



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:05 PM GMT

PDB ID : 1IBL  
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL SUBUNIT IN COMPLEX WITH A MESSENGER RNA FRAGMENT AND COGNATE TRANSFER RNA ANTICODON STEM-LOOP BOUND AT THE A SITE AND WITH THE ANTIBIOTIC PAROMOMYCIN  
Authors : Ogle, J.M.; Brodersen, D.E.; Clemons Jr., W.M.; Tarry, M.J.; Carter, A.P.; Ramakrishnan, V.  
Deposited on : 2001-03-28  
Resolution : 3.11 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

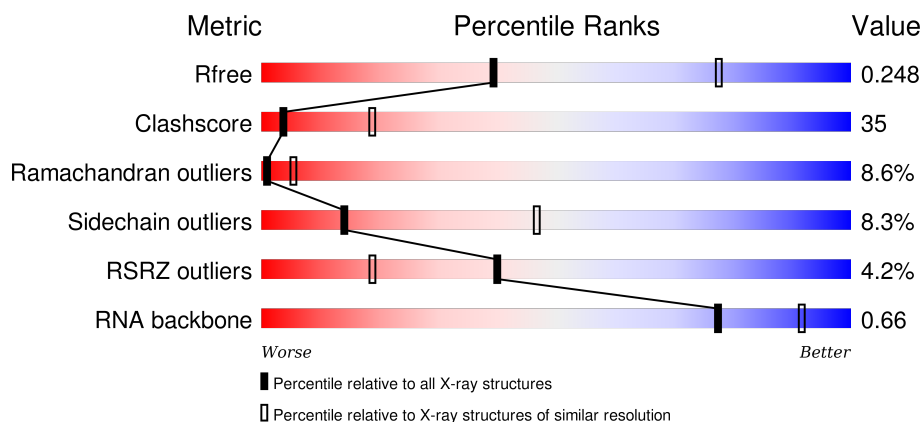
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1112 (3.16-3.08)                                      |
| Clashscore            | 102246                      | 1218 (3.16-3.08)                                      |
| Ramachandran outliers | 100387                      | 1175 (3.16-3.08)                                      |
| Sidechain outliers    | 100360                      | 1175 (3.16-3.08)                                      |
| RSRZ outliers         | 91569                       | 1114 (3.16-3.08)                                      |
| RNA backbone          | 2183                        | 1010 (3.54-2.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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   | A     | 1522   | <div> <div>31%</div> <div>55%</div> <div>11%</div> <div>..</div> </div>  |
| 2   | X     | 6      | <div> <div>33%</div> <div>100%</div> </div>                              |
| 3   | Y     | 15     | <div> <div>40%</div> <div>53%</div> <div>7%</div> </div>                 |
| 4   | Z     | 4      | <div> <div>25%</div> <div>25%</div> <div>50%</div> <div>25%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | B     | 256    |                  |
| 6   | C     | 239    |                  |
| 7   | D     | 209    |                  |
| 8   | E     | 162    |                  |
| 9   | F     | 101    |                  |
| 10  | G     | 156    |                  |
| 11  | H     | 138    |                  |
| 12  | I     | 128    |                  |
| 13  | J     | 105    |                  |
| 14  | K     | 129    |                  |
| 15  | L     | 135    |                  |
| 16  | M     | 126    |                  |
| 17  | N     | 61     |                  |
| 18  | O     | 89     |                  |
| 19  | P     | 88     |                  |
| 20  | Q     | 105    |                  |
| 21  | R     | 88     |                  |
| 22  | S     | 93     |                  |
| 23  | T     | 106    |                  |
| 24  | V     | 26     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25  | PAR  | A     | 1545 | -         | -        | -       | X                |
| 26  | MG   | A     | 1561 | -         | -        | -       | X                |
| 26  | MG   | A     | 1562 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 26  | MG   | A     | 1564 | -         | -        | -       | X                |
| 26  | MG   | A     | 1589 | -         | -        | -       | X                |
| 26  | MG   | A     | 1601 | -         | -        | -       | X                |
| 26  | MG   | A     | 1608 | -         | -        | -       | X                |
| 26  | MG   | A     | 1623 | -         | -        | -       | X                |
| 26  | MG   | A     | 1633 | -         | -        | -       | X                |
| 26  | MG   | A     | 1646 | -         | -        | -       | X                |
| 26  | MG   | A     | 1648 | -         | -        | -       | X                |
| 26  | MG   | A     | 1651 | -         | -        | -       | X                |
| 26  | MG   | A     | 211  | -         | -        | -       | X                |

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52270 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   | A     | 1507     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32391 | 14418 | 6002 | 10465 | 1506 |         |         |       |

- Molecule 2 is a RNA chain called P-SITE MESSENGER RNA FRAGMENT.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2   | X     | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 117   | 54 | 14 | 44 | 5 |         |         |       |

- Molecule 3 is a RNA chain called ANTICODON STEM-LOOP OF PHENYLALANINE TRANSFER RNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 3   | Y     | 15       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 319   | 144 | 60 | 101 | 14 |         |         |       |

- Molecule 4 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 4   | Z     | 4        | Total | C  | N | O  | P | 0       | 0       | 0     |
|     |       |          | 77    | 36 | 8 | 30 | 3 |         |         |       |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 12  | I     | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |  |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | J     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 792   | 498 | 156 | 137 | 1 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | M     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment           | Reference   |
|-------|---------|----------|--------|-------------------|-------------|
| P     | ?       | -        | PHE    | CONFLICT/DELETION | GB 12056104 |
| P     | ?       | -        | HIS    | CONFLICT/DELETION | GB 12056104 |
| P     | ?       | -        | TYR    | CONFLICT/DELETION | GB 12056104 |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | S     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 674   | 430 | 126 | 116 | 2 |         |         |       |

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S20.

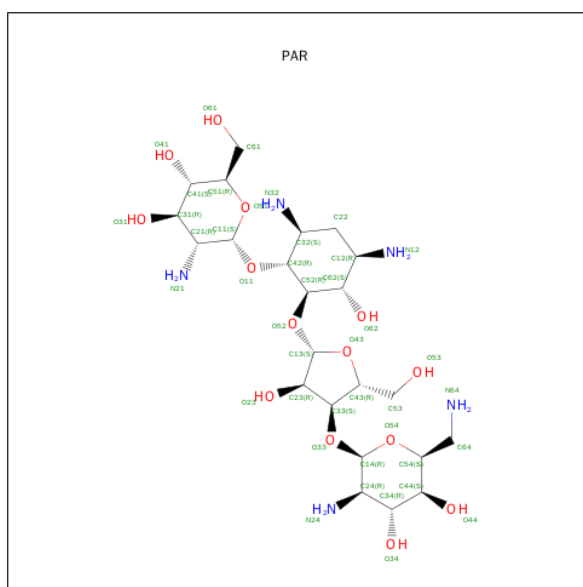
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | T     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 |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

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 25 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).





| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 25  | A     | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 26  | J     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 26  | A     | 120      | Total | Mg  | 0       | 0       |
|     |       |          | 120   | 120 |         |         |
| 26  | D     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 26  | Y     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

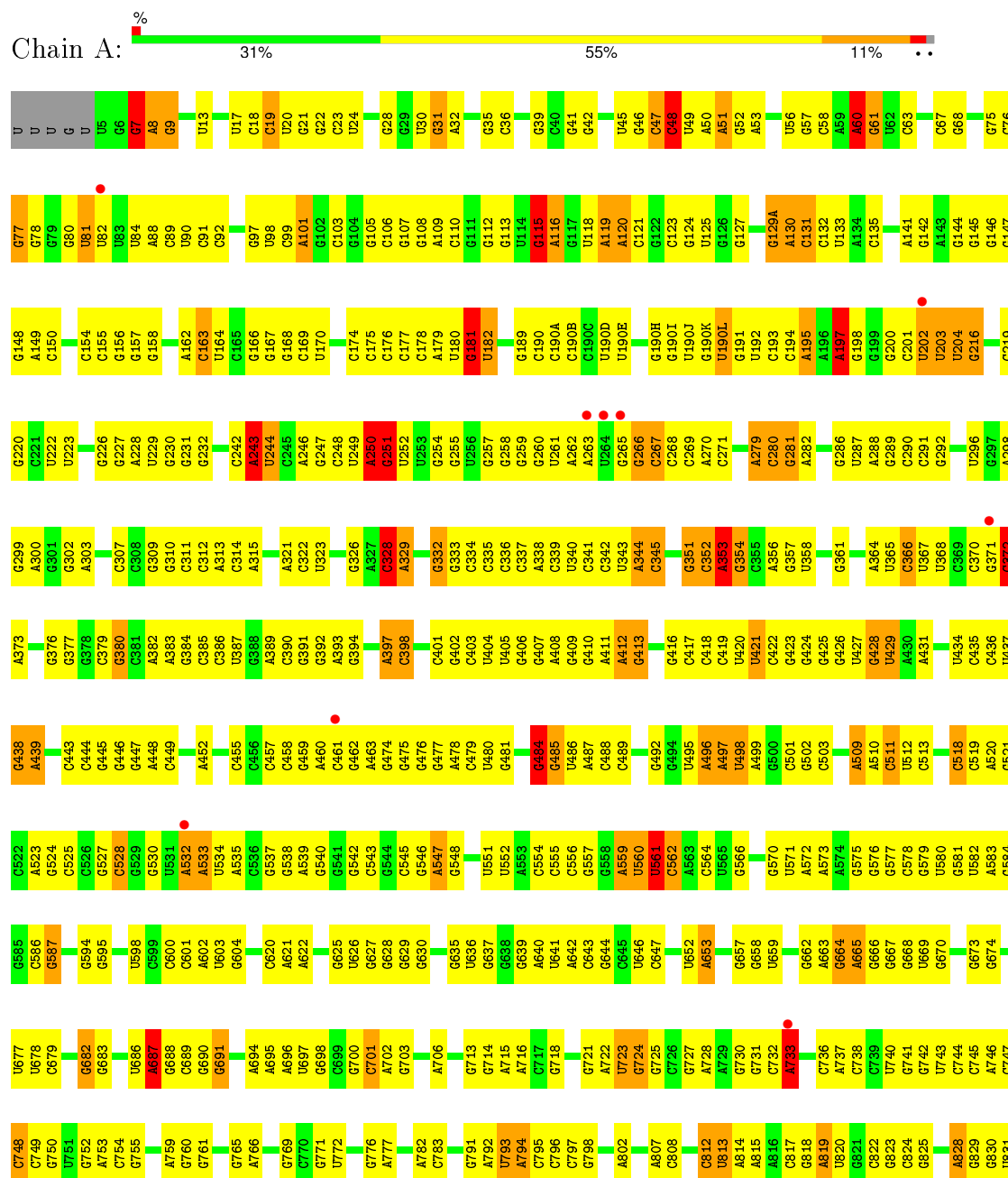
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

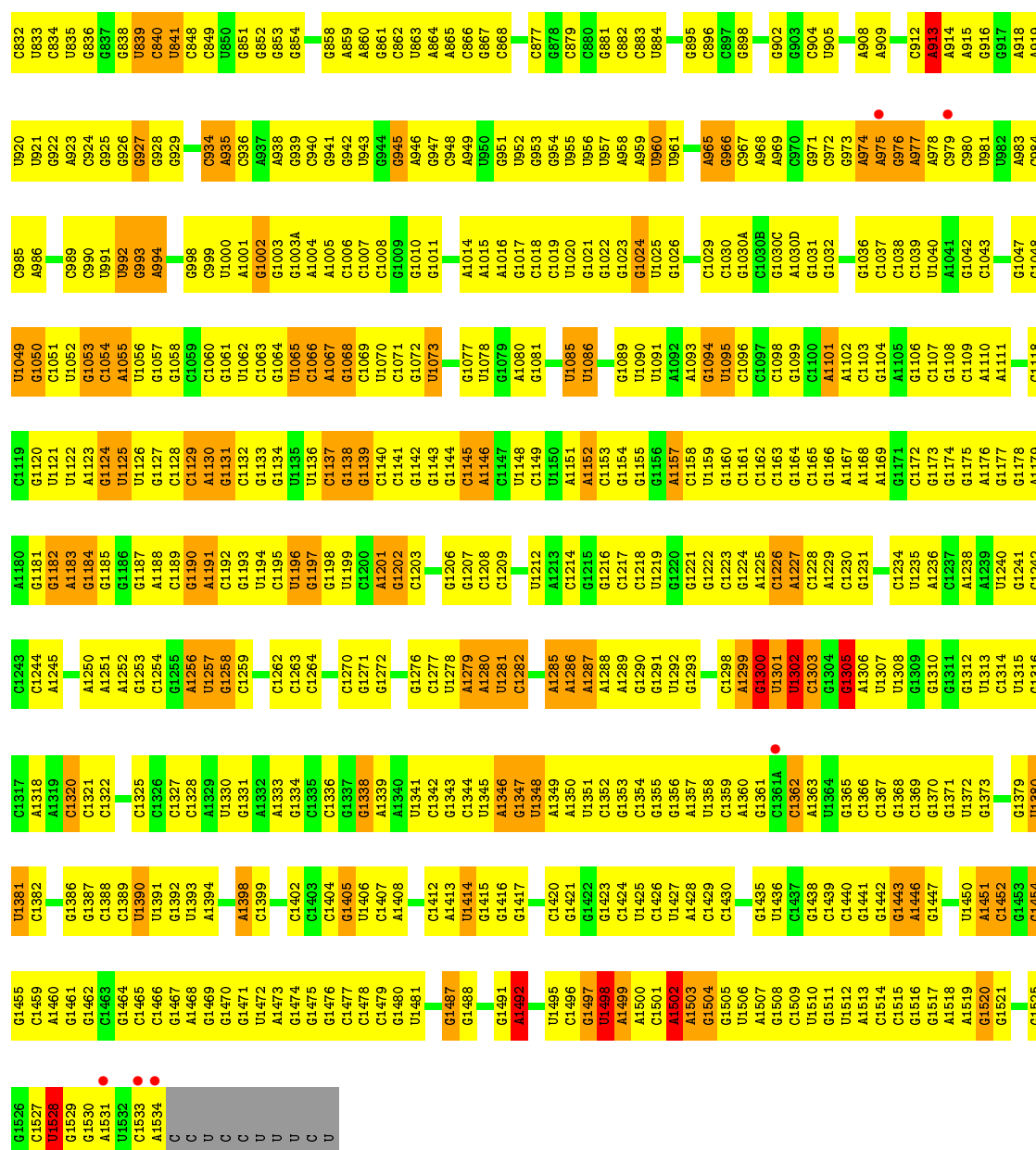
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 27  | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 27  | N     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

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

#### • Molecule 1: 16S RIBOSOMAL RNA

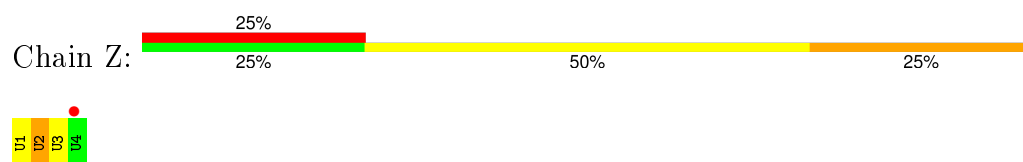




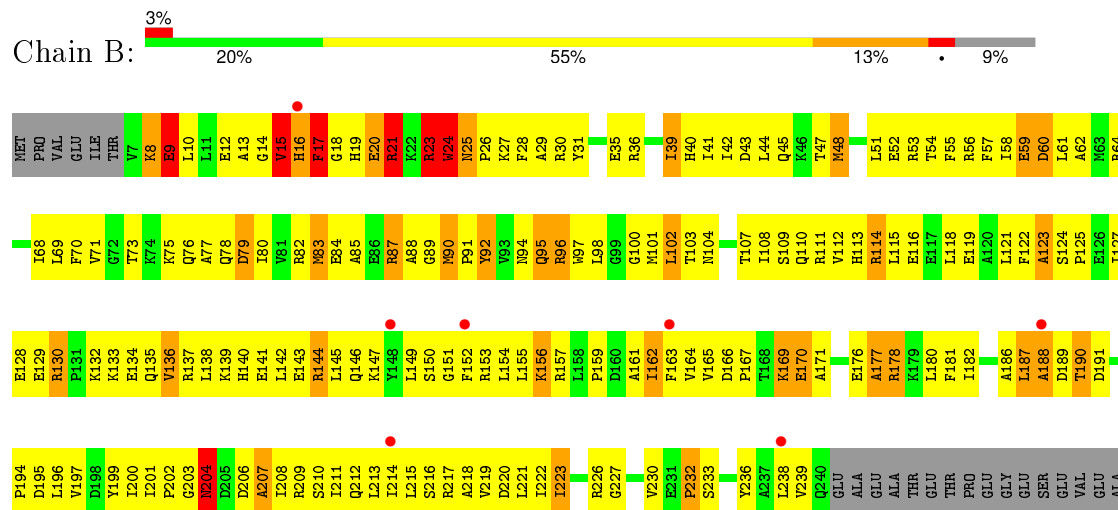
● Molecule 2: P-SITE MESSENGER RNA FRAGMENT

● Molecule 3: ANTICODON STEM-LOOP OF PHENYLALANINE TRANSFER RNA

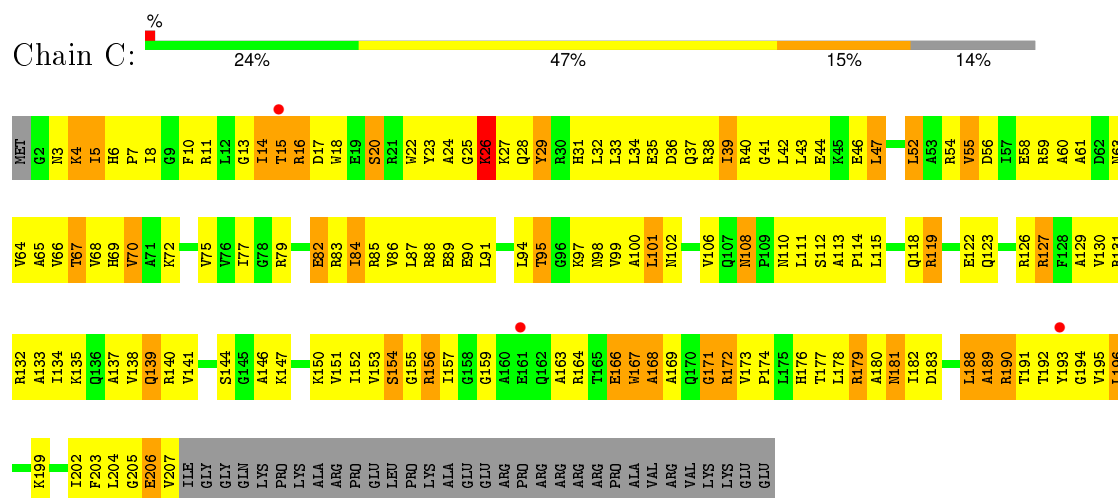
● Molecule 4: A-SITE MESSENGER RNA FRAGMENT



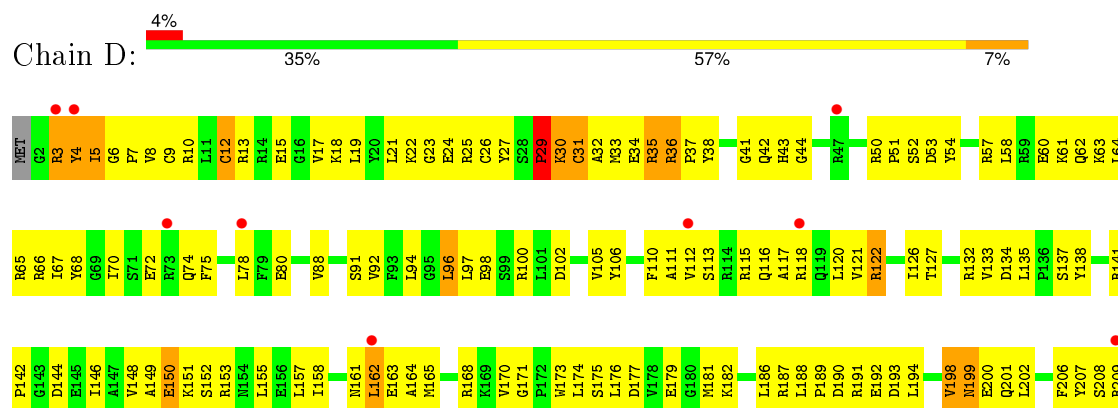
• Molecule 5: 30S RIBOSOMAL PROTEIN S2



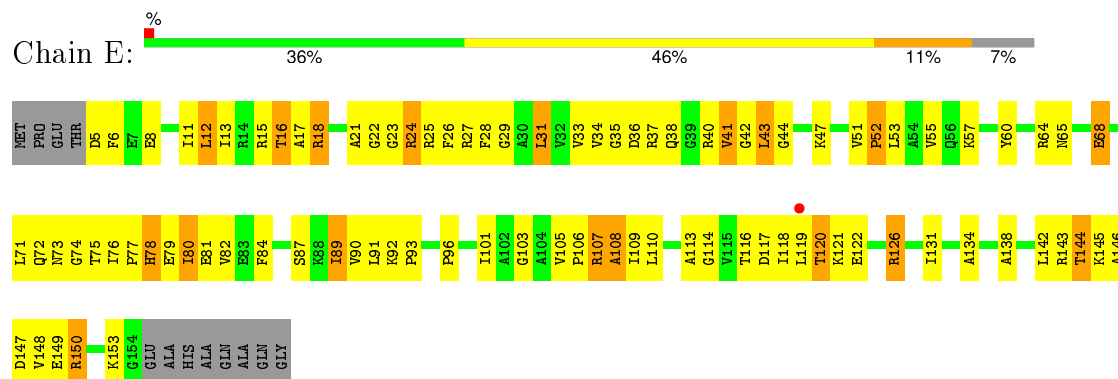
• Molecule 6: 30S RIBOSOMAL PROTEIN S3



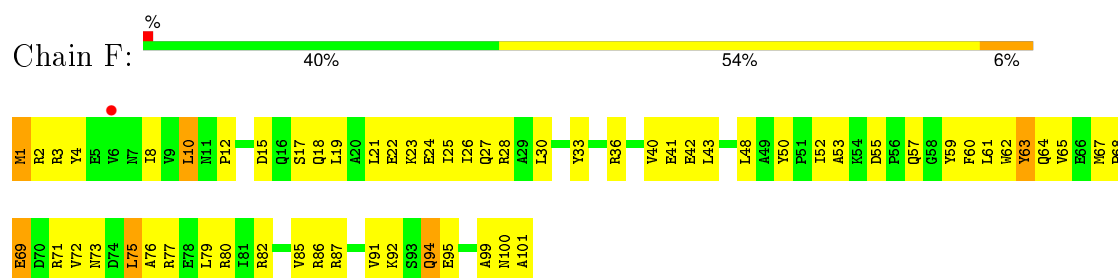
- Molecule 7: 30S RIBOSOMAL PROTEIN S4



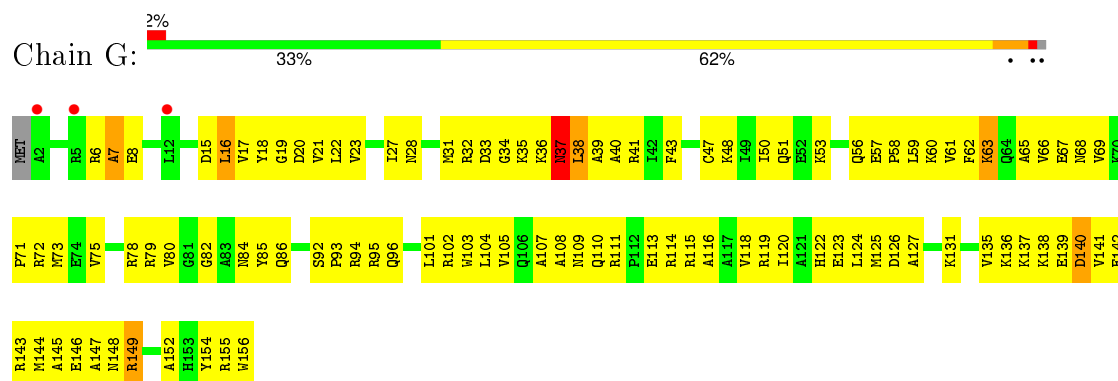
- Molecule 8: 30S RIBOSOMAL PROTEIN S5



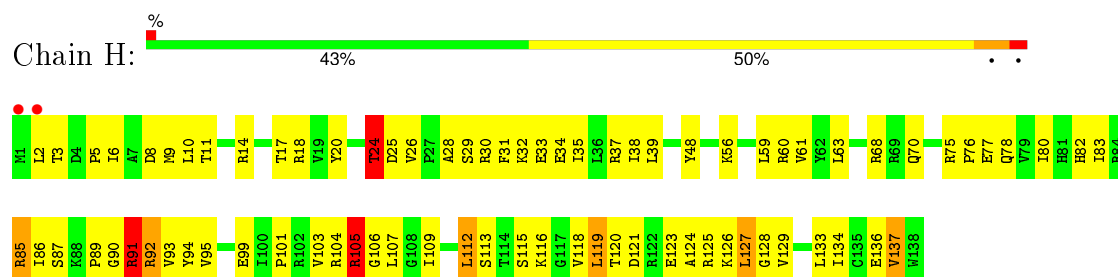
- Molecule 9: 30S RIBOSOMAL PROTEIN S6



- Molecule 10: 30S RIBOSOMAL PROTEIN S7

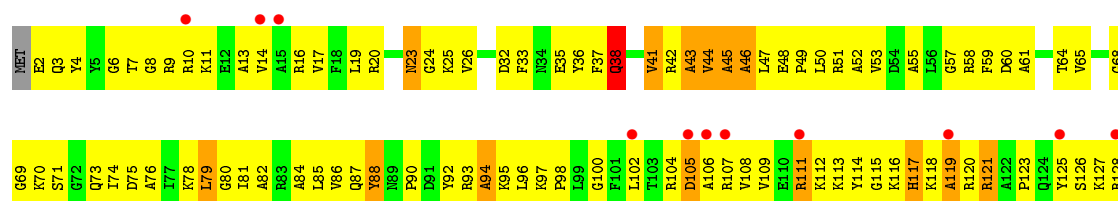


- Molecule 11: 30S RIBOSOMAL PROTEIN S8

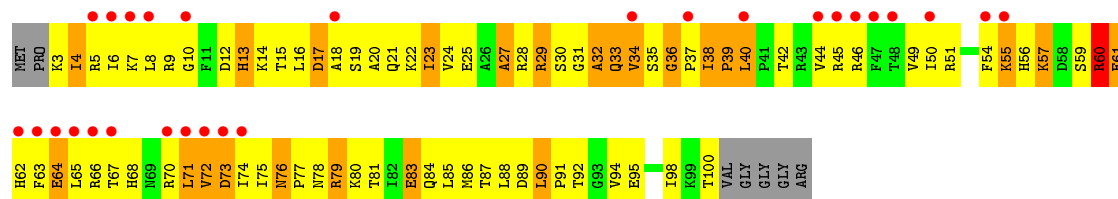
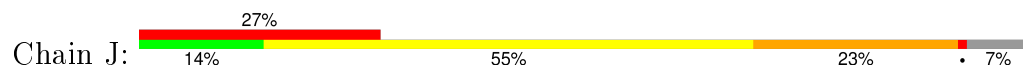


- Molecule 12: 30S RIBOSOMAL PROTEIN S9

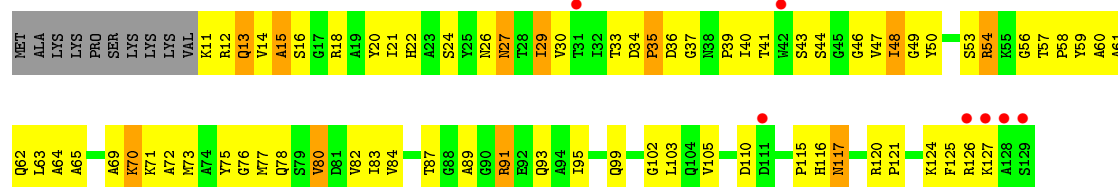




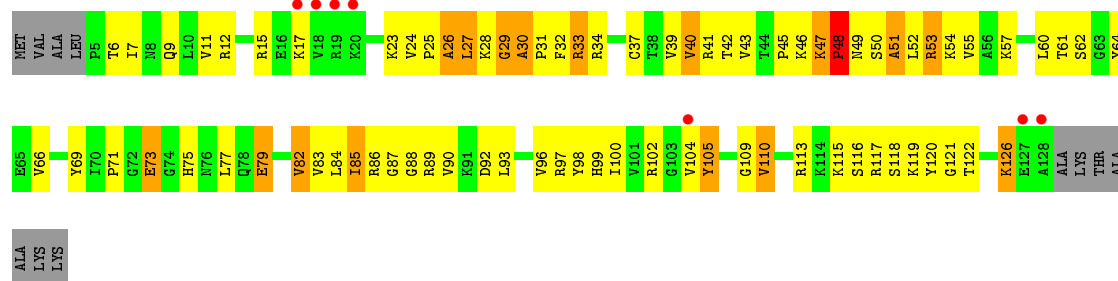
• Molecule 13: 30S RIBOSOMAL PROTEIN S10



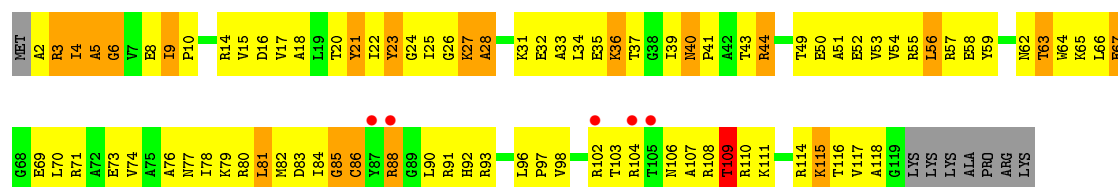
• Molecule 14: 30S RIBOSOMAL PROTEIN S11



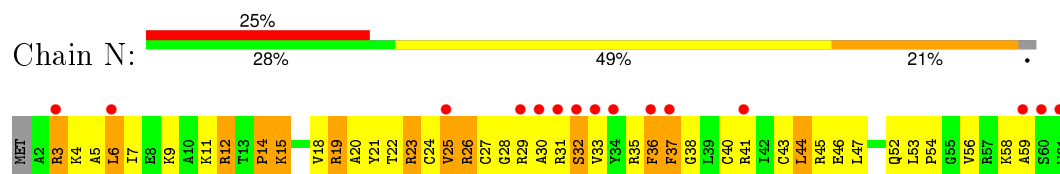
• Molecule 15: 30S RIBOSOMAL PROTEIN S12



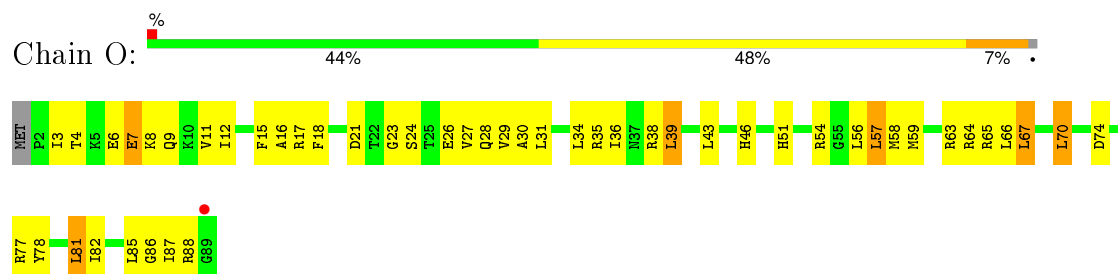
• Molecule 16: 30S RIBOSOMAL PROTEIN S13



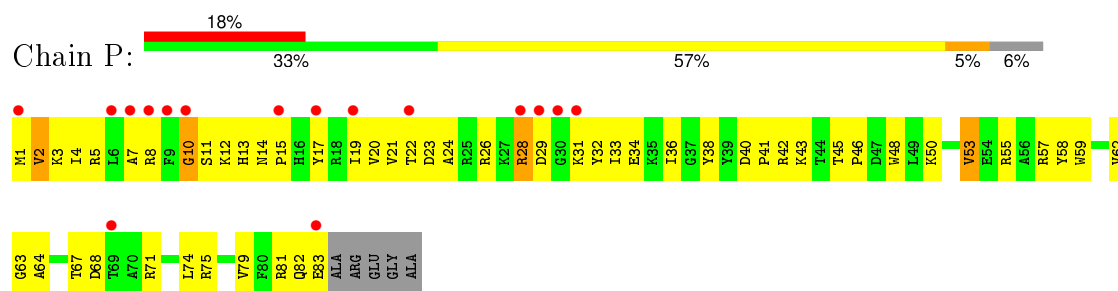
- Molecule 17: 30S RIBOSOMAL PROTEIN S14



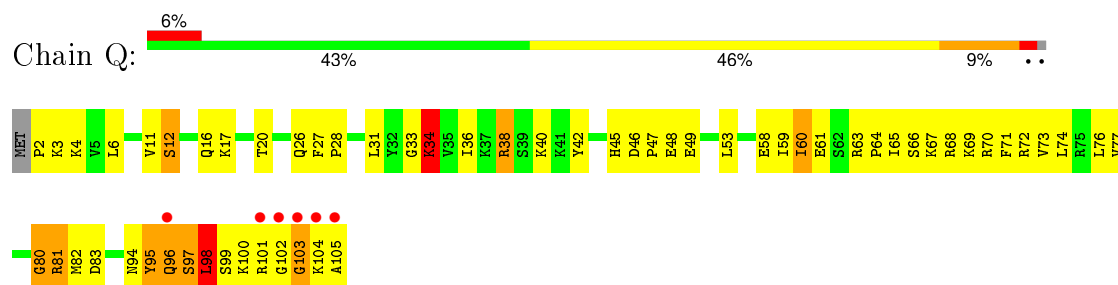
- Molecule 18: 30S RIBOSOMAL PROTEIN S15



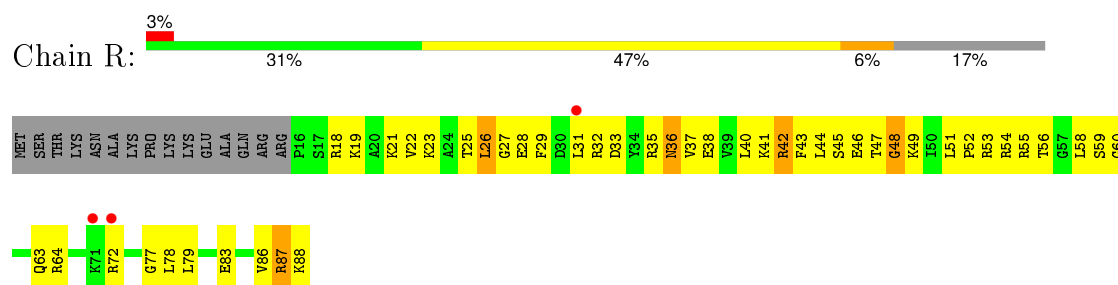
- Molecule 19: 30S RIBOSOMAL PROTEIN S16



- Molecule 20: 30S RIBOSOMAL PROTEIN S17

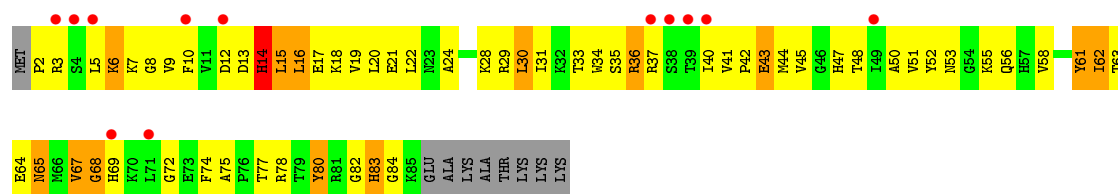


- Molecule 21: 30S RIBOSOMAL PROTEIN S18

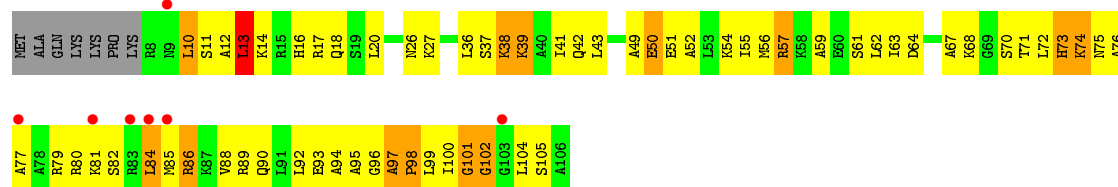


- Molecule 22: 30S RIBOSOMAL PROTEIN S19





• Molecule 23: 30S RIBOSOMAL PROTEIN S20



• Molecule 24: 30S RIBOSOMAL PROTEIN THX





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 400.80Å 400.80Å 175.88Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 316.23 – 3.11<br>200.40 – 3.11                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.9 (316.23-3.11)<br>89.8 (200.40-3.11)                    | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.12  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.36 (at 3.13Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.232 , 0.275<br>0.212 , 0.248                              | Depositor<br>DCC |
| $R_{free}$ test set   | 11493 reflections (5.32%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.7  | Xtriage          |
| Anisotropy  | 0.163   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 83.1   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 0 of 227639 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.84  | EDS              |
| Total number of atoms   | 52270   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 71.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.54         | 0/36259        | 0.74        | 34/56593 (0.1%) |
| 2   | X     | 0.45         | 0/128          | 0.64        | 0/196           |
| 3   | Y     | 0.36         | 0/357          | 0.66        | 0/555           |
| 4   | Z     | 0.42         | 0/84           | 0.81        | 0/128           |
| 5   | B     | 0.33         | 0/1935         | 0.62        | 0/2609          |
| 6   | C     | 0.36         | 0/1636         | 0.63        | 0/2205          |
| 7   | D     | 0.47         | 2/1733 (0.1%)  | 0.65        | 1/2318 (0.0%)   |
| 8   | E     | 0.47         | 0/1162         | 0.71        | 0/1564          |
| 9   | F     | 0.31         | 0/856          | 0.62        | 0/1154          |
| 10  | G     | 0.35         | 0/1276         | 0.59        | 0/1709          |
| 11  | H     | 0.44         | 0/1136         | 0.77        | 0/1527          |
| 12  | I     | 0.35         | 0/1029         | 0.64        | 0/1378          |
| 13  | J     | 0.37         | 0/805          | 0.68        | 1/1082 (0.1%)   |
| 14  | K     | 0.41         | 0/900          | 0.73        | 0/1213          |
| 15  | L     | 0.47         | 0/986          | 0.80        | 2/1320 (0.2%)   |
| 16  | M     | 0.34         | 0/947          | 0.64        | 0/1270          |
| 17  | N     | 0.44         | 0/501          | 0.74        | 0/664           |
| 18  | O     | 0.39         | 0/745          | 0.60        | 0/992           |
| 19  | P     | 0.46         | 0/716          | 0.73        | 0/963           |
| 20  | Q     | 0.48         | 0/870          | 0.74        | 0/1159          |
| 21  | R     | 0.36         | 0/603          | 0.63        | 0/799           |
| 22  | S     | 0.32         | 0/689          | 0.67        | 0/926           |
| 23  | T     | 0.44         | 0/765          | 0.75        | 1/1007 (0.1%)   |
| 24  | V     | 0.41         | 0/212          | 0.67        | 0/277           |
| All | All   | 0.50         | 2/56330 (0.0%) | 0.72        | 39/83608 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 3                   | 34                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | D     | 198 | VAL  | C-N   | -8.29 | 1.15        | 1.34     |
| 7   | D     | 200 | GLU  | C-N   | 5.60  | 1.47        | 1.34     |

The worst 5 of 39 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 10.07 | 131.65      | 109.50   |
| 1   | A     | 243  | A    | C2'-C3'-O3' | 9.49  | 130.37      | 109.50   |
| 1   | A     | 281  | G    | C2'-C3'-O3' | 9.34  | 130.05      | 109.50   |
| 1   | A     | 484  | G    | C2'-C3'-O3' | 8.78  | 128.82      | 109.50   |
| 1   | A     | 1302 | U    | C2'-C3'-O3' | 8.65  | 128.53      | 109.50   |

All (3) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | A     | 243  | A    | C3'  |
| 1   | A     | 281  | G    | C3'  |
| 1   | A     | 1528 | U    | C3'  |

5 of 34 planarity outliers are listed below:

| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 1   | A     | 19     | C    | Sidechain |
| 1   | A     | 190(L) | U    | Sidechain |
| 1   | A     | 197    | A    | Sidechain |
| 1   | A     | 250    | A    | Sidechain |
| 1   | A     | 77     | G    | 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   | A     | 32391 | 0        | 16349    | 1145    | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | X     | 117   | 0        | 64       | 0       | 0            |
| 3   | Y     | 319   | 0        | 164      | 12      | 0            |
| 4   | Z     | 77    | 0        | 42       | 6       | 0            |
| 5   | B     | 1900  | 0        | 1951     | 280     | 0            |
| 6   | C     | 1612  | 0        | 1677     | 244     | 0            |
| 7   | D     | 1703  | 0        | 1763     | 153     | 0            |
| 8   | E     | 1146  | 0        | 1207     | 111     | 0            |
| 9   | F     | 843   | 0        | 857      | 85      | 0            |
| 10  | G     | 1257  | 0        | 1296     | 101     | 0            |
| 11  | H     | 1116  | 0        | 1177     | 105     | 0            |
| 12  | I     | 1011  | 0        | 1043     | 133     | 0            |
| 13  | J     | 792   | 0        | 835      | 149     | 1            |
| 14  | K     | 885   | 0        | 904      | 86      | 0            |
| 15  | L     | 970   | 0        | 1057     | 126     | 0            |
| 16  | M     | 937   | 0        | 995      | 130     | 0            |
| 17  | N     | 492   | 0        | 529      | 79      | 0            |
| 18  | O     | 734   | 0        | 771      | 53      | 0            |
| 19  | P     | 700   | 0        | 720      | 57      | 0            |
| 20  | Q     | 857   | 0        | 930      | 93      | 0            |
| 21  | R     | 597   | 0        | 668      | 77      | 0            |
| 22  | S     | 674   | 0        | 699      | 88      | 0            |
| 23  | T     | 763   | 0        | 861      | 90      | 0            |
| 24  | V     | 208   | 0        | 221      | 20      | 0            |
| 25  | A     | 42    | 0        | 45       | 2       | 0            |
| 26  | A     | 120   | 0        | 0        | 0       | 0            |
| 26  | D     | 2     | 0        | 0        | 0       | 0            |
| 26  | J     | 2     | 0        | 0        | 0       | 0            |
| 26  | Y     | 1     | 0        | 0        | 0       | 0            |
| 27  | D     | 1     | 0        | 0        | 0       | 0            |
| 27  | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 52270 | 0        | 36825    | 3136    | 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 35.

The worst 5 of 3136 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) |
|----------------|-----------------|--------------------------|-------------------|
| 5:B:132:LYS:HA | 5:B:135:GLN:HB3 | 1.20                     | 1.14              |
| 7:D:36:ARG:H   | 7:D:37:PRO:HD3  | 1.09                     | 1.13              |
| 1:A:975:A:H4'  | 1:A:976:G:H5''  | 1.25                     | 1.12              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:1286:A:H3'  | 1:A:1287:A:H5'' | 1.28                     | 1.12              |
| 8:E:80:ILE:HD11 | 8:E:91:LEU:HB2  | 1.31                     | 1.11              |

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) |
|----------------|-----------------------|--------------------------|-------------------|
| 13:J:79:ARG:CD | 13:J:79:ARG:CD[8_665] | 2.14                     | 0.06              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 5   | B     | 232/256 (91%) | 145 (62%) | 59 (25%) | 28 (12%) | 0           | 2   |
| 6   | C     | 204/239 (85%) | 126 (62%) | 51 (25%) | 27 (13%) | 0           | 1   |
| 7   | D     | 206/209 (99%) | 160 (78%) | 32 (16%) | 14 (7%)  | 1           | 9   |
| 8   | E     | 148/162 (91%) | 132 (89%) | 13 (9%)  | 3 (2%)   | 9           | 39  |
| 9   | F     | 99/101 (98%)  | 82 (83%)  | 17 (17%) | 0        | 100         | 100 |
| 10  | G     | 153/156 (98%) | 118 (77%) | 28 (18%) | 7 (5%)   | 3           | 18  |
| 11  | H     | 136/138 (99%) | 112 (82%) | 20 (15%) | 4 (3%)   | 6           | 30  |
| 12  | I     | 125/128 (98%) | 94 (75%)  | 18 (14%) | 13 (10%) | 1           | 3   |
| 13  | J     | 96/105 (91%)  | 59 (62%)  | 17 (18%) | 20 (21%) | 0           | 0   |
| 14  | K     | 117/129 (91%) | 88 (75%)  | 20 (17%) | 9 (8%)   | 1           | 7   |
| 15  | L     | 122/135 (90%) | 96 (79%)  | 13 (11%) | 13 (11%) | 0           | 3   |
| 16  | M     | 116/126 (92%) | 77 (66%)  | 23 (20%) | 16 (14%) | 0           | 1   |
| 17  | N     | 58/61 (95%)   | 37 (64%)  | 11 (19%) | 10 (17%) | 0           | 0   |
| 18  | O     | 86/89 (97%)   | 67 (78%)  | 17 (20%) | 2 (2%)   | 8           | 36  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 19  | P     | 81/88 (92%)     | 71 (88%)   | 9 (11%)   | 1 (1%)   | 16          | 53 |
| 20  | Q     | 102/105 (97%)   | 78 (76%)   | 15 (15%)  | 9 (9%)   | 1           | 5  |
| 21  | R     | 71/88 (81%)     | 59 (83%)   | 8 (11%)   | 4 (6%)   | 2           | 13 |
| 22  | S     | 82/93 (88%)     | 53 (65%)   | 18 (22%)  | 11 (13%) | 0           | 1  |
| 23  | T     | 97/106 (92%)    | 61 (63%)   | 26 (27%)  | 10 (10%) | 1           | 3  |
| 24  | V     | 22/26 (85%)     | 15 (68%)   | 5 (23%)   | 2 (9%)   | 1           | 5  |
| All | All   | 2353/2540 (93%) | 1730 (74%) | 420 (18%) | 203 (9%) | 1           | 5  |

5 of 203 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | B     | 8   | LYS  |
| 5   | B     | 15  | VAL  |
| 5   | B     | 16  | HIS  |
| 5   | B     | 17  | PHE  |
| 5   | B     | 23  | ARG  |

### 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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5   | B     | 202/220 (92%)  | 176 (87%) | 26 (13%) | 5           | 22 |
| 6   | C     | 160/188 (85%)  | 146 (91%) | 14 (9%)  | 12          | 43 |
| 7   | D     | 180/181 (99%)  | 171 (95%) | 9 (5%)   | 30          | 68 |
| 8   | E     | 115/123 (94%)  | 98 (85%)  | 17 (15%) | 4           | 16 |
| 9   | F     | 90/90 (100%)   | 83 (92%)  | 7 (8%)   | 16          | 50 |
| 10  | G     | 126/127 (99%)  | 119 (94%) | 7 (6%)   | 26          | 63 |
| 11  | H     | 119/119 (100%) | 108 (91%) | 11 (9%)  | 11          | 40 |
| 12  | I     | 98/99 (99%)    | 92 (94%)  | 6 (6%)   | 23          | 60 |
| 13  | J     | 87/92 (95%)    | 79 (91%)  | 8 (9%)   | 11          | 40 |
| 14  | K     | 90/99 (91%)    | 84 (93%)  | 6 (7%)   | 20          | 56 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 15  | L     | 104/111 (94%)   | 97 (93%)   | 7 (7%)   | 20          | 56  |
| 16  | M     | 94/101 (93%)    | 85 (90%)   | 9 (10%)  | 10          | 37  |
| 17  | N     | 49/50 (98%)     | 44 (90%)   | 5 (10%)  | 9           | 33  |
| 18  | O     | 79/80 (99%)     | 71 (90%)   | 8 (10%)  | 9           | 34  |
| 19  | P     | 72/74 (97%)     | 68 (94%)   | 4 (6%)   | 26          | 63  |
| 20  | Q     | 96/97 (99%)     | 91 (95%)   | 5 (5%)   | 29          | 65  |
| 21  | R     | 64/77 (83%)     | 62 (97%)   | 2 (3%)   | 47          | 80  |
| 22  | S     | 73/80 (91%)     | 65 (89%)   | 8 (11%)  | 8           | 30  |
| 23  | T     | 76/82 (93%)     | 69 (91%)   | 7 (9%)   | 11          | 40  |
| 24  | V     | 19/21 (90%)     | 19 (100%)  | 0        | 100         | 100 |
| All | All   | 1993/2111 (94%) | 1827 (92%) | 166 (8%) | 14          | 47  |

5 of 166 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | G     | 37  | ASN  |
| 12  | I     | 23  | ASN  |
| 22  | S     | 15  | LEU  |
| 10  | G     | 136 | LYS  |
| 11  | H     | 85  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | F     | 73  | ASN  |
| 10  | G     | 122 | HIS  |
| 22  | S     | 23  | ASN  |
| 9   | F     | 94  | GLN  |
| 10  | G     | 37  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1506/1522 (98%) | 200 (13%)         | 67 (4%)         |
| 2   | X     | 5/6 (83%)       | 0                 | 0               |
| 3   | Y     | 14/15 (93%)     | 1 (7%)            | 0               |

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| Mol | Chain | Analysed          | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 4   | Z     | 3 / 4 (75%)       | 1 (33%)           | 0               |
| All | All   | 1528 / 1547 (98%) | 202 (13%)         | 67 (4%)         |

5 of 202 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | A    |
| 1   | A     | 9   | G    |
| 1   | A     | 31  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 39  | G    |

5 of 67 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 575  | G    |
| 1   | A     | 913  | A    |
| 1   | A     | 1346 | A    |
| 1   | A     | 687  | A    |
| 1   | A     | 793  | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 127 are monoatomic - leaving 1 for Mogul analysis.

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



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | PAR  | A     | 1545 | -    | 45,45,45     | 1.35 | 7 (15%)  | 59,67,67    | 1.18 | 5 (8%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 25  | PAR  | A     | 1545 | -    | -       | 0/18/94/94 | 0/4/4/4 |

The worst 5 of 7 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 25  | A     | 1545 | PAR  | O51-C11 | 2.20 | 1.47        | 1.41     |
| 25  | A     | 1545 | PAR  | O33-C14 | 2.26 | 1.47        | 1.41     |
| 25  | A     | 1545 | PAR  | C52-C42 | 2.33 | 1.57        | 1.52     |
| 25  | A     | 1545 | PAR  | C31-C21 | 2.34 | 1.56        | 1.53     |
| 25  | A     | 1545 | PAR  | C64-C54 | 2.48 | 1.58        | 1.52     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 25  | A     | 1545 | PAR  | O11-C11-C21 | 2.85 | 113.24      | 107.96   |
| 25  | A     | 1545 | PAR  | C14-O54-C54 | 2.89 | 119.35      | 113.75   |
| 25  | A     | 1545 | PAR  | O33-C14-C24 | 2.93 | 113.39      | 107.96   |
| 25  | A     | 1545 | PAR  | O52-C13-C23 | 3.00 | 114.00      | 107.75   |
| 25  | A     | 1545 | PAR  | O54-C54-C64 | 3.51 | 112.96      | 106.10   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | A     | 1545 | PAR  | 2       | 0            |

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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   | A     | 1507/1522 (99%) | 0.37   | 15 (0%) 84 70 | 22, 56, 140, 201      | 0     |
| 2   | X     | 6/6 (100%)      | 1.66   | 2 (33%) 0 0   | 47, 59, 141, 164      | 0     |
| 3   | Y     | 15/15 (100%)    | 0.62   | 0 100 100     | 58, 100, 200, 201     | 0     |
| 4   | Z     | 4/4 (100%)      | 1.31   | 1 (25%) 1 0   | 69, 71, 82, 141       | 0     |
| 5   | B     | 234/256 (91%)   | 0.25   | 7 (2%) 54 30  | 30, 94, 172, 201      | 0     |
| 6   | C     | 206/239 (86%)   | 0.03   | 3 (1%) 76 58  | 38, 81, 170, 192      | 0     |
| 7   | D     | 208/209 (99%)   | 0.39   | 9 (4%) 39 18  | 25, 62, 145, 181      | 0     |
| 8   | E     | 150/162 (92%)   | 0.03   | 1 (0%) 89 79  | 21, 47, 109, 164      | 0     |
| 9   | F     | 101/101 (100%)  | -0.10  | 1 (0%) 84 70  | 45, 90, 145, 176      | 0     |
| 10  | G     | 155/156 (99%)   | -0.12  | 3 (1%) 70 48  | 38, 73, 150, 191      | 0     |
| 11  | H     | 138/138 (100%)  | 0.16   | 2 (1%) 78 61  | 17, 43, 103, 150      | 0     |
| 12  | I     | 127/128 (99%)   | 0.52   | 11 (8%) 13 4  | 34, 89, 151, 180      | 0     |
| 13  | J     | 98/105 (93%)    | 1.27   | 28 (28%) 1 0  | 36, 114, 185, 201     | 0     |
| 14  | K     | 119/129 (92%)   | 0.59   | 7 (5%) 26 10  | 24, 60, 123, 201      | 0     |
| 15  | L     | 124/135 (91%)   | 0.35   | 7 (5%) 28 11  | 16, 55, 125, 192      | 0     |
| 16  | M     | 118/126 (93%)   | 0.11   | 5 (4%) 40 19  | 36, 74, 131, 165      | 0     |
| 17  | N     | 60/61 (98%)     | 1.20   | 15 (25%) 1 0  | 44, 76, 139, 194      | 0     |
| 18  | O     | 88/89 (98%)     | 0.04   | 1 (1%) 82 67  | 26, 56, 137, 199      | 0     |
| 19  | P     | 83/88 (94%)     | 0.90   | 16 (19%) 2 1  | 22, 47, 77, 158       | 0     |
| 20  | Q     | 104/105 (99%)   | 0.89   | 6 (5%) 26 11  | 13, 45, 137, 201      | 0     |
| 21  | R     | 73/88 (82%)     | 0.42   | 3 (4%) 41 19  | 33, 71, 165, 201      | 0     |
| 22  | S     | 84/93 (90%)     | 0.70   | 12 (14%) 4 2  | 54, 100, 165, 201     | 0     |
| 23  | T     | 99/106 (93%)    | 0.68   | 7 (7%) 19 7   | 25, 57, 127, 198      | 0     |
| 24  | V     | 24/26 (92%)     | 1.19   | 2 (8%) 14 5   | 42, 61, 113, 188      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| All | All   | 3925/4087 (96%) | 0.38   | 164 (4%) | 40 | 19 | 13, 63, 153, 201      | 0     |

The worst 5 of 164 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 14  | K     | 129 | SER  | 26.9 |
| 22  | S     | 3   | ARG  | 13.9 |
| 20  | Q     | 103 | GLY  | 12.6 |
| 14  | K     | 128 | ALA  | 11.5 |
| 20  | Q     | 104 | LYS  | 10.3 |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 26  | MG   | A     | 1608 | 1/1   | 0.89 | 0.31 | 22.79 | 20,20,20,20                | 1     |
| 26  | MG   | A     | 1646 | 1/1   | 0.85 | 0.36 | 18.85 | 20,20,20,20                | 1     |
| 26  | MG   | A     | 1651 | 1/1   | 0.93 | 0.43 | 12.78 | 20,20,20,20                | 1     |
| 26  | MG   | A     | 1623 | 1/1   | 0.81 | 0.33 | 7.36  | 20,20,20,20                | 1     |
| 26  | MG   | A     | 1589 | 1/1   | 0.88 | 0.35 | 6.36  | 20,20,20,20                | 1     |
| 26  | MG   | A     | 1648 | 1/1   | 0.91 | 0.68 | 4.98  | 20,20,20,20                | 1     |
| 26  | MG   | A     | 211  | 1/1   | 0.75 | 0.32 | 4.82  | 20,20,20,20                | 1     |
| 26  | MG   | A     | 1601 | 1/1   | 0.92 | 0.25 | 4.13  | 20,20,20,20                | 1     |
| 26  | MG   | A     | 1561 | 1/1   | 0.98 | 0.26 | 3.82  | 20,20,20,20                | 0     |
| 26  | MG   | A     | 1564 | 1/1   | 0.96 | 0.37 | 3.08  | 20,20,20,20                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 25  | PAR  | A     | 1545 | 42/42 | 0.92 | 0.29 | 2.68  | 59,59,59,59                 | 0     |
| 26  | MG   | A     | 1562 | 1/1   | 0.95 | 0.24 | 2.40  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 441  | 1/1   | 0.40 | 0.21 | 1.92  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1596 | 1/1   | 0.97 | 0.28 | 1.88  | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1597 | 1/1   | 0.89 | 0.23 | 1.85  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1642 | 1/1   | 0.79 | 0.20 | 1.62  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1653 | 1/1   | 0.79 | 0.23 | 1.60  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1622 | 1/1   | 0.62 | 0.23 | 1.59  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1633 | 1/1   | 0.49 | 0.41 | 1.07  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1573 | 1/1   | 0.98 | 0.26 | 1.03  | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1552 | 1/1   | 0.95 | 0.28 | 0.87  | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1572 | 1/1   | 0.96 | 0.36 | 0.81  | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1579 | 1/1   | 0.98 | 0.25 | 0.64  | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1600 | 1/1   | 0.95 | 0.25 | 0.29  | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1592 | 1/1   | 0.98 | 0.21 | 0.04  | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1598 | 1/1   | 0.88 | 0.24 | -0.16 | 20,20,20,20                 | 1     |
| 27  | ZN   | N     | 307  | 1/1   | 0.99 | 0.18 | -0.53 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1644 | 1/1   | 0.83 | 0.20 | -0.59 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1556 | 1/1   | 0.87 | 0.24 | -0.70 | 20,20,20,20                 | 0     |
| 26  | MG   | D     | 215  | 1/1   | 0.66 | 0.18 | -0.84 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1546 | 1/1   | 0.99 | 0.20 | -1.08 | 20,20,20,20                 | 0     |
| 26  | MG   | J     | 422  | 1/1   | 0.98 | 0.20 | -1.13 | 20,20,20,20                 | 0     |
| 26  | MG   | J     | 449  | 1/1   | 0.96 | 0.25 | -1.13 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 210  | 1/1   | 0.75 | 0.17 | -1.40 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1575 | 1/1   | 0.97 | 0.20 | -1.40 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1593 | 1/1   | 0.99 | 0.20 | -1.52 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1609 | 1/1   | 0.87 | 0.14 | -1.63 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1599 | 1/1   | 0.94 | 0.18 | -1.73 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1635 | 1/1   | 0.82 | 0.22 | -1.81 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1588 | 1/1   | 0.95 | 0.20 | -1.82 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1625 | 1/1   | 0.90 | 0.18 | -2.27 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1604 | 1/1   | 0.92 | 0.16 | -3.37 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1637 | 1/1   | 0.91 | 0.10 | -3.50 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1559 | 1/1   | 0.95 | 0.17 | -3.51 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1656 | 1/1   | 0.77 | 0.12 | -3.57 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1634 | 1/1   | 0.93 | 0.11 | -3.82 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1581 | 1/1   | 0.96 | 0.16 | -4.40 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1605 | 1/1   | 0.87 | 0.15 | -4.47 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1638 | 1/1   | 0.89 | 0.22 | -5.01 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1614 | 1/1   | 0.94 | 0.09 | -5.35 | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1585 | 1/1   | 0.98 | 0.12 | -6.35 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1594 | 1/1   | 0.94 | 0.08 | -9.12 | 20,20,20,20                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 26  | MG   | A     | 1565 | 1/1   | 0.93 | 0.10 | -11.19 | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1616 | 1/1   | 0.90 | 0.44 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1568 | 1/1   | 0.94 | 0.25 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1570 | 1/1   | 0.94 | 0.29 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1583 | 1/1   | 0.90 | 0.32 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1586 | 1/1   | 0.98 | 0.21 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1610 | 1/1   | 0.91 | 0.40 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1617 | 1/1   | 0.82 | 0.37 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1652 | 1/1   | 0.95 | 0.45 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1603 | 1/1   | 0.94 | 0.21 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 87   | 1/1   | 0.94 | 0.41 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1619 | 1/1   | 0.92 | 0.39 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1567 | 1/1   | 0.92 | 0.28 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1650 | 1/1   | 0.95 | 0.14 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1590 | 1/1   | 0.81 | 0.30 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1643 | 1/1   | 0.63 | 0.38 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1548 | 1/1   | 0.89 | 0.13 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1549 | 1/1   | 0.67 | 0.32 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1632 | 1/1   | 0.95 | 0.14 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1630 | 1/1   | 0.76 | 0.20 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1602 | 1/1   | 0.95 | 0.37 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1639 | 1/1   | 0.90 | 0.32 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1655 | 1/1   | 0.92 | 0.14 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1563 | 1/1   | 0.90 | 0.14 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1547 | 1/1   | 0.96 | 0.24 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1553 | 1/1   | 0.95 | 0.29 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1560 | 1/1   | 0.97 | 0.36 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1641 | 1/1   | 0.89 | 0.14 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1577 | 1/1   | 0.96 | 0.20 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1554 | 1/1   | 0.98 | 0.36 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1626 | 1/1   | 0.91 | 0.25 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1566 | 1/1   | 0.97 | 0.34 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1654 | 1/1   | 0.96 | 0.20 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1618 | 1/1   | 0.79 | 0.25 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1550 | 1/1   | 0.91 | 0.26 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | D     | 210  | 1/1   | 0.96 | 0.33 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1606 | 1/1   | 0.91 | 0.19 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1645 | 1/1   | 0.70 | 0.43 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1615 | 1/1   | 0.76 | 0.37 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1613 | 1/1   | 0.94 | 0.08 | -      | 20,20,20,20                 | 0     |
| 26  | MG   | Y     | 456  | 1/1   | 0.25 | 0.33 | -      | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1582 | 1/1   | 0.98 | 0.32 | -      | 20,20,20,20                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 26  | MG   | A     | 1591 | 1/1   | 0.93 | 0.40 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1578 | 1/1   | 0.89 | 0.36 | -    | 20,20,20,20                 | 1     |
| 27  | ZN   | D     | 306  | 1/1   | 0.97 | 0.35 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1584 | 1/1   | 0.91 | 0.26 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1629 | 1/1   | 0.87 | 0.20 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 71   | 1/1   | 0.93 | 0.28 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1558 | 1/1   | 0.97 | 0.29 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1631 | 1/1   | 0.81 | 0.46 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1557 | 1/1   | 0.95 | 0.40 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1569 | 1/1   | 0.89 | 0.43 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1611 | 1/1   | 0.96 | 0.28 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1657 | 1/1   | 0.83 | 0.25 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1628 | 1/1   | 0.82 | 0.46 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1649 | 1/1   | 0.90 | 0.29 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 86   | 1/1   | 0.97 | 0.28 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1647 | 1/1   | 0.86 | 0.34 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1607 | 1/1   | 0.97 | 0.21 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1624 | 1/1   | 0.92 | 0.27 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1555 | 1/1   | 0.79 | 0.22 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1627 | 1/1   | 0.90 | 0.29 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1640 | 1/1   | 0.69 | 0.21 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1580 | 1/1   | 0.92 | 0.17 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1571 | 1/1   | 0.96 | 0.14 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1636 | 1/1   | 0.91 | 0.27 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1595 | 1/1   | 0.94 | 0.31 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 214  | 1/1   | 0.88 | 0.15 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1620 | 1/1   | 0.84 | 0.22 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1587 | 1/1   | 0.98 | 0.23 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 1551 | 1/1   | 0.95 | 0.23 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1576 | 1/1   | 0.97 | 0.26 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1612 | 1/1   | 0.98 | 0.25 | -    | 20,20,20,20                 | 0     |
| 26  | MG   | A     | 213  | 1/1   | 0.97 | 0.26 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1621 | 1/1   | 0.88 | 0.29 | -    | 20,20,20,20                 | 1     |
| 26  | MG   | A     | 1574 | 1/1   | 0.90 | 0.24 | -    | 20,20,20,20                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.