



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 01:27 AM EDT

PDB ID : 5J8B / pdb\_00005j8b  
Title : Crystal structure of Elongation Factor 4 (EF-4/LepA) in complex with  
GDP-CP bound to the Thermus thermophilus 70S ribosome  
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.  
Deposited on : 2016-04-07  
Resolution : 2.60 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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

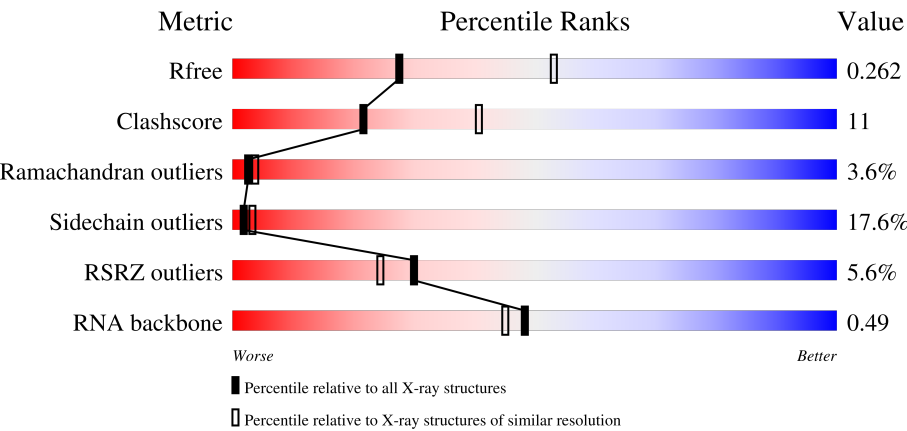
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



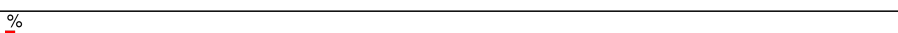
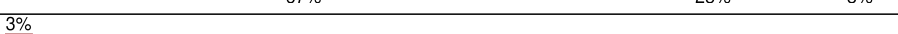
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 4008 (2.60-2.60)                                      |
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |
| RNA backbone          | 3983                        | 1014 (2.84-2.36)                                      |

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   | A     | 2915   | <div><div>4%</div><div><div></div><div>59%</div><div>31%</div><div>8%</div><div>.</div></div></div>    |
| 2   | B     | 121    | <div><div>%</div><div><div></div><div>60%</div><div>35%</div><div>.</div><div>.</div></div></div>      |
| 3   | C     | 228    | <div><div>26%</div><div><div></div><div>22%</div><div>29%</div><div>9%</div><div>40%</div></div></div> |
| 4   | D     | 276    | <div><div>%</div><div><div></div><div>66%</div><div>25%</div><div>8%</div></div></div>                 |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 206    |    |
| 6   | F     | 210    |    |
| 7   | G     | 182    |    |
| 8   | H     | 180    |    |
| 9   | J     | 173    |    |
| 10  | K     | 147    |    |
| 11  | N     | 140    |    |
| 12  | O     | 122    |    |
| 13  | P     | 150    |    |
| 14  | Q     | 141    |    |
| 15  | R     | 118    |    |
| 16  | S     | 112    |    |
| 17  | T     | 146    |  |
| 18  | U     | 118    |  |
| 19  | V     | 101    |  |
| 20  | W     | 113    |  |
| 21  | X     | 96     |  |
| 22  | Y     | 110    |  |
| 23  | Z     | 206    |  |
| 24  | 0     | 85     |  |
| 25  | 1     | 98     |  |
| 26  | 2     | 72     |  |
| 27  | 3     | 60     |  |
| 28  | 4     | 71     |  |
| 29  | 5     | 60     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30  | 6     | 54     |                  |
| 31  | 7     | 49     |                  |
| 32  | 8     | 65     |                  |
| 33  | 9     | 37     |                  |
| 34  | a     | 1521   |                  |
| 35  | b     | 256    |                  |
| 36  | c     | 239    |                  |
| 37  | d     | 209    |                  |
| 38  | e     | 162    |                  |
| 39  | f     | 101    |                  |
| 40  | g     | 156    |                  |
| 41  | h     | 138    |                  |
| 42  | i     | 128    |                  |
| 43  | j     | 105    |                  |
| 44  | k     | 129    |                  |
| 45  | l     | 132    |                  |
| 46  | m     | 126    |                  |
| 47  | n     | 61     |                  |
| 48  | o     | 89     |                  |
| 49  | p     | 88     |                  |
| 50  | q     | 105    |                  |
| 51  | r     | 88     |                  |
| 52  | s     | 93     |                  |
| 53  | t     | 106    |                  |
| 54  | u     | 27     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55  | v     | 24     |                  |
| 56  | w     | 76     |                  |
| 57  | x     | 77     |                  |
| 58  | y     | 76     |                  |
| 59  | z     | 679    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 62  | SF4  | d     | 302 | -         | -        | X       | -                |

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155465 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 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | A     | 2874     | Total | C     | N     | O     | P    | 11      | 0       | 0     |
|     |       |          | 61902 | 27550 | 11582 | 19897 | 2873 |         |         |       |

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | B     | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 136      | Total | C   | N   | O   | S | 1       | 0       | 0     |
|     |       |          | 1024  | 644 | 190 | 189 | 1 |         |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | F     | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1584  | 1009 | 298 | 275 | 2 |         |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1425  | 914 | 256 | 251 | 4 |         |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 174      | Total | C   | N   | O   | S | 1       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | J     | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 641   | 381 | 130 | 130 |   |         |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | K     | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1025  | 653 | 181 | 186 | 5 |         |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | N     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | O     | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | P     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | Q     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | R     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 16  | S     | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |         |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | T     | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1091  | 680 | 225 | 185 | 1 |         |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | U     | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | V     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | W     | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L23.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | X     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | Y     | 107      | Total | C   | N   | O   | S | 1       | 0       | 0     |
|     |       |          | 806   | 517 | 152 | 131 | 6 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | Z     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 784   | 499 | 150 | 134 | 1 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 24  | 0     | 74       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 591   | 366 | 126 | 98 | 1 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | 1     | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 475 | 148 | 131 | 1 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | 2     | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 27  | 3     | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | 4     | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 557   | 350 | 101 | 101 | 5 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29  | 5     | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | 6     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 31  | 7     | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32  | 8     | 64       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 511   | 328 | 99 | 82 | 2 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 33  | 9     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 34  | a     | 1498     | Total | C     | N    | O     | P    | 4       | 0       | 0     |
|     |       |          | 32207 | 14334 | 5973 | 10402 | 1498 |         |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35  | b     | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1850  | 1181 | 331 | 333 | 5 |         |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | c     | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1550  | 974 | 302 | 273 | 1 |         |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 37  | d     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1655  | 1038 | 326 | 284 | 7 |         |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | e     | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 213 | 198 | 4 |         |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | f     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 511 | 143 | 149 | 3 |         |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | g     | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1227  | 764 | 242 | 215 | 6 |         |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | h     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | i     | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 983   | 623 | 193 | 167 |         |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43  | j     | 96       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 698   | 434 | 134 | 130 |         |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | k     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 829   | 516 | 155 | 155 | 3 |         |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | l     | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 930   | 585 | 185 | 159 | 1 |         |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | m     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 924   | 570 | 192 | 160 | 2 |         |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 47  | n     | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | o     | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 456 | 144 | 126 | 2 |         |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | p     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 433 | 134 | 113 | 1 |         |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | q     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 51  | r     | 68       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |         |         |       |

- Molecule 52 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | s     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 650   | 415 | 120 | 113 | 2 |         |         |       |

- Molecule 53 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | t     | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 724   | 443 | 155 | 124 | 2 |         |         |       |

- Molecule 54 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 54  | u     | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |

- Molecule 55 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 55  | v     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 277   | 125 | 51 | 88 | 13 |         |         |       |

- Molecule 56 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 56  | w     | 74       | Total | C   | N   | O   | P  | S | 1       | 0       | 0     |
|     |       |          | 1586  | 713 | 285 | 513 | 73 | 2 |         |         |       |

- Molecule 57 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 57  | x     | 77       | Total | C   | N   | O   | P  | S | 3       | 0       | 0     |
|     |       |          | 1645  | 734 | 297 | 536 | 77 | 1 |         |         |       |

- Molecule 58 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 58  | y     | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1580  | 706 | 285 | 515 | 73 | 1 |         |         |       |

- Molecule 59 is a protein called GDPCP fused to the N-terminus of the ribosomal protein L9,Elongation factor 4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 59  | z     | 671      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 5200  | 3333 | 897 | 961 | 9 |         |         |       |

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 60  | A     | 644      | Total | Mg  | 0       | 0       |
|     |       |          | 644   | 644 |         |         |
| 60  | B     | 18       | Total | Mg  | 0       | 0       |
|     |       |          | 18    | 18  |         |         |
| 60  | D     | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 60  | E     | 5        | Total | Mg  | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 60  | F     | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 60  | G     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | H     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | N     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | O     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 60  | P     | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 60  | Q     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | R     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | U     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | V     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | W     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | X     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | Z     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | 0     | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 60  | 5     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | 6     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | 7     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | 8     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | 9     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | a     | 188      | Total<br>188 | Mg<br>188 | 0       | 0       |
| 60  | d     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | e     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | f     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | l     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | m     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | n     | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |

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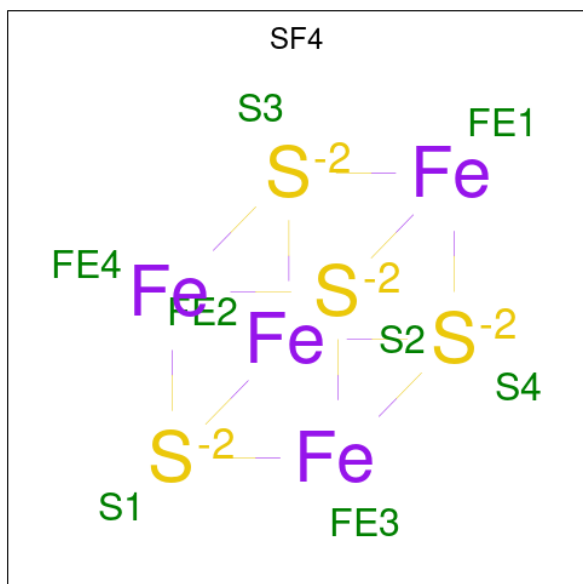
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60  | v     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 60  | x     | 9        | Total | Mg | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 60  | z     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 61  | Y     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 4     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 5     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 6     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 9     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | n     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

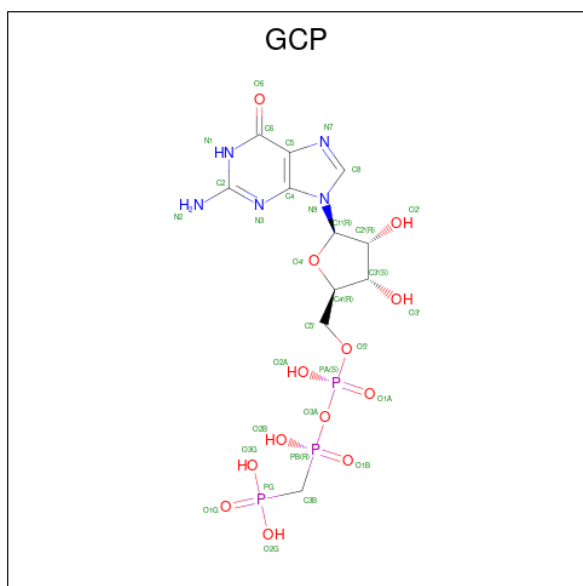
- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 62  | d     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 63 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 63  | z     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |

- Molecule 64 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 64  | A     | 715      | Total | O   | 0       | 0       |
|     |       |          | 715   | 715 |         |         |
| 64  | B     | 32       | Total | O   | 0       | 0       |
|     |       |          | 32    | 32  |         |         |
| 64  | D     | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 64  | E     | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 64  | F     | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 64  | H     | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 64  | N     | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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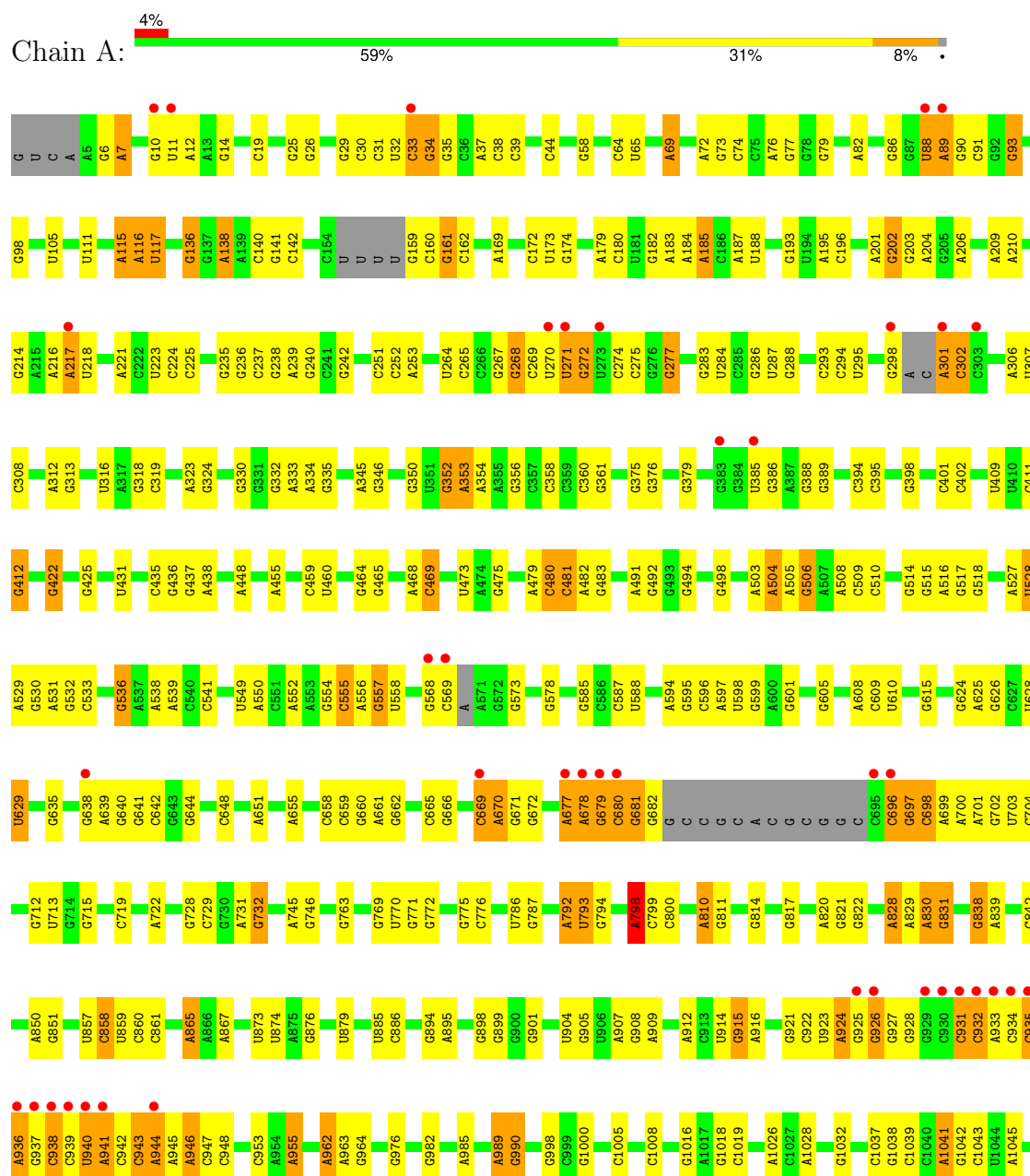
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 64  | O     | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 64  | P     | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 64  | Q     | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 64  | T     | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 64  | U     | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 64  | V     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 64  | 0     | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 64  | 1     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 64  | 3     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 64  | 7     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 64  | 8     | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 64  | a     | 165      | Total<br>165 | O<br>165 | 0       | 0       |
| 64  | l     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 64  | p     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 64  | v     | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 64  | w     | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 64  | z     | 1        | Total<br>1   | O<br>1   | 0       | 0       |

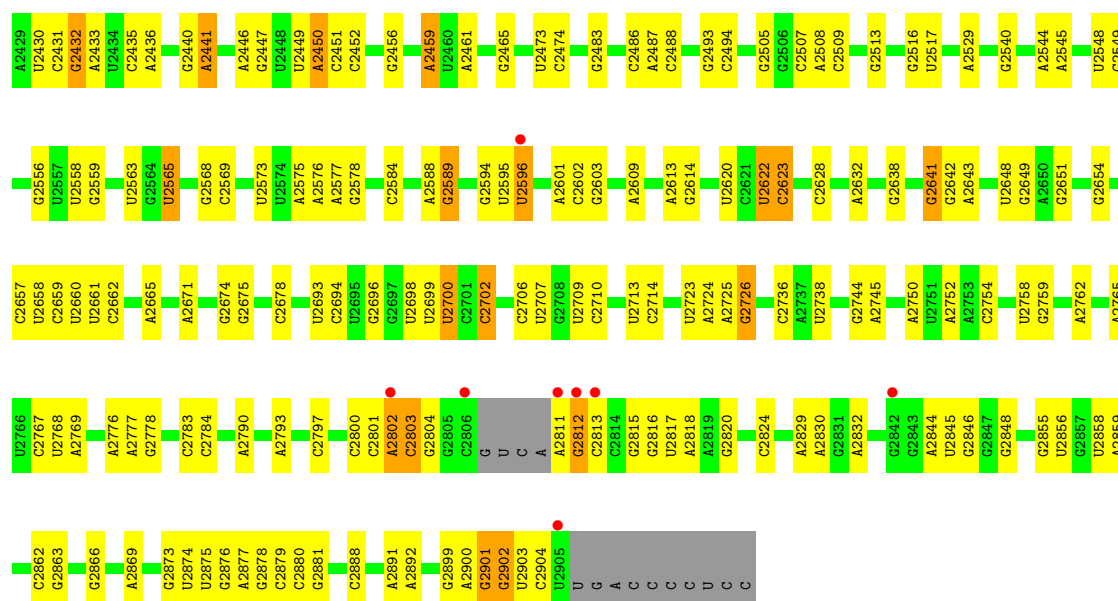
### 3 Residue-property plots

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

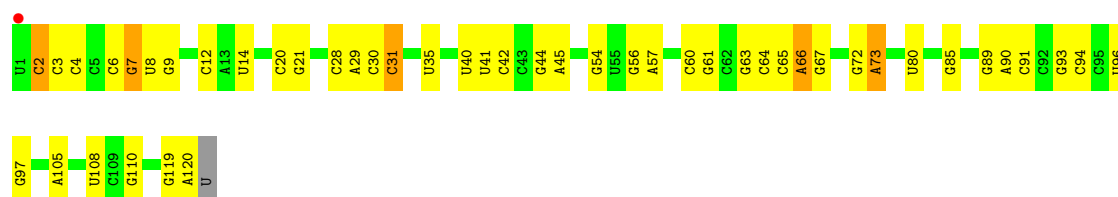
#### • Molecule 1: 23S Ribosomal RNA



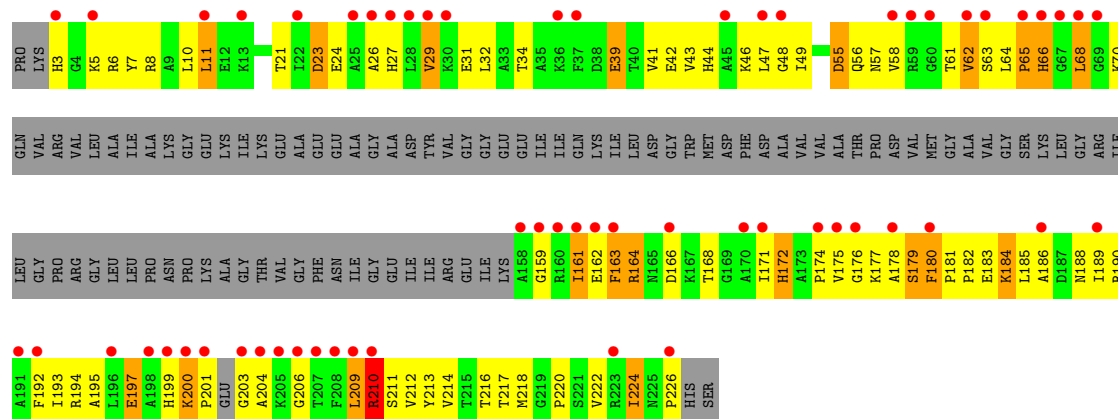
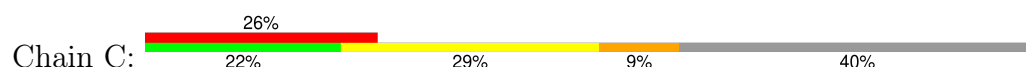
|       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2330 | G2212 | G2152 | G2053 | C1830 | U1739 | C1621 | G1529 | G1425 | A1299 | G1209 | C1124 | C1050 |
| A2331 | G2213 | G2153 | A2054 | G1831 | U1739 | U1622 | G1530 | A1429 | U1300 | U1210 | C1125 | C1051 |
| A2332 | G2214 | U2055 | G2056 | A1833 | G1742 | C1623 | A1531 | A1430 | C1301 | C1126 | C1126 | A1054 |
| G2333 |       | G2154 |       | A1833 | G1742 | C1623 | G1532 | C1431 | C1302 | U1127 | U1127 |       |
| G2334 | C2217 | A2155 | A2063 | U1835 | G1743 | A1625 | G1537 | C1432 | C1303 | U1128 | U1128 |       |
| G2335 | U2218 | A2156 | C2064 | U1835 | A1744 | A1626 | C1538 |       | G1305 | A1129 | A1129 | U1057 |
| G2336 | A2219 | C2157 |       | A1839 | G1745 | G1627 | U1538 |       | G1305 | A1130 | A1130 | C1058 |
| G2337 | A2220 | C2158 |       | A1840 | A1746 | A1628 | A1540 |       | C1306 | A1131 | A1131 | C1059 |
| A2338 | G2221 | C2159 | C2076 |       |       | C1629 | A1541 |       | A1307 | G1132 | G1132 | U1060 |
| A2339 |       | C2160 | G2077 | G1844 | U1758 | C1630 | A1541 |       |       |       |       |       |
| G2340 | G2226 | U2161 |       | A1845 | C1760 | A1631 | G1545 |       | A1310 | A1133 | A1133 | U1064 |
| G2345 | A2227 | C2164 | A2081 | A1846 | G1761 | A1632 |       |       |       | A1134 | A1134 |       |
| A2346 | G2228 | U2165 | A2082 | A1846 | G1761 | C1633 |       |       | A1311 | U1135 | U1135 | A1065 |
| A2347 | U2229 | G2166 | A2083 | G1847 | G1762 | C1634 |       |       | U1312 | U1136 | U1136 | A1066 |
| G2348 | G2230 | A1953 | A2084 | U1848 | U1764 | U1635 | U1548 |       | A1313 | G1137 | G1137 | G1087 |
|       |       | C2167 | C2085 | A1848 | U1764 | G1636 | C1549 |       | G1316 | U1138 | U1138 | U1088 |
|       |       | C2168 | C2086 | U1850 | G1765 | C1637 | A1552 |       | U1317 | C1223 | C1223 | A1069 |
|       |       | G2169 |       | A1851 | A1766 | G1638 | A1553 |       | U1318 | C1224 | C1224 | G1070 |
| C2354 | G2235 | G2170 | G2090 | G1852 | U1767 | G1639 | C1554 |       | A1319 | G1228 | U1142 | A1072 |
| U2355 | C2237 | U2171 |       |       | G1768 |       | A1555 |       |       |       | A1143 | A1073 |
|       |       | C2172 | G2093 | G1856 | U1769 | C1643 | A1556 |       | U1333 | G1231 | A1148 |       |
|       |       | G2173 | U2107 | C1857 | A1769 | C1648 | G1557 |       | C1334 | U1232 | U1150 |       |
|       |       | G2174 | G2108 | G1858 | C1771 | A1648 | U1561 |       | C1335 | A1233 | G1149 | A1076 |
|       |       | G2175 |       | A1859 | C1772 | C1649 | G1569 |       | C1336 | A1238 | U1148 | U1078 |
|       |       | C2176 | U2113 | U1863 | C1773 | C1652 |       |       | U1337 |       | U1151 |       |
|       |       | C2177 | G2114 |       | C1774 | A1653 | G1578 |       | G1344 | C1245 | G1152 | G1084 |
|       |       | A2178 |       | G1869 | G1775 | A1654 | G1587 |       | U1345 | A1248 | U1153 | A1090 |
|       |       | U2179 |       | U1883 | G1776 | A1655 | A1588 |       | A1346 | U1249 | U1154 | A1091 |
| U2254 | U2254 | C1988 | C2118 | A1883 | G1777 | A1655 | G1589 |       | C1360 | G1250 | G1155 | A1092 |
| A2371 | U2255 | U1989 | U2119 | A1884 | G1778 | A1659 | G1597 |       |       | C1251 | A1156 | A1093 |
| A2372 | U2256 | A1990 | U2120 | G1885 | G1779 |       | C1598 |       | G1372 | C1265 | G1170 |       |
| A2373 | U2257 | A1991 | U2121 | G1886 | A1779 |       | G1598 |       |       | C1266 | A1173 |       |
| C2374 | G2261 | A1992 | G2122 | G1887 |       | C1662 | A1599 |       |       | C1267 | A1174 |       |
| G2375 |       | A1993 | U2123 | G1888 | C1784 |       | G1599 |       | G1389 | G1268 | U1175 |       |
| G2376 |       | G2013 | C2124 | U1888 | G1785 | G1667 | C1599 |       |       | A1264 | G1179 |       |
| A2388 | A2280 | U2186 | G2125 | A1888 | G1786 |       | C1599 |       |       | C1265 | G1180 |       |
| A2389 | G2282 | U2188 | C2126 | G1885 | U1787 | G1670 | A1588 |       |       | A1264 | G1181 |       |
|       | U2283 | G2189 | G2127 | G1886 | G1788 | G1671 | A1589 |       |       | C1266 | G1182 |       |
| G2394 | U2284 | A2190 | C2128 | G1887 | G1789 |       | G1599 |       |       | C1267 | G1183 |       |
| G2395 | A2284 | A2026 | U2130 | G1888 | G1794 | C1682 | C1599 |       |       | G1268 | G1184 |       |
| G2396 | C2286 | G2193 | U2131 | G1889 | G1799 | U1685 | C1597 |       |       | A1264 | G1185 |       |
|       | G2287 | U2133 | C2132 | U1894 | A1803 | C1686 | G1598 |       |       | C1265 | U1186 |       |
| A2399 | G2288 | U2133 | G2133 | G1895 |       |       | A1599 |       |       | A1271 | A1187 |       |
| G2400 | A2289 | C2196 | U2134 | C1896 |       | C1690 | A1599 |       |       |       | G1194 |       |
|       | G2290 | C2197 | A2135 | A1897 | A1810 | C1694 | A1600 |       |       |       | G1198 |       |
|       |       | C2198 | G2136 | A1898 | C1811 | C1694 | G1601 |       |       |       | G1199 |       |
|       |       | C2199 | G2137 | A1899 | C1812 |       | C1602 |       |       |       | A1200 |       |
|       |       | C2200 | A2138 | C1813 | C1813 | G1689 | G1603 |       |       |       | G1295 |       |
|       | C2294 | C2200 | A2139 | A1814 | A1814 | A1700 | A1604 |       |       |       | A1423 |       |
|       |       | U2201 | U2139 | G1904 |       |       | G1605 |       |       |       |       |       |
|       | A2287 | G2202 | A2140 | A1905 |       | A1711 | G1606 |       |       |       | G1289 |       |
| G2415 | A2298 | G2203 | G2141 | A1906 | C1820 | G1712 | A1612 |       |       |       | G1293 |       |
| G2416 |       | C2204 | G2142 | C2045 | A1821 |       | G1613 |       |       |       | U1294 |       |
| G2418 | A2316 | C2204 | U2143 | G2046 | U1824 | G1720 | A1614 |       |       |       | G1199 |       |
|       |       | G2205 | G2144 | C2047 | U1825 |       | A1615 |       |       |       | A1201 |       |
|       | G2318 | G2206 | G2145 | G2048 | U1826 | G1732 | G1616 |       |       |       | A1202 |       |
| G2421 | G2319 | G2207 | G2146 | U2049 | U1827 |       | A1617 |       |       |       |       |       |
|       |       | G2208 | G2146 | U2049 | U1828 | G1734 |       |       |       |       |       |       |
|       |       | C2209 | A2147 | G2050 | U1828 | U1734 |       |       |       |       |       |       |
| G2425 |       | U2210 | G2148 | A2051 | G1829 | A1735 |       |       |       |       |       |       |
| G2428 |       | G2323 |       | A2052 |       |       |       |       |       |       |       |       |
|       |       | G2329 |       |       |       |       |       |       |       |       |       |       |



• Molecule 2: 5S Ribosomal RNA

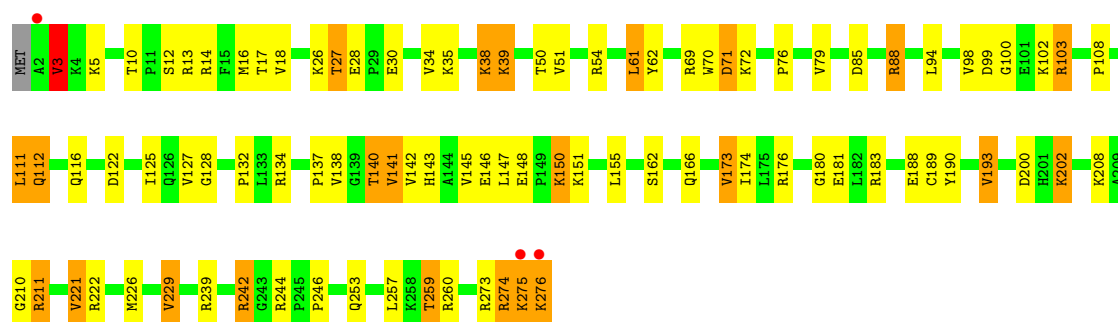


• Molecule 3: 50S ribosomal protein L1

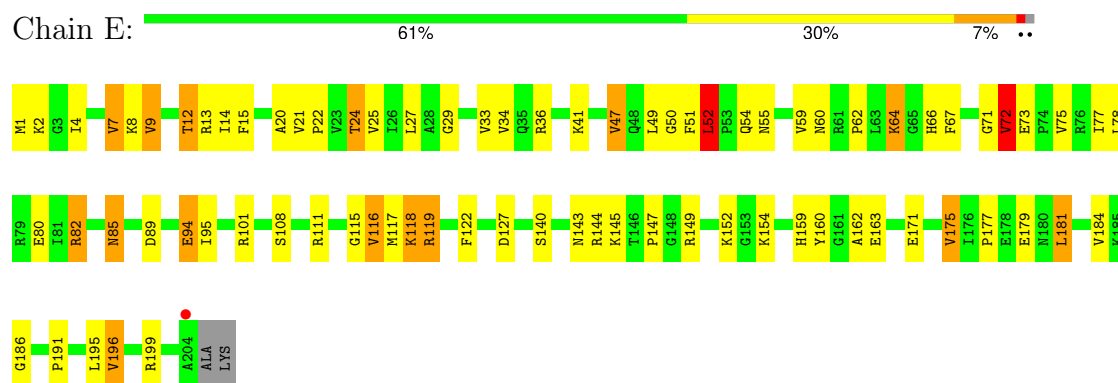


• Molecule 4: 50S ribosomal protein L2

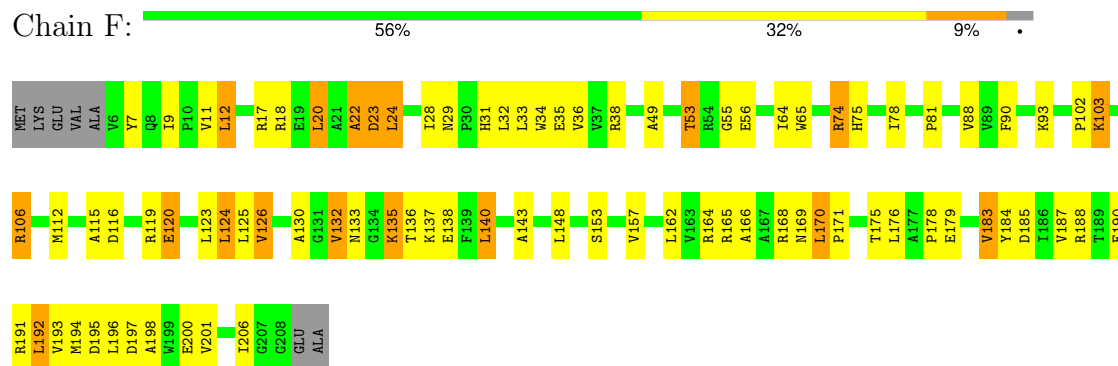




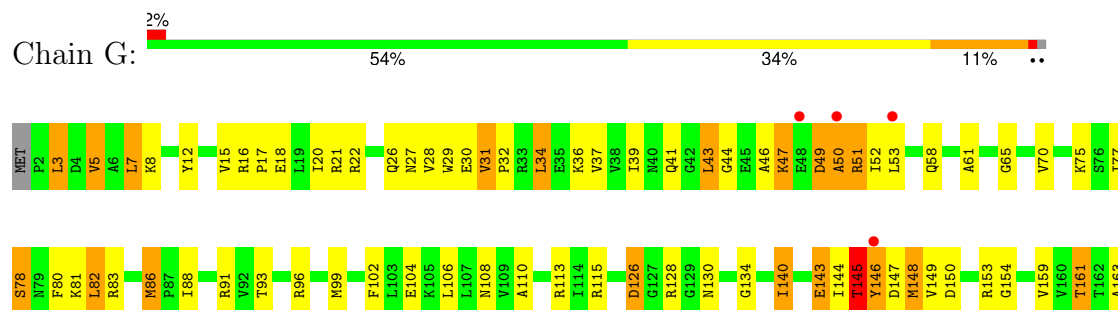
• Molecule 5: 50S ribosomal protein L3



• Molecule 6: 50S ribosomal protein L4

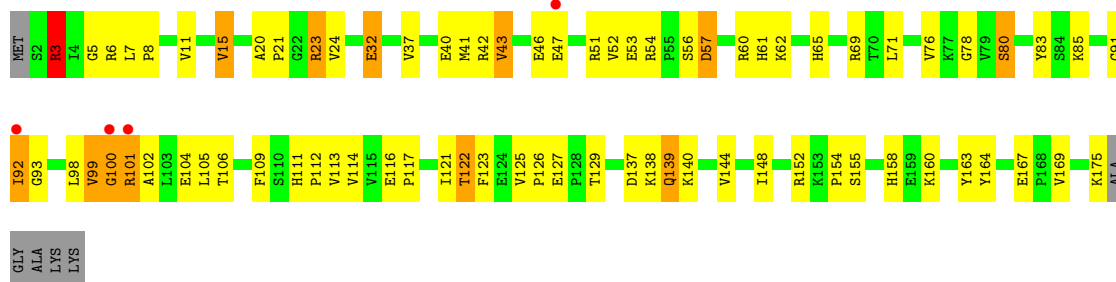


• Molecule 7: 50S ribosomal protein L5

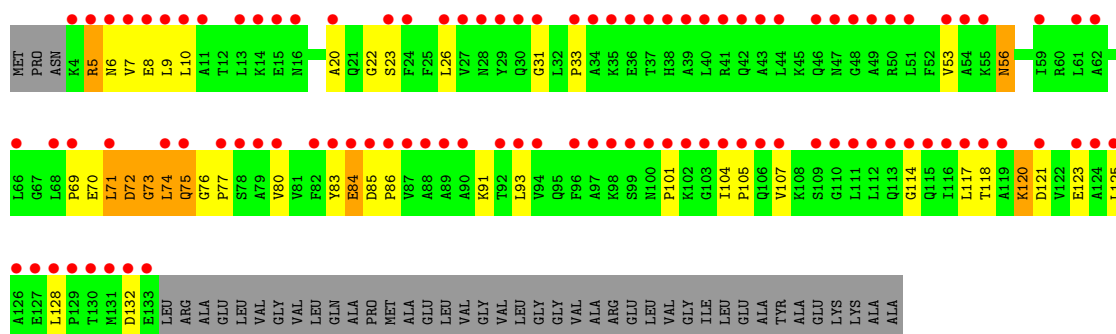




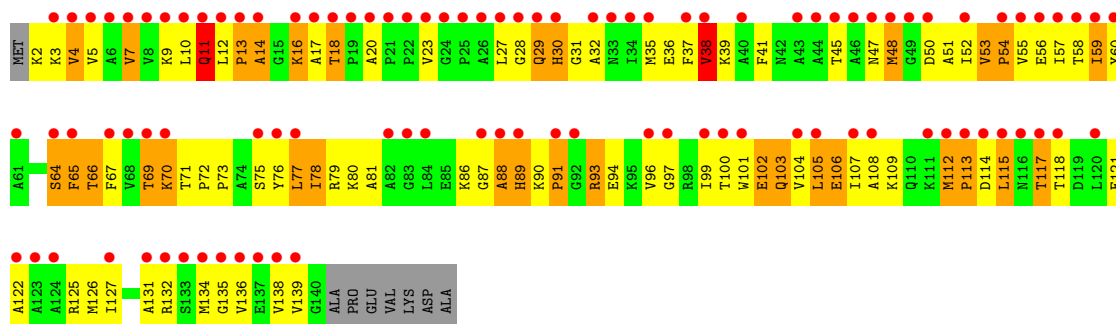
• Molecule 8: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L10

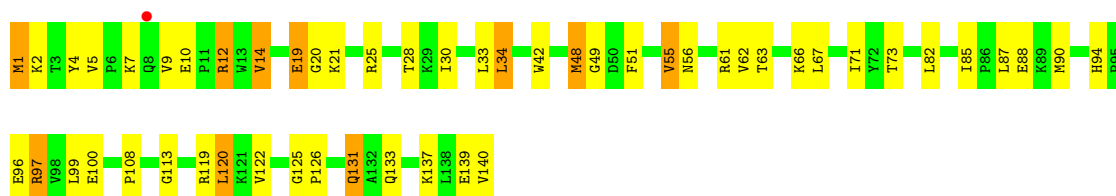


• Molecule 10: 50S ribosomal protein L11



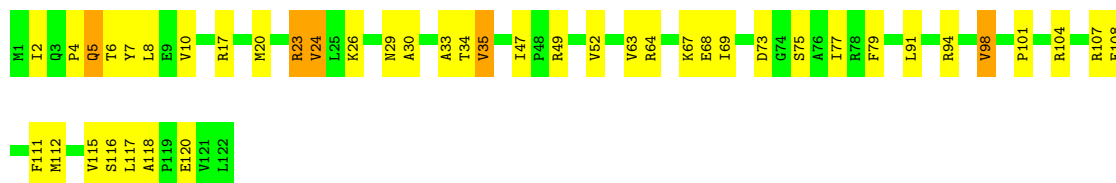
• Molecule 11: 50S ribosomal protein L13





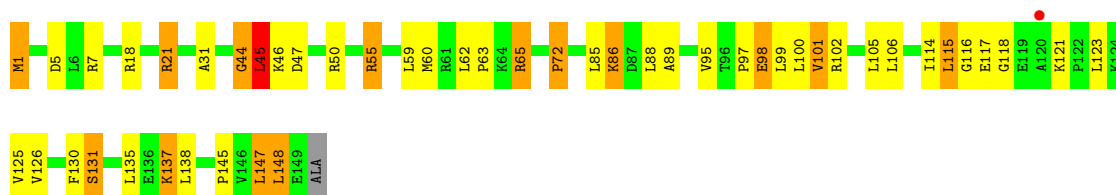
• Molecule 12: 50S ribosomal protein L14

Chain O: 65% 31%



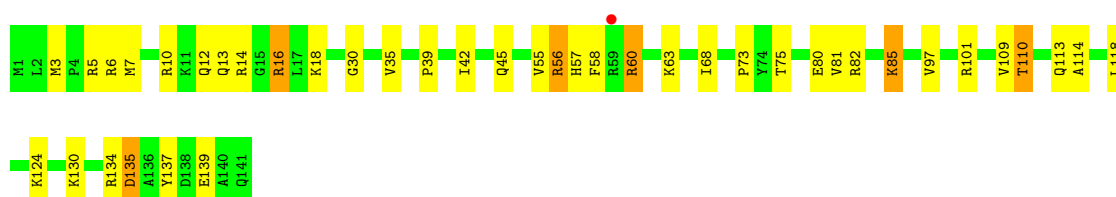
• Molecule 13: 50S ribosomal protein L15

Chain P: 67% 22% 9%



• Molecule 14: 50S ribosomal protein L16

Chain Q: 71% 25%



• Molecule 15: 50S ribosomal protein L17

Chain R: 75% 20% 5%



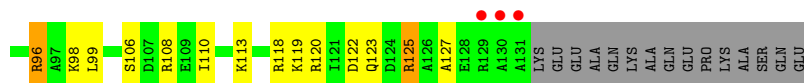
• Molecule 16: 50S ribosomal protein L18

Chain S: 71% 19% 7%





- Molecule 17: 50S ribosomal protein L19



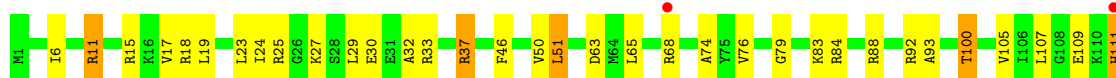
- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21



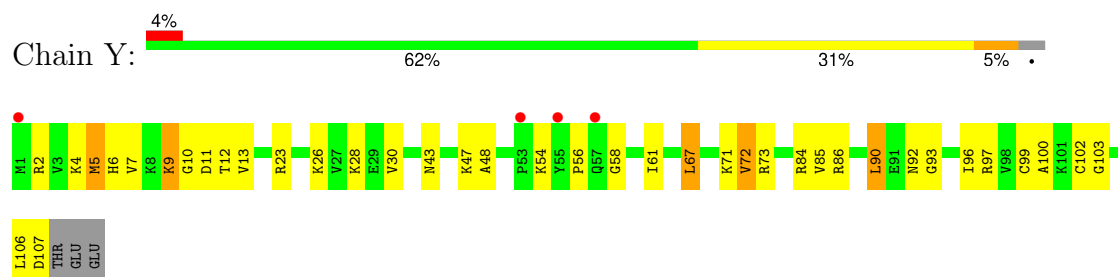
- Molecule 20: 50S ribosomal protein L22



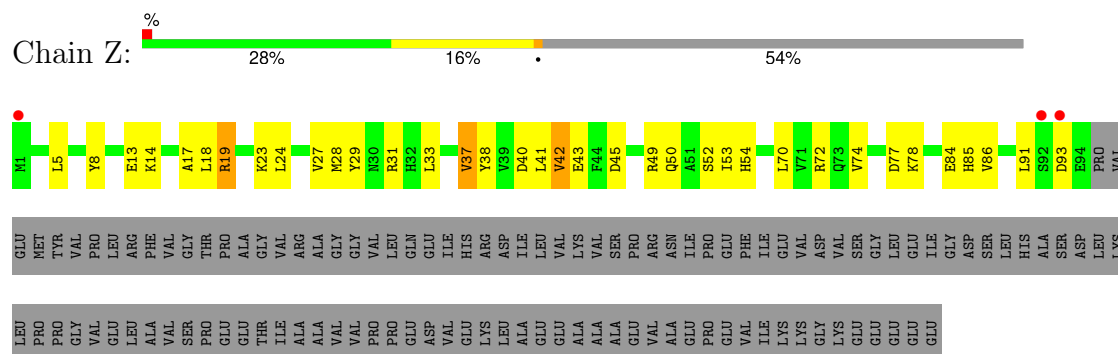
- Molecule 21: 50S ribosomal protein L23



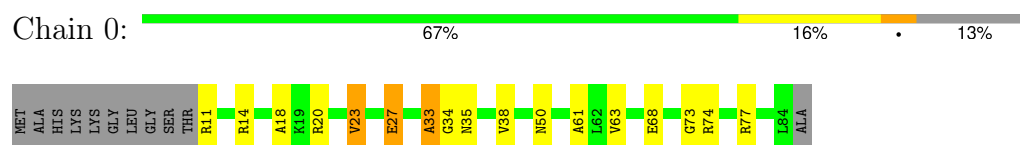
## • Molecule 22: 50S ribosomal protein L24



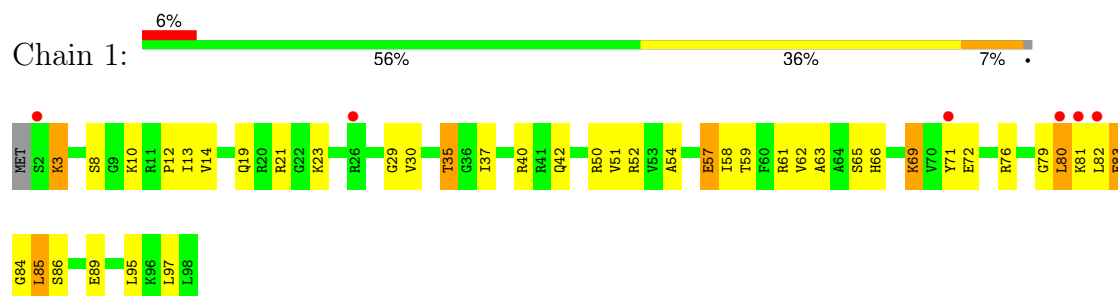
## • Molecule 23: 50S ribosomal protein L25



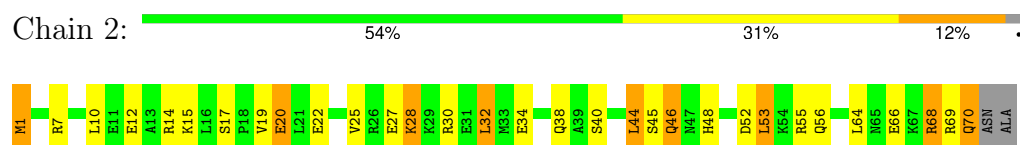
## • Molecule 24: 50S ribosomal protein L27



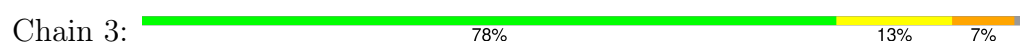
## • Molecule 25: 50S ribosomal protein L28

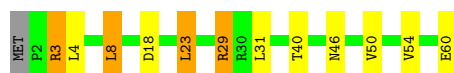


## • Molecule 26: 50S ribosomal protein L29

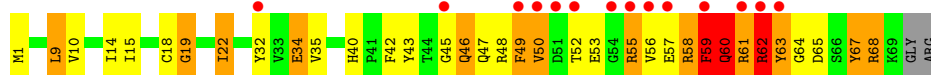


## • Molecule 27: 50S ribosomal protein L30





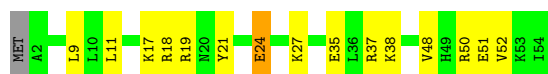
- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35

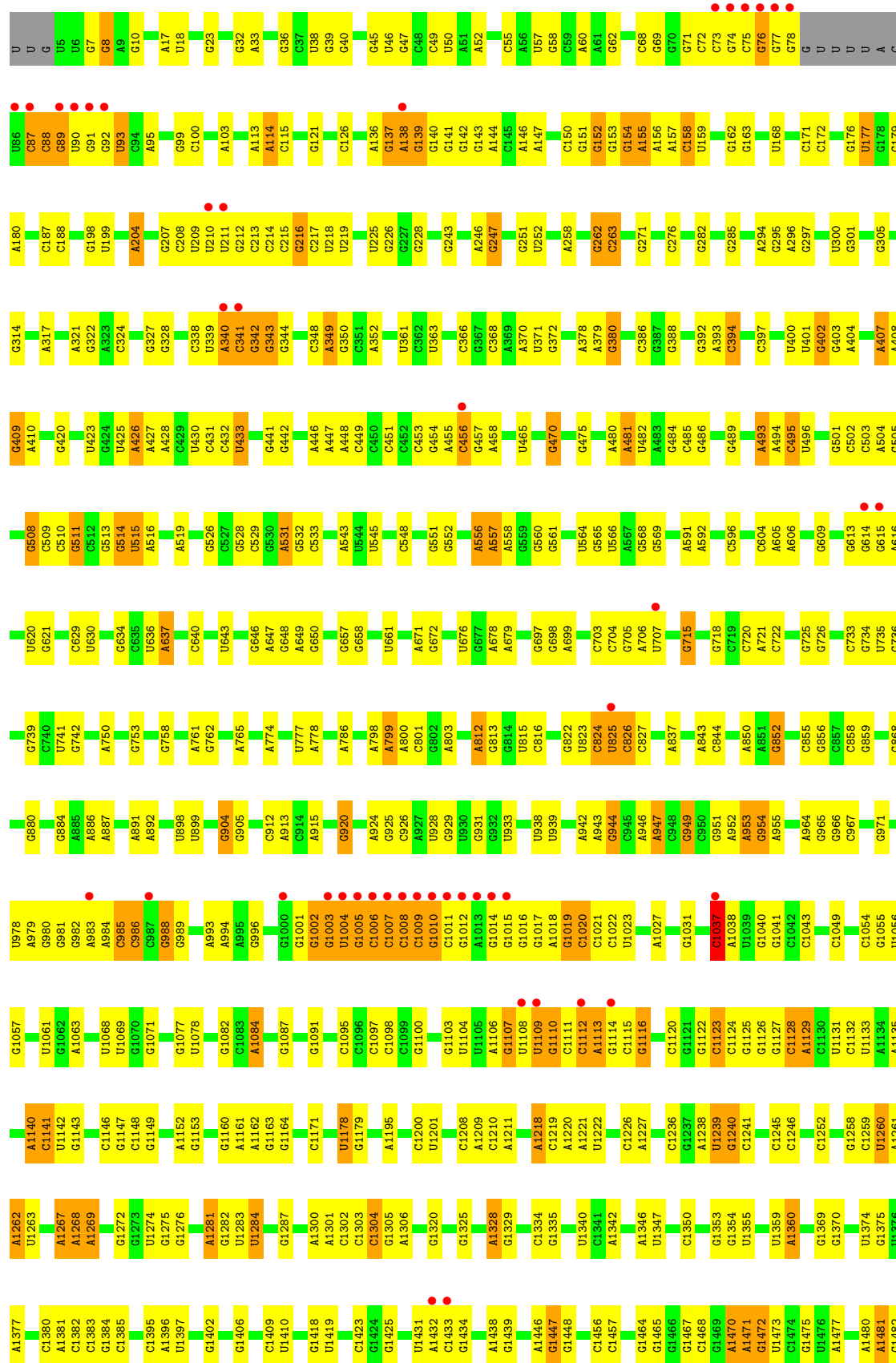


- Molecule 33: 50S ribosomal protein L36



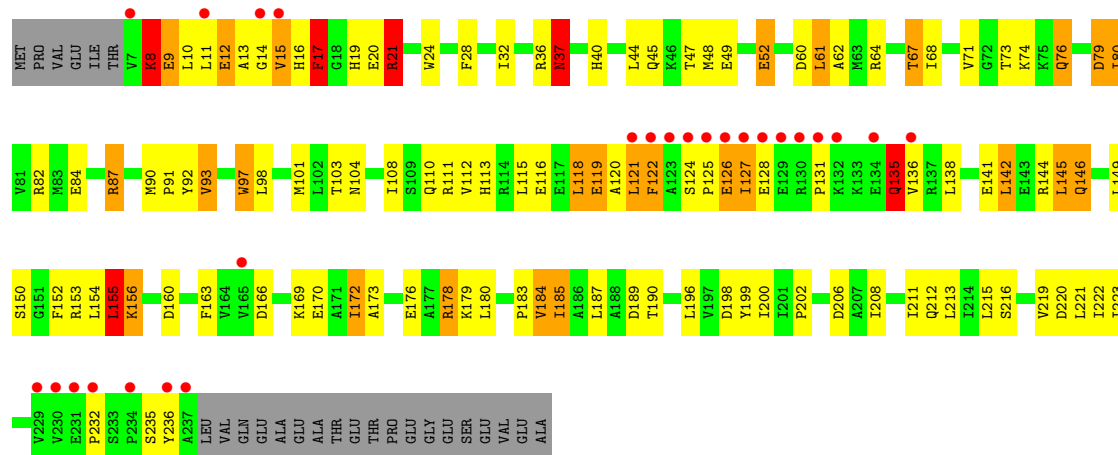
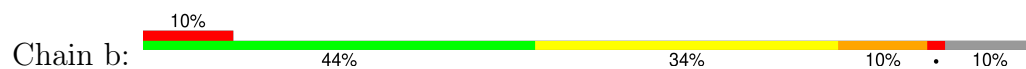
- Molecule 34: 16S Ribosomal RNA



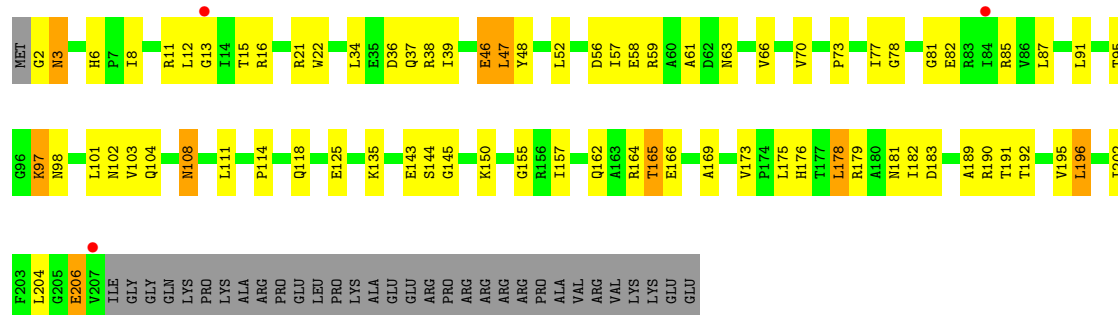




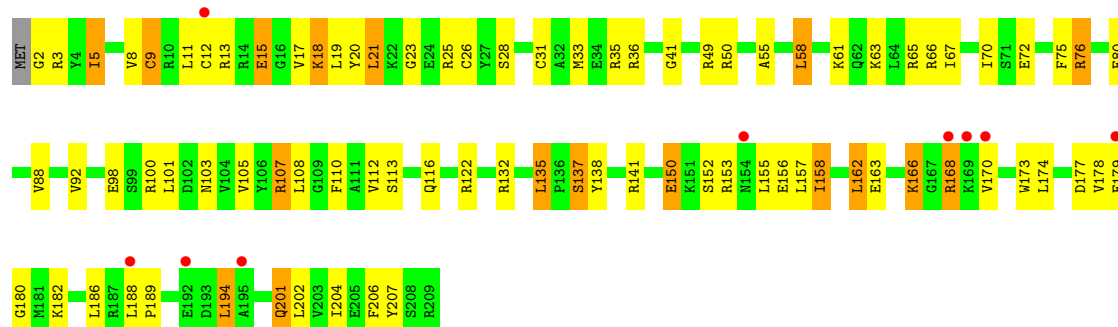
• Molecule 35: 30S ribosomal protein S2



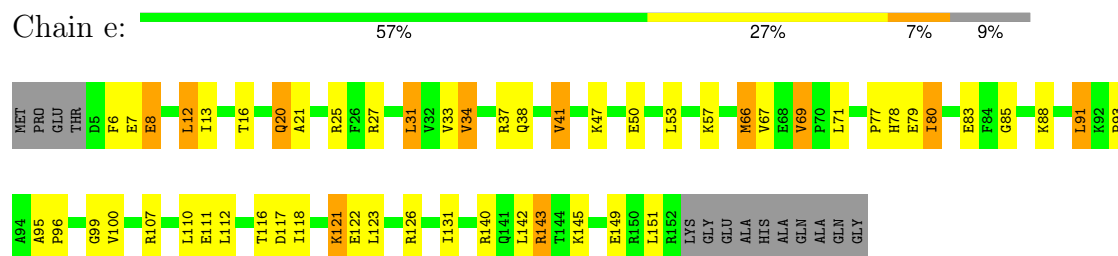
• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4



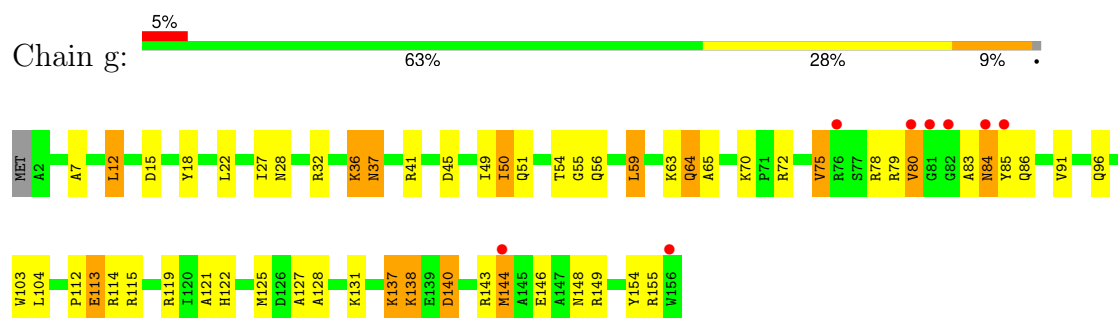
- Molecule 38: 30S ribosomal protein S5



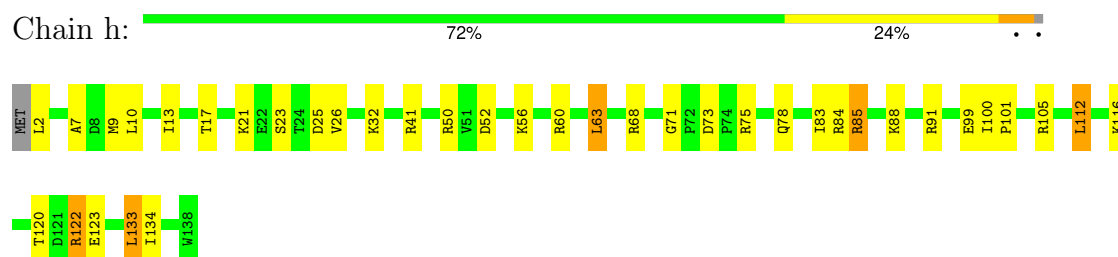
- Molecule 39: 30S ribosomal protein S6



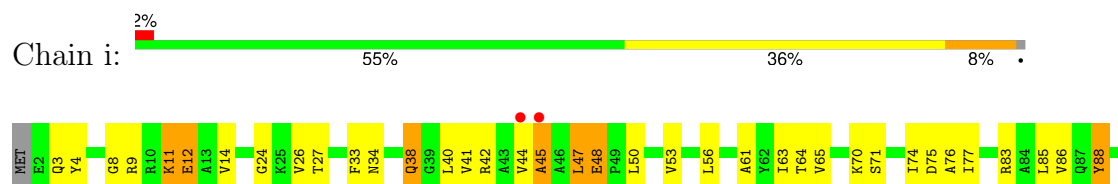
- Molecule 40: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S8

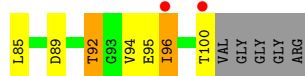


- Molecule 42: 30S ribosomal protein S9





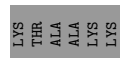
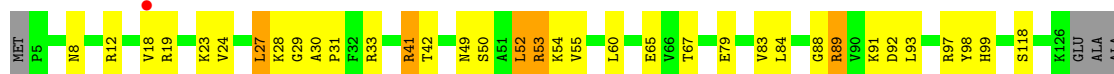
• Molecule 43: 30S ribosomal protein S10



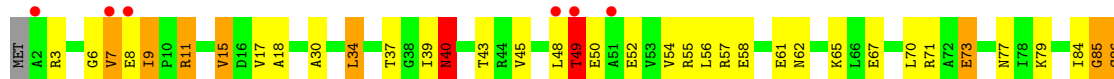
• Molecule 44: 30S ribosomal protein S11



• Molecule 45: 30S ribosomal protein S12



• Molecule 46: 30S ribosomal protein S13



• Molecule 47: 30S ribosomal protein S14 type Z

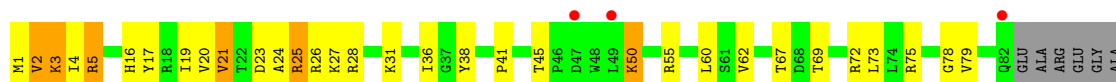




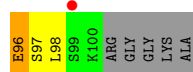
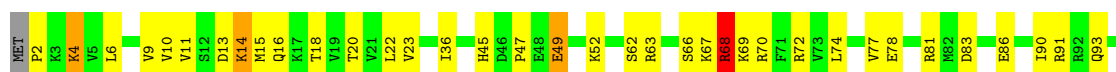
- Molecule 48: 30S ribosomal protein S15



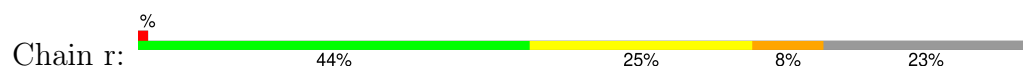
- Molecule 49: 30S ribosomal protein S16



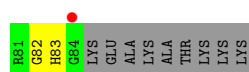
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19

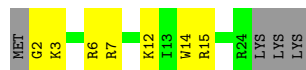




- Molecule 53: 30S ribosomal protein S20



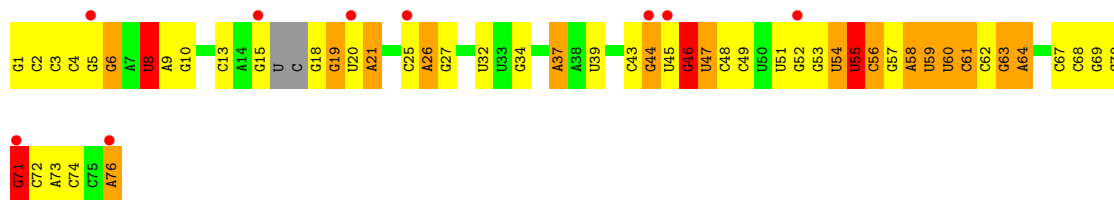
- Molecule 54: 30S ribosomal protein Thx



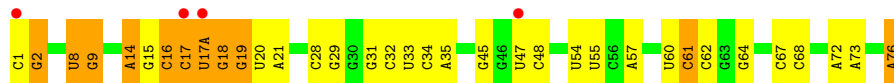
- Molecule 55: mRNA



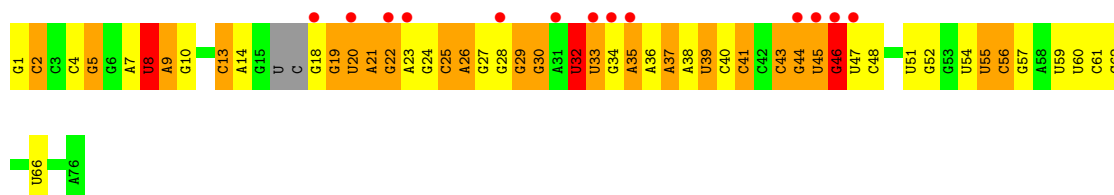
- Molecule 56: A-site tRNA



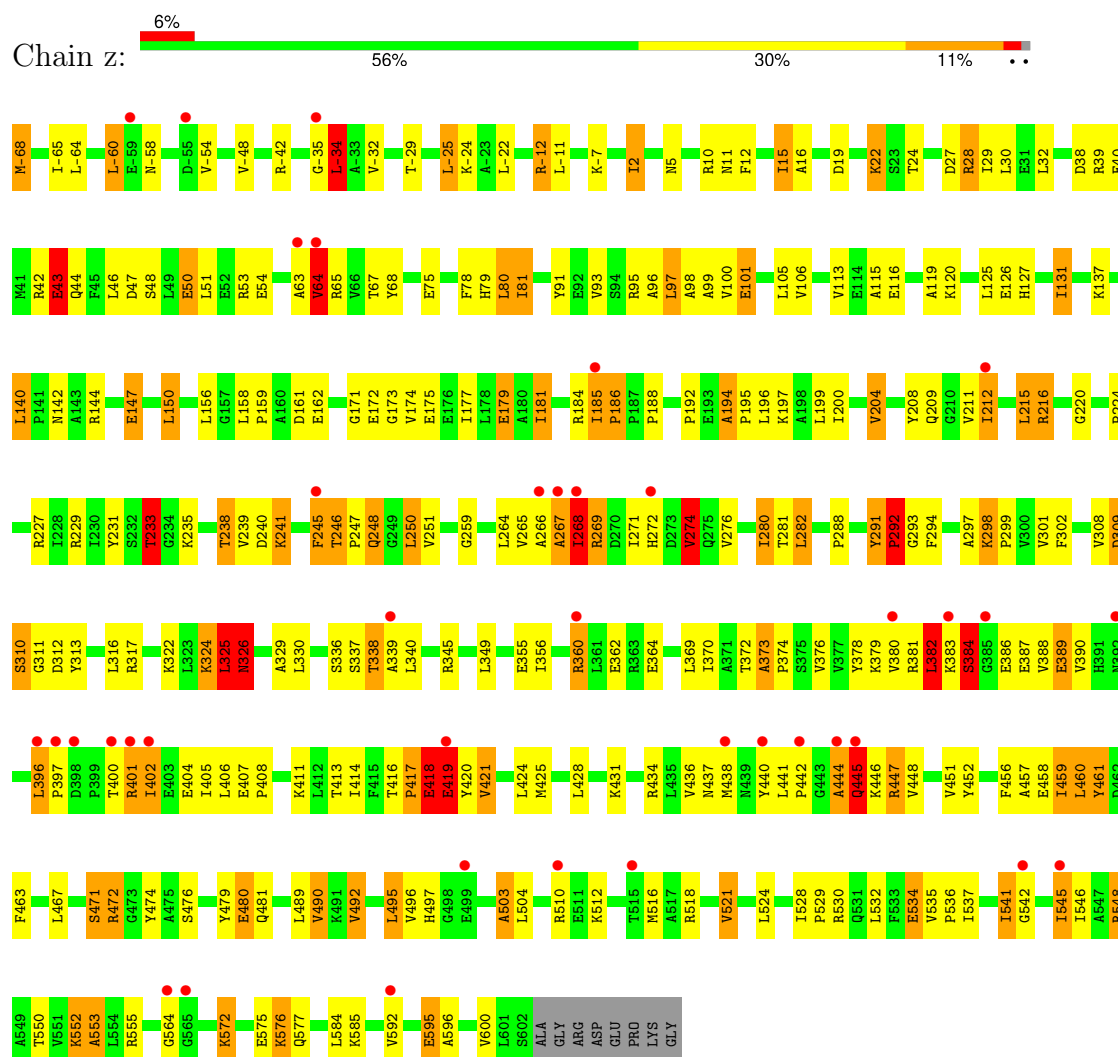
- Molecule 57: P-site tRNA



- Molecule 58: E-site tRNA



- Molecule 59: GDPCP fused to the N-terminus of the ribosomal protein L9, Elongation factor 4



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 213.12Å 271.72Å 436.83Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.52 – 2.60<br>49.52 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.4 (49.52-2.60)<br>99.4 (49.52-2.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.26                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.00 (at 2.58Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.10.1-2155                                          | Depositor        |
| R, $R_{free}$                                                           | 0.192 , 0.261<br>0.195 , 0.262                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 38580 reflections (4.97%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 47.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.255                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 49.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 155465                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 51.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GCP, 5MU, PSU, MIA, 7MG, ZN, 5MC, 4SU, SF4

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     | 0.39         | 0/69327     | 0.61        | 8/108217 (0.0%) |
| 2   | B     | 0.29         | 0/2878      | 0.49        | 0/4490          |
| 3   | C     | 0.35         | 0/1044      | 0.75        | 2/1413 (0.1%)   |
| 4   | D     | 0.43         | 0/2186      | 0.72        | 2/2944 (0.1%)   |
| 5   | E     | 0.40         | 0/1592      | 0.69        | 2/2149 (0.1%)   |
| 6   | F     | 0.40         | 0/1619      | 0.67        | 0/2193          |
| 7   | G     | 0.33         | 0/1450      | 0.63        | 0/1959          |
| 8   | H     | 0.36         | 0/1356      | 0.65        | 0/1834          |
| 9   | J     | 0.37         | 0/640       | 0.67        | 1/889 (0.1%)    |
| 10  | K     | 0.41         | 0/1044      | 0.75        | 1/1416 (0.1%)   |
| 11  | N     | 0.36         | 0/1144      | 0.62        | 0/1543          |
| 12  | O     | 0.43         | 0/943       | 0.64        | 0/1269          |
| 13  | P     | 0.42         | 0/1152      | 0.76        | 2/1533 (0.1%)   |
| 14  | Q     | 0.38         | 0/1143      | 0.60        | 0/1527          |
| 15  | R     | 0.35         | 0/982       | 0.61        | 0/1312          |
| 16  | S     | 0.33         | 0/887       | 0.61        | 0/1180          |
| 17  | T     | 0.39         | 0/1105      | 0.62        | 0/1477          |
| 18  | U     | 0.40         | 0/977       | 0.68        | 0/1301          |
| 19  | V     | 0.40         | 0/782       | 0.64        | 0/1049          |
| 20  | W     | 0.40         | 0/897       | 0.63        | 0/1205          |
| 21  | X     | 0.35         | 0/764       | 0.61        | 0/1025          |
| 22  | Y     | 0.35         | 0/819       | 0.69        | 0/1095          |
| 23  | Z     | 0.30         | 0/801       | 0.52        | 0/1079          |
| 24  | 0     | 0.36         | 0/599       | 0.64        | 0/798           |
| 25  | 1     | 0.47         | 0/762       | 0.72        | 0/1014          |
| 26  | 2     | 0.35         | 0/590       | 0.57        | 0/781           |
| 27  | 3     | 0.34         | 0/474       | 0.62        | 0/635           |
| 28  | 4     | 0.34         | 0/570       | 0.82        | 1/768 (0.1%)    |
| 29  | 5     | 0.39         | 0/473       | 0.63        | 0/639           |
| 30  | 6     | 0.40         | 0/460       | 0.62        | 0/613           |
| 31  | 7     | 0.44         | 0/438       | 0.71        | 0/575           |
| 32  | 8     | 0.43         | 0/519       | 0.67        | 0/684           |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 33  | g     | 0.44         | 0/310           | 0.73        | 0/407            |
| 34  | a     | 0.35         | 0/36053         | 0.57        | 1/56270 (0.0%)   |
| 35  | b     | 0.32         | 0/1885          | 0.64        | 2/2547 (0.1%)    |
| 36  | c     | 0.35         | 1/1574 (0.1%)   | 0.60        | 0/2127           |
| 37  | d     | 0.33         | 0/1685          | 0.56        | 0/2262           |
| 38  | e     | 0.38         | 0/1145          | 0.63        | 0/1543           |
| 39  | f     | 0.31         | 0/819           | 0.57        | 0/1111           |
| 40  | g     | 0.31         | 0/1246          | 0.55        | 0/1674           |
| 41  | h     | 0.34         | 0/1108          | 0.53        | 0/1494           |
| 42  | i     | 0.34         | 0/1002          | 0.62        | 0/1346           |
| 43  | j     | 0.33         | 0/711           | 0.60        | 0/968            |
| 44  | k     | 0.32         | 0/844           | 0.55        | 0/1145           |
| 45  | l     | 0.43         | 0/946           | 0.73        | 0/1274           |
| 46  | m     | 0.36         | 0/934           | 0.70        | 0/1256           |
| 47  | n     | 0.39         | 0/501           | 0.67        | 0/664            |
| 48  | o     | 0.34         | 0/739           | 0.60        | 0/985            |
| 49  | p     | 0.33         | 0/697           | 0.62        | 0/939            |
| 50  | q     | 0.36         | 0/836           | 0.69        | 0/1117           |
| 51  | r     | 0.33         | 0/560           | 0.56        | 0/746            |
| 52  | s     | 0.35         | 0/665           | 0.74        | 2/897 (0.2%)     |
| 53  | t     | 0.37         | 0/726           | 0.71        | 0/961            |
| 54  | u     | 0.44         | 0/203           | 0.61        | 0/266            |
| 55  | v     | 0.37         | 0/310           | 0.59        | 0/480            |
| 56  | w     | 0.34         | 1/1602 (0.1%)   | 0.59        | 2/2493 (0.1%)    |
| 57  | x     | 0.40         | 0/1747          | 0.63        | 0/2723           |
| 58  | y     | 0.35         | 1/1628 (0.1%)   | 0.62        | 2/2534 (0.1%)    |
| 59  | z     | 0.34         | 0/5296          | 0.68        | 11/7179 (0.2%)   |
| All | All   | 0.37         | 3/166189 (0.0%) | 0.61        | 39/248014 (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 |
|-----|-------|---------------------|---------------------|
| 10  | K     | 0                   | 1                   |
| 19  | V     | 0                   | 1                   |
| 26  | 2     | 0                   | 1                   |
| 28  | 4     | 0                   | 1                   |
| 37  | d     | 0                   | 1                   |
| 39  | f     | 0                   | 1                   |
| 42  | i     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 52  | s     | 0                   | 2                   |
| 53  | t     | 0                   | 1                   |
| 59  | z     | 0                   | 6                   |
| All | All   | 0                   | 17                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 36  | c     | 173 | VAL  | C-N   | -5.48 | 1.21        | 1.33     |
| 58  | y     | 8   | 4SU  | O3'-P | 5.07  | 1.61        | 1.56     |
| 56  | w     | 8   | 4SU  | O3'-P | 5.07  | 1.61        | 1.56     |

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

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 13  | P     | 44   | GLY  | CA-C-N      | 8.48 | 136.96      | 121.70   |
| 13  | P     | 44   | GLY  | C-N-CA      | 8.48 | 136.96      | 121.70   |
| 1   | A     | 2013 | G    | C2'-C3'-O3' | 8.13 | 121.70      | 109.50   |
| 4   | D     | 274  | ARG  | CA-C-N      | 7.77 | 135.69      | 121.70   |
| 4   | D     | 274  | ARG  | C-N-CA      | 7.77 | 135.69      | 121.70   |

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 26  | 2     | 44  | LEU  | Peptide |
| 28  | 4     | 65  | ASP  | Peptide |
| 10  | K     | 70  | LYS  | Peptide |
| 19  | V     | 43  | GLU  | Peptide |
| 37  | d     | 179 | GLU  | Peptide |

## 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     | 61902 | 0        | 31210    | 816     | 1            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B     | 2573  | 0        | 1306     | 30      | 0            |
| 3   | C     | 1024  | 0        | 1007     | 84      | 0            |
| 4   | D     | 2136  | 0        | 2218     | 68      | 0            |
| 5   | E     | 1559  | 0        | 1618     | 48      | 0            |
| 6   | F     | 1584  | 0        | 1625     | 53      | 0            |
| 7   | G     | 1425  | 0        | 1443     | 63      | 0            |
| 8   | H     | 1330  | 0        | 1407     | 48      | 0            |
| 9   | J     | 641   | 0        | 309      | 20      | 0            |
| 10  | K     | 1025  | 0        | 1066     | 68      | 0            |
| 11  | N     | 1117  | 0        | 1184     | 27      | 0            |
| 12  | O     | 933   | 0        | 996      | 29      | 0            |
| 13  | P     | 1135  | 0        | 1212     | 40      | 0            |
| 14  | Q     | 1122  | 0        | 1179     | 28      | 0            |
| 15  | R     | 968   | 0        | 1033     | 12      | 0            |
| 16  | S     | 877   | 0        | 938      | 31      | 0            |
| 17  | T     | 1091  | 0        | 1151     | 34      | 0            |
| 18  | U     | 959   | 0        | 1019     | 26      | 0            |
| 19  | V     | 771   | 0        | 830      | 20      | 0            |
| 20  | W     | 886   | 0        | 940      | 24      | 1            |
| 21  | X     | 750   | 0        | 814      | 20      | 0            |
| 22  | Y     | 806   | 0        | 881      | 19      | 0            |
| 23  | Z     | 784   | 0        | 796      | 20      | 0            |
| 24  | 0     | 591   | 0        | 607      | 15      | 0            |
| 25  | 1     | 755   | 0        | 826      | 22      | 0            |
| 26  | 2     | 588   | 0        | 643      | 16      | 0            |
| 27  | 3     | 469   | 0        | 518      | 8       | 0            |
| 28  | 4     | 557   | 0        | 535      | 34      | 0            |
| 29  | 5     | 459   | 0        | 476      | 13      | 0            |
| 30  | 6     | 453   | 0        | 473      | 8       | 0            |
| 31  | 7     | 430   | 0        | 480      | 9       | 0            |
| 32  | 8     | 511   | 0        | 571      | 19      | 0            |
| 33  | 9     | 307   | 0        | 335      | 13      | 0            |
| 34  | a     | 32207 | 0        | 16255    | 394     | 0            |
| 35  | b     | 1850  | 0        | 1871     | 72      | 0            |
| 36  | c     | 1550  | 0        | 1539     | 47      | 0            |
| 37  | d     | 1655  | 0        | 1673     | 61      | 0            |
| 38  | e     | 1129  | 0        | 1185     | 28      | 0            |
| 39  | f     | 806   | 0        | 793      | 25      | 0            |
| 40  | g     | 1227  | 0        | 1232     | 34      | 0            |
| 41  | h     | 1088  | 0        | 1126     | 19      | 0            |
| 42  | i     | 983   | 0        | 986      | 34      | 0            |
| 43  | j     | 698   | 0        | 637      | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | k     | 829   | 0        | 825      | 17      | 0            |
| 45  | l     | 930   | 0        | 980      | 19      | 0            |
| 46  | m     | 924   | 0        | 960      | 33      | 0            |
| 47  | n     | 492   | 0        | 529      | 16      | 0            |
| 48  | o     | 728   | 0        | 760      | 21      | 0            |
| 49  | p     | 681   | 0        | 697      | 17      | 0            |
| 50  | q     | 823   | 0        | 891      | 21      | 0            |
| 51  | r     | 555   | 0        | 618      | 20      | 0            |
| 52  | s     | 650   | 0        | 655      | 24      | 0            |
| 53  | t     | 724   | 0        | 787      | 13      | 0            |
| 54  | u     | 199   | 0        | 208      | 5       | 0            |
| 55  | v     | 277   | 0        | 140      | 8       | 0            |
| 56  | w     | 1586  | 0        | 819      | 62      | 0            |
| 57  | x     | 1645  | 0        | 839      | 25      | 0            |
| 58  | y     | 1580  | 0        | 801      | 55      | 0            |
| 59  | z     | 5200  | 0        | 5309     | 192     | 0            |
| 60  | 0     | 4     | 0        | 0        | 0       | 0            |
| 60  | 5     | 2     | 0        | 0        | 0       | 0            |
| 60  | 6     | 2     | 0        | 0        | 0       | 0            |
| 60  | 7     | 1     | 0        | 0        | 0       | 0            |
| 60  | 8     | 1     | 0        | 0        | 0       | 0            |
| 60  | 9     | 1     | 0        | 0        | 0       | 0            |
| 60  | A     | 644   | 0        | 0        | 0       | 0            |
| 60  | B     | 18    | 0        | 0        | 0       | 0            |
| 60  | D     | 6     | 0        | 0        | 0       | 0            |
| 60  | E     | 5     | 0        | 0        | 0       | 0            |
| 60  | F     | 6     | 0        | 0        | 0       | 0            |
| 60  | G     | 2     | 0        | 0        | 0       | 0            |
| 60  | H     | 1     | 0        | 0        | 0       | 0            |
| 60  | N     | 1     | 0        | 0        | 0       | 0            |
| 60  | O     | 2     | 0        | 0        | 0       | 0            |
| 60  | P     | 3     | 0        | 0        | 0       | 0            |
| 60  | Q     | 2     | 0        | 0        | 0       | 0            |
| 60  | R     | 2     | 0        | 0        | 0       | 0            |
| 60  | U     | 1     | 0        | 0        | 0       | 0            |
| 60  | V     | 2     | 0        | 0        | 0       | 0            |
| 60  | W     | 1     | 0        | 0        | 0       | 0            |
| 60  | X     | 1     | 0        | 0        | 0       | 0            |
| 60  | Z     | 1     | 0        | 0        | 0       | 0            |
| 60  | a     | 188   | 0        | 0        | 0       | 0            |
| 60  | d     | 1     | 0        | 0        | 0       | 0            |
| 60  | e     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | f     | 1      | 0        | 0        | 0       | 0            |
| 60  | l     | 1      | 0        | 0        | 0       | 0            |
| 60  | m     | 2      | 0        | 0        | 0       | 0            |
| 60  | n     | 3      | 0        | 0        | 0       | 0            |
| 60  | v     | 2      | 0        | 0        | 0       | 0            |
| 60  | x     | 9      | 0        | 0        | 0       | 0            |
| 60  | z     | 2      | 0        | 0        | 0       | 0            |
| 61  | 4     | 1      | 0        | 0        | 0       | 0            |
| 61  | 5     | 1      | 0        | 0        | 0       | 0            |
| 61  | 6     | 1      | 0        | 0        | 0       | 0            |
| 61  | 9     | 1      | 0        | 0        | 0       | 0            |
| 61  | Y     | 1      | 0        | 0        | 0       | 0            |
| 61  | n     | 1      | 0        | 0        | 0       | 0            |
| 62  | d     | 8      | 0        | 0        | 3       | 0            |
| 63  | z     | 32     | 0        | 14       | 4       | 0            |
| 64  | 0     | 3      | 0        | 0        | 0       | 0            |
| 64  | 1     | 1      | 0        | 0        | 0       | 0            |
| 64  | 3     | 1      | 0        | 0        | 0       | 0            |
| 64  | 7     | 1      | 0        | 0        | 0       | 0            |
| 64  | 8     | 4      | 0        | 0        | 0       | 0            |
| 64  | A     | 715    | 0        | 0        | 37      | 0            |
| 64  | B     | 32     | 0        | 0        | 0       | 0            |
| 64  | D     | 4      | 0        | 0        | 0       | 0            |
| 64  | E     | 6      | 0        | 0        | 1       | 0            |
| 64  | F     | 5      | 0        | 0        | 0       | 0            |
| 64  | H     | 1      | 0        | 0        | 0       | 0            |
| 64  | N     | 1      | 0        | 0        | 0       | 0            |
| 64  | O     | 3      | 0        | 0        | 0       | 0            |
| 64  | P     | 8      | 0        | 0        | 0       | 0            |
| 64  | Q     | 3      | 0        | 0        | 0       | 0            |
| 64  | T     | 2      | 0        | 0        | 0       | 0            |
| 64  | U     | 3      | 0        | 0        | 0       | 0            |
| 64  | V     | 1      | 0        | 0        | 0       | 0            |
| 64  | a     | 165    | 0        | 0        | 4       | 0            |
| 64  | l     | 1      | 0        | 0        | 0       | 0            |
| 64  | p     | 1      | 0        | 0        | 0       | 0            |
| 64  | v     | 3      | 0        | 0        | 0       | 0            |
| 64  | w     | 1      | 0        | 0        | 0       | 0            |
| 64  | z     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 155465 | 0        | 104775   | 2687    | 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 11.

The worst 5 of 2687 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:C:201:PRO:C   | 3:C:203:GLY:HA2  | 1.75                     | 1.11              |
| 58:y:22:G:N7    | 58:y:46:G:N2     | 1.98                     | 1.09              |
| 3:C:199:HIS:O   | 3:C:201:PRO:HD3  | 1.57                     | 1.03              |
| 37:d:12:CYS:SG  | 37:d:19:LEU:HB2  | 1.98                     | 1.02              |
| 10:K:109:LYS:HA | 10:K:112:MET:HE3 | 1.40                     | 1.02              |

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) |
|---------------|-----------------------|--------------------------|-------------------|
| 1:A:1519:G:N2 | 20:W:111:HIS:O[4_557] | 2.15                     | 0.05              |

## 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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3   | C     | 130/228 (57%) | 94 (72%)  | 25 (19%) | 11 (8%)  | 0           | 0  |
| 4   | D     | 273/276 (99%) | 255 (93%) | 15 (6%)  | 3 (1%)   | 11          | 25 |
| 5   | E     | 202/206 (98%) | 188 (93%) | 11 (5%)  | 3 (2%)   | 8           | 18 |
| 6   | F     | 201/210 (96%) | 184 (92%) | 12 (6%)  | 5 (2%)   | 4           | 8  |
| 7   | G     | 179/182 (98%) | 162 (90%) | 10 (6%)  | 7 (4%)   | 2           | 3  |
| 8   | H     | 172/180 (96%) | 148 (86%) | 17 (10%) | 7 (4%)   | 2           | 3  |
| 9   | J     | 128/173 (74%) | 76 (59%)  | 22 (17%) | 30 (23%) | 0           | 0  |
| 10  | K     | 137/147 (93%) | 85 (62%)  | 31 (23%) | 21 (15%) | 0           | 0  |
| 11  | N     | 138/140 (99%) | 129 (94%) | 5 (4%)   | 4 (3%)   | 3           | 6  |
| 12  | O     | 120/122 (98%) | 112 (93%) | 7 (6%)   | 1 (1%)   | 16          | 34 |
| 13  | P     | 147/150 (98%) | 129 (88%) | 16 (11%) | 2 (1%)   | 9           | 19 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14  | Q     | 139/141 (99%) | 131 (94%) | 7 (5%)   | 1 (1%)   | 18          | 38  |
| 15  | R     | 116/118 (98%) | 111 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 16  | S     | 108/112 (96%) | 96 (89%)  | 10 (9%)  | 2 (2%)   | 6           | 13  |
| 17  | T     | 129/146 (88%) | 123 (95%) | 5 (4%)   | 1 (1%)   | 16          | 34  |
| 18  | U     | 114/118 (97%) | 113 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 19  | V     | 99/101 (98%)  | 94 (95%)  | 3 (3%)   | 2 (2%)   | 6           | 12  |
| 20  | W     | 110/113 (97%) | 105 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 21  | X     | 93/96 (97%)   | 89 (96%)  | 3 (3%)   | 1 (1%)   | 11          | 25  |
| 22  | Y     | 105/110 (96%) | 89 (85%)  | 12 (11%) | 4 (4%)   | 2           | 3   |
| 23  | Z     | 92/206 (45%)  | 84 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 24  | 0     | 72/85 (85%)   | 67 (93%)  | 3 (4%)   | 2 (3%)   | 4           | 6   |
| 25  | 1     | 95/98 (97%)   | 86 (90%)  | 6 (6%)   | 3 (3%)   | 3           | 5   |
| 26  | 2     | 68/72 (94%)   | 65 (96%)  | 2 (3%)   | 1 (2%)   | 8           | 18  |
| 27  | 3     | 57/60 (95%)   | 52 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 28  | 4     | 67/71 (94%)   | 45 (67%)  | 15 (22%) | 7 (10%)  | 0           | 0   |
| 29  | 5     | 57/60 (95%)   | 54 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 30  | 6     | 51/54 (94%)   | 50 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 31  | 7     | 47/49 (96%)   | 44 (94%)  | 1 (2%)   | 2 (4%)   | 2           | 2   |
| 32  | 8     | 62/65 (95%)   | 61 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 33  | 9     | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 35  | b     | 229/256 (90%) | 192 (84%) | 23 (10%) | 14 (6%)  | 1           | 1   |
| 36  | c     | 204/239 (85%) | 177 (87%) | 20 (10%) | 7 (3%)   | 3           | 4   |
| 37  | d     | 206/209 (99%) | 187 (91%) | 16 (8%)  | 3 (2%)   | 8           | 18  |
| 38  | e     | 146/162 (90%) | 130 (89%) | 13 (9%)  | 3 (2%)   | 5           | 11  |
| 39  | f     | 98/101 (97%)  | 84 (86%)  | 11 (11%) | 3 (3%)   | 3           | 5   |
| 40  | g     | 153/156 (98%) | 135 (88%) | 13 (8%)  | 5 (3%)   | 3           | 5   |
| 41  | h     | 135/138 (98%) | 130 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 42  | i     | 125/128 (98%) | 113 (90%) | 5 (4%)   | 7 (6%)   | 1           | 1   |
| 43  | j     | 94/105 (90%)  | 79 (84%)  | 6 (6%)   | 9 (10%)  | 0           | 0   |
| 44  | k     | 112/129 (87%) | 107 (96%) | 4 (4%)   | 1 (1%)   | 14          | 30  |
| 45  | l     | 120/132 (91%) | 112 (93%) | 7 (6%)   | 1 (1%)   | 16          | 34  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 46  | m     | 117/126 (93%)   | 102 (87%)  | 9 (8%)   | 6 (5%)   | 1           | 2   |
| 47  | n     | 58/61 (95%)     | 57 (98%)   | 0        | 1 (2%)   | 7           | 15  |
| 48  | o     | 86/89 (97%)     | 78 (91%)   | 5 (6%)   | 3 (4%)   | 3           | 4   |
| 49  | p     | 80/88 (91%)     | 72 (90%)   | 7 (9%)   | 1 (1%)   | 9           | 21  |
| 50  | q     | 97/105 (92%)    | 86 (89%)   | 8 (8%)   | 3 (3%)   | 3           | 5   |
| 51  | r     | 66/88 (75%)     | 60 (91%)   | 6 (9%)   | 0        | 100         | 100 |
| 52  | s     | 81/93 (87%)     | 72 (89%)   | 4 (5%)   | 5 (6%)   | 1           | 1   |
| 53  | t     | 94/106 (89%)    | 84 (89%)   | 4 (4%)   | 6 (6%)   | 1           | 1   |
| 54  | u     | 21/27 (78%)     | 19 (90%)   | 2 (10%)  | 0        | 100         | 100 |
| 59  | z     | 669/679 (98%)   | 568 (85%)  | 62 (9%)  | 39 (6%)  | 1           | 1   |
| All | All   | 6534/7143 (92%) | 5800 (89%) | 497 (8%) | 237 (4%) | 2           | 4   |

5 of 237 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 65  | PRO  |
| 3   | C     | 172 | HIS  |
| 3   | C     | 224 | ILE  |
| 4   | D     | 275 | LYS  |
| 6   | F     | 130 | ALA  |

### 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 |   |
|-----|-------|---------------|-----------|----------|-------------|---|
| 3   | C     | 103/180 (57%) | 76 (74%)  | 27 (26%) | 0           | 1 |
| 4   | D     | 215/218 (99%) | 182 (85%) | 33 (15%) | 3           | 5 |
| 5   | E     | 164/166 (99%) | 134 (82%) | 30 (18%) | 2           | 3 |
| 6   | F     | 160/166 (96%) | 130 (81%) | 30 (19%) | 1           | 2 |
| 7   | G     | 143/156 (92%) | 115 (80%) | 28 (20%) | 1           | 2 |
| 8   | H     | 144/148 (97%) | 123 (85%) | 21 (15%) | 3           | 6 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 10  | K     | 104/111 (94%)  | 70 (67%)  | 34 (33%) | 0           | 0  |
| 11  | N     | 118/119 (99%)  | 93 (79%)  | 25 (21%) | 1           | 2  |
| 12  | O     | 100/100 (100%) | 88 (88%)  | 12 (12%) | 5           | 10 |
| 13  | P     | 115/116 (99%)  | 99 (86%)  | 16 (14%) | 3           | 7  |
| 14  | Q     | 111/111 (100%) | 93 (84%)  | 18 (16%) | 2           | 4  |
| 15  | R     | 101/101 (100%) | 83 (82%)  | 18 (18%) | 2           | 3  |
| 16  | S     | 87/88 (99%)    | 73 (84%)  | 14 (16%) | 2           | 4  |
| 17  | T     | 115/127 (91%)  | 97 (84%)  | 18 (16%) | 2           | 4  |
| 18  | U     | 93/94 (99%)    | 80 (86%)  | 13 (14%) | 3           | 6  |
| 19  | V     | 80/82 (98%)    | 66 (82%)  | 14 (18%) | 2           | 3  |
| 20  | W     | 90/92 (98%)    | 78 (87%)  | 12 (13%) | 4           | 8  |
| 21  | X     | 77/78 (99%)    | 66 (86%)  | 11 (14%) | 3           | 6  |
| 22  | Y     | 85/91 (93%)    | 74 (87%)  | 11 (13%) | 4           | 8  |
| 23  | Z     | 84/179 (47%)   | 71 (84%)  | 13 (16%) | 2           | 5  |
| 24  | 0     | 59/67 (88%)    | 55 (93%)  | 4 (7%)   | 14          | 32 |
| 25  | 1     | 80/83 (96%)    | 64 (80%)  | 16 (20%) | 1           | 2  |
| 26  | 2     | 65/67 (97%)    | 50 (77%)  | 15 (23%) | 1           | 1  |
| 27  | 3     | 51/52 (98%)    | 43 (84%)  | 8 (16%)  | 2           | 4  |
| 28  | 4     | 60/63 (95%)    | 45 (75%)  | 15 (25%) | 0           | 1  |
| 29  | 5     | 51/52 (98%)    | 44 (86%)  | 7 (14%)  | 3           | 7  |
| 30  | 6     | 51/52 (98%)    | 46 (90%)  | 5 (10%)  | 7           | 17 |
| 31  | 7     | 42/42 (100%)   | 34 (81%)  | 8 (19%)  | 1           | 2  |
| 32  | 8     | 53/55 (96%)    | 48 (91%)  | 5 (9%)   | 8           | 18 |
| 33  | 9     | 34/34 (100%)   | 29 (85%)  | 5 (15%)  | 3           | 6  |
| 35  | b     | 193/220 (88%)  | 145 (75%) | 48 (25%) | 0           | 1  |
| 36  | c     | 142/188 (76%)  | 126 (89%) | 16 (11%) | 5           | 12 |
| 37  | d     | 169/181 (93%)  | 143 (85%) | 26 (15%) | 2           | 5  |
| 38  | e     | 113/123 (92%)  | 92 (81%)  | 21 (19%) | 1           | 3  |
| 39  | f     | 83/90 (92%)    | 63 (76%)  | 20 (24%) | 1           | 1  |
| 40  | g     | 118/127 (93%)  | 95 (80%)  | 23 (20%) | 1           | 2  |
| 41  | h     | 114/119 (96%)  | 97 (85%)  | 17 (15%) | 3           | 5  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 42  | i     | 90/99 (91%)     | 77 (86%)   | 13 (14%)  | 3           | 6  |
| 43  | j     | 65/92 (71%)     | 52 (80%)   | 13 (20%)  | 1           | 2  |
| 44  | k     | 82/99 (83%)     | 73 (89%)   | 9 (11%)   | 6           | 13 |
| 45  | l     | 97/109 (89%)    | 83 (86%)   | 14 (14%)  | 3           | 6  |
| 46  | m     | 89/101 (88%)    | 74 (83%)   | 15 (17%)  | 2           | 4  |
| 47  | n     | 49/50 (98%)     | 40 (82%)   | 9 (18%)   | 1           | 3  |
| 48  | o     | 78/80 (98%)     | 69 (88%)   | 9 (12%)   | 5           | 11 |
| 49  | p     | 69/74 (93%)     | 56 (81%)   | 13 (19%)  | 1           | 2  |
| 50  | q     | 94/97 (97%)     | 79 (84%)   | 15 (16%)  | 2           | 4  |
| 51  | r     | 59/77 (77%)     | 47 (80%)   | 12 (20%)  | 1           | 2  |
| 52  | s     | 68/80 (85%)     | 57 (84%)   | 11 (16%)  | 2           | 4  |
| 53  | t     | 69/82 (84%)     | 60 (87%)   | 9 (13%)   | 4           | 8  |
| 54  | u     | 18/22 (82%)     | 16 (89%)   | 2 (11%)   | 6           | 12 |
| 59  | z     | 542/560 (97%)   | 424 (78%)  | 118 (22%) | 1           | 2  |
| All | All   | 5236/5760 (91%) | 4317 (82%) | 919 (18%) | 2           | 3  |

5 of 919 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | 6     | 17  | LYS  |
| 59  | z     | 405 | ILE  |
| 37  | d     | 188 | LEU  |
| 59  | z     | 360 | ARG  |
| 54  | u     | 7   | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | f     | 100 | ASN  |
| 48  | o     | 9   | GLN  |
| 40  | g     | 68  | ASN  |
| 43  | j     | 69  | ASN  |
| 52  | s     | 57  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 2868/2915 (98%) | 470 (16%)         | 42 (1%)         |
| 2   | B     | 119/121 (98%)   | 14 (11%)          | 0               |
| 34  | a     | 1496/1521 (98%) | 245 (16%)         | 0               |
| 55  | v     | 12/24 (50%)     | 1 (8%)            | 0               |
| 56  | w     | 72/76 (94%)     | 26 (36%)          | 0               |
| 57  | x     | 76/77 (98%)     | 13 (17%)          | 0               |
| 58  | y     | 72/76 (94%)     | 29 (40%)          | 0               |
| All | All   | 4715/4810 (98%) | 798 (16%)         | 42 (0%)         |

5 of 798 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | A    |
| 1   | A     | 10  | G    |
| 1   | A     | 14  | G    |
| 1   | A     | 34  | G    |
| 1   | A     | 44  | C    |

5 of 42 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1699 | G    |
| 1   | A     | 2417 | U    |
| 1   | A     | 2013 | G    |
| 1   | A     | 2202 | G    |
| 1   | A     | 2433 | A    |

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

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 | $\# Z  > 2$ |
| 56  | PSU  | w     | 55  | 56   | 18,21,22     | 1.36 | 2 (11%)     | 21,30,33    | 1.89 | 4 (19%)     |
| 56  | MIA  | w     | 37  | 56   | 27,29,32     | 2.35 | 7 (25%)     | 38,41,47    | 2.91 | 15 (39%)    |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 57  | PSU  | x     | 55  | 57    | 18,21,22     | 1.43 | 3 (16%)  | 21,30,33    | 1.99  | 5 (23%)  |
| 58  | PSU  | y     | 39  | 58    | 18,21,22     | 1.50 | 2 (11%)  | 21,30,33    | 1.95  | 6 (28%)  |
| 58  | 5MU  | y     | 54  | 58    | 19,22,23     | 1.44 | 6 (31%)  | 27,32,35    | 2.00  | 9 (33%)  |
| 58  | PSU  | y     | 55  | 58    | 18,21,22     | 1.41 | 2 (11%)  | 21,30,33    | 2.04  | 4 (19%)  |
| 56  | 5MU  | w     | 54  | 56    | 19,22,23     | 1.40 | 4 (21%)  | 27,32,35    | 1.82  | 7 (25%)  |
| 57  | 5MU  | x     | 54  | 60,57 | 19,22,23     | 1.29 | 4 (21%)  | 27,32,35    | 2.14  | 6 (22%)  |
| 58  | 4SU  | y     | 8   | 58    | 18,21,22     | 4.77 | 7 (38%)  | 25,30,33    | 12.20 | 8 (32%)  |
| 56  | PSU  | w     | 39  | 56    | 18,21,22     | 1.30 | 2 (11%)  | 21,30,33    | 2.06  | 5 (23%)  |
| 58  | MIA  | y     | 37  | 58,34 | 21,24,32     | 1.71 | 4 (19%)  | 30,35,47    | 2.04  | 7 (23%)  |
| 56  | PSU  | w     | 32  | 56    | 18,21,22     | 1.46 | 2 (11%)  | 21,30,33    | 2.02  | 5 (23%)  |
| 57  | 5MC  | x     | 32  | 57    | 19,22,23     | 1.60 | 3 (15%)  | 26,32,35    | 1.15  | 2 (7%)   |
| 56  | 7MG  | w     | 46  | 56    | 23,26,27     | 1.39 | 5 (21%)  | 27,39,42    | 2.50  | 6 (22%)  |
| 58  | PSU  | y     | 32  | 58    | 18,21,22     | 1.43 | 3 (16%)  | 21,30,33    | 1.94  | 3 (14%)  |
| 56  | 4SU  | w     | 8   | 56    | 18,21,22     | 1.91 | 5 (27%)  | 25,30,33    | 2.00  | 5 (20%)  |
| 57  | 4SU  | x     | 8   | 57    | 18,21,22     | 2.19 | 6 (33%)  | 25,30,33    | 2.11  | 5 (20%)  |

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   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 56  | PSU  | w     | 55  | 56    | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | MIA  | w     | 37  | 56    | -       | 6/14/31/34 | 0/3/3/3 |
| 57  | PSU  | x     | 55  | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | PSU  | y     | 39  | 58    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | 5MU  | y     | 54  | 58    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | PSU  | y     | 55  | 58    | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | 5MU  | w     | 54  | 56    | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | 5MU  | x     | 54  | 60,57 | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | 4SU  | y     | 8   | 58    | -       | 2/7/25/26  | 0/2/2/2 |
| 56  | PSU  | w     | 39  | 56    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | MIA  | y     | 37  | 58,34 | -       | 2/7/25/34  | 0/3/3/3 |
| 56  | PSU  | w     | 32  | 56    | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | 5MC  | x     | 32  | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | 7MG  | w     | 46  | 56    | -       | 3/7/37/38  | 0/3/3/3 |
| 58  | PSU  | y     | 32  | 58    | -       | 4/7/25/26  | 0/2/2/2 |
| 56  | 4SU  | w     | 8   | 56    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 57  | 4SU  | x     | 8   | 57   | -       | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 67 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 58  | y     | 8   | 4SU  | O2-C2   | -12.93 | 1.00        | 1.23     |
| 58  | y     | 8   | 4SU  | C4-N3   | 11.35  | 1.49        | 1.37     |
| 56  | w     | 37  | MIA  | C2-S10  | -7.46  | 1.69        | 1.75     |
| 56  | w     | 37  | MIA  | C13-C14 | 6.61   | 1.52        | 1.32     |
| 57  | x     | 8   | 4SU  | C4-N3   | -6.00  | 1.31        | 1.37     |

The worst 5 of 102 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 58  | y     | 8   | 4SU  | O2-C2-N1 | -41.14 | 69.25       | 122.80   |
| 58  | y     | 8   | 4SU  | O2-C2-N3 | -40.19 | 47.40       | 121.49   |
| 58  | y     | 8   | 4SU  | C6-C5-C4 | -12.81 | 108.86      | 119.95   |
| 58  | y     | 8   | 4SU  | C5-C4-N3 | 11.16  | 125.13      | 114.75   |
| 56  | w     | 46  | 7MG  | N9-C4-N3 | 8.55   | 137.99      | 125.46   |

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | w     | 37  | MIA  | C5-C6-N6-C12    |
| 56  | w     | 37  | MIA  | C12-C13-C14-C15 |
| 56  | w     | 37  | MIA  | C12-C13-C14-C16 |
| 58  | y     | 32  | PSU  | C2'-C1'-C5-C4   |
| 58  | y     | 32  | PSU  | C2'-C1'-C5-C6   |

There are no ring outliers.

10 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56  | w     | 55  | PSU  | 1       | 0            |
| 56  | w     | 37  | MIA  | 1       | 0            |
| 58  | y     | 39  | PSU  | 2       | 0            |
| 58  | y     | 55  | PSU  | 1       | 0            |
| 56  | w     | 54  | 5MU  | 2       | 0            |
| 58  | y     | 8   | 4SU  | 4       | 0            |
| 56  | w     | 46  | 7MG  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 58  | y     | 32  | PSU  | 2       | 0            |
| 56  | w     | 8   | 4SU  | 2       | 0            |
| 57  | x     | 8   | 4SU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 927 ligands modelled in this entry, 925 are monoatomic - leaving 2 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 | $\# Z  > 2$ |
| 63  | GCP  | z     | 703 | 60   | 32,34,34     | 2.17 | 11 (34%)    | 49,54,54    | 1.97 | 13 (26%)    |
| 62  | SF4  | d     | 302 | 37   | 0,12,12      | -    | -           | -           | -    | -           |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 63  | GCP  | z     | 703 | 60   | -       | 10/19/38/38 | 0/3/3/3 |
| 62  | SF4  | d     | 302 | 37   | -       | -           | 0/6/5/5 |

The worst 5 of 11 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 63  | z     | 703 | GCP  | PB-O2B | -6.10 | 1.41        | 1.56     |
| 63  | z     | 703 | GCP  | PG-O3G | -4.45 | 1.45        | 1.55     |
| 63  | z     | 703 | GCP  | C6-N1  | -3.87 | 1.31        | 1.38     |
| 63  | z     | 703 | GCP  | C5-N7  | -3.30 | 1.32        | 1.39     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 63  | z     | 703 | GCP  | PB-O1B | 2.83 | 1.58        | 1.51     |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 63  | z     | 703 | GCP  | C5-C4-N3    | -6.41 | 118.19      | 128.39   |
| 63  | z     | 703 | GCP  | N9-C4-N3    | 5.30  | 136.55      | 125.95   |
| 63  | z     | 703 | GCP  | C2-N3-C4    | 5.11  | 121.10      | 112.30   |
| 63  | z     | 703 | GCP  | O3'-C3'-C2' | -2.81 | 102.79      | 111.82   |
| 63  | z     | 703 | GCP  | C6-C5-N7    | 2.81  | 135.41      | 130.29   |

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

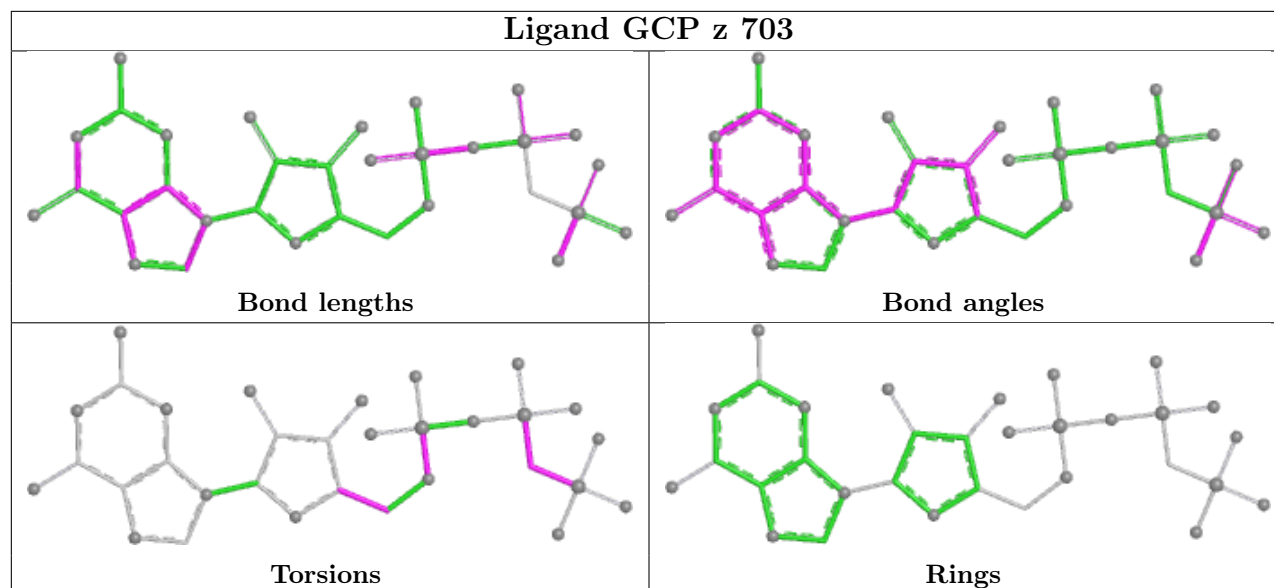
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 63  | z     | 703 | GCP  | PB-C3B-PG-O1G   |
| 63  | z     | 703 | GCP  | PB-C3B-PG-O2G   |
| 63  | z     | 703 | GCP  | PG-C3B-PB-O1B   |
| 63  | z     | 703 | GCP  | C5'-O5'-PA-O2A  |
| 63  | z     | 703 | GCP  | O4'-C4'-C5'-O5' |

There are no ring outliers.

2 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 63  | z     | 703 | GCP  | 4       | 0            |
| 62  | d     | 302 | SF4  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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     | 2874/2915 (98%) | -0.43  | 114 (3%) 42 37 | 20, 37, 80, 93        | 403 (14%) |
| 2   | B     | 120/121 (99%)   | -0.04  | 1 (0%) 82 80   | 33, 53, 65, 83        | 14 (11%)  |
| 3   | C     | 136/228 (59%)   | 2.03   | 59 (43%) 0 0   | 35, 74, 85, 96        | 104 (76%) |
| 4   | D     | 275/276 (99%)   | -0.35  | 3 (1%) 78 74   | 16, 35, 45, 53        | 36 (13%)  |
| 5   | E     | 204/206 (99%)   | -0.17  | 1 (0%) 87 85   | 19, 39, 59, 74        | 35 (17%)  |
| 6   | F     | 203/210 (96%)   | -0.01  | 0 100 100      | 21, 48, 68, 82        | 30 (14%)  |
| 7   | G     | 181/182 (99%)   | 0.53   | 4 (2%) 62 57   | 40, 54, 70, 77        | 35 (19%)  |
| 8   | H     | 174/180 (96%)   | 0.17   | 4 (2%) 61 55   | 34, 51, 63, 69        | 29 (16%)  |
| 9   | J     | 130/173 (75%)   | 2.81   | 102 (78%) 0 0  | 81, 134, 176, 200     | 9 (6%)    |
| 10  | K     | 139/147 (94%)   | 2.77   | 99 (71%) 0 0   | 60, 83, 95, 103       | 112 (80%) |
| 11  | N     | 140/140 (100%)  | -0.12  | 1 (0%) 84 82   | 23, 40, 58, 74        | 21 (15%)  |
| 12  | O     | 122/122 (100%)  | -0.38  | 0 100 100      | 25, 37, 47, 60        | 6 (4%)    |
| 13  | P     | 149/150 (99%)   | 0.03   | 1 (0%) 84 82   | 20, 45, 60, 78        | 34 (22%)  |
| 14  | Q     | 141/141 (100%)  | -0.23  | 1 (0%) 84 82   | 24, 39, 54, 70        | 34 (24%)  |
| 15  | R     | 118/118 (100%)  | -0.18  | 0 100 100      | 24, 42, 51, 62        | 15 (12%)  |
| 16  | S     | 110/112 (98%)   | 0.24   | 1 (0%) 81 78   | 39, 49, 59, 70        | 23 (20%)  |
| 17  | T     | 131/146 (89%)   | 0.02   | 5 (3%) 44 38   | 31, 43, 65, 87        | 19 (14%)  |
| 18  | U     | 116/118 (98%)   | -0.26  | 0 100 100      | 24, 37, 47, 52        | 21 (18%)  |
| 19  | V     | 101/101 (100%)  | -0.14  | 1 (0%) 79 76   | 26, 45, 55, 65        | 11 (10%)  |
| 20  | W     | 112/113 (99%)   | 0.01   | 3 (2%) 56 50   | 26, 39, 54, 72        | 21 (18%)  |
| 21  | X     | 95/96 (98%)     | 0.31   | 2 (2%) 63 58   | 36, 47, 66, 76        | 13 (13%)  |
| 22  | Y     | 107/110 (97%)   | 0.45   | 4 (3%) 45 39   | 43, 51, 72, 82        | 19 (17%)  |
| 23  | Z     | 94/206 (45%)    | 0.36   | 3 (3%) 50 44   | 40, 56, 69, 85        | 14 (14%)  |
| 24  | 0     | 74/85 (87%)     | -0.26  | 0 100 100      | 25, 38, 48, 64        | 13 (17%)  |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9     |
|-----|-------|-----------------|--------|---------------|-----------------------|-----------|
| 25  | 1     | 97/98 (98%)     | 0.16   | 6 (6%) 26 21  | 21, 38, 66, 72        | 20 (20%)  |
| 26  | 2     | 70/72 (97%)     | 0.28   | 0 100 100     | 40, 54, 62, 77        | 12 (17%)  |
| 27  | 3     | 59/60 (98%)     | -0.21  | 0 100 100     | 28, 42, 61, 66        | 9 (15%)   |
| 28  | 4     | 69/71 (97%)     | 1.22   | 14 (20%) 3 2  | 48, 67, 78, 80        | 25 (36%)  |
| 29  | 5     | 59/60 (98%)     | -0.19  | 0 100 100     | 21, 41, 58, 65        | 8 (13%)   |
| 30  | 6     | 53/54 (98%)     | -0.22  | 0 100 100     | 31, 38, 45, 50        | 11 (20%)  |
| 31  | 7     | 49/49 (100%)    | -0.28  | 3 (6%) 27 22  | 24, 28, 40, 59        | 9 (18%)   |
| 32  | 8     | 64/65 (98%)     | -0.34  | 0 100 100     | 24, 32, 36, 42        | 7 (10%)   |
| 33  | 9     | 37/37 (100%)    | -0.04  | 0 100 100     | 29, 36, 45, 52        | 9 (24%)   |
| 34  | a     | 1498/1521 (98%) | -0.30  | 46 (3%) 51 45 | 26, 43, 79, 93        | 194 (12%) |
| 35  | b     | 231/256 (90%)   | 0.94   | 26 (11%) 10 8 | 44, 66, 80, 92        | 54 (23%)  |
| 36  | c     | 206/239 (86%)   | 0.28   | 3 (1%) 72 68  | 37, 54, 70, 82        | 16 (7%)   |
| 37  | d     | 208/209 (99%)   | 0.62   | 9 (4%) 40 34  | 42, 56, 72, 81        | 45 (21%)  |
| 38  | e     | 148/162 (91%)   | -0.07  | 0 100 100     | 33, 45, 54, 69        | 22 (14%)  |
| 39  | f     | 100/101 (99%)   | 0.52   | 3 (3%) 52 47  | 47, 62, 72, 82        | 16 (16%)  |
| 40  | g     | 155/156 (99%)   | 0.43   | 8 (5%) 33 27  | 37, 54, 75, 85        | 38 (24%)  |
| 41  | h     | 137/138 (99%)   | -0.18  | 0 100 100     | 36, 45, 53, 61        | 13 (9%)   |
| 42  | i     | 127/128 (99%)   | 0.51   | 3 (2%) 59 54  | 32, 59, 73, 77        | 13 (10%)  |
| 43  | j     | 96/105 (91%)    | 0.78   | 13 (13%) 7 5  | 30, 61, 82, 86        | 22 (22%)  |
| 44  | k     | 114/129 (88%)   | 0.15   | 2 (1%) 67 63  | 31, 50, 63, 68        | 16 (14%)  |
| 45  | l     | 122/132 (92%)   | -0.22  | 1 (0%) 82 80  | 26, 38, 52, 61        | 17 (13%)  |
| 46  | m     | 119/126 (94%)   | 0.48   | 7 (5%) 28 23  | 28, 53, 71, 73        | 22 (18%)  |
| 47  | n     | 60/61 (98%)     | -0.03  | 1 (1%) 69 64  | 31, 42, 52, 57        | 4 (6%)    |
| 48  | o     | 88/89 (98%)     | 0.08   | 0 100 100     | 33, 46, 59, 65        | 20 (22%)  |
| 49  | p     | 82/88 (93%)     | 0.52   | 3 (3%) 45 39  | 38, 53, 64, 70        | 13 (15%)  |
| 50  | q     | 99/105 (94%)    | 0.03   | 1 (1%) 79 76  | 37, 47, 56, 60        | 17 (17%)  |
| 51  | r     | 68/88 (77%)     | 0.16   | 1 (1%) 72 68  | 42, 54, 71, 81        | 13 (19%)  |
| 52  | s     | 83/93 (89%)     | 0.39   | 3 (3%) 46 40  | 34, 51, 68, 76        | 11 (13%)  |
| 53  | t     | 96/106 (90%)    | 0.39   | 7 (7%) 21 17  | 36, 46, 54, 69        | 15 (15%)  |
| 54  | u     | 23/27 (85%)     | 0.18   | 0 100 100     | 32, 43, 47, 47        | 3 (13%)   |
| 55  | v     | 13/24 (54%)     | 0.33   | 3 (23%) 2 1   | 34, 45, 58, 71        | 4 (30%)   |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9      |
|-----|-------|-------------------|--------|----------------|-----------------------|------------|
| 56  | w     | 67/76 (88%)       | 1.14   | 9 (13%) 7 5    | 41, 75, 83, 86        | 52 (77%)   |
| 57  | x     | 73/77 (94%)       | -0.15  | 4 (5%) 30 25   | 25, 46, 64, 70        | 13 (17%)   |
| 58  | y     | 68/76 (89%)       | 0.93   | 13 (19%) 3 2   | 27, 75, 91, 94        | 39 (57%)   |
| 59  | z     | 671/679 (98%)     | 0.68   | 38 (5%) 29 24  | 25, 61, 78, 90        | 154 (22%)  |
| All | All   | 11355/11953 (94%) | 0.06   | 636 (5%) 30 24 | 16, 46, 80, 200       | 2027 (17%) |

The worst 5 of 636 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 28  | 4     | 56  | VAL  | 7.2  |
| 28  | 4     | 49  | PHE  | 6.5  |
| 40  | g     | 82  | GLY  | 6.4  |
| 1   | A     | 932 | C    | 6.3  |
| 9   | J     | 37  | THR  | 5.9  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 56  | PSU  | w     | 55  | 20/21 | 0.52 | 0.14 | 96,105,110,111             | 13    |
| 58  | PSU  | y     | 32  | 20/21 | 0.71 | 0.15 | 92,98,106,108              | 11    |
| 56  | 7MG  | w     | 46  | 24/25 | 0.73 | 0.14 | 91,97,102,104              | 13    |
| 58  | MIA  | y     | 37  | 22/30 | 0.77 | 0.15 | 75,84,87,89                | 8     |
| 56  | 5MU  | w     | 54  | 21/22 | 0.78 | 0.14 | 94,99,101,104              | 14    |
| 58  | PSU  | y     | 39  | 20/21 | 0.78 | 0.13 | 85,93,96,96                | 8     |
| 58  | PSU  | y     | 55  | 20/21 | 0.81 | 0.13 | 68,75,84,88                | 11    |
| 58  | 5MU  | y     | 54  | 21/22 | 0.84 | 0.13 | 67,72,82,83                | 11    |
| 58  | 4SU  | y     | 8   | 20/21 | 0.86 | 0.12 | 78,95,101,102              | 10    |
| 56  | 4SU  | w     | 8   | 20/21 | 0.87 | 0.10 | 86,92,95,95                | 12    |
| 56  | PSU  | w     | 32  | 20/21 | 0.91 | 0.09 | 54,61,66,72                | 2     |
| 56  | PSU  | w     | 39  | 20/21 | 0.93 | 0.10 | 54,63,69,70                | 7     |
| 56  | MIA  | w     | 37  | 27/30 | 0.93 | 0.10 | 42,47,52,52                | 8     |
| 57  | 4SU  | x     | 8   | 20/21 | 0.95 | 0.08 | 41,49,54,54                | 7     |
| 57  | 5MU  | x     | 54  | 21/22 | 0.95 | 0.09 | 40,51,55,61                | 10    |
| 57  | PSU  | x     | 55  | 20/21 | 0.96 | 0.08 | 39,51,54,57                | 7     |
| 57  | 5MC  | x     | 32  | 21/22 | 0.97 | 0.09 | 33,40,44,46                | 4     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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. 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  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | B     | 206  | 1/1   | 0.50 | 0.18 | 86,86,86,86                 | 0     |
| 60  | MG   | A     | 3586 | 1/1   | 0.60 | 0.18 | 75,75,75,75                 | 0     |
| 60  | MG   | A     | 3255 | 1/1   | 0.60 | 0.15 | 94,94,94,94                 | 0     |
| 60  | MG   | A     | 3068 | 1/1   | 0.64 | 0.29 | 69,69,69,69                 | 0     |
| 60  | MG   | A     | 3290 | 1/1   | 0.68 | 0.17 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3394 | 1/1   | 0.71 | 0.11 | 81,81,81,81                 | 0     |
| 60  | MG   | A     | 3498 | 1/1   | 0.72 | 0.16 | 68,68,68,68                 | 0     |
| 60  | MG   | B     | 211  | 1/1   | 0.72 | 0.30 | 69,69,69,69                 | 0     |
| 60  | MG   | B     | 215  | 1/1   | 0.72 | 0.11 | 75,75,75,75                 | 1     |
| 60  | MG   | a     | 1614 | 1/1   | 0.72 | 0.14 | 75,75,75,75                 | 0     |
| 60  | MG   | A     | 3517 | 1/1   | 0.73 | 0.20 | 85,85,85,85                 | 0     |
| 60  | MG   | A     | 3151 | 1/1   | 0.73 | 0.19 | 72,72,72,72                 | 0     |
| 60  | MG   | A     | 3514 | 1/1   | 0.73 | 0.16 | 69,69,69,69                 | 0     |
| 60  | MG   | a     | 1758 | 1/1   | 0.74 | 0.17 | 72,72,72,72                 | 0     |
| 60  | MG   | A     | 3275 | 1/1   | 0.75 | 0.20 | 55,55,55,55                 | 1     |
| 60  | MG   | A     | 3155 | 1/1   | 0.75 | 0.14 | 65,65,65,65                 | 0     |
| 60  | MG   | a     | 1636 | 1/1   | 0.75 | 0.25 | 59,59,59,59                 | 0     |
| 60  | MG   | a     | 1705 | 1/1   | 0.75 | 0.15 | 72,72,72,72                 | 0     |
| 60  | MG   | A     | 3130 | 1/1   | 0.75 | 0.10 | 55,55,55,55                 | 0     |
| 60  | MG   | e     | 201  | 1/1   | 0.75 | 0.09 | 78,78,78,78                 | 0     |
| 60  | MG   | x     | 109  | 1/1   | 0.75 | 0.20 | 77,77,77,77                 | 0     |
| 60  | MG   | a     | 1601 | 1/1   | 0.76 | 0.14 | 68,68,68,68                 | 0     |
| 60  | MG   | a     | 1603 | 1/1   | 0.76 | 0.21 | 67,67,67,67                 | 0     |
| 60  | MG   | A     | 3492 | 1/1   | 0.76 | 0.17 | 64,64,64,64                 | 1     |
| 60  | MG   | A     | 3049 | 1/1   | 0.76 | 0.20 | 68,68,68,68                 | 0     |
| 60  | MG   | A     | 3209 | 1/1   | 0.77 | 0.28 | 72,72,72,72                 | 0     |
| 60  | MG   | a     | 1626 | 1/1   | 0.77 | 0.14 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3520 | 1/1   | 0.77 | 0.25 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1690 | 1/1   | 0.77 | 0.20 | 69,69,69,69                 | 0     |
| 60  | MG   | A     | 3050 | 1/1   | 0.78 | 0.20 | 60,60,60,60                 | 0     |
| 60  | MG   | V     | 202  | 1/1   | 0.78 | 0.22 | 73,73,73,73                 | 0     |
| 60  | MG   | A     | 3236 | 1/1   | 0.78 | 0.24 | 47,47,47,47                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3246 | 1/1   | 0.78 | 0.18 | 66,66,66,66                 | 0     |
| 60  | MG   | A     | 3508 | 1/1   | 0.79 | 0.10 | 68,68,68,68                 | 0     |
| 60  | MG   | a     | 1641 | 1/1   | 0.79 | 0.17 | 68,68,68,68                 | 0     |
| 60  | MG   | a     | 1689 | 1/1   | 0.79 | 0.26 | 74,74,74,74                 | 0     |
| 60  | MG   | A     | 3610 | 1/1   | 0.79 | 0.11 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3144 | 1/1   | 0.79 | 0.17 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3063 | 1/1   | 0.79 | 0.22 | 49,49,49,49                 | 0     |
| 60  | MG   | a     | 1623 | 1/1   | 0.79 | 0.16 | 46,46,46,46                 | 1     |
| 60  | MG   | A     | 3253 | 1/1   | 0.79 | 0.13 | 67,67,67,67                 | 0     |
| 60  | MG   | A     | 3061 | 1/1   | 0.80 | 0.12 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3556 | 1/1   | 0.80 | 0.11 | 35,35,35,35                 | 1     |
| 60  | MG   | A     | 3423 | 1/1   | 0.80 | 0.14 | 73,73,73,73                 | 0     |
| 60  | MG   | A     | 3441 | 1/1   | 0.80 | 0.15 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3630 | 1/1   | 0.80 | 0.21 | 34,34,34,34                 | 1     |
| 60  | MG   | A     | 3252 | 1/1   | 0.80 | 0.15 | 76,76,76,76                 | 0     |
| 60  | MG   | A     | 3496 | 1/1   | 0.80 | 0.24 | 33,33,33,33                 | 1     |
| 60  | MG   | A     | 3277 | 1/1   | 0.80 | 0.15 | 47,47,47,47                 | 1     |
| 60  | MG   | A     | 3282 | 1/1   | 0.80 | 0.20 | 68,68,68,68                 | 0     |
| 60  | MG   | A     | 3157 | 1/1   | 0.80 | 0.30 | 40,40,40,40                 | 1     |
| 60  | MG   | A     | 3295 | 1/1   | 0.80 | 0.23 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3551 | 1/1   | 0.81 | 0.15 | 71,71,71,71                 | 0     |
| 60  | MG   | A     | 3333 | 1/1   | 0.81 | 0.14 | 61,61,61,61                 | 1     |
| 60  | MG   | A     | 3572 | 1/1   | 0.81 | 0.12 | 58,58,58,58                 | 0     |
| 60  | MG   | a     | 1662 | 1/1   | 0.81 | 0.13 | 53,53,53,53                 | 0     |
| 60  | MG   | 5     | 102  | 1/1   | 0.81 | 0.17 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3358 | 1/1   | 0.81 | 0.15 | 46,46,46,46                 | 1     |
| 60  | MG   | A     | 3234 | 1/1   | 0.81 | 0.13 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3283 | 1/1   | 0.81 | 0.12 | 41,41,41,41                 | 0     |
| 60  | MG   | a     | 1759 | 1/1   | 0.81 | 0.15 | 53,53,53,53                 | 0     |
| 60  | MG   | a     | 1765 | 1/1   | 0.81 | 0.10 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1782 | 1/1   | 0.81 | 0.30 | 62,62,62,62                 | 0     |
| 60  | MG   | a     | 1615 | 1/1   | 0.81 | 0.18 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3525 | 1/1   | 0.81 | 0.10 | 37,37,37,37                 | 0     |
| 60  | MG   | 6     | 101  | 1/1   | 0.82 | 0.20 | 42,42,42,42                 | 1     |
| 60  | MG   | A     | 3188 | 1/1   | 0.82 | 0.20 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3344 | 1/1   | 0.82 | 0.15 | 70,70,70,70                 | 0     |
| 60  | MG   | A     | 3011 | 1/1   | 0.82 | 0.25 | 53,53,53,53                 | 0     |
| 60  | MG   | a     | 1732 | 1/1   | 0.82 | 0.12 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3249 | 1/1   | 0.82 | 0.14 | 72,72,72,72                 | 0     |
| 60  | MG   | A     | 3554 | 1/1   | 0.82 | 0.14 | 67,67,67,67                 | 0     |
| 60  | MG   | A     | 3420 | 1/1   | 0.82 | 0.12 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1779 | 1/1   | 0.82 | 0.16 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3559 | 1/1   | 0.82 | 0.17 | 38,38,38,38                 | 1     |
| 60  | MG   | a     | 1787 | 1/1   | 0.82 | 0.33 | 40,40,40,40                 | 1     |
| 60  | MG   | A     | 3179 | 1/1   | 0.82 | 0.22 | 61,61,61,61                 | 0     |
| 60  | MG   | a     | 1653 | 1/1   | 0.82 | 0.20 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3464 | 1/1   | 0.83 | 0.11 | 56,56,56,56                 | 0     |
| 60  | MG   | a     | 1664 | 1/1   | 0.83 | 0.24 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3194 | 1/1   | 0.83 | 0.12 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3578 | 1/1   | 0.83 | 0.15 | 60,60,60,60                 | 0     |
| 60  | MG   | a     | 1701 | 1/1   | 0.83 | 0.10 | 66,66,66,66                 | 0     |
| 60  | MG   | A     | 3052 | 1/1   | 0.83 | 0.13 | 51,51,51,51                 | 1     |
| 60  | MG   | a     | 1612 | 1/1   | 0.83 | 0.09 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3531 | 1/1   | 0.83 | 0.10 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3537 | 1/1   | 0.83 | 0.09 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3548 | 1/1   | 0.83 | 0.15 | 65,65,65,65                 | 0     |
| 60  | MG   | A     | 3154 | 1/1   | 0.83 | 0.14 | 67,67,67,67                 | 0     |
| 60  | MG   | A     | 3278 | 1/1   | 0.83 | 0.11 | 56,56,56,56                 | 0     |
| 60  | MG   | a     | 1638 | 1/1   | 0.83 | 0.14 | 53,53,53,53                 | 0     |
| 60  | MG   | F     | 301  | 1/1   | 0.83 | 0.07 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3146 | 1/1   | 0.83 | 0.17 | 72,72,72,72                 | 0     |
| 60  | MG   | A     | 3054 | 1/1   | 0.84 | 0.12 | 48,48,48,48                 | 0     |
| 60  | MG   | a     | 1643 | 1/1   | 0.84 | 0.22 | 58,58,58,58                 | 0     |
| 60  | MG   | a     | 1648 | 1/1   | 0.84 | 0.16 | 58,58,58,58                 | 0     |
| 60  | MG   | R     | 202  | 1/1   | 0.84 | 0.11 | 62,62,62,62                 | 0     |
| 60  | MG   | a     | 1661 | 1/1   | 0.84 | 0.17 | 69,69,69,69                 | 0     |
| 60  | MG   | V     | 201  | 1/1   | 0.84 | 0.18 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3256 | 1/1   | 0.84 | 0.13 | 62,62,62,62                 | 0     |
| 60  | MG   | Z     | 301  | 1/1   | 0.84 | 0.13 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3262 | 1/1   | 0.84 | 0.11 | 50,50,50,50                 | 1     |
| 60  | MG   | A     | 3573 | 1/1   | 0.84 | 0.19 | 34,34,34,34                 | 1     |
| 60  | MG   | A     | 3169 | 1/1   | 0.84 | 0.16 | 44,44,44,44                 | 1     |
| 60  | MG   | a     | 1715 | 1/1   | 0.84 | 0.19 | 58,58,58,58                 | 0     |
| 60  | MG   | a     | 1729 | 1/1   | 0.84 | 0.14 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3580 | 1/1   | 0.84 | 0.10 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3002 | 1/1   | 0.84 | 0.16 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3450 | 1/1   | 0.84 | 0.20 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3335 | 1/1   | 0.84 | 0.14 | 59,59,59,59                 | 1     |
| 60  | MG   | A     | 3343 | 1/1   | 0.84 | 0.11 | 64,64,64,64                 | 0     |
| 60  | MG   | B     | 207  | 1/1   | 0.84 | 0.09 | 76,76,76,76                 | 0     |
| 60  | MG   | a     | 1635 | 1/1   | 0.84 | 0.09 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3119 | 1/1   | 0.84 | 0.13 | 68,68,68,68                 | 0     |
| 60  | MG   | A     | 3356 | 1/1   | 0.84 | 0.10 | 50,50,50,50                 | 0     |
| 60  | MG   | z     | 701  | 1/1   | 0.84 | 0.13 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3606 | 1/1   | 0.85 | 0.12 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3167 | 1/1   | 0.85 | 0.14 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3618 | 1/1   | 0.85 | 0.12 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3248 | 1/1   | 0.85 | 0.17 | 48,48,48,48                 | 1     |
| 60  | MG   | A     | 3141 | 1/1   | 0.85 | 0.14 | 42,42,42,42                 | 1     |
| 60  | MG   | A     | 3081 | 1/1   | 0.85 | 0.23 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3094 | 1/1   | 0.85 | 0.16 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3189 | 1/1   | 0.85 | 0.27 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3107 | 1/1   | 0.85 | 0.19 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1667 | 1/1   | 0.85 | 0.11 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3195 | 1/1   | 0.85 | 0.26 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3364 | 1/1   | 0.85 | 0.10 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3263 | 1/1   | 0.85 | 0.10 | 67,67,67,67                 | 0     |
| 60  | MG   | A     | 3266 | 1/1   | 0.85 | 0.10 | 67,67,67,67                 | 0     |
| 60  | MG   | 5     | 101  | 1/1   | 0.85 | 0.14 | 44,44,44,44                 | 1     |
| 60  | MG   | A     | 3267 | 1/1   | 0.85 | 0.10 | 64,64,64,64                 | 0     |
| 60  | MG   | A     | 3108 | 1/1   | 0.85 | 0.22 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3448 | 1/1   | 0.85 | 0.20 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3225 | 1/1   | 0.85 | 0.14 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3576 | 1/1   | 0.85 | 0.09 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3034 | 1/1   | 0.85 | 0.15 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3010 | 1/1   | 0.85 | 0.14 | 32,32,32,32                 | 1     |
| 60  | MG   | a     | 1620 | 1/1   | 0.85 | 0.18 | 47,47,47,47                 | 0     |
| 60  | MG   | d     | 301  | 1/1   | 0.85 | 0.27 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3240 | 1/1   | 0.85 | 0.10 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3603 | 1/1   | 0.85 | 0.17 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3605 | 1/1   | 0.85 | 0.22 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3604 | 1/1   | 0.86 | 0.17 | 64,64,64,64                 | 0     |
| 60  | MG   | A     | 3259 | 1/1   | 0.86 | 0.13 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3323 | 1/1   | 0.86 | 0.16 | 72,72,72,72                 | 0     |
| 60  | MG   | A     | 3029 | 1/1   | 0.86 | 0.12 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3097 | 1/1   | 0.86 | 0.18 | 56,56,56,56                 | 0     |
| 60  | MG   | a     | 1642 | 1/1   | 0.86 | 0.20 | 70,70,70,70                 | 0     |
| 60  | MG   | A     | 3265 | 1/1   | 0.86 | 0.23 | 64,64,64,64                 | 0     |
| 60  | MG   | B     | 203  | 1/1   | 0.86 | 0.08 | 56,56,56,56                 | 0     |
| 60  | MG   | B     | 204  | 1/1   | 0.86 | 0.21 | 63,63,63,63                 | 0     |
| 60  | MG   | a     | 1659 | 1/1   | 0.86 | 0.13 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1660 | 1/1   | 0.86 | 0.11 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3057 | 1/1   | 0.86 | 0.21 | 72,72,72,72                 | 0     |
| 60  | MG   | A     | 3353 | 1/1   | 0.86 | 0.11 | 60,60,60,60                 | 0     |
| 60  | MG   | a     | 1663 | 1/1   | 0.86 | 0.18 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3208 | 1/1   | 0.86 | 0.17 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3536 | 1/1   | 0.86 | 0.21 | 57,57,57,57                 | 0     |
| 60  | MG   | a     | 1675 | 1/1   | 0.86 | 0.15 | 61,61,61,61                 | 0     |
| 60  | MG   | a     | 1676 | 1/1   | 0.86 | 0.12 | 58,58,58,58                 | 0     |
| 60  | MG   | a     | 1680 | 1/1   | 0.86 | 0.24 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3269 | 1/1   | 0.86 | 0.22 | 64,64,64,64                 | 0     |
| 60  | MG   | A     | 3271 | 1/1   | 0.86 | 0.22 | 71,71,71,71                 | 0     |
| 60  | MG   | A     | 3083 | 1/1   | 0.86 | 0.10 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3418 | 1/1   | 0.86 | 0.09 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3276 | 1/1   | 0.86 | 0.08 | 51,51,51,51                 | 1     |
| 60  | MG   | a     | 1717 | 1/1   | 0.86 | 0.22 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3557 | 1/1   | 0.86 | 0.12 | 70,70,70,70                 | 0     |
| 60  | MG   | A     | 3250 | 1/1   | 0.86 | 0.23 | 64,64,64,64                 | 0     |
| 60  | MG   | A     | 3432 | 1/1   | 0.86 | 0.13 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3223 | 1/1   | 0.86 | 0.21 | 52,52,52,52                 | 0     |
| 60  | MG   | a     | 1761 | 1/1   | 0.86 | 0.11 | 55,55,55,55                 | 1     |
| 60  | MG   | A     | 3442 | 1/1   | 0.86 | 0.23 | 60,60,60,60                 | 0     |
| 60  | MG   | a     | 1604 | 1/1   | 0.86 | 0.15 | 64,64,64,64                 | 0     |
| 60  | MG   | a     | 1611 | 1/1   | 0.86 | 0.11 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3110 | 1/1   | 0.86 | 0.22 | 25,25,25,25                 | 1     |
| 60  | MG   | A     | 3231 | 1/1   | 0.86 | 0.20 | 68,68,68,68                 | 0     |
| 60  | MG   | A     | 3284 | 1/1   | 0.86 | 0.10 | 39,39,39,39                 | 1     |
| 60  | MG   | x     | 102  | 1/1   | 0.86 | 0.21 | 77,77,77,77                 | 0     |
| 60  | MG   | x     | 108  | 1/1   | 0.86 | 0.20 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3594 | 1/1   | 0.86 | 0.15 | 85,85,85,85                 | 0     |
| 60  | MG   | A     | 3085 | 1/1   | 0.86 | 0.17 | 70,70,70,70                 | 0     |
| 60  | MG   | O     | 201  | 1/1   | 0.87 | 0.10 | 55,55,55,55                 | 0     |
| 60  | MG   | P     | 201  | 1/1   | 0.87 | 0.14 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3244 | 1/1   | 0.87 | 0.12 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3088 | 1/1   | 0.87 | 0.12 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3511 | 1/1   | 0.87 | 0.14 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3579 | 1/1   | 0.87 | 0.10 | 50,50,50,50                 | 0     |
| 60  | MG   | 0     | 103  | 1/1   | 0.87 | 0.16 | 53,53,53,53                 | 0     |
| 60  | MG   | a     | 1669 | 1/1   | 0.87 | 0.24 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3072 | 1/1   | 0.87 | 0.09 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3406 | 1/1   | 0.87 | 0.17 | 74,74,74,74                 | 0     |
| 60  | MG   | A     | 3006 | 1/1   | 0.87 | 0.17 | 52,52,52,52                 | 1     |
| 60  | MG   | A     | 3600 | 1/1   | 0.87 | 0.09 | 53,53,53,53                 | 0     |
| 60  | MG   | a     | 1602 | 1/1   | 0.87 | 0.12 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3307 | 1/1   | 0.87 | 0.12 | 60,60,60,60                 | 0     |
| 60  | MG   | a     | 1703 | 1/1   | 0.87 | 0.13 | 57,57,57,57                 | 1     |
| 60  | MG   | A     | 3530 | 1/1   | 0.87 | 0.13 | 38,38,38,38                 | 1     |
| 60  | MG   | A     | 3309 | 1/1   | 0.87 | 0.12 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3321 | 1/1   | 0.87 | 0.10 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3438 | 1/1   | 0.87 | 0.15 | 77,77,77,77                 | 0     |
| 60  | MG   | A     | 3612 | 1/1   | 0.87 | 0.09 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3541 | 1/1   | 0.87 | 0.08 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3098 | 1/1   | 0.87 | 0.11 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3636 | 1/1   | 0.87 | 0.19 | 37,37,37,37                 | 1     |
| 60  | MG   | a     | 1627 | 1/1   | 0.87 | 0.14 | 47,47,47,47                 | 0     |
| 60  | MG   | a     | 1632 | 1/1   | 0.87 | 0.16 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3233 | 1/1   | 0.87 | 0.10 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3066 | 1/1   | 0.87 | 0.17 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3235 | 1/1   | 0.87 | 0.08 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3205 | 1/1   | 0.87 | 0.10 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3237 | 1/1   | 0.87 | 0.15 | 43,43,43,43                 | 1     |
| 60  | MG   | A     | 3563 | 1/1   | 0.87 | 0.09 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3022 | 1/1   | 0.87 | 0.17 | 59,59,59,59                 | 0     |
| 60  | MG   | N     | 201  | 1/1   | 0.87 | 0.16 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3184 | 1/1   | 0.88 | 0.24 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3075 | 1/1   | 0.88 | 0.11 | 60,60,60,60                 | 1     |
| 60  | MG   | A     | 3581 | 1/1   | 0.88 | 0.10 | 63,63,63,63                 | 0     |
| 60  | MG   | a     | 1686 | 1/1   | 0.88 | 0.15 | 61,61,61,61                 | 0     |
| 60  | MG   | a     | 1618 | 1/1   | 0.88 | 0.28 | 54,54,54,54                 | 0     |
| 60  | MG   | D     | 305  | 1/1   | 0.88 | 0.20 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3493 | 1/1   | 0.88 | 0.12 | 48,48,48,48                 | 1     |
| 60  | MG   | F     | 303  | 1/1   | 0.88 | 0.11 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3588 | 1/1   | 0.88 | 0.18 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3332 | 1/1   | 0.88 | 0.11 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3058 | 1/1   | 0.88 | 0.09 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3056 | 1/1   | 0.88 | 0.09 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3555 | 1/1   | 0.88 | 0.16 | 63,63,63,63                 | 0     |
| 60  | MG   | a     | 1755 | 1/1   | 0.88 | 0.08 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3039 | 1/1   | 0.88 | 0.21 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3513 | 1/1   | 0.88 | 0.20 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3257 | 1/1   | 0.88 | 0.10 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3291 | 1/1   | 0.88 | 0.17 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1772 | 1/1   | 0.88 | 0.16 | 62,62,62,62                 | 0     |
| 60  | MG   | a     | 1778 | 1/1   | 0.88 | 0.09 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3613 | 1/1   | 0.88 | 0.22 | 67,67,67,67                 | 0     |
| 60  | MG   | A     | 3564 | 1/1   | 0.88 | 0.10 | 52,52,52,52                 | 0     |
| 60  | MG   | a     | 1786 | 1/1   | 0.88 | 0.17 | 38,38,38,38                 | 1     |
| 60  | MG   | A     | 3274 | 1/1   | 0.88 | 0.14 | 66,66,66,66                 | 0     |
| 60  | MG   | A     | 3148 | 1/1   | 0.88 | 0.10 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3449 | 1/1   | 0.88 | 0.09 | 29,29,29,29                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3577 | 1/1   | 0.88 | 0.16 | 60,60,60,60                 | 0     |
| 60  | MG   | a     | 1606 | 1/1   | 0.88 | 0.10 | 48,48,48,48                 | 0     |
| 60  | MG   | a     | 1609 | 1/1   | 0.88 | 0.23 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3126 | 1/1   | 0.88 | 0.09 | 28,28,28,28                 | 1     |
| 60  | MG   | A     | 3436 | 1/1   | 0.89 | 0.07 | 43,43,43,43                 | 0     |
| 60  | MG   | 0     | 101  | 1/1   | 0.89 | 0.12 | 39,39,39,39                 | 0     |
| 60  | MG   | 0     | 102  | 1/1   | 0.89 | 0.09 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3016 | 1/1   | 0.89 | 0.20 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3254 | 1/1   | 0.89 | 0.19 | 62,62,62,62                 | 0     |
| 60  | MG   | a     | 1665 | 1/1   | 0.89 | 0.17 | 47,47,47,47                 | 1     |
| 60  | MG   | A     | 3545 | 1/1   | 0.89 | 0.08 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3132 | 1/1   | 0.89 | 0.14 | 43,43,43,43                 | 1     |
| 60  | MG   | a     | 1671 | 1/1   | 0.89 | 0.17 | 48,48,48,48                 | 0     |
| 60  | MG   | 7     | 101  | 1/1   | 0.89 | 0.12 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3175 | 1/1   | 0.89 | 0.12 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3207 | 1/1   | 0.89 | 0.21 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3082 | 1/1   | 0.89 | 0.15 | 43,43,43,43                 | 1     |
| 60  | MG   | A     | 3454 | 1/1   | 0.89 | 0.13 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3099 | 1/1   | 0.89 | 0.10 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3467 | 1/1   | 0.89 | 0.09 | 37,37,37,37                 | 0     |
| 60  | MG   | B     | 201  | 1/1   | 0.89 | 0.08 | 53,53,53,53                 | 1     |
| 60  | MG   | A     | 3561 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3217 | 1/1   | 0.89 | 0.16 | 56,56,56,56                 | 1     |
| 60  | MG   | A     | 3289 | 1/1   | 0.89 | 0.12 | 59,59,59,59                 | 0     |
| 60  | MG   | a     | 1718 | 1/1   | 0.89 | 0.13 | 55,55,55,55                 | 1     |
| 60  | MG   | A     | 3569 | 1/1   | 0.89 | 0.07 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3220 | 1/1   | 0.89 | 0.15 | 45,45,45,45                 | 0     |
| 60  | MG   | a     | 1733 | 1/1   | 0.89 | 0.21 | 51,51,51,51                 | 0     |
| 60  | MG   | a     | 1751 | 1/1   | 0.89 | 0.16 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3362 | 1/1   | 0.89 | 0.15 | 47,47,47,47                 | 0     |
| 60  | MG   | a     | 1625 | 1/1   | 0.89 | 0.17 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3064 | 1/1   | 0.89 | 0.14 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3374 | 1/1   | 0.89 | 0.21 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3292 | 1/1   | 0.89 | 0.13 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3164 | 1/1   | 0.89 | 0.18 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3301 | 1/1   | 0.89 | 0.14 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3227 | 1/1   | 0.89 | 0.20 | 63,63,63,63                 | 0     |
| 60  | MG   | a     | 1640 | 1/1   | 0.89 | 0.20 | 68,68,68,68                 | 0     |
| 60  | MG   | a     | 1785 | 1/1   | 0.89 | 0.25 | 53,53,53,53                 | 0     |
| 60  | MG   | P     | 202  | 1/1   | 0.89 | 0.18 | 59,59,59,59                 | 0     |
| 60  | MG   | P     | 203  | 1/1   | 0.89 | 0.09 | 45,45,45,45                 | 1     |
| 60  | MG   | A     | 3191 | 1/1   | 0.89 | 0.08 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | a     | 1646 | 1/1   | 0.89 | 0.12 | 52,52,52,52                 | 0     |
| 60  | MG   | n     | 101  | 1/1   | 0.89 | 0.32 | 64,64,64,64                 | 0     |
| 60  | MG   | A     | 3316 | 1/1   | 0.89 | 0.13 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3435 | 1/1   | 0.89 | 0.09 | 51,51,51,51                 | 0     |
| 60  | MG   | a     | 1657 | 1/1   | 0.89 | 0.10 | 57,57,57,57                 | 0     |
| 60  | MG   | W     | 201  | 1/1   | 0.89 | 0.22 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3535 | 1/1   | 0.90 | 0.12 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3142 | 1/1   | 0.90 | 0.08 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3143 | 1/1   | 0.90 | 0.17 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3228 | 1/1   | 0.90 | 0.15 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3428 | 1/1   | 0.90 | 0.08 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3027 | 1/1   | 0.90 | 0.07 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3550 | 1/1   | 0.90 | 0.31 | 65,65,65,65                 | 0     |
| 60  | MG   | a     | 1649 | 1/1   | 0.90 | 0.26 | 67,67,67,67                 | 0     |
| 60  | MG   | a     | 1651 | 1/1   | 0.90 | 0.20 | 64,64,64,64                 | 0     |
| 60  | MG   | B     | 214  | 1/1   | 0.90 | 0.11 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3076 | 1/1   | 0.90 | 0.33 | 33,33,33,33                 | 1     |
| 60  | MG   | A     | 3553 | 1/1   | 0.90 | 0.10 | 51,51,51,51                 | 1     |
| 60  | MG   | A     | 3118 | 1/1   | 0.90 | 0.13 | 64,64,64,64                 | 0     |
| 60  | MG   | F     | 302  | 1/1   | 0.90 | 0.16 | 32,32,32,32                 | 1     |
| 60  | MG   | A     | 3437 | 1/1   | 0.90 | 0.10 | 30,30,30,30                 | 1     |
| 60  | MG   | F     | 306  | 1/1   | 0.90 | 0.12 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3320 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3149 | 1/1   | 0.90 | 0.12 | 54,54,54,54                 | 0     |
| 60  | MG   | a     | 1666 | 1/1   | 0.90 | 0.29 | 68,68,68,68                 | 0     |
| 60  | MG   | A     | 3044 | 1/1   | 0.90 | 0.14 | 25,25,25,25                 | 1     |
| 60  | MG   | A     | 3443 | 1/1   | 0.90 | 0.12 | 41,41,41,41                 | 0     |
| 60  | MG   | a     | 1670 | 1/1   | 0.90 | 0.08 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3562 | 1/1   | 0.90 | 0.09 | 67,67,67,67                 | 0     |
| 60  | MG   | a     | 1673 | 1/1   | 0.90 | 0.11 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3270 | 1/1   | 0.90 | 0.10 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3100 | 1/1   | 0.90 | 0.12 | 66,66,66,66                 | 0     |
| 60  | MG   | A     | 3568 | 1/1   | 0.90 | 0.08 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3196 | 1/1   | 0.90 | 0.14 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3452 | 1/1   | 0.90 | 0.08 | 69,69,69,69                 | 0     |
| 60  | MG   | A     | 3336 | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 60  | MG   | a     | 1700 | 1/1   | 0.90 | 0.16 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3574 | 1/1   | 0.90 | 0.09 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3462 | 1/1   | 0.90 | 0.10 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3342 | 1/1   | 0.90 | 0.20 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3197 | 1/1   | 0.90 | 0.09 | 48,48,48,48                 | 1     |
| 60  | MG   | A     | 3470 | 1/1   | 0.90 | 0.14 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3485 | 1/1   | 0.90 | 0.12 | 59,59,59,59                 | 0     |
| 60  | MG   | 9     | 101  | 1/1   | 0.90 | 0.19 | 50,50,50,50                 | 0     |
| 60  | MG   | a     | 1731 | 1/1   | 0.90 | 0.10 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3199 | 1/1   | 0.90 | 0.13 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3350 | 1/1   | 0.90 | 0.10 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3101 | 1/1   | 0.90 | 0.11 | 47,47,47,47                 | 0     |
| 60  | MG   | a     | 1753 | 1/1   | 0.90 | 0.23 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3589 | 1/1   | 0.90 | 0.07 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1605 | 1/1   | 0.90 | 0.09 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3591 | 1/1   | 0.90 | 0.12 | 39,39,39,39                 | 1     |
| 60  | MG   | A     | 3593 | 1/1   | 0.90 | 0.08 | 70,70,70,70                 | 0     |
| 60  | MG   | A     | 3131 | 1/1   | 0.90 | 0.18 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3597 | 1/1   | 0.90 | 0.17 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3158 | 1/1   | 0.90 | 0.14 | 38,38,38,38                 | 1     |
| 60  | MG   | A     | 3602 | 1/1   | 0.90 | 0.14 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3160 | 1/1   | 0.90 | 0.32 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3214 | 1/1   | 0.90 | 0.11 | 44,44,44,44                 | 1     |
| 60  | MG   | A     | 3102 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3382 | 1/1   | 0.90 | 0.14 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3519 | 1/1   | 0.90 | 0.11 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3388 | 1/1   | 0.90 | 0.08 | 31,31,31,31                 | 0     |
| 60  | MG   | a     | 1629 | 1/1   | 0.90 | 0.09 | 44,44,44,44                 | 0     |
| 60  | MG   | a     | 1631 | 1/1   | 0.90 | 0.16 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3391 | 1/1   | 0.90 | 0.20 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3135 | 1/1   | 0.90 | 0.17 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3036 | 1/1   | 0.90 | 0.11 | 25,25,25,25                 | 1     |
| 60  | MG   | A     | 3463 | 1/1   | 0.91 | 0.28 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3607 | 1/1   | 0.91 | 0.11 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3305 | 1/1   | 0.91 | 0.06 | 38,38,38,38                 | 0     |
| 60  | MG   | A     | 3092 | 1/1   | 0.91 | 0.11 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3468 | 1/1   | 0.91 | 0.09 | 37,37,37,37                 | 1     |
| 60  | MG   | A     | 3268 | 1/1   | 0.91 | 0.08 | 52,52,52,52                 | 0     |
| 60  | MG   | a     | 1674 | 1/1   | 0.91 | 0.24 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3624 | 1/1   | 0.91 | 0.31 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3628 | 1/1   | 0.91 | 0.19 | 35,35,35,35                 | 0     |
| 60  | MG   | a     | 1677 | 1/1   | 0.91 | 0.08 | 63,63,63,63                 | 0     |
| 60  | MG   | a     | 1679 | 1/1   | 0.91 | 0.13 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3482 | 1/1   | 0.91 | 0.13 | 38,38,38,38                 | 0     |
| 60  | MG   | A     | 3633 | 1/1   | 0.91 | 0.17 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3242 | 1/1   | 0.91 | 0.23 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3644 | 1/1   | 0.91 | 0.13 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1691 | 1/1   | 0.91 | 0.16 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3488 | 1/1   | 0.91 | 0.11 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3395 | 1/1   | 0.91 | 0.12 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3147 | 1/1   | 0.91 | 0.19 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3180 | 1/1   | 0.91 | 0.17 | 44,44,44,44                 | 0     |
| 60  | MG   | a     | 1713 | 1/1   | 0.91 | 0.20 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3215 | 1/1   | 0.91 | 0.18 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3328 | 1/1   | 0.91 | 0.10 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3121 | 1/1   | 0.91 | 0.10 | 38,38,38,38                 | 1     |
| 60  | MG   | A     | 3008 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 60  | MG   | B     | 216  | 1/1   | 0.91 | 0.08 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3221 | 1/1   | 0.91 | 0.23 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3106 | 1/1   | 0.91 | 0.11 | 46,46,46,46                 | 1     |
| 60  | MG   | a     | 1741 | 1/1   | 0.91 | 0.17 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3280 | 1/1   | 0.91 | 0.21 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3012 | 1/1   | 0.91 | 0.10 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3523 | 1/1   | 0.91 | 0.08 | 31,31,31,31                 | 0     |
| 60  | MG   | G     | 201  | 1/1   | 0.91 | 0.15 | 48,48,48,48                 | 0     |
| 60  | MG   | H     | 201  | 1/1   | 0.91 | 0.10 | 62,62,62,62                 | 0     |
| 60  | MG   | A     | 3084 | 1/1   | 0.91 | 0.13 | 56,56,56,56                 | 0     |
| 60  | MG   | a     | 1762 | 1/1   | 0.91 | 0.11 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3528 | 1/1   | 0.91 | 0.10 | 51,51,51,51                 | 0     |
| 60  | MG   | a     | 1770 | 1/1   | 0.91 | 0.19 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3585 | 1/1   | 0.91 | 0.21 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3133 | 1/1   | 0.91 | 0.09 | 36,36,36,36                 | 1     |
| 60  | MG   | A     | 3060 | 1/1   | 0.91 | 0.07 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3532 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3111 | 1/1   | 0.91 | 0.09 | 46,46,46,46                 | 0     |
| 60  | MG   | a     | 1656 | 1/1   | 0.91 | 0.11 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3114 | 1/1   | 0.91 | 0.17 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3203 | 1/1   | 0.91 | 0.22 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3451 | 1/1   | 0.91 | 0.13 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3542 | 1/1   | 0.91 | 0.20 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3543 | 1/1   | 0.91 | 0.08 | 51,51,51,51                 | 0     |
| 60  | MG   | x     | 107  | 1/1   | 0.91 | 0.11 | 69,69,69,69                 | 0     |
| 60  | MG   | A     | 3117 | 1/1   | 0.91 | 0.11 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3367 | 1/1   | 0.91 | 0.06 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3032 | 1/1   | 0.91 | 0.17 | 50,50,50,50                 | 0     |
| 60  | MG   | a     | 1678 | 1/1   | 0.92 | 0.15 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3173 | 1/1   | 0.92 | 0.19 | 37,37,37,37                 | 0     |
| 60  | MG   | a     | 1621 | 1/1   | 0.92 | 0.10 | 64,64,64,64                 | 0     |
| 60  | MG   | a     | 1681 | 1/1   | 0.92 | 0.15 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1683 | 1/1   | 0.92 | 0.21 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | E     | 303  | 1/1   | 0.92 | 0.18 | 32,32,32,32                 | 1     |
| 60  | MG   | A     | 3544 | 1/1   | 0.92 | 0.18 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3297 | 1/1   | 0.92 | 0.10 | 35,35,35,35                 | 1     |
| 60  | MG   | A     | 3421 | 1/1   | 0.92 | 0.10 | 57,57,57,57                 | 0     |
| 60  | MG   | a     | 1693 | 1/1   | 0.92 | 0.21 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3422 | 1/1   | 0.92 | 0.15 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3599 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3232 | 1/1   | 0.92 | 0.11 | 35,35,35,35                 | 0     |
| 60  | MG   | a     | 1704 | 1/1   | 0.92 | 0.14 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3212 | 1/1   | 0.92 | 0.07 | 46,46,46,46                 | 0     |
| 60  | MG   | a     | 1711 | 1/1   | 0.92 | 0.06 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3355 | 1/1   | 0.92 | 0.14 | 61,61,61,61                 | 0     |
| 60  | MG   | a     | 1714 | 1/1   | 0.92 | 0.15 | 54,54,54,54                 | 0     |
| 60  | MG   | a     | 1637 | 1/1   | 0.92 | 0.19 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3434 | 1/1   | 0.92 | 0.07 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3115 | 1/1   | 0.92 | 0.21 | 27,27,27,27                 | 1     |
| 60  | MG   | A     | 3505 | 1/1   | 0.92 | 0.06 | 41,41,41,41                 | 0     |
| 60  | MG   | a     | 1730 | 1/1   | 0.92 | 0.19 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3128 | 1/1   | 0.92 | 0.08 | 37,37,37,37                 | 0     |
| 60  | MG   | U     | 201  | 1/1   | 0.92 | 0.21 | 30,30,30,30                 | 1     |
| 60  | MG   | a     | 1644 | 1/1   | 0.92 | 0.14 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3560 | 1/1   | 0.92 | 0.15 | 58,58,58,58                 | 0     |
| 60  | MG   | a     | 1748 | 1/1   | 0.92 | 0.07 | 46,46,46,46                 | 0     |
| 60  | MG   | a     | 1749 | 1/1   | 0.92 | 0.18 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3360 | 1/1   | 0.92 | 0.11 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3361 | 1/1   | 0.92 | 0.12 | 64,64,64,64                 | 0     |
| 60  | MG   | a     | 1754 | 1/1   | 0.92 | 0.08 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3089 | 1/1   | 0.92 | 0.12 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3622 | 1/1   | 0.92 | 0.28 | 57,57,57,57                 | 0     |
| 60  | MG   | a     | 1655 | 1/1   | 0.92 | 0.18 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3218 | 1/1   | 0.92 | 0.22 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3182 | 1/1   | 0.92 | 0.23 | 43,43,43,43                 | 0     |
| 60  | MG   | a     | 1764 | 1/1   | 0.92 | 0.17 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3183 | 1/1   | 0.92 | 0.17 | 21,21,21,21                 | 0     |
| 60  | MG   | a     | 1767 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3264 | 1/1   | 0.92 | 0.12 | 23,23,23,23                 | 1     |
| 60  | MG   | A     | 3384 | 1/1   | 0.92 | 0.08 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3637 | 1/1   | 0.92 | 0.25 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3091 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3041 | 1/1   | 0.92 | 0.06 | 38,38,38,38                 | 0     |
| 60  | MG   | a     | 1783 | 1/1   | 0.92 | 0.30 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3453 | 1/1   | 0.92 | 0.13 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3055 | 1/1   | 0.92 | 0.08 | 47,47,47,47                 | 0     |
| 60  | MG   | B     | 205  | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3190 | 1/1   | 0.92 | 0.24 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3404 | 1/1   | 0.92 | 0.18 | 35,35,35,35                 | 0     |
| 60  | MG   | B     | 209  | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 60  | MG   | A     | 3229 | 1/1   | 0.92 | 0.09 | 39,39,39,39                 | 0     |
| 60  | MG   | B     | 213  | 1/1   | 0.92 | 0.11 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3540 | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3465 | 1/1   | 0.92 | 0.09 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3408 | 1/1   | 0.92 | 0.10 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3431 | 1/1   | 0.93 | 0.16 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3570 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 60  | MG   | a     | 1616 | 1/1   | 0.93 | 0.14 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3238 | 1/1   | 0.93 | 0.07 | 38,38,38,38                 | 0     |
| 60  | MG   | A     | 3433 | 1/1   | 0.93 | 0.08 | 27,27,27,27                 | 1     |
| 60  | MG   | a     | 1692 | 1/1   | 0.93 | 0.17 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3123 | 1/1   | 0.93 | 0.09 | 30,30,30,30                 | 1     |
| 60  | MG   | a     | 1695 | 1/1   | 0.93 | 0.21 | 40,40,40,40                 | 0     |
| 60  | MG   | a     | 1696 | 1/1   | 0.93 | 0.27 | 52,52,52,52                 | 0     |
| 60  | MG   | B     | 212  | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3357 | 1/1   | 0.93 | 0.17 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3518 | 1/1   | 0.93 | 0.07 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3219 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 60  | MG   | a     | 1628 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 60  | MG   | a     | 1710 | 1/1   | 0.93 | 0.10 | 53,53,53,53                 | 1     |
| 60  | MG   | A     | 3359 | 1/1   | 0.93 | 0.09 | 63,63,63,63                 | 0     |
| 60  | MG   | a     | 1712 | 1/1   | 0.93 | 0.10 | 54,54,54,54                 | 0     |
| 60  | MG   | D     | 304  | 1/1   | 0.93 | 0.12 | 36,36,36,36                 | 1     |
| 60  | MG   | A     | 3124 | 1/1   | 0.93 | 0.10 | 32,32,32,32                 | 1     |
| 60  | MG   | A     | 3037 | 1/1   | 0.93 | 0.07 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3145 | 1/1   | 0.93 | 0.19 | 61,61,61,61                 | 0     |
| 60  | MG   | A     | 3127 | 1/1   | 0.93 | 0.09 | 24,24,24,24                 | 1     |
| 60  | MG   | A     | 3312 | 1/1   | 0.93 | 0.06 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3368 | 1/1   | 0.93 | 0.12 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3534 | 1/1   | 0.93 | 0.12 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3201 | 1/1   | 0.93 | 0.18 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3381 | 1/1   | 0.93 | 0.15 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3319 | 1/1   | 0.93 | 0.09 | 43,43,43,43                 | 0     |
| 60  | MG   | a     | 1744 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3538 | 1/1   | 0.93 | 0.12 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3251 | 1/1   | 0.93 | 0.08 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3386 | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | Q     | 201  | 1/1   | 0.93 | 0.19 | 47,47,47,47                 | 0     |
| 60  | MG   | R     | 201  | 1/1   | 0.93 | 0.15 | 50,50,50,50                 | 0     |
| 60  | MG   | a     | 1654 | 1/1   | 0.93 | 0.09 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3461 | 1/1   | 0.93 | 0.08 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3024 | 1/1   | 0.93 | 0.10 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3104 | 1/1   | 0.93 | 0.14 | 25,25,25,25                 | 0     |
| 60  | MG   | A     | 3087 | 1/1   | 0.93 | 0.07 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3014 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3402 | 1/1   | 0.93 | 0.16 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3071 | 1/1   | 0.93 | 0.19 | 61,61,61,61                 | 0     |
| 60  | MG   | a     | 1768 | 1/1   | 0.93 | 0.18 | 43,43,43,43                 | 0     |
| 60  | MG   | a     | 1769 | 1/1   | 0.93 | 0.10 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3134 | 1/1   | 0.93 | 0.09 | 25,25,25,25                 | 0     |
| 60  | MG   | a     | 1771 | 1/1   | 0.93 | 0.07 | 67,67,67,67                 | 0     |
| 60  | MG   | A     | 3474 | 1/1   | 0.93 | 0.15 | 44,44,44,44                 | 0     |
| 60  | MG   | a     | 1773 | 1/1   | 0.93 | 0.10 | 58,58,58,58                 | 0     |
| 60  | MG   | a     | 1777 | 1/1   | 0.93 | 0.09 | 32,32,32,32                 | 1     |
| 60  | MG   | 0     | 104  | 1/1   | 0.93 | 0.11 | 36,36,36,36                 | 1     |
| 60  | MG   | A     | 3043 | 1/1   | 0.93 | 0.08 | 39,39,39,39                 | 0     |
| 60  | MG   | a     | 1780 | 1/1   | 0.93 | 0.10 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3623 | 1/1   | 0.93 | 0.23 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3260 | 1/1   | 0.93 | 0.12 | 44,44,44,44                 | 1     |
| 60  | MG   | a     | 1784 | 1/1   | 0.93 | 0.24 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3285 | 1/1   | 0.93 | 0.08 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3558 | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3632 | 1/1   | 0.93 | 0.10 | 35,35,35,35                 | 1     |
| 60  | MG   | A     | 3491 | 1/1   | 0.93 | 0.18 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3261 | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3347 | 1/1   | 0.93 | 0.07 | 37,37,37,37                 | 1     |
| 60  | MG   | n     | 103  | 1/1   | 0.93 | 0.14 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3639 | 1/1   | 0.93 | 0.11 | 36,36,36,36                 | 0     |
| 60  | MG   | x     | 103  | 1/1   | 0.93 | 0.07 | 62,62,62,62                 | 0     |
| 60  | MG   | x     | 104  | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3140 | 1/1   | 0.93 | 0.18 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3122 | 1/1   | 0.93 | 0.10 | 51,51,51,51                 | 1     |
| 60  | MG   | A     | 3430 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3506 | 1/1   | 0.93 | 0.06 | 41,41,41,41                 | 0     |
| 60  | MG   | a     | 1694 | 1/1   | 0.94 | 0.15 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3105 | 1/1   | 0.94 | 0.13 | 28,28,28,28                 | 1     |
| 60  | MG   | a     | 1617 | 1/1   | 0.94 | 0.14 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3028 | 1/1   | 0.94 | 0.06 | 57,57,57,57                 | 0     |
| 60  | MG   | a     | 1619 | 1/1   | 0.94 | 0.06 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3051 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3466 | 1/1   | 0.94 | 0.11 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3065 | 1/1   | 0.94 | 0.18 | 64,64,64,64                 | 0     |
| 60  | MG   | a     | 1706 | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 60  | MG   | a     | 1624 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3392 | 1/1   | 0.94 | 0.07 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3007 | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 0     |
| 60  | MG   | B     | 208  | 1/1   | 0.94 | 0.12 | 64,64,64,64                 | 0     |
| 60  | MG   | A     | 3053 | 1/1   | 0.94 | 0.08 | 35,35,35,35                 | 0     |
| 60  | MG   | B     | 210  | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3476 | 1/1   | 0.94 | 0.07 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3159 | 1/1   | 0.94 | 0.09 | 45,45,45,45                 | 1     |
| 60  | MG   | a     | 1724 | 1/1   | 0.94 | 0.13 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1725 | 1/1   | 0.94 | 0.13 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3040 | 1/1   | 0.94 | 0.10 | 31,31,31,31                 | 1     |
| 60  | MG   | A     | 3093 | 1/1   | 0.94 | 0.21 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3204 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3409 | 1/1   | 0.94 | 0.07 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3411 | 1/1   | 0.94 | 0.10 | 39,39,39,39                 | 0     |
| 60  | MG   | a     | 1737 | 1/1   | 0.94 | 0.16 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3494 | 1/1   | 0.94 | 0.07 | 35,35,35,35                 | 0     |
| 60  | MG   | a     | 1743 | 1/1   | 0.94 | 0.10 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3416 | 1/1   | 0.94 | 0.07 | 31,31,31,31                 | 0     |
| 60  | MG   | a     | 1746 | 1/1   | 0.94 | 0.06 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3417 | 1/1   | 0.94 | 0.11 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3503 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3504 | 1/1   | 0.94 | 0.09 | 25,25,25,25                 | 0     |
| 60  | MG   | a     | 1752 | 1/1   | 0.94 | 0.19 | 43,43,43,43                 | 0     |
| 60  | MG   | a     | 1647 | 1/1   | 0.94 | 0.06 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3334 | 1/1   | 0.94 | 0.11 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3137 | 1/1   | 0.94 | 0.16 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3206 | 1/1   | 0.94 | 0.07 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3138 | 1/1   | 0.94 | 0.05 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3116 | 1/1   | 0.94 | 0.14 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3427 | 1/1   | 0.94 | 0.10 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3025 | 1/1   | 0.94 | 0.12 | 51,51,51,51                 | 1     |
| 60  | MG   | A     | 3247 | 1/1   | 0.94 | 0.10 | 46,46,46,46                 | 1     |
| 60  | MG   | A     | 3210 | 1/1   | 0.94 | 0.22 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3177 | 1/1   | 0.94 | 0.17 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3521 | 1/1   | 0.94 | 0.07 | 35,35,35,35                 | 1     |
| 60  | MG   | A     | 3354 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3178 | 1/1   | 0.94 | 0.20 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3526 | 1/1   | 0.94 | 0.13 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3527 | 1/1   | 0.94 | 0.11 | 45,45,45,45                 | 0     |
| 60  | MG   | a     | 1775 | 1/1   | 0.94 | 0.11 | 53,53,53,53                 | 1     |
| 60  | MG   | A     | 3042 | 1/1   | 0.94 | 0.08 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3033 | 1/1   | 0.94 | 0.07 | 59,59,59,59                 | 1     |
| 60  | MG   | A     | 3181 | 1/1   | 0.94 | 0.22 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3079 | 1/1   | 0.94 | 0.08 | 18,18,18,18                 | 0     |
| 60  | MG   | A     | 3026 | 1/1   | 0.94 | 0.12 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3293 | 1/1   | 0.94 | 0.14 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3048 | 1/1   | 0.94 | 0.05 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3444 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3015 | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3620 | 1/1   | 0.94 | 0.06 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3365 | 1/1   | 0.94 | 0.08 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3299 | 1/1   | 0.94 | 0.12 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3224 | 1/1   | 0.94 | 0.09 | 34,34,34,34                 | 0     |
| 60  | MG   | A     | 3371 | 1/1   | 0.94 | 0.06 | 40,40,40,40                 | 0     |
| 60  | MG   | v     | 101  | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 1     |
| 60  | MG   | x     | 101  | 1/1   | 0.94 | 0.16 | 29,29,29,29                 | 1     |
| 60  | MG   | A     | 3303 | 1/1   | 0.94 | 0.09 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3380 | 1/1   | 0.94 | 0.08 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3458 | 1/1   | 0.94 | 0.11 | 38,38,38,38                 | 0     |
| 60  | MG   | x     | 105  | 1/1   | 0.94 | 0.06 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3549 | 1/1   | 0.94 | 0.09 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3062 | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3638 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 60  | MG   | A     | 3226 | 1/1   | 0.94 | 0.20 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3239 | 1/1   | 0.95 | 0.26 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3445 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 1     |
| 60  | MG   | a     | 1697 | 1/1   | 0.95 | 0.11 | 34,34,34,34                 | 0     |
| 60  | MG   | a     | 1699 | 1/1   | 0.95 | 0.10 | 56,56,56,56                 | 0     |
| 60  | MG   | a     | 1610 | 1/1   | 0.95 | 0.23 | 32,32,32,32                 | 1     |
| 60  | MG   | A     | 3447 | 1/1   | 0.95 | 0.11 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3533 | 1/1   | 0.95 | 0.15 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3187 | 1/1   | 0.95 | 0.17 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3373 | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 0     |
| 60  | MG   | A     | 3310 | 1/1   | 0.95 | 0.14 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3080 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3315 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3243 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3317 | 1/1   | 0.95 | 0.06 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3385 | 1/1   | 0.95 | 0.05 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3460 | 1/1   | 0.95 | 0.05 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3641 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 1     |
| 60  | MG   | A     | 3643 | 1/1   | 0.95 | 0.14 | 34,34,34,34                 | 0     |
| 60  | MG   | a     | 1722 | 1/1   | 0.95 | 0.14 | 51,51,51,51                 | 0     |
| 60  | MG   | a     | 1723 | 1/1   | 0.95 | 0.12 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3216 | 1/1   | 0.95 | 0.17 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3272 | 1/1   | 0.95 | 0.17 | 55,55,55,55                 | 0     |
| 60  | MG   | a     | 1727 | 1/1   | 0.95 | 0.06 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3113 | 1/1   | 0.95 | 0.16 | 29,29,29,29                 | 1     |
| 60  | MG   | A     | 3322 | 1/1   | 0.95 | 0.06 | 42,42,42,42                 | 1     |
| 60  | MG   | a     | 1630 | 1/1   | 0.95 | 0.19 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3393 | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3059 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 1     |
| 60  | MG   | a     | 1734 | 1/1   | 0.95 | 0.04 | 33,33,33,33                 | 0     |
| 60  | MG   | a     | 1736 | 1/1   | 0.95 | 0.05 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3165 | 1/1   | 0.95 | 0.17 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1740 | 1/1   | 0.95 | 0.08 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3399 | 1/1   | 0.95 | 0.09 | 44,44,44,44                 | 0     |
| 60  | MG   | a     | 1742 | 1/1   | 0.95 | 0.09 | 58,58,58,58                 | 0     |
| 60  | MG   | A     | 3400 | 1/1   | 0.95 | 0.13 | 42,42,42,42                 | 0     |
| 60  | MG   | A     | 3166 | 1/1   | 0.95 | 0.08 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3475 | 1/1   | 0.95 | 0.07 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3129 | 1/1   | 0.95 | 0.10 | 35,35,35,35                 | 1     |
| 60  | MG   | A     | 3477 | 1/1   | 0.95 | 0.06 | 21,21,21,21                 | 0     |
| 60  | MG   | a     | 1750 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3001 | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 60  | MG   | A     | 3483 | 1/1   | 0.95 | 0.05 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3484 | 1/1   | 0.95 | 0.19 | 41,41,41,41                 | 0     |
| 60  | MG   | D     | 302  | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3281 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 60  | MG   | a     | 1757 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3487 | 1/1   | 0.95 | 0.05 | 35,35,35,35                 | 0     |
| 60  | MG   | a     | 1650 | 1/1   | 0.95 | 0.20 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3566 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 60  | MG   | A     | 3170 | 1/1   | 0.95 | 0.20 | 33,33,33,33                 | 0     |
| 60  | MG   | a     | 1763 | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 1     |
| 60  | MG   | A     | 3489 | 1/1   | 0.95 | 0.09 | 27,27,27,27                 | 0     |
| 60  | MG   | A     | 3337 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 60  | MG   | a     | 1766 | 1/1   | 0.95 | 0.16 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3414 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 60  | MG   | A     | 3339 | 1/1   | 0.95 | 0.09 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3103 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3575 | 1/1   | 0.95 | 0.07 | 39,39,39,39                 | 1     |
| 60  | MG   | A     | 3074 | 1/1   | 0.95 | 0.09 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3202 | 1/1   | 0.95 | 0.05 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3499 | 1/1   | 0.95 | 0.10 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3500 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3502 | 1/1   | 0.95 | 0.08 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3345 | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3286 | 1/1   | 0.95 | 0.25 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3176 | 1/1   | 0.95 | 0.06 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3352 | 1/1   | 0.95 | 0.13 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3067 | 1/1   | 0.95 | 0.08 | 34,34,34,34                 | 0     |
| 60  | MG   | A     | 3590 | 1/1   | 0.95 | 0.10 | 63,63,63,63                 | 0     |
| 60  | MG   | X     | 101  | 1/1   | 0.95 | 0.07 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3510 | 1/1   | 0.95 | 0.13 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3258 | 1/1   | 0.95 | 0.07 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3096 | 1/1   | 0.95 | 0.04 | 27,27,27,27                 | 0     |
| 60  | MG   | A     | 3023 | 1/1   | 0.95 | 0.10 | 34,34,34,34                 | 0     |
| 60  | MG   | A     | 3152 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 60  | MG   | n     | 102  | 1/1   | 0.95 | 0.10 | 28,28,28,28                 | 0     |
| 60  | MG   | A     | 3296 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3077 | 1/1   | 0.95 | 0.10 | 24,24,24,24                 | 1     |
| 60  | MG   | a     | 1682 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3109 | 1/1   | 0.95 | 0.09 | 25,25,25,25                 | 1     |
| 60  | MG   | A     | 3139 | 1/1   | 0.95 | 0.09 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3522 | 1/1   | 0.95 | 0.06 | 28,28,28,28                 | 0     |
| 60  | MG   | A     | 3211 | 1/1   | 0.95 | 0.13 | 50,50,50,50                 | 0     |
| 60  | MG   | x     | 106  | 1/1   | 0.95 | 0.11 | 56,56,56,56                 | 1     |
| 60  | MG   | A     | 3440 | 1/1   | 0.95 | 0.06 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3304 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3069 | 1/1   | 0.95 | 0.09 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3306 | 1/1   | 0.95 | 0.15 | 33,33,33,33                 | 0     |
| 60  | MG   | z     | 702  | 1/1   | 0.95 | 0.06 | 57,57,57,57                 | 0     |
| 60  | MG   | D     | 301  | 1/1   | 0.96 | 0.04 | 21,21,21,21                 | 0     |
| 60  | MG   | a     | 1634 | 1/1   | 0.96 | 0.27 | 53,53,53,53                 | 0     |
| 60  | MG   | a     | 1719 | 1/1   | 0.96 | 0.16 | 48,48,48,48                 | 0     |
| 60  | MG   | a     | 1720 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3150 | 1/1   | 0.96 | 0.15 | 54,54,54,54                 | 0     |
| 60  | MG   | D     | 303  | 1/1   | 0.96 | 0.12 | 24,24,24,24                 | 1     |
| 60  | MG   | A     | 3161 | 1/1   | 0.96 | 0.08 | 34,34,34,34                 | 1     |
| 60  | MG   | A     | 3539 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |
| 60  | MG   | a     | 1639 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3162 | 1/1   | 0.96 | 0.05 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3592 | 1/1   | 0.96 | 0.12 | 41,41,41,41                 | 1     |
| 60  | MG   | A     | 3136 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3245 | 1/1   | 0.96 | 0.05 | 45,45,45,45                 | 0     |
| 60  | MG   | F     | 305  | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3596 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 1     |
| 60  | MG   | a     | 1735 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3038 | 1/1   | 0.96 | 0.08 | 29,29,29,29                 | 0     |
| 60  | MG   | G     | 202  | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3598 | 1/1   | 0.96 | 0.14 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3338 | 1/1   | 0.96 | 0.07 | 20,20,20,20                 | 0     |
| 60  | MG   | A     | 3410 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3546 | 1/1   | 0.96 | 0.07 | 53,53,53,53                 | 0     |
| 60  | MG   | A     | 3547 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 60  | MG   | a     | 1745 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3366 | 1/1   | 0.96 | 0.08 | 19,19,19,19                 | 1     |
| 60  | MG   | A     | 3412 | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3413 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3273 | 1/1   | 0.96 | 0.11 | 37,37,37,37                 | 1     |
| 60  | MG   | A     | 3552 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3611 | 1/1   | 0.96 | 0.09 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3456 | 1/1   | 0.96 | 0.09 | 46,46,46,46                 | 1     |
| 60  | MG   | A     | 3340 | 1/1   | 0.96 | 0.09 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3616 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 60  | MG   | a     | 1756 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3370 | 1/1   | 0.96 | 0.14 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3509 | 1/1   | 0.96 | 0.19 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3341 | 1/1   | 0.96 | 0.10 | 30,30,30,30                 | 0     |
| 60  | MG   | a     | 1760 | 1/1   | 0.96 | 0.05 | 38,38,38,38                 | 0     |
| 60  | MG   | A     | 3047 | 1/1   | 0.96 | 0.05 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3512 | 1/1   | 0.96 | 0.07 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3625 | 1/1   | 0.96 | 0.04 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3626 | 1/1   | 0.96 | 0.09 | 30,30,30,30                 | 1     |
| 60  | MG   | A     | 3078 | 1/1   | 0.96 | 0.13 | 27,27,27,27                 | 1     |
| 60  | MG   | 6     | 103  | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3377 | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 60  | MG   | 8     | 101  | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3222 | 1/1   | 0.96 | 0.05 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3425 | 1/1   | 0.96 | 0.16 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3073 | 1/1   | 0.96 | 0.07 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3346 | 1/1   | 0.96 | 0.09 | 57,57,57,57                 | 0     |
| 60  | MG   | A     | 3567 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 1     |
| 60  | MG   | a     | 1774 | 1/1   | 0.96 | 0.04 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3030 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 60  | MG   | a     | 1685 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3640 | 1/1   | 0.96 | 0.05 | 30,30,30,30                 | 1     |
| 60  | MG   | a     | 1687 | 1/1   | 0.96 | 0.09 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3471 | 1/1   | 0.96 | 0.08 | 65,65,65,65                 | 0     |
| 60  | MG   | a     | 1781 | 1/1   | 0.96 | 0.05 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3642 | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 1     |
| 60  | MG   | A     | 3472 | 1/1   | 0.96 | 0.18 | 25,25,25,25                 | 0     |
| 60  | MG   | A     | 3571 | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 1     |
| 60  | MG   | A     | 3349 | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |
| 60  | MG   | B     | 202  | 1/1   | 0.96 | 0.10 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3279 | 1/1   | 0.96 | 0.07 | 30,30,30,30                 | 1     |
| 60  | MG   | A     | 3172 | 1/1   | 0.96 | 0.17 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3390 | 1/1   | 0.96 | 0.05 | 36,36,36,36                 | 0     |
| 60  | MG   | f     | 201  | 1/1   | 0.96 | 0.12 | 53,53,53,53                 | 0     |
| 60  | MG   | l     | 201  | 1/1   | 0.96 | 0.11 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3529 | 1/1   | 0.96 | 0.05 | 59,59,59,59                 | 0     |
| 60  | MG   | A     | 3478 | 1/1   | 0.96 | 0.18 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3300 | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1702 | 1/1   | 0.96 | 0.21 | 42,42,42,42                 | 0     |
| 60  | MG   | v     | 102  | 1/1   | 0.96 | 0.10 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1622 | 1/1   | 0.96 | 0.05 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3005 | 1/1   | 0.96 | 0.09 | 31,31,31,31                 | 1     |
| 60  | MG   | A     | 3325 | 1/1   | 0.96 | 0.04 | 23,23,23,23                 | 0     |
| 60  | MG   | A     | 3327 | 1/1   | 0.96 | 0.07 | 30,30,30,30                 | 0     |
| 60  | MG   | a     | 1707 | 1/1   | 0.96 | 0.07 | 34,34,34,34                 | 0     |
| 60  | MG   | A     | 3583 | 1/1   | 0.96 | 0.12 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3584 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3302 | 1/1   | 0.96 | 0.07 | 22,22,22,22                 | 0     |
| 60  | MG   | A     | 3397 | 1/1   | 0.96 | 0.12 | 38,38,38,38                 | 0     |
| 60  | MG   | A     | 3587 | 1/1   | 0.96 | 0.09 | 23,23,23,23                 | 1     |
| 60  | MG   | B     | 218  | 1/1   | 0.96 | 0.11 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3330 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 1     |
| 60  | MG   | A     | 3595 | 1/1   | 0.97 | 0.05 | 27,27,27,27                 | 0     |
| 60  | MG   | a     | 1668 | 1/1   | 0.97 | 0.04 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3387 | 1/1   | 0.97 | 0.05 | 26,26,26,26                 | 0     |
| 60  | MG   | A     | 3009 | 1/1   | 0.97 | 0.10 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3389 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 60  | MG   | a     | 1672 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3003 | 1/1   | 0.97 | 0.11 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3013 | 1/1   | 0.97 | 0.08 | 24,24,24,24                 | 0     |
| 60  | MG   | A     | 3429 | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3153 | 1/1   | 0.97 | 0.12 | 45,45,45,45                 | 0     |
| 60  | MG   | a     | 1613 | 1/1   | 0.97 | 0.13 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3185 | 1/1   | 0.97 | 0.12 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3516 | 1/1   | 0.97 | 0.11 | 25,25,25,25                 | 1     |
| 60  | MG   | A     | 3469 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3090 | 1/1   | 0.97 | 0.12 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3608 | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3609 | 1/1   | 0.97 | 0.08 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3171 | 1/1   | 0.97 | 0.09 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3017 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 60  | MG   | E     | 301  | 1/1   | 0.97 | 0.06 | 33,33,33,33                 | 0     |
| 60  | MG   | E     | 302  | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3398 | 1/1   | 0.97 | 0.05 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3288 | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3614 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3615 | 1/1   | 0.97 | 0.10 | 34,34,34,34                 | 0     |
| 60  | MG   | F     | 304  | 1/1   | 0.97 | 0.15 | 28,28,28,28                 | 1     |
| 60  | MG   | A     | 3070 | 1/1   | 0.97 | 0.04 | 10,10,10,10                 | 0     |
| 60  | MG   | A     | 3617 | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 60  | MG   | A     | 3018 | 1/1   | 0.97 | 0.10 | 27,27,27,27                 | 0     |
| 60  | MG   | a     | 1698 | 1/1   | 0.97 | 0.18 | 49,49,49,49                 | 0     |
| 60  | MG   | A     | 3439 | 1/1   | 0.97 | 0.09 | 50,50,50,50                 | 0     |
| 60  | MG   | a     | 1633 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3621 | 1/1   | 0.97 | 0.21 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3479 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 60  | MG   | a     | 1776 | 1/1   | 0.97 | 0.13 | 52,52,52,52                 | 0     |
| 60  | MG   | A     | 3480 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 60  | MG   | O     | 202  | 1/1   | 0.97 | 0.05 | 50,50,50,50                 | 0     |
| 60  | MG   | A     | 3403 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 60  | MG   | A     | 3192 | 1/1   | 0.97 | 0.05 | 26,26,26,26                 | 0     |
| 60  | MG   | A     | 3405 | 1/1   | 0.97 | 0.12 | 32,32,32,32                 | 0     |
| 60  | MG   | a     | 1709 | 1/1   | 0.97 | 0.05 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3193 | 1/1   | 0.97 | 0.05 | 27,27,27,27                 | 0     |
| 60  | MG   | Q     | 202  | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3486 | 1/1   | 0.97 | 0.08 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3631 | 1/1   | 0.97 | 0.20 | 24,24,24,24                 | 1     |
| 60  | MG   | a     | 1645 | 1/1   | 0.97 | 0.11 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1788 | 1/1   | 0.97 | 0.06 | 43,43,43,43                 | 1     |
| 60  | MG   | A     | 3213 | 1/1   | 0.97 | 0.06 | 34,34,34,34                 | 1     |
| 60  | MG   | A     | 3035 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 1     |
| 60  | MG   | A     | 3634 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 1     |
| 60  | MG   | A     | 3635 | 1/1   | 0.97 | 0.16 | 29,29,29,29                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | m     | 201  | 1/1   | 0.97 | 0.19 | 38,38,38,38                 | 1     |
| 60  | MG   | m     | 202  | 1/1   | 0.97 | 0.12 | 56,56,56,56                 | 0     |
| 60  | MG   | A     | 3446 | 1/1   | 0.97 | 0.06 | 26,26,26,26                 | 0     |
| 60  | MG   | A     | 3490 | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3095 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3375 | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3019 | 1/1   | 0.97 | 0.09 | 20,20,20,20                 | 0     |
| 60  | MG   | A     | 3378 | 1/1   | 0.97 | 0.11 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3046 | 1/1   | 0.97 | 0.11 | 29,29,29,29                 | 0     |
| 60  | MG   | a     | 1658 | 1/1   | 0.97 | 0.08 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3497 | 1/1   | 0.97 | 0.07 | 38,38,38,38                 | 1     |
| 60  | MG   | A     | 3351 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3021 | 1/1   | 0.97 | 0.07 | 34,34,34,34                 | 0     |
| 60  | MG   | A     | 3200 | 1/1   | 0.97 | 0.06 | 39,39,39,39                 | 0     |
| 60  | MG   | A     | 3419 | 1/1   | 0.97 | 0.05 | 30,30,30,30                 | 1     |
| 60  | MG   | A     | 3457 | 1/1   | 0.97 | 0.04 | 24,24,24,24                 | 0     |
| 60  | MG   | A     | 3329 | 1/1   | 0.97 | 0.06 | 33,33,33,33                 | 1     |
| 60  | MG   | a     | 1739 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 61  | ZN   | 4     | 501  | 1/1   | 0.97 | 0.05 | 79,79,79,79                 | 0     |
| 62  | SF4  | d     | 302  | 8/8   | 0.97 | 0.05 | 60,65,70,71                 | 2     |
| 63  | GCP  | z     | 703  | 32/32 | 0.97 | 0.07 | 47,57,62,63                 | 13    |
| 60  | MG   | A     | 3407 | 1/1   | 0.98 | 0.06 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3379 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3582 | 1/1   | 0.98 | 0.04 | 21,21,21,21                 | 1     |
| 60  | MG   | D     | 306  | 1/1   | 0.98 | 0.06 | 25,25,25,25                 | 0     |
| 60  | MG   | A     | 3507 | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 60  | MG   | a     | 1607 | 1/1   | 0.98 | 0.12 | 42,42,42,42                 | 1     |
| 60  | MG   | a     | 1608 | 1/1   | 0.98 | 0.08 | 23,23,23,23                 | 0     |
| 60  | MG   | a     | 1708 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3331 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3120 | 1/1   | 0.98 | 0.16 | 26,26,26,26                 | 0     |
| 60  | MG   | E     | 304  | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 60  | MG   | E     | 305  | 1/1   | 0.98 | 0.04 | 23,23,23,23                 | 1     |
| 60  | MG   | A     | 3627 | 1/1   | 0.98 | 0.09 | 25,25,25,25                 | 0     |
| 60  | MG   | A     | 3112 | 1/1   | 0.98 | 0.06 | 44,44,44,44                 | 0     |
| 60  | MG   | A     | 3311 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 60  | MG   | a     | 1716 | 1/1   | 0.98 | 0.04 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3294 | 1/1   | 0.98 | 0.08 | 25,25,25,25                 | 1     |
| 60  | MG   | A     | 3313 | 1/1   | 0.98 | 0.07 | 29,29,29,29                 | 0     |
| 60  | MG   | A     | 3314 | 1/1   | 0.98 | 0.05 | 48,48,48,48                 | 0     |
| 60  | MG   | A     | 3515 | 1/1   | 0.98 | 0.12 | 47,47,47,47                 | 0     |
| 60  | MG   | a     | 1721 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3241 | 1/1   | 0.98 | 0.05 | 20,20,20,20                 | 0     |
| 60  | MG   | A     | 3481 | 1/1   | 0.98 | 0.05 | 46,46,46,46                 | 0     |
| 60  | MG   | A     | 3186 | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3230 | 1/1   | 0.98 | 0.13 | 40,40,40,40                 | 0     |
| 60  | MG   | a     | 1726 | 1/1   | 0.98 | 0.04 | 43,43,43,43                 | 0     |
| 60  | MG   | A     | 3363 | 1/1   | 0.98 | 0.06 | 35,35,35,35                 | 0     |
| 60  | MG   | a     | 1728 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3298 | 1/1   | 0.98 | 0.07 | 34,34,34,34                 | 0     |
| 60  | MG   | A     | 3045 | 1/1   | 0.98 | 0.14 | 20,20,20,20                 | 0     |
| 60  | MG   | A     | 3198 | 1/1   | 0.98 | 0.07 | 20,20,20,20                 | 0     |
| 60  | MG   | A     | 3524 | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 1     |
| 60  | MG   | A     | 3601 | 1/1   | 0.98 | 0.03 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3424 | 1/1   | 0.98 | 0.11 | 20,20,20,20                 | 0     |
| 60  | MG   | A     | 3455 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |
| 60  | MG   | A     | 3168 | 1/1   | 0.98 | 0.09 | 23,23,23,23                 | 0     |
| 60  | MG   | A     | 3565 | 1/1   | 0.98 | 0.03 | 35,35,35,35                 | 0     |
| 60  | MG   | a     | 1738 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3426 | 1/1   | 0.98 | 0.05 | 36,36,36,36                 | 0     |
| 60  | MG   | a     | 1684 | 1/1   | 0.98 | 0.05 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3396 | 1/1   | 0.98 | 0.04 | 26,26,26,26                 | 0     |
| 60  | MG   | A     | 3031 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3324 | 1/1   | 0.98 | 0.06 | 38,38,38,38                 | 0     |
| 60  | MG   | a     | 1688 | 1/1   | 0.98 | 0.03 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3495 | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3287 | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 60  | MG   | A     | 3372 | 1/1   | 0.98 | 0.12 | 41,41,41,41                 | 0     |
| 60  | MG   | A     | 3401 | 1/1   | 0.98 | 0.13 | 36,36,36,36                 | 0     |
| 60  | MG   | A     | 3348 | 1/1   | 0.98 | 0.04 | 30,30,30,30                 | 0     |
| 60  | MG   | A     | 3004 | 1/1   | 0.98 | 0.15 | 40,40,40,40                 | 1     |
| 60  | MG   | A     | 3501 | 1/1   | 0.98 | 0.05 | 24,24,24,24                 | 0     |
| 60  | MG   | A     | 3125 | 1/1   | 0.98 | 0.12 | 22,22,22,22                 | 1     |
| 60  | MG   | B     | 217  | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 60  | MG   | A     | 3163 | 1/1   | 0.98 | 0.04 | 26,26,26,26                 | 0     |
| 61  | ZN   | 5     | 103  | 1/1   | 0.98 | 0.03 | 54,54,54,54                 | 0     |
| 60  | MG   | A     | 3619 | 1/1   | 0.98 | 0.08 | 16,16,16,16                 | 0     |
| 60  | MG   | A     | 3156 | 1/1   | 0.98 | 0.08 | 26,26,26,26                 | 0     |
| 60  | MG   | A     | 3174 | 1/1   | 0.99 | 0.13 | 25,25,25,25                 | 0     |
| 60  | MG   | A     | 3086 | 1/1   | 0.99 | 0.10 | 21,21,21,21                 | 0     |
| 60  | MG   | a     | 1747 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 60  | MG   | A     | 3383 | 1/1   | 0.99 | 0.03 | 28,28,28,28                 | 0     |
| 60  | MG   | A     | 3326 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 60  | MG   | A     | 3376 | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |

*Continued on next page...*

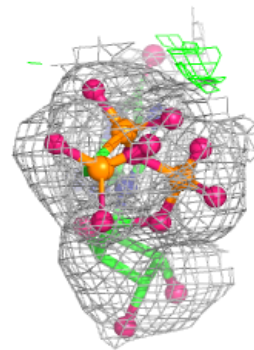
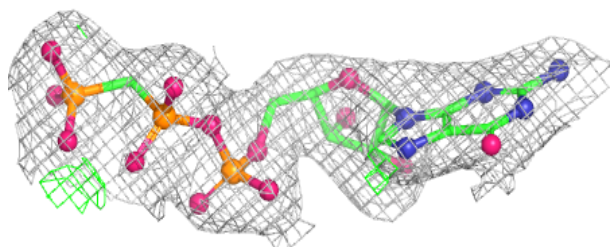
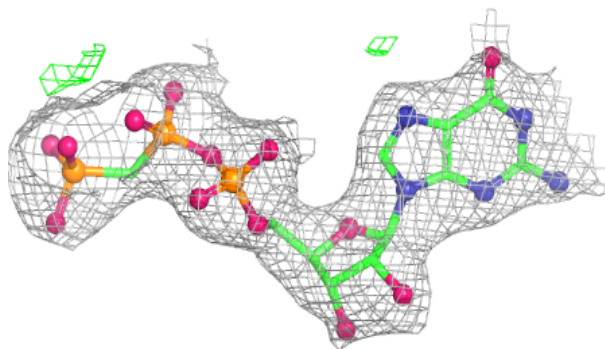
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | MG   | A     | 3459 | 1/1   | 0.99 | 0.11 | 33,33,33,33                 | 0     |
| 60  | MG   | A     | 3369 | 1/1   | 0.99 | 0.03 | 31,31,31,31                 | 0     |
| 60  | MG   | A     | 3308 | 1/1   | 0.99 | 0.09 | 14,14,14,14                 | 0     |
| 60  | MG   | A     | 3020 | 1/1   | 0.99 | 0.05 | 26,26,26,26                 | 0     |
| 61  | ZN   | Y     | 501  | 1/1   | 0.99 | 0.02 | 63,63,63,63                 | 0     |
| 60  | MG   | A     | 3473 | 1/1   | 0.99 | 0.04 | 27,27,27,27                 | 0     |
| 60  | MG   | A     | 3318 | 1/1   | 0.99 | 0.07 | 42,42,42,42                 | 1     |
| 61  | ZN   | 6     | 102  | 1/1   | 0.99 | 0.15 | 72,72,72,72                 | 0     |
| 61  | ZN   | 9     | 102  | 1/1   | 0.99 | 0.12 | 49,49,49,49                 | 1     |
| 61  | ZN   | n     | 104  | 1/1   | 0.99 | 0.02 | 44,44,44,44                 | 0     |
| 60  | MG   | a     | 1652 | 1/1   | 0.99 | 0.08 | 20,20,20,20                 | 0     |
| 60  | MG   | A     | 3629 | 1/1   | 0.99 | 0.03 | 21,21,21,21                 | 0     |
| 60  | MG   | A     | 3415 | 1/1   | 1.00 | 0.04 | 34,34,34,34                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GCP z 703:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.