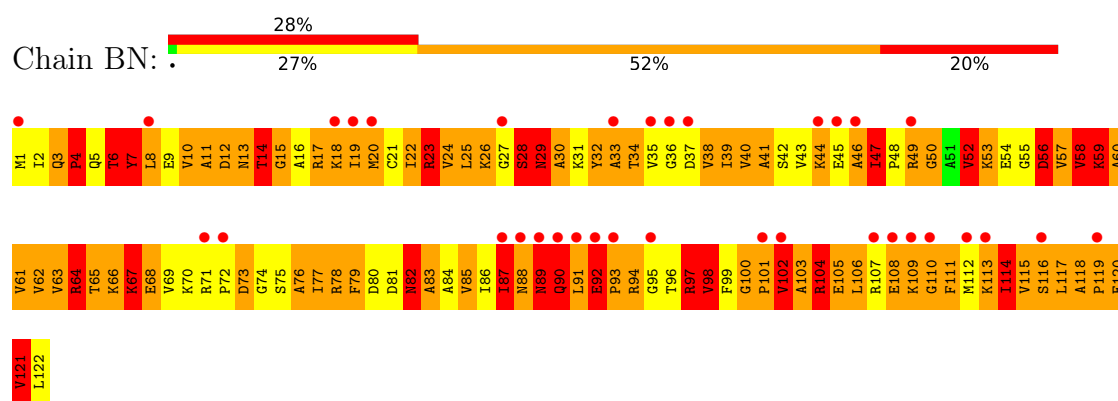
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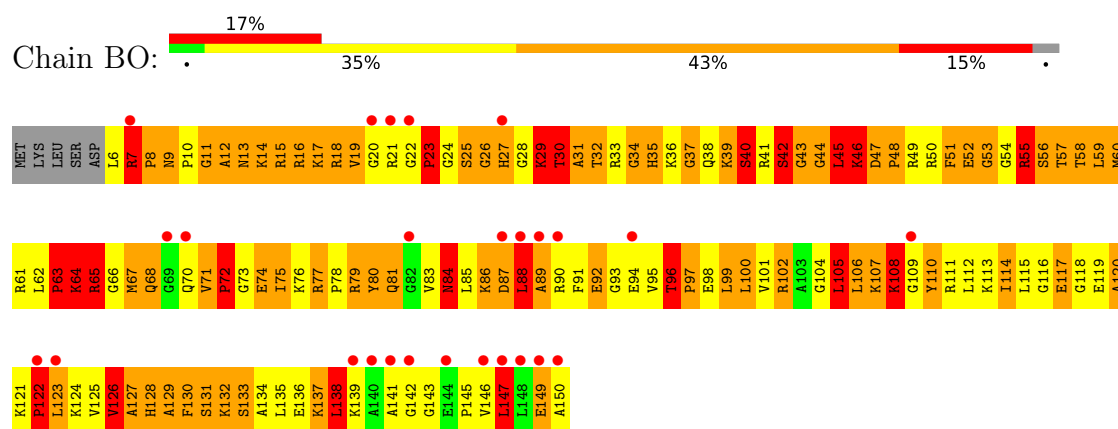
• Molecule 34: 50S ribosomal protein L13



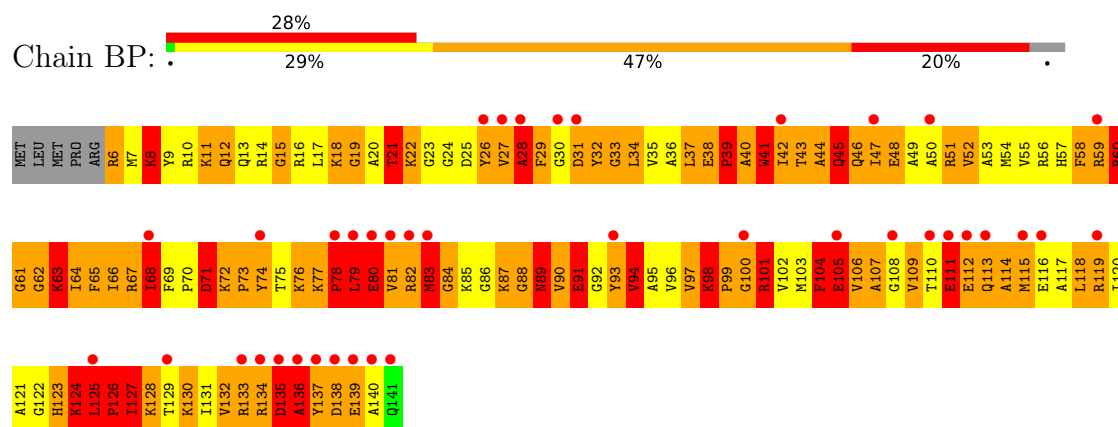
• Molecule 35: 50S ribosomal protein L14



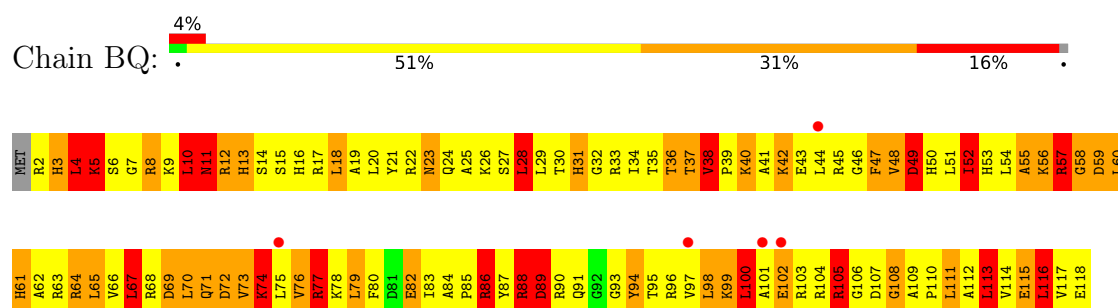
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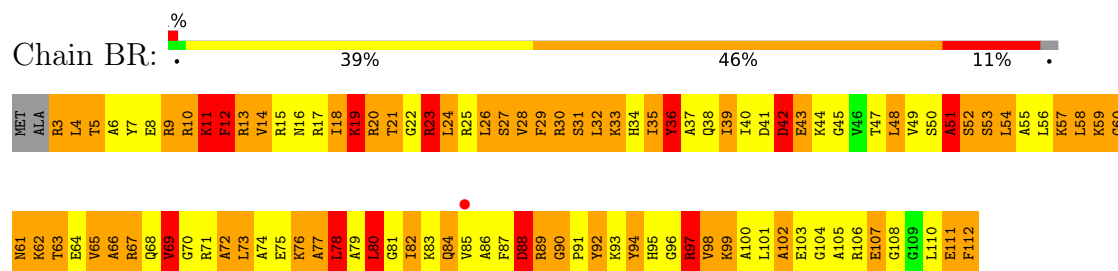
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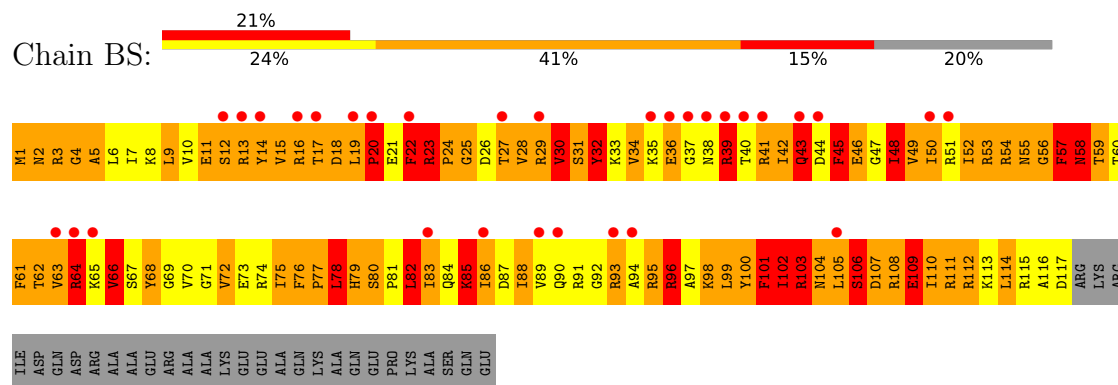
• Molecule 38: 50S ribosomal protein L17



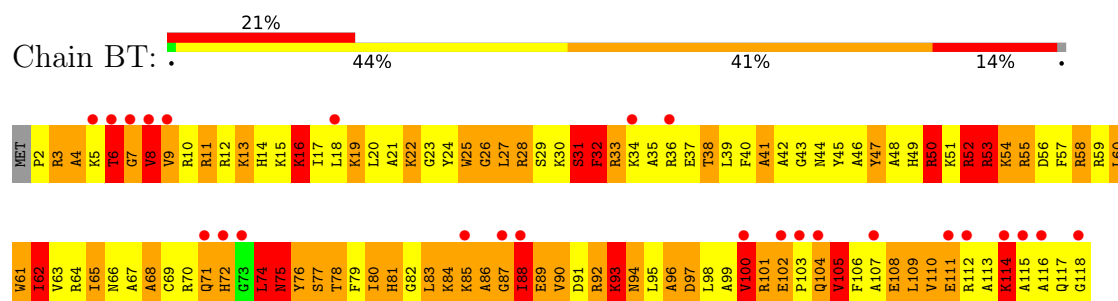
- Molecule 39: 50S ribosomal protein L18



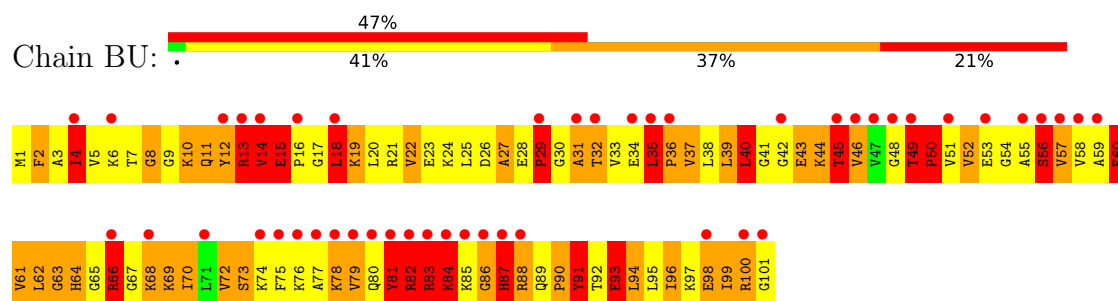
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20

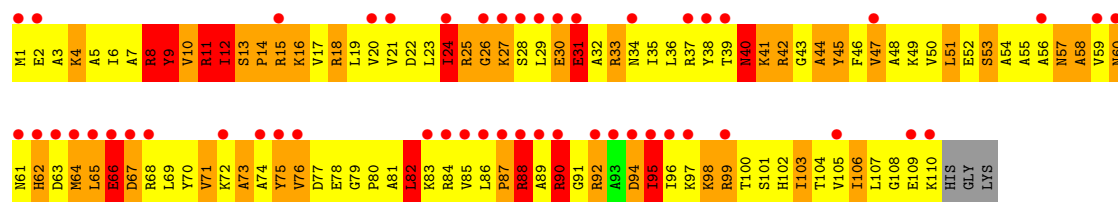


- Molecule 42: 50S ribosomal protein L21

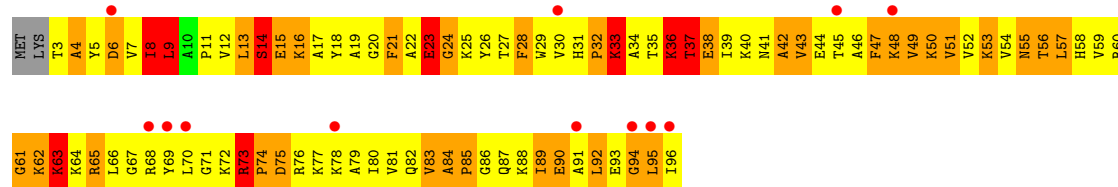


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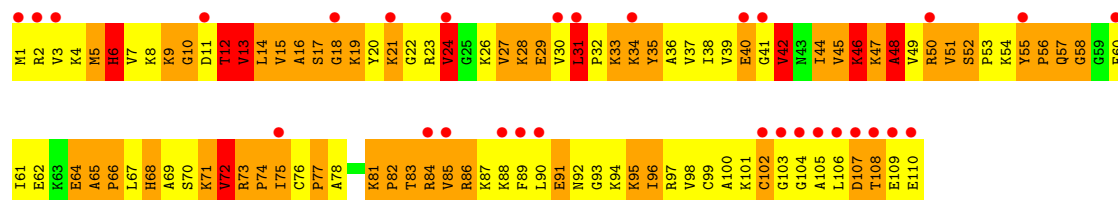




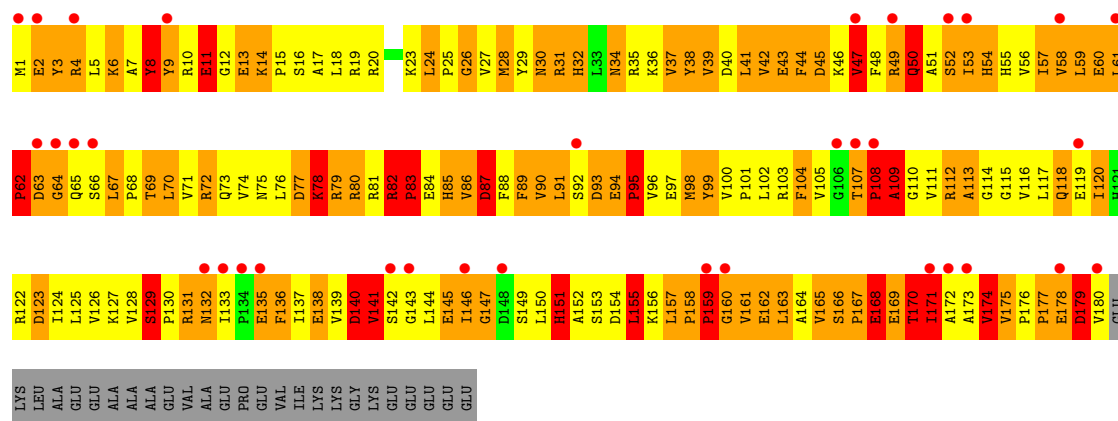
• Molecule 44: 50S ribosomal protein L23



• Molecule 45: 50S ribosomal protein L24

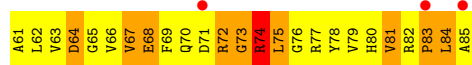


• Molecule 46: 50S ribosomal protein L25

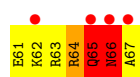
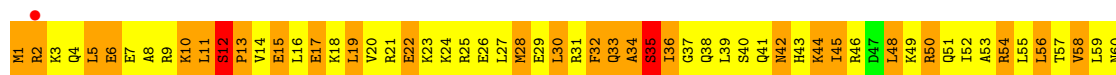
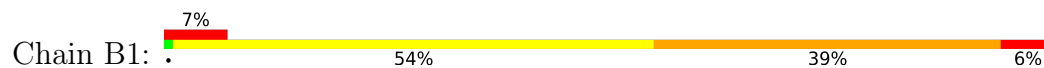


• Molecule 47: Ribosomal protein L27

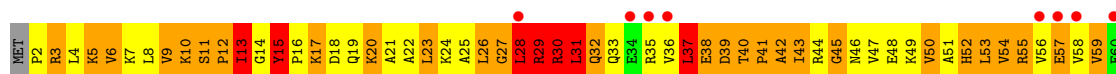




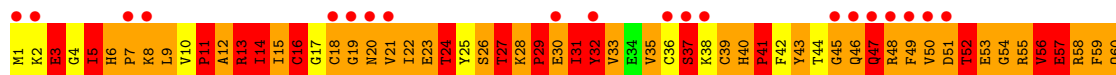
• Molecule 48: 50S ribosomal protein L29



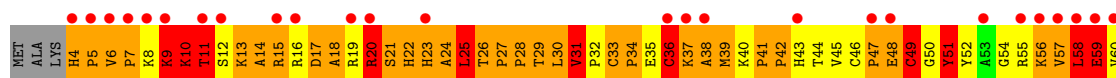
• Molecule 49: 50S ribosomal protein L30



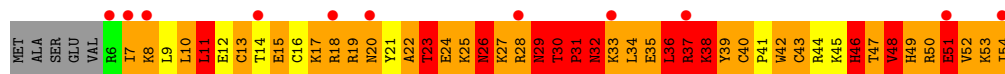
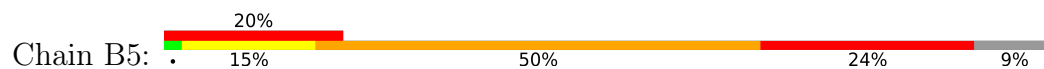
• Molecule 50: 50S ribosomal protein L31



• Molecule 51: 50S ribosomal protein L32



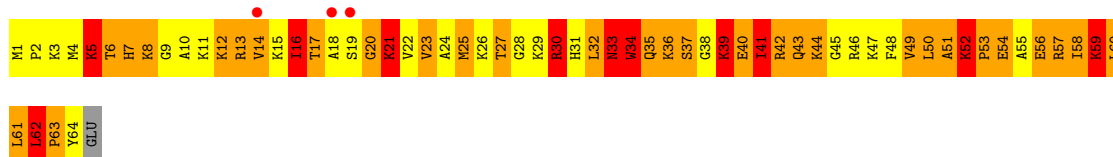
• Molecule 52: 50S ribosomal protein L33



• Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | I 4 2 2                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 508.54Å 508.54Å 806.29Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 300.00 – 5.50<br>300.00 – 5.50                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.7 (300.00-5.50)<br>99.0 (300.00-5.50)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.00 (at 4.88Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.243 , 0.326<br>0.245 , 0.301                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10840 reflections (4.78%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 108.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.045                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.12 , 80.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 151691                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 226.0                                                       | wwPDB-VP         |

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 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   | AA    | 0.59         | 2/36438 (0.0%)  | 0.98        | 148/56869 (0.3%)  |
| 2   | A1    | 0.49         | 0/1133          | 0.93        | 5/1753 (0.3%)     |
| 3   | AB    | 0.52         | 0/1813          | 0.95        | 10/2823 (0.4%)    |
| 3   | AC    | 0.62         | 0/1813          | 0.97        | 4/2823 (0.1%)     |
| 3   | AD    | 0.50         | 0/1813          | 0.88        | 3/2823 (0.1%)     |
| 4   | AE    | 0.87         | 1/1935 (0.1%)   | 1.50        | 38/2609 (1.5%)    |
| 5   | AF    | 0.70         | 0/1636          | 1.33        | 21/2205 (1.0%)    |
| 6   | AG    | 0.89         | 3/1733 (0.2%)   | 1.42        | 27/2318 (1.2%)    |
| 7   | AH    | 0.86         | 0/1162          | 1.47        | 22/1564 (1.4%)    |
| 8   | AI    | 0.85         | 0/856           | 1.28        | 7/1154 (0.6%)     |
| 9   | AJ    | 0.77         | 0/1276          | 1.37        | 21/1709 (1.2%)    |
| 10  | AK    | 0.85         | 0/1136          | 1.34        | 13/1527 (0.9%)    |
| 11  | AL    | 0.75         | 0/1029          | 1.16        | 9/1379 (0.7%)     |
| 12  | AM    | 0.69         | 0/807           | 1.33        | 10/1085 (0.9%)    |
| 13  | AN    | 0.85         | 0/900           | 1.58        | 23/1213 (1.9%)    |
| 14  | AO    | 0.78         | 0/986           | 1.49        | 21/1320 (1.6%)    |
| 15  | AP    | 0.67         | 0/1008          | 1.28        | 14/1347 (1.0%)    |
| 16  | AQ    | 0.72         | 0/501           | 1.34        | 8/664 (1.2%)      |
| 17  | AR    | 0.83         | 0/745           | 1.33        | 9/992 (0.9%)      |
| 18  | AS    | 0.87         | 0/716           | 1.35        | 12/963 (1.2%)     |
| 19  | AT    | 0.98         | 1/870 (0.1%)    | 1.51        | 20/1159 (1.7%)    |
| 20  | AU    | 0.79         | 0/603           | 1.61        | 13/799 (1.6%)     |
| 21  | AV    | 0.67         | 0/661           | 1.22        | 4/890 (0.4%)      |
| 22  | AW    | 0.93         | 0/765           | 1.28        | 8/1007 (0.8%)     |
| 23  | AX    | 0.57         | 0/212           | 1.26        | 3/277 (1.1%)      |
| 24  | BA    | 0.66         | 16/69685 (0.0%) | 1.05        | 370/108786 (0.3%) |
| 25  | BB    | 0.56         | 0/2954          | 0.95        | 5/4606 (0.1%)     |
| 26  | BC    | 0.79         | 0/1775          | 1.36        | 32/2393 (1.3%)    |
| 27  | BD    | 0.97         | 1/2174 (0.0%)   | 1.76        | 57/2927 (1.9%)    |
| 28  | BE    | 1.06         | 5/1611 (0.3%)   | 1.66        | 43/2171 (2.0%)    |
| 29  | BF    | 0.84         | 0/1660          | 1.51        | 35/2247 (1.6%)    |
| 30  | BG    | 0.83         | 1/1507 (0.1%)   | 1.53        | 34/2027 (1.7%)    |
| 31  | BH    | 0.82         | 2/1354 (0.1%)   | 1.48        | 28/1831 (1.5%)    |
| 32  | BK    | 0.85         | 1/1170 (0.1%)   | 1.61        | 36/1581 (2.3%)    |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 33  | BL    | 0.94         | 0/1044           | 1.49        | 27/1415 (1.9%)     |
| 34  | BM    | 1.02         | 1/1140 (0.1%)    | 1.64        | 30/1537 (2.0%)     |
| 35  | BN    | 1.24         | 3/942 (0.3%)     | 1.97        | 48/1268 (3.8%)     |
| 36  | BO    | 1.00         | 2/1123 (0.2%)    | 1.63        | 33/1493 (2.2%)     |
| 37  | BP    | 0.99         | 0/1100           | 1.76        | 35/1470 (2.4%)     |
| 38  | BQ    | 0.98         | 1/974 (0.1%)     | 1.60        | 28/1302 (2.2%)     |
| 39  | BR    | 1.00         | 0/887            | 1.66        | 28/1180 (2.4%)     |
| 40  | BS    | 1.14         | 2/990 (0.2%)     | 1.85        | 34/1325 (2.6%)     |
| 41  | BT    | 1.03         | 1/982 (0.1%)     | 1.50        | 21/1306 (1.6%)     |
| 42  | BU    | 1.16         | 3/790 (0.4%)     | 1.93        | 32/1057 (3.0%)     |
| 43  | BV    | 0.89         | 1/886 (0.1%)     | 1.52        | 17/1189 (1.4%)     |
| 44  | BW    | 0.77         | 0/756            | 1.38        | 16/1015 (1.6%)     |
| 45  | BX    | 0.75         | 0/857            | 1.57        | 21/1142 (1.8%)     |
| 46  | BY    | 0.92         | 1/1467 (0.1%)    | 1.78        | 55/1992 (2.8%)     |
| 47  | BZ    | 0.86         | 0/679            | 1.59        | 20/902 (2.2%)      |
| 48  | B1    | 0.83         | 0/569            | 1.31        | 8/751 (1.1%)       |
| 49  | B2    | 0.86         | 1/474 (0.2%)     | 1.62        | 13/635 (2.0%)      |
| 50  | B3    | 1.10         | 0/594            | 1.85        | 26/795 (3.3%)      |
| 51  | B4    | 1.03         | 2/459 (0.4%)     | 1.76        | 20/621 (3.2%)      |
| 52  | B5    | 1.10         | 0/433            | 1.88        | 15/576 (2.6%)      |
| 53  | B6    | 0.97         | 0/438            | 1.35        | 4/575 (0.7%)       |
| 54  | B7    | 0.83         | 0/523            | 1.62        | 18/690 (2.6%)      |
| 55  | B8    | 0.81         | 0/310            | 1.56        | 6/407 (1.5%)       |
| All | All   | 0.72         | 51/164854 (0.0%) | 1.18        | 1668/246484 (0.7%) |

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                   | 175                 |
| 2   | A1    | 0                   | 3                   |
| 3   | AB    | 0                   | 6                   |
| 3   | AC    | 0                   | 8                   |
| 3   | AD    | 0                   | 8                   |
| 6   | AG    | 0                   | 1                   |
| 8   | AI    | 0                   | 1                   |
| 13  | AN    | 0                   | 1                   |
| 15  | AP    | 0                   | 1                   |
| 16  | AQ    | 0                   | 1                   |
| 24  | BA    | 0                   | 463                 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 25  | BB    | 0                   | 18                  |
| 26  | BC    | 0                   | 1                   |
| 28  | BE    | 0                   | 1                   |
| 34  | BM    | 0                   | 1                   |
| 37  | BP    | 0                   | 1                   |
| 40  | BS    | 0                   | 1                   |
| 42  | BU    | 0                   | 1                   |
| 50  | B3    | 0                   | 1                   |
| 51  | B4    | 0                   | 1                   |
| All | All   | 0                   | 694                 |

The worst 5 of 51 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 24  | BA    | 1203 | G    | O3'-P | -27.76 | 1.19        | 1.61     |
| 6   | AG    | 146  | ILE  | CA-CB | -13.42 | 1.45        | 1.55     |
| 24  | BA    | 2500 | U    | O3'-P | -12.13 | 1.43        | 1.61     |
| 24  | BA    | 2448 | A    | O3'-P | -11.53 | 1.43        | 1.61     |
| 24  | BA    | 1240 | U    | O3'-P | -10.77 | 1.45        | 1.61     |

The worst 5 of 1668 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 24  | BA    | 2448 | A    | C5'-C4'-O4' | -21.85 | 76.33       | 109.10   |
| 24  | BA    | 1203 | G    | P-O3'-C3'   | 21.82  | 152.94      | 120.20   |
| 1   | AA    | 1064 | G    | N1-C2-N2    | -21.50 | 51.71       | 116.20   |
| 5   | AF    | 48   | TYR  | N-CA-C      | -21.19 | 86.17       | 113.72   |
| 40  | BS    | 66   | VAL  | N-CA-C      | -17.80 | 82.48       | 108.12   |

There are no chirality outliers.

5 of 694 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 12  | U    | Sidechain |
| 1   | AA    | 17  | U    | Sidechain |
| 1   | AA    | 31  | G    | Sidechain |
| 1   | AA    | 37  | U    | Sidechain |
| 1   | AA    | 45  | U    | Sidechain |

## 5.2 Too-close contacts

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        | 16431    | 6725    | 0            |
| 2   | A1    | 1025  | 0        | 511      | 175     | 0            |
| 3   | AB    | 1623  | 0        | 821      | 224     | 0            |
| 3   | AC    | 1623  | 0        | 821      | 321     | 0            |
| 3   | AD    | 1623  | 0        | 821      | 289     | 0            |
| 4   | AE    | 1900  | 0        | 1951     | 1080    | 0            |
| 5   | AF    | 1612  | 0        | 1677     | 745     | 0            |
| 6   | AG    | 1703  | 0        | 1763     | 900     | 0            |
| 7   | AH    | 1146  | 0        | 1207     | 602     | 0            |
| 8   | AI    | 843   | 0        | 857      | 404     | 0            |
| 9   | AJ    | 1257  | 0        | 1296     | 600     | 0            |
| 10  | AK    | 1116  | 0        | 1177     | 742     | 0            |
| 11  | AL    | 1010  | 0        | 1037     | 485     | 0            |
| 12  | AM    | 794   | 0        | 840      | 367     | 0            |
| 13  | AN    | 885   | 0        | 904      | 478     | 0            |
| 14  | AO    | 970   | 0        | 1057     | 524     | 0            |
| 15  | AP    | 997   | 0        | 1072     | 535     | 0            |
| 16  | AQ    | 492   | 0        | 529      | 286     | 0            |
| 17  | AR    | 734   | 0        | 771      | 346     | 0            |
| 18  | AS    | 700   | 0        | 720      | 365     | 0            |
| 19  | AT    | 857   | 0        | 930      | 471     | 0            |
| 20  | AU    | 597   | 0        | 668      | 383     | 0            |
| 21  | AV    | 647   | 0        | 673      | 320     | 0            |
| 22  | AW    | 763   | 0        | 861      | 383     | 0            |
| 23  | AX    | 208   | 0        | 221      | 84      | 0            |
| 24  | BA    | 62218 | 0        | 31356    | 15266   | 0            |
| 25  | BB    | 2641  | 0        | 1337     | 603     | 1            |
| 26  | BC    | 1742  | 0        | 1796     | 749     | 0            |
| 27  | BD    | 2124  | 0        | 2207     | 1521    | 0            |
| 28  | BE    | 1578  | 0        | 1647     | 1118    | 0            |
| 29  | BF    | 1625  | 0        | 1666     | 841     | 0            |
| 30  | BG    | 1482  | 0        | 1546     | 923     | 0            |
| 31  | BH    | 1328  | 0        | 1408     | 716     | 0            |
| 32  | BK    | 1155  | 0        | 1244     | 517     | 0            |
| 33  | BL    | 1025  | 0        | 1074     | 454     | 0            |
| 34  | BM    | 1113  | 0        | 1183     | 809     | 0            |
| 35  | BN    | 932   | 0        | 994      | 731     | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 36  | BO    | 1106   | 0        | 1183     | 809     | 0            |
| 37  | BP    | 1080   | 0        | 1127     | 769     | 0            |
| 38  | BQ    | 960    | 0        | 1021     | 612     | 0            |
| 39  | BR    | 877    | 0        | 938      | 538     | 0            |
| 40  | BS    | 976    | 0        | 1033     | 654     | 0            |
| 41  | BT    | 964    | 0        | 1022     | 755     | 0            |
| 42  | BU    | 779    | 0        | 852      | 584     | 0            |
| 43  | BV    | 876    | 0        | 941      | 468     | 0            |
| 44  | BW    | 742    | 0        | 800      | 376     | 0            |
| 45  | BX    | 844    | 0        | 930      | 433     | 0            |
| 46  | BY    | 1435   | 0        | 1463     | 750     | 0            |
| 47  | BZ    | 670    | 0        | 700      | 360     | 0            |
| 48  | B1    | 567    | 0        | 621      | 327     | 0            |
| 49  | B2    | 469    | 0        | 518      | 329     | 0            |
| 50  | B3    | 581    | 0        | 577      | 403     | 0            |
| 51  | B4    | 445    | 0        | 459      | 282     | 0            |
| 52  | B5    | 426    | 0        | 452      | 286     | 0            |
| 53  | B6    | 430    | 0        | 480      | 282     | 0            |
| 54  | B7    | 515    | 0        | 587      | 403     | 0            |
| 55  | B8    | 307    | 0        | 335      | 154     | 0            |
| All | All   | 151691 | 0        | 103113   | 47112   | 1            |

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 186.

The worst 5 of 47112 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) |
|------------------|------------------|--------------------------|-------------------|
| 24:BA:2447:G:C8  | 24:BA:2500:U:H3' | 1.23                     | 1.61              |
| 24:BA:1202:C:C5  | 24:BA:1203:G:H1' | 1.39                     | 1.55              |
| 24:BA:1203:G:O6  | 24:BA:1240:U:C2  | 1.66                     | 1.48              |
| 24:BA:2459:A:N3  | 24:BA:2460:U:H1' | 1.38                     | 1.38              |
| 24:BA:2596:U:H2' | 27:BD:242:ARG:CZ | 1.55                     | 1.35              |

All (1) 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) |
|---------------|-----------------------|--------------------------|-------------------|
| 25:BB:0:A:OP1 | 25:BB:0:A:OP1[15_545] | 2.18                     | 0.02              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 4   | AE    | 232/256 (91%) | 114 (49%) | 42 (18%) | 76 (33%) | 0           | 0 |
| 5   | AF    | 204/239 (85%) | 107 (52%) | 46 (22%) | 51 (25%) | 0           | 1 |
| 6   | AG    | 206/209 (99%) | 96 (47%)  | 57 (28%) | 53 (26%) | 0           | 1 |
| 7   | AH    | 148/162 (91%) | 93 (63%)  | 38 (26%) | 17 (12%) | 0           | 5 |
| 8   | AI    | 99/101 (98%)  | 58 (59%)  | 19 (19%) | 22 (22%) | 0           | 1 |
| 9   | AJ    | 153/156 (98%) | 73 (48%)  | 45 (29%) | 35 (23%) | 0           | 1 |
| 10  | AK    | 136/138 (99%) | 68 (50%)  | 35 (26%) | 33 (24%) | 0           | 1 |
| 11  | AL    | 125/128 (98%) | 62 (50%)  | 33 (26%) | 30 (24%) | 0           | 1 |
| 12  | AM    | 96/105 (91%)  | 52 (54%)  | 20 (21%) | 24 (25%) | 0           | 1 |
| 13  | AN    | 117/129 (91%) | 65 (56%)  | 29 (25%) | 23 (20%) | 0           | 2 |
| 14  | AO    | 122/132 (92%) | 50 (41%)  | 30 (25%) | 42 (34%) | 0           | 0 |
| 15  | AP    | 123/126 (98%) | 56 (46%)  | 34 (28%) | 33 (27%) | 0           | 0 |
| 16  | AQ    | 58/61 (95%)   | 24 (41%)  | 16 (28%) | 18 (31%) | 0           | 0 |
| 17  | AR    | 86/89 (97%)   | 36 (42%)  | 35 (41%) | 15 (17%) | 0           | 2 |
| 18  | AS    | 81/88 (92%)   | 42 (52%)  | 24 (30%) | 15 (18%) | 0           | 2 |
| 19  | AT    | 102/105 (97%) | 62 (61%)  | 23 (22%) | 17 (17%) | 0           | 2 |
| 20  | AU    | 71/88 (81%)   | 26 (37%)  | 26 (37%) | 19 (27%) | 0           | 0 |
| 21  | AV    | 78/93 (84%)   | 32 (41%)  | 23 (30%) | 23 (30%) | 0           | 0 |
| 22  | AW    | 97/106 (92%)  | 38 (39%)  | 32 (33%) | 27 (28%) | 0           | 0 |
| 23  | AX    | 22/27 (82%)   | 9 (41%)   | 6 (27%)  | 7 (32%)  | 0           | 0 |
| 26  | BC    | 226/229 (99%) | 155 (69%) | 41 (18%) | 30 (13%) | 0           | 3 |
| 27  | BD    | 270/276 (98%) | 125 (46%) | 59 (22%) | 86 (32%) | 0           | 0 |
| 28  | BE    | 204/206 (99%) | 117 (57%) | 31 (15%) | 56 (28%) | 0           | 0 |
| 29  | BF    | 206/210 (98%) | 109 (53%) | 46 (22%) | 51 (25%) | 0           | 1 |
| 30  | BG    | 180/182 (99%) | 79 (44%)  | 47 (26%) | 54 (30%) | 0           | 0 |

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| Mol | Chain | Analysed        | Favoured   | Allowed    | Outliers   | Percentiles |   |
|-----|-------|-----------------|------------|------------|------------|-------------|---|
| 31  | BH    | 172/180 (96%)   | 80 (46%)   | 46 (27%)   | 46 (27%)   | 0           | 0 |
| 32  | BK    | 146/148 (99%)   | 91 (62%)   | 30 (20%)   | 25 (17%)   | 0           | 2 |
| 33  | BL    | 136/147 (92%)   | 69 (51%)   | 38 (28%)   | 29 (21%)   | 0           | 2 |
| 34  | BM    | 137/140 (98%)   | 64 (47%)   | 28 (20%)   | 45 (33%)   | 0           | 0 |
| 35  | BN    | 120/122 (98%)   | 59 (49%)   | 23 (19%)   | 38 (32%)   | 0           | 0 |
| 36  | BO    | 143/150 (95%)   | 57 (40%)   | 36 (25%)   | 50 (35%)   | 0           | 0 |
| 37  | BP    | 134/141 (95%)   | 49 (37%)   | 33 (25%)   | 52 (39%)   | 0           | 0 |
| 38  | BQ    | 115/118 (98%)   | 57 (50%)   | 39 (34%)   | 19 (16%)   | 0           | 2 |
| 39  | BR    | 108/112 (96%)   | 48 (44%)   | 29 (27%)   | 31 (29%)   | 0           | 0 |
| 40  | BS    | 115/146 (79%)   | 52 (45%)   | 26 (23%)   | 37 (32%)   | 0           | 0 |
| 41  | BT    | 115/118 (98%)   | 35 (30%)   | 50 (44%)   | 30 (26%)   | 0           | 1 |
| 42  | BU    | 99/101 (98%)    | 52 (52%)   | 19 (19%)   | 28 (28%)   | 0           | 0 |
| 43  | BV    | 108/113 (96%)   | 63 (58%)   | 24 (22%)   | 21 (19%)   | 0           | 2 |
| 44  | BW    | 92/96 (96%)     | 57 (62%)   | 16 (17%)   | 19 (21%)   | 0           | 2 |
| 45  | BX    | 108/110 (98%)   | 43 (40%)   | 32 (30%)   | 33 (31%)   | 0           | 0 |
| 46  | BY    | 178/206 (86%)   | 95 (53%)   | 44 (25%)   | 39 (22%)   | 0           | 1 |
| 47  | BZ    | 83/85 (98%)     | 52 (63%)   | 21 (25%)   | 10 (12%)   | 0           | 4 |
| 48  | B1    | 65/67 (97%)     | 36 (55%)   | 20 (31%)   | 9 (14%)    | 0           | 3 |
| 49  | B2    | 57/60 (95%)     | 34 (60%)   | 8 (14%)    | 15 (26%)   | 0           | 1 |
| 50  | B3    | 69/71 (97%)     | 23 (33%)   | 16 (23%)   | 30 (44%)   | 0           | 0 |
| 51  | B4    | 55/60 (92%)     | 14 (26%)   | 19 (34%)   | 22 (40%)   | 0           | 0 |
| 52  | B5    | 47/54 (87%)     | 14 (30%)   | 7 (15%)    | 26 (55%)   | 0           | 0 |
| 53  | B6    | 47/49 (96%)     | 20 (43%)   | 12 (26%)   | 15 (32%)   | 0           | 0 |
| 54  | B7    | 62/65 (95%)     | 23 (37%)   | 18 (29%)   | 21 (34%)   | 0           | 0 |
| 55  | B8    | 35/37 (95%)     | 20 (57%)   | 5 (14%)    | 10 (29%)   | 0           | 0 |
| All | All   | 5988/6337 (94%) | 2955 (49%) | 1476 (25%) | 1557 (26%) | 0           | 1 |

5 of 1557 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AE    | 8   | LYS  |
| 4   | AE    | 11  | LEU  |
| 4   | AE    | 13  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AE    | 15  | VAL  |
| 4   | AE    | 16  | HIS  |

### 5.3.2 Protein sidechains ⓘ

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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4   | AE    | 202/220 (92%)  | 133 (66%) | 69 (34%) | 0           | 1  |
| 5   | AF    | 160/188 (85%)  | 121 (76%) | 39 (24%) | 1           | 4  |
| 6   | AG    | 180/181 (99%)  | 129 (72%) | 51 (28%) | 0           | 3  |
| 7   | AH    | 115/123 (94%)  | 76 (66%)  | 39 (34%) | 0           | 2  |
| 8   | AI    | 90/90 (100%)   | 62 (69%)  | 28 (31%) | 0           | 2  |
| 9   | AJ    | 126/127 (99%)  | 93 (74%)  | 33 (26%) | 0           | 3  |
| 10  | AK    | 119/119 (100%) | 85 (71%)  | 34 (29%) | 0           | 3  |
| 11  | AL    | 98/99 (99%)    | 74 (76%)  | 24 (24%) | 1           | 4  |
| 12  | AM    | 88/92 (96%)    | 67 (76%)  | 21 (24%) | 1           | 5  |
| 13  | AN    | 90/99 (91%)    | 75 (83%)  | 15 (17%) | 2           | 11 |
| 14  | AO    | 104/109 (95%)  | 79 (76%)  | 25 (24%) | 1           | 5  |
| 15  | AP    | 100/101 (99%)  | 75 (75%)  | 25 (25%) | 0           | 4  |
| 16  | AQ    | 49/50 (98%)    | 37 (76%)  | 12 (24%) | 1           | 4  |
| 17  | AR    | 79/80 (99%)    | 62 (78%)  | 17 (22%) | 1           | 6  |
| 18  | AS    | 72/74 (97%)    | 47 (65%)  | 25 (35%) | 0           | 1  |
| 19  | AT    | 96/97 (99%)    | 69 (72%)  | 27 (28%) | 0           | 3  |
| 20  | AU    | 64/77 (83%)    | 51 (80%)  | 13 (20%) | 1           | 7  |
| 21  | AV    | 71/80 (89%)    | 58 (82%)  | 13 (18%) | 2           | 9  |
| 22  | AW    | 76/82 (93%)    | 59 (78%)  | 17 (22%) | 1           | 6  |
| 23  | AX    | 19/22 (86%)    | 17 (90%)  | 2 (10%)  | 6           | 22 |
| 26  | BC    | 180/181 (99%)  | 147 (82%) | 33 (18%) | 2           | 9  |
| 27  | BD    | 215/218 (99%)  | 150 (70%) | 65 (30%) | 0           | 2  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |  |
|-----|-------|-----------------|------------|------------|-------------|----|--|
| 28  | BE    | 166/166 (100%)  | 102 (61%)  | 64 (39%)   | 0           | 1  |  |
| 29  | BF    | 164/166 (99%)   | 103 (63%)  | 61 (37%)   | 0           | 1  |  |
| 30  | BG    | 156/156 (100%)  | 111 (71%)  | 45 (29%)   | 0           | 2  |  |
| 31  | BH    | 143/148 (97%)   | 102 (71%)  | 41 (29%)   | 0           | 3  |  |
| 32  | BK    | 124/124 (100%)  | 89 (72%)   | 35 (28%)   | 0           | 3  |  |
| 33  | BL    | 105/111 (95%)   | 87 (83%)   | 18 (17%)   | 2           | 10 |  |
| 34  | BM    | 118/119 (99%)   | 73 (62%)   | 45 (38%)   | 0           | 1  |  |
| 35  | BN    | 100/100 (100%)  | 62 (62%)   | 38 (38%)   | 0           | 1  |  |
| 36  | BO    | 111/116 (96%)   | 74 (67%)   | 37 (33%)   | 0           | 2  |  |
| 37  | BP    | 106/111 (96%)   | 65 (61%)   | 41 (39%)   | 0           | 1  |  |
| 38  | BQ    | 100/101 (99%)   | 70 (70%)   | 30 (30%)   | 0           | 2  |  |
| 39  | BR    | 87/88 (99%)     | 63 (72%)   | 24 (28%)   | 0           | 3  |  |
| 40  | BS    | 105/127 (83%)   | 67 (64%)   | 38 (36%)   | 0           | 1  |  |
| 41  | BT    | 93/94 (99%)     | 64 (69%)   | 29 (31%)   | 0           | 2  |  |
| 42  | BU    | 82/82 (100%)    | 58 (71%)   | 24 (29%)   | 0           | 2  |  |
| 43  | BV    | 90/92 (98%)     | 62 (69%)   | 28 (31%)   | 0           | 2  |  |
| 44  | BW    | 76/78 (97%)     | 54 (71%)   | 22 (29%)   | 0           | 2  |  |
| 45  | BX    | 91/91 (100%)    | 72 (79%)   | 19 (21%)   | 1           | 7  |  |
| 46  | BY    | 159/179 (89%)   | 116 (73%)  | 43 (27%)   | 0           | 3  |  |
| 47  | BZ    | 67/67 (100%)    | 49 (73%)   | 18 (27%)   | 0           | 3  |  |
| 48  | B1    | 62/62 (100%)    | 44 (71%)   | 18 (29%)   | 0           | 2  |  |
| 49  | B2    | 51/52 (98%)     | 36 (71%)   | 15 (29%)   | 0           | 2  |  |
| 50  | B3    | 63/63 (100%)    | 43 (68%)   | 20 (32%)   | 0           | 2  |  |
| 51  | B4    | 50/52 (96%)     | 33 (66%)   | 17 (34%)   | 0           | 1  |  |
| 52  | B5    | 48/52 (92%)     | 31 (65%)   | 17 (35%)   | 0           | 1  |  |
| 53  | B6    | 42/42 (100%)    | 30 (71%)   | 12 (29%)   | 0           | 3  |  |
| 54  | B7    | 54/55 (98%)     | 39 (72%)   | 15 (28%)   | 0           | 3  |  |
| 55  | B8    | 34/34 (100%)    | 28 (82%)   | 6 (18%)    | 2           | 10 |  |
| All | All   | 5040/5237 (96%) | 3593 (71%) | 1447 (29%) | 0           | 3  |  |

5 of 1447 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | BM    | 91  | LEU  |
| 41  | BT    | 16  | LYS  |
| 35  | BN    | 52  | VAL  |
| 34  | BM    | 90  | MET  |
| 37  | BP    | 105 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | BM    | 38  | HIS  |
| 43  | BV    | 34  | ASN  |
| 35  | BN    | 90  | GLN  |
| 39  | BR    | 38  | GLN  |
| 44  | BW    | 87  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1515/1522 (99%) | 463 (30%)         | 137 (9%)        |
| 2   | A1    | 49/50 (98%)     | 21 (42%)          | 4 (8%)          |
| 24  | BA    | 2888/2916 (99%) | 1206 (41%)        | 253 (8%)        |
| 25  | BB    | 122/123 (99%)   | 46 (37%)          | 3 (2%)          |
| 3   | AB    | 75/76 (98%)     | 32 (42%)          | 1 (1%)          |
| 3   | AC    | 75/76 (98%)     | 23 (30%)          | 4 (5%)          |
| 3   | AD    | 75/76 (98%)     | 23 (30%)          | 1 (1%)          |
| All | All   | 4799/4839 (99%) | 1814 (37%)        | 403 (8%)        |

5 of 1814 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 6   | G    |
| 1   | AA    | 8   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 14  | U    |
| 1   | AA    | 19  | C    |

5 of 403 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 973  | A    |
| 24  | BA    | 1603 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2893 | G    |
| 24  | BA    | 1064 | C    |
| 24  | BA    | 1250 | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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 |
|-----|-------|------------------|
| 24  | BA    | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | BA    | 2756:U    | O3'    | 2757:A    | P      | 1.77         |
| 1     | BA    | 1203:G    | O3'    | 1204:A    | P      | 1.19         |

## 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<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | AA    | 1515/1522 (99%) | 0.58   | 201 (13%) 7 14 | 145, 221, 302, 356    | 0     |
| 2   | A1    | 50/50 (100%)    | 4.44   | 38 (76%) 0 1   | 200, 320, 348, 357    | 0     |
| 3   | AB    | 76/76 (100%)    | 2.91   | 54 (71%) 0 2   | 288, 351, 370, 374    | 0     |
| 3   | AC    | 76/76 (100%)    | 0.12   | 4 (5%) 32 33   | 167, 214, 260, 284    | 0     |
| 3   | AD    | 76/76 (100%)    | 0.61   | 9 (11%) 9 16   | 222, 271, 293, 316    | 0     |
| 4   | AE    | 234/256 (91%)   | 2.29   | 91 (38%) 1 4   | 189, 226, 271, 304    | 0     |
| 5   | AF    | 206/239 (86%)   | 2.46   | 94 (45%) 0 3   | 222, 244, 266, 277    | 0     |
| 6   | AG    | 208/209 (99%)   | 1.66   | 74 (35%) 1 4   | 168, 215, 233, 242    | 0     |
| 7   | AH    | 150/162 (92%)   | 2.70   | 72 (48%) 0 3   | 174, 210, 235, 257    | 0     |
| 8   | AI    | 101/101 (100%)  | 3.26   | 62 (61%) 0 2   | 191, 223, 236, 261    | 0     |
| 9   | AJ    | 155/156 (99%)   | 1.84   | 56 (36%) 1 4   | 210, 240, 256, 275    | 0     |
| 10  | AK    | 138/138 (100%)  | 2.01   | 48 (34%) 1 5   | 186, 208, 225, 232    | 0     |
| 11  | AL    | 127/128 (99%)   | 1.34   | 37 (29%) 1 6   | 222, 261, 276, 287    | 0     |
| 12  | AM    | 98/105 (93%)    | 1.12   | 23 (23%) 2 7   | 230, 260, 274, 282    | 0     |
| 13  | AN    | 119/129 (92%)   | 1.50   | 34 (28%) 1 6   | 193, 212, 245, 267    | 0     |
| 14  | AO    | 124/132 (93%)   | 1.87   | 41 (33%) 1 5   | 179, 199, 233, 267    | 0     |
| 15  | AP    | 125/126 (99%)   | 0.68   | 15 (12%) 9 15  | 223, 243, 272, 278    | 0     |
| 16  | AQ    | 60/61 (98%)     | 0.87   | 12 (20%) 3 9   | 215, 248, 259, 263    | 0     |
| 17  | AR    | 88/89 (98%)     | 1.79   | 32 (36%) 1 4   | 186, 207, 231, 238    | 0     |
| 18  | AS    | 83/88 (94%)     | 0.78   | 16 (19%) 3 9   | 180, 201, 226, 249    | 0     |
| 19  | AT    | 104/105 (99%)   | 1.08   | 22 (21%) 2 8   | 164, 193, 244, 277    | 0     |
| 20  | AU    | 73/88 (82%)     | 3.42   | 40 (54%) 0 3   | 184, 209, 258, 287    | 0     |
| 21  | AV    | 80/93 (86%)     | 0.74   | 11 (13%) 6 14  | 226, 252, 266, 270    | 0     |
| 22  | AW    | 99/106 (93%)    | 1.26   | 26 (26%) 1 6   | 167, 195, 225, 241    | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 23  | AX    | 24/27 (88%)     | -0.50  | 0 100 100     | 230, 249, 280, 288    | 0     |
| 24  | BA    | 2889/2916 (99%) | 0.80   | 567 (19%) 3 9 | 129, 215, 297, 342    | 0     |
| 25  | BB    | 123/123 (100%)  | -0.44  | 1 (0%) 82 71  | 199, 259, 293, 316    | 0     |
| 26  | BC    | 228/229 (99%)   | 1.84   | 84 (36%) 1 4  | 250, 281, 300, 313    | 0     |
| 27  | BD    | 272/276 (98%)   | 1.06   | 55 (20%) 3 9  | 130, 199, 221, 259    | 0     |
| 28  | BE    | 206/206 (100%)  | 2.13   | 88 (42%) 0 3  | 148, 186, 232, 269    | 0     |
| 29  | BF    | 208/210 (99%)   | 2.18   | 77 (37%) 1 4  | 164, 238, 263, 276    | 0     |
| 30  | BG    | 182/182 (100%)  | 0.72   | 25 (13%) 6 14 | 212, 246, 268, 276    | 0     |
| 31  | BH    | 174/180 (96%)   | 1.84   | 66 (37%) 1 4  | 196, 241, 260, 271    | 0     |
| 32  | BK    | 148/148 (100%)  | 2.09   | 65 (43%) 0 3  | 202, 227, 249, 257    | 0     |
| 33  | BL    | 138/147 (93%)   | 2.92   | 72 (52%) 0 3  | 271, 298, 312, 327    | 0     |
| 34  | BM    | 139/140 (99%)   | 1.24   | 41 (29%) 1 6  | 167, 198, 224, 235    | 0     |
| 35  | BN    | 122/122 (100%)  | 1.64   | 34 (27%) 1 6  | 148, 177, 209, 221    | 0     |
| 36  | BO    | 145/150 (96%)   | 0.80   | 26 (17%) 3 10 | 166, 247, 276, 315    | 0     |
| 37  | BP    | 136/141 (96%)   | 1.37   | 39 (28%) 1 6  | 166, 208, 234, 241    | 0     |
| 38  | BQ    | 117/118 (99%)   | 0.15   | 5 (4%) 40 38  | 168, 192, 219, 226    | 0     |
| 39  | BR    | 110/112 (98%)   | -0.03  | 1 (0%) 81 69  | 186, 235, 263, 289    | 0     |
| 40  | BS    | 117/146 (80%)   | 1.44   | 31 (26%) 1 6  | 164, 194, 227, 242    | 0     |
| 41  | BT    | 117/118 (99%)   | 1.15   | 25 (21%) 2 8  | 183, 202, 220, 232    | 0     |
| 42  | BU    | 101/101 (100%)  | 2.33   | 47 (46%) 0 3  | 168, 225, 246, 257    | 0     |
| 43  | BV    | 110/113 (97%)   | 2.25   | 50 (45%) 0 3  | 180, 209, 237, 248    | 0     |
| 44  | BW    | 94/96 (97%)     | 0.60   | 12 (12%) 7 14 | 212, 232, 280, 288    | 0     |
| 45  | BX    | 110/110 (100%)  | 1.23   | 30 (27%) 1 6  | 221, 255, 287, 305    | 0     |
| 46  | BY    | 180/206 (87%)   | 0.98   | 34 (18%) 3 10 | 208, 246, 268, 279    | 0     |
| 47  | BZ    | 85/85 (100%)    | 0.40   | 10 (11%) 9 16 | 211, 229, 242, 271    | 0     |
| 48  | B1    | 67/67 (100%)    | 0.49   | 5 (7%) 20 25  | 218, 243, 263, 268    | 0     |
| 49  | B2    | 59/60 (98%)     | 0.86   | 8 (13%) 7 14  | 204, 224, 249, 259    | 0     |
| 50  | B3    | 71/71 (100%)    | 2.30   | 27 (38%) 1 4  | 199, 223, 238, 246    | 0     |
| 51  | B4    | 57/60 (95%)     | 1.77   | 26 (45%) 0 3  | 164, 209, 264, 289    | 0     |
| 52  | B5    | 49/54 (90%)     | 1.00   | 11 (22%) 2 8  | 206, 232, 242, 252    | 0     |
| 53  | B6    | 49/49 (100%)    | 0.56   | 6 (12%) 8 15  | 162, 209, 221, 235    | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 54  | B7    | 64/65 (98%)       | 0.16   | 3 (4%) 36 36   | 164, 195, 225, 242    | 0     |
| 55  | B8    | 37/37 (100%)      | 0.93   | 6 (16%) 4 11   | 205, 215, 224, 226    | 0     |
| All | All   | 10893/11176 (97%) | 1.19   | 2689 (24%) 2 7 | 129, 223, 295, 374    | 0     |

The worst 5 of 2689 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | AF    | 207 | VAL  | 27.0 |
| 7   | AH    | 154 | GLY  | 25.9 |
| 20  | AU    | 16  | PRO  | 21.9 |
| 8   | AI    | 101 | ALA  | 20.2 |
| 4   | AE    | 7   | VAL  | 19.6 |

## 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 oligosaccharides 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.