



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 01:56 AM UTC

PDB ID : 4WZO / pdb\_00004wzo  
Title : Complex of 70S ribosome with tRNA-fMet and mRNA  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-11-20  
Resolution : 3.30 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  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

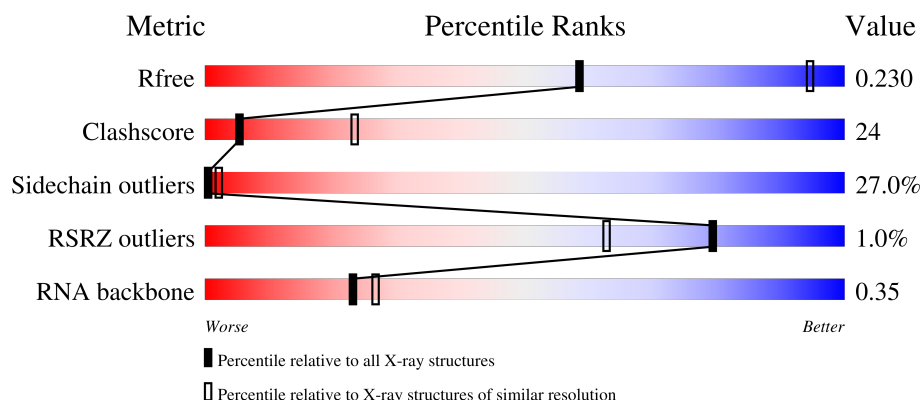
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



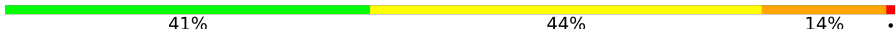
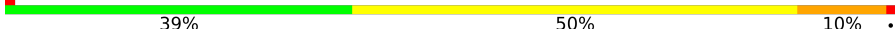
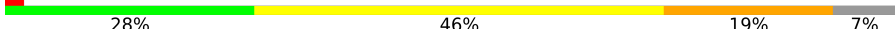
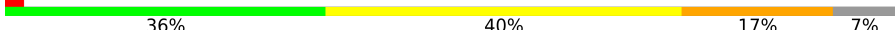
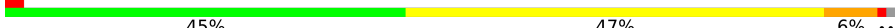
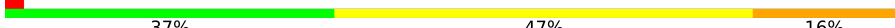
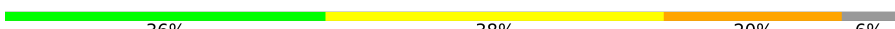
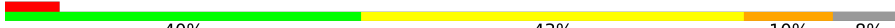
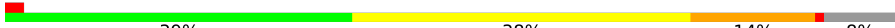
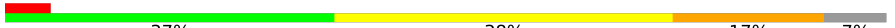
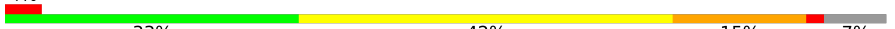
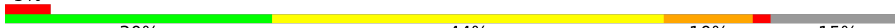
| Metric             | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|--------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$         | 180053                      | 1169 (3.32-3.28)                                      |
| Clashscore         | 190562                      | 1209 (3.32-3.28)                                      |
| Sidechain outliers | 187428                      | 1187 (3.32-3.28)                                      |
| RSRZ outliers      | 180081                      | 1169 (3.32-3.28)                                      |
| RNA backbone       | 3983                        | 1048 (3.60-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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   | 13    | 1522   | <div> <div>29%</div> <div>50%</div> <div>19%</div> <div>.</div> </div>                |
| 1   | 1G    | 1522   | <div> <div>27%</div> <div>53%</div> <div>18%</div> <div>.</div> </div>                |
| 2   | 12    | 256    | <div> <div>2%</div> <div>31%</div> <div>45%</div> <div>15%</div> <div>7%</div> </div> |
| 2   | 1E    | 256    | <div> <div>37%</div> <div>38%</div> <div>16%</div> <div>7%</div> </div>               |
| 3   | 22    | 239    | <div> <div>%</div> <div>34%</div> <div>38%</div> <div>15%</div> <div>14%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | 2E    | 239    |    |
| 4   | 32    | 209    |    |
| 4   | 3E    | 209    |    |
| 5   | 42    | 162    |    |
| 5   | 4E    | 162    |    |
| 6   | 52    | 101    |    |
| 6   | 5E    | 101    |    |
| 7   | 62    | 156    |    |
| 7   | 6E    | 156    |    |
| 8   | 72    | 138    |    |
| 8   | 7E    | 138    |    |
| 9   | 82    | 128    |   |
| 9   | 8E    | 128    |  |
| 10  | 1A    | 105    |  |
| 10  | 1I    | 105    |  |
| 11  | 2A    | 129    |  |
| 11  | 2I    | 129    |  |
| 12  | 3A    | 132    |  |
| 12  | 3I    | 132    |  |
| 13  | 4A    | 126    |  |
| 13  | 4I    | 126    |  |
| 14  | 5A    | 61     |  |
| 14  | 5I    | 61     |  |
| 15  | 6A    | 89     |  |
| 15  | 6I    | 89     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16  | 7A    | 88     |                  |
| 16  | 7I    | 88     |                  |
| 17  | 8A    | 105    |                  |
| 17  | 8I    | 105    |                  |
| 18  | 9A    | 88     |                  |
| 18  | 9I    | 88     |                  |
| 19  | AA    | 93     |                  |
| 19  | AI    | 93     |                  |
| 20  | BA    | 106    |                  |
| 20  | BI    | 106    |                  |
| 21  | 1B    | 27     |                  |
| 21  | 1F    | 27     |                  |
| 22  | 1K    | 77     |                  |
| 23  | 2K    | 77     |                  |
| 24  | 3K    | 76     |                  |
| 24  | 3L    | 76     |                  |
| 25  | 4K    | 27     |                  |
| 25  | 4L    | 27     |                  |
| 26  | 14    | 2917   |                  |
| 26  | 1H    | 2917   |                  |
| 27  | 16    | 122    |                  |
| 27  | 1J    | 122    |                  |
| 28  | 7I    | 229    |                  |
| 29  | 11    | 276    |                  |
| 29  | 19    | 276    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30  | 21    | 206    |                  |
| 30  | 29    | 206    |                  |
| 31  | 31    | 210    |                  |
| 31  | 39    | 210    |                  |
| 32  | 41    | 182    |                  |
| 32  | 49    | 182    |                  |
| 33  | 51    | 180    |                  |
| 33  | 59    | 180    |                  |
| 34  | 61    | 148    |                  |
| 34  | 69    | 148    |                  |
| 35  | 15    | 140    |                  |
| 35  | 58    | 140    |                  |
| 36  | 25    | 122    |                  |
| 36  | 68    | 122    |                  |
| 37  | 35    | 150    |                  |
| 37  | 78    | 150    |                  |
| 38  | 45    | 141    |                  |
| 38  | 88    | 141    |                  |
| 39  | 55    | 118    |                  |
| 39  | 98    | 118    |                  |
| 40  | 65    | 112    |                  |
| 40  | A8    | 112    |                  |
| 41  | 75    | 146    |                  |
| 41  | B8    | 146    |                  |
| 42  | 85    | 118    |                  |

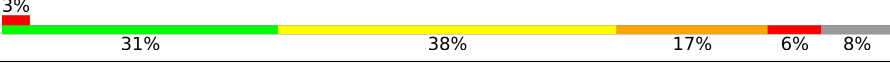
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 42  | C8    | 118    |                  |
| 43  | 95    | 101    |                  |
| 43  | D8    | 101    |                  |
| 44  | A5    | 113    |                  |
| 44  | E8    | 113    |                  |
| 45  | B5    | 96     |                  |
| 45  | F8    | 96     |                  |
| 46  | C5    | 110    |                  |
| 46  | G8    | 110    |                  |
| 47  | D5    | 206    |                  |
| 47  | H8    | 206    |                  |
| 48  | E5    | 85     |                  |
| 48  | I8    | 85     |                  |
| 49  | F5    | 98     |                  |
| 49  | J8    | 98     |                  |
| 50  | G5    | 72     |                  |
| 50  | K8    | 72     |                  |
| 51  | H5    | 60     |                  |
| 51  | L8    | 60     |                  |
| 52  | I5    | 71     |                  |
| 52  | M8    | 71     |                  |
| 53  | J5    | 60     |                  |
| 53  | N8    | 60     |                  |
| 54  | L5    | 49     |                  |
| 54  | P8    | 49     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 55  | M5    | 65     |  |
| 55  | Q8    | 65     |  |
| 56  | 2L    | 77     |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | 1G    | 1641 | -         | -        | -       | X                |
| 57  | MG   | 1H    | 3191 | -         | -        | -       | X                |
| 57  | MG   | 1J    | 201  | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 295920 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | 13    | 1497     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32185 | 14324 | 5968 | 10396 | 1497 |         |         |       |
| 1   | 1G    | 1497     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32182 | 14324 | 5968 | 10394 | 1496 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | 1E    | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1924  | 1228 | 344 | 347 | 5 |         |         |       |
| 2   | 12    | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1924  | 1228 | 344 | 347 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | 2E    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1011 | 313 | 280 | 1 |         |         |       |
| 3   | 22    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | 3E    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1702  | 1066 | 339 | 290 | 7 |         |         |       |
| 4   | 32    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1702  | 1066 | 339 | 290 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | 4E    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |
| 5   | 42    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | 5E    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 842   | 531 | 155 | 153 | 3 |         |         |       |
| 6   | 52    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 842   | 531 | 155 | 153 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | 6E    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1256  | 781 | 252 | 217 | 6 |         |         |       |
| 7   | 62    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1194  | 744 | 237 | 207 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 7E    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1115  | 705 | 215 | 192 | 3 |         |         |       |
| 8   | 72    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1115  | 705 | 215 | 192 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | 8E    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1009  | 639 | 197 | 173 |         |         |       |
| 9   | 82    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1009  | 639 | 197 | 173 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | 1I    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | 1A    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 522   | 327 | 99 | 95 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | 2I    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 884   | 549 | 168 | 164 | 3 |         |         |       |
| 11  | 2A    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 864   | 537 | 164 | 160 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | 3I    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 956   | 603 | 193 | 159 | 1 |         |         |       |
| 12  | 3A    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 956   | 603 | 193 | 159 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | 4I    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 577 | 192 | 162 | 2 |         |         |       |
| 13  | 4A    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 577 | 192 | 162 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | 5I    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 312 | 104 | 71 | 4 |         |         |       |
| 14  | 5A    | 52       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 262 | 90  | 62 | 4 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | 6I    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 459 | 147 | 125 | 2 |         |         |       |
| 15  | 6A    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 459 | 147 | 125 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | 7I    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |
| 16  | 7A    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | 8I    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |
| 17  | 8A    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | 9I    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 590   | 376 | 117 | 97 |         |         |       |
| 18  | 9A    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 590   | 376 | 117 | 97 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AI    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 647   | 413 | 119 | 113 | 2 |         |         |       |
| 19  | AA    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 624   | 398 | 115 | 109 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | BI    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 470 | 162 | 128 | 2 |         |         |       |
| 20  | BA    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 470 | 162 | 128 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | 1F    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |
| 21  | 1B    | 22       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 188   | 116 | 44 | 28 |         |         |       |

- Molecule 22 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | 1K    | 70       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1497  | 669 | 274 | 485 | 69 |         |         |       |

- Molecule 23 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23  | 2K    | 77       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1646  | 735 | 298 | 535 | 77 | 1 |         |         |       |

- Molecule 24 is a RNA chain called tRNA-Phe.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 24  | 3K    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1627  | 730 | 290 | 530 | 75 | 2 |         |         |       |
| 24  | 3L    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1627  | 730 | 290 | 530 | 75 | 2 |         |         |       |

- Molecule 25 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 25  | 4K    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 285   | 129 | 62 | 81 | 13 |         |         |       |
| 25  | 4L    | 9        | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 197   | 89  | 42 | 57 | 9  |         |         |       |

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26  | 1H    | 2902     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62497 | 27816 | 11684 | 20095 | 2902 |         |         |       |
| 26  | 14    | 2877     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61968 | 27579 | 11594 | 19918 | 2877 |         |         |       |

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 27  | 16    | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2617  | 1166 | 486 | 844 | 121 |         |         |       |
| 27  | 1J    | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2617  | 1166 | 486 | 844 | 121 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 28  | 71    | 93       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 737   | 465 | 139 | 133 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | 11    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |
| 29  | 19    | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2120  | 1338 | 421 | 358 | 3 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | 21    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 30  | 29    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 31  | 31    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |
| 31  | 39    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 301 | 281 | 2 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | 41    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1473  | 942 | 268 | 259 | 4 |         |         |       |
| 32  | 49    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1473  | 942 | 268 | 259 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | 51    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1336  | 848 | 251 | 236 | 1 |         |         |       |
| 33  | 59    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | 61    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |
| 34  | 69    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | 58    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 35  | 15    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | 68    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 588 | 171 | 169 | 4 |         |         |       |
| 36  | 25    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 588 | 171 | 169 | 4 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | 78    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1144  | 712 | 232 | 197 | 3 |         |         |       |
| 37  | 35    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 698 | 229 | 192 | 3 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | 88    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1077  | 688 | 206 | 177 | 6 |         |         |       |
| 38  | 45    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 715 | 212 | 187 | 7 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | 98    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 967   | 604 | 203 | 159 | 1 |         |         |       |
| 39  | 55    | 117      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 959   | 599 | 202 | 158 |   |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40  | A8    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 881   | 556 | 176 | 149 |         |         |       |
| 40  | 65    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 881   | 556 | 176 | 149 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | B8    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 41  | 75    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | C8    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 963   | 610 | 202 | 150 | 1 |         |         |       |
| 42  | 85    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 963   | 610 | 202 | 150 | 1 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | D8    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 778   | 501 | 142 | 134 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | 95    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 778   | 501 | 142 | 134 | 1 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | E8    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 899   | 566 | 177 | 154 | 2 |         |         |       |
| 44  | A5    | 111      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 558 | 174 | 152 | 2 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | F8    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 742   | 482 | 134 | 125 | 1 |         |         |       |
| 45  | B5    | 92       | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |   |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | G8    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 791   | 510 | 149 | 127 | 5 |         |         |       |
| 46  | C5    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 794   | 510 | 152 | 127 | 5 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | H8    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 714 | 202 | 192 | 2 |         |         |       |
| 47  | D5    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1126  | 725 | 202 | 197 | 2 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | I8    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 626   | 388 | 132 | 105 | 1 |         |         |       |
| 48  | E5    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 612   | 379 | 129 | 103 | 1 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| I8    | 6       | ALA      | GLY    | conflict | UNP P60493 |
| I8    | 8       | ALA      | GLY    | conflict | UNP P60493 |
| E5    | 6       | ALA      | GLY    | conflict | UNP P60493 |
| E5    | 8       | ALA      | GLY    | conflict | UNP P60493 |

- Molecule 49 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | J8    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 481 | 150 | 130 | 1 |         |         |       |
| 49  | F5    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 737   | 463 | 146 | 127 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 50  | K8    | 67       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 563   | 349 | 114 | 99 | 1 |         |         |       |
| 50  | G5    | 66       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 558   | 346 | 113 | 98 | 1 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 51  | L8    | 57       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 452   | 288 | 88 | 76 |  |         |         |       |
| 51  | H5    | 59       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 468   | 298 | 90 | 80 |  |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | M8    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 533   | 335 | 96 | 97 | 5 |         |         |       |
| 52  | I5    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 515   | 326 | 93 | 91 | 5 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | N8    | 54       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 422   | 264 | 85 | 68 | 5 |         |         |       |
| 53  | J5    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 434   | 272 | 87 | 70 | 5 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | P8    | 47       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 409   | 251 | 102 | 54 | 2 |         |         |       |
| 54  | L5    | 46       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 398   | 245 | 98  | 53 | 2 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55  | Q8    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 480   | 306 | 98 | 74 | 2 |         |         |       |
| 55  | M5    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 477   | 303 | 98 | 74 | 2 |         |         |       |

- Molecule 56 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 56  | 2L    | 77       | Total | C   | N   | O   | P  | S       | 0       | 0     |
|     |       |          | 1645  | 734 | 298 | 535 | 77 | 1       |         |       |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | 13    | 99       | Total | Mg  | 0       | 0       |
|     |       |          | 99    | 99  |         |         |
| 57  | 3E    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | 4E    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | 4I    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | 2K    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 57  | 1H    | 444      | Total | Mg  | 0       | 0       |
|     |       |          | 444   | 444 |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | 16    | 11       | Total<br>11  | Mg<br>11  | 0       | 0       |
| 57  | 11    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 41    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 68    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 78    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 88    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 98    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | I8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | J8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | L8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | P8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1G    | 72       | Total<br>72  | Mg<br>72  | 0       | 0       |
| 57  | 2L    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 3L    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 14    | 327      | Total<br>327 | Mg<br>327 | 0       | 0       |
| 57  | 1J    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 29    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 25    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 35    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 45    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 55    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57  | M5    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 58  | 3E    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 58  | 5I    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 58  | G8    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 58  | 32    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 58  | 5A    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 58  | C5    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 59 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 59  | 13    | 144      | Total<br>144 | O<br>144 | 0       | 0       |
| 59  | 3E    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | 1I    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | 3I    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | 5I    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | 2K    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 59  | 4K    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | 1H    | 933      | Total<br>933 | O<br>933 | 0       | 0       |
| 59  | 16    | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 59  | 11    | 11       | Total<br>11  | O<br>11  | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 59  | 21    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | 31    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 59  | 78    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 59  | D8    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | F8    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | G8    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | I8    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 59  | J8    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | L8    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | P8    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | Q8    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | 1G    | 48       | Total<br>48  | O<br>48  | 0       | 0       |
| 59  | 14    | 592      | Total<br>592 | O<br>592 | 0       | 0       |
| 59  | 19    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 59  | 29    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 59  | 39    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 59  | 25    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 59  | 35    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | 55    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | 75    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | A5    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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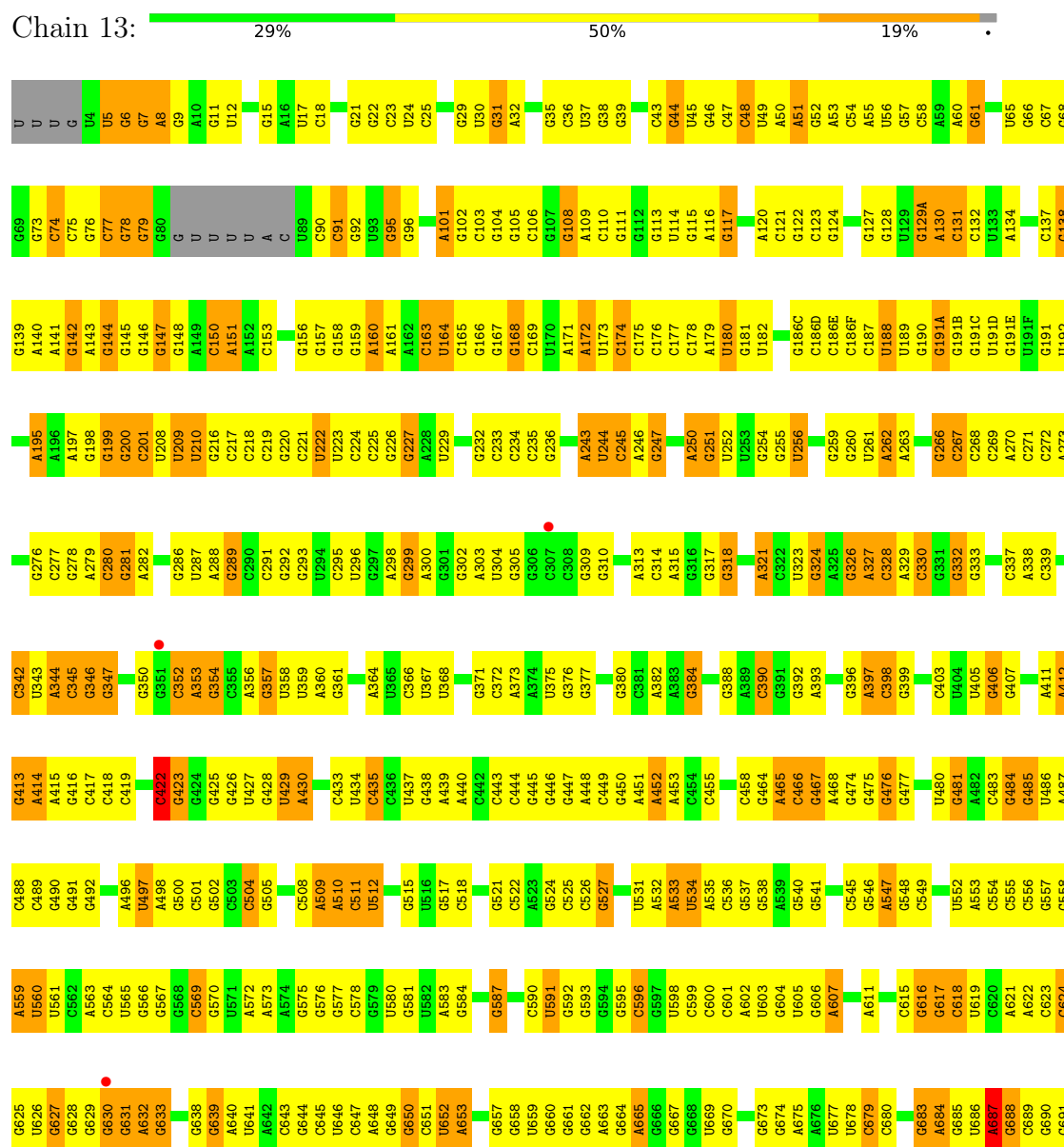
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 59  | H5    | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 59  | L5    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 59  | M5    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

### 3 Residue-property plots [i](#)

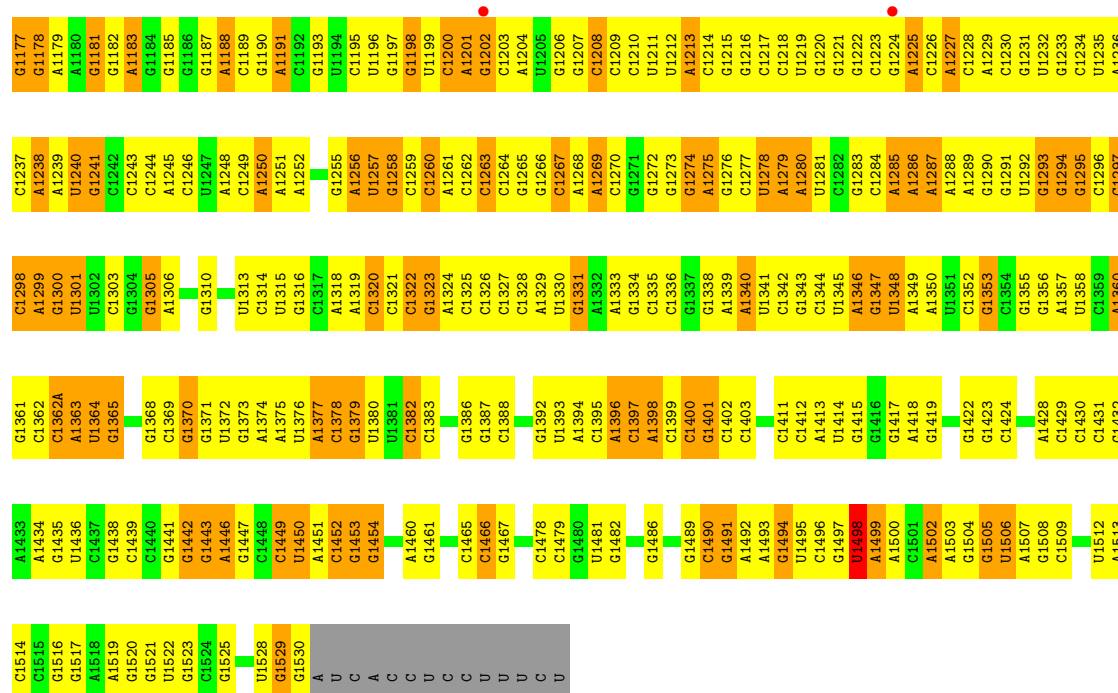
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 16S ribosomal RNA



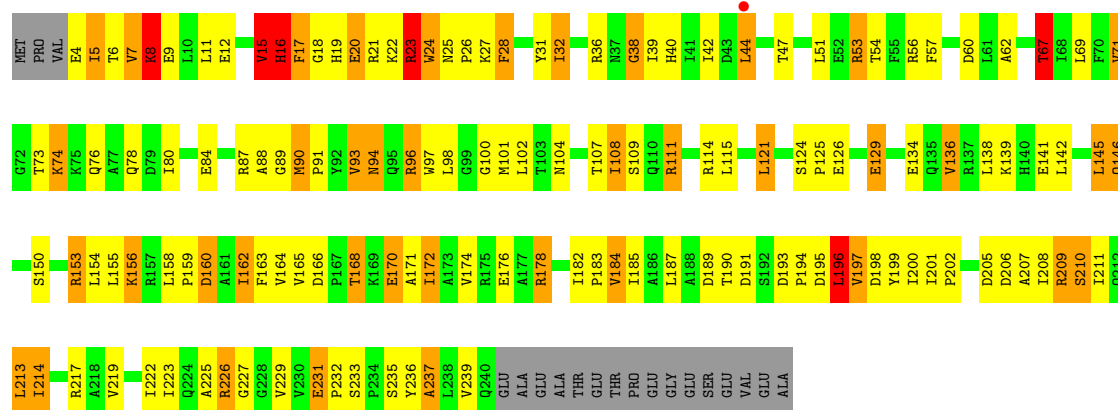


|       |       |        |      |      |      |      |      |      |      |      |      |      |       |       |
|-------|-------|--------|------|------|------|------|------|------|------|------|------|------|-------|-------|
| C1112 | A1044 | A986   | G922 | C848 | A767 | A695 | U626 | G557 | C489 | G416 | G340 | C267 | U191F | C137  |
| C1115 | C1045 | G987   | A923 | C849 | A768 | G698 | G627 | G558 | G490 | C417 | C341 | C271 | G191  | G138  |
| C1116 | A1046 |        | G925 | G855 | G769 | G699 | G628 | A589 | G491 | C418 | C342 | C272 | U192  | G139  |
| G1117 | G1047 | U991   | G926 | G856 | G770 | G699 | G629 | U560 | G492 | C419 |      | C273 | G194  | A140  |
| C1118 | G1048 | U992   | G927 | C857 | G771 | A704 | G630 | U561 | C345 | U420 | G346 | A274 | A195  | G141  |
|       | G1049 | G993   | G927 | C858 | U772 |      | G631 | C562 | A495 | U421 |      | G275 | A196  | G142  |
| U1121 | G1050 | A994   |      | G859 | G773 |      | A632 | C564 | A496 | C422 |      |      | A197  | A143  |
| U1122 | C1051 | C995   | C932 | A859 | G774 | C707 | G633 | U565 | A497 | C423 |      | G278 | G198  | G144  |
| A1123 | U1052 | A996   | G933 | A860 | G775 | C708 | C634 | U566 | A498 | G424 |      |      | G199  | G145  |
| G1124 | G1053 | U997   | C934 | C861 | G776 | G709 | G635 | G566 | G500 | A425 |      | A279 | G199  | G146  |
| U1125 | C1054 | G998   | A935 | C862 | A777 | G710 | U636 | G567 | C501 | G426 |      | C280 | G200  | G147  |
| U1126 | A1055 | C998A  | C936 | U863 | G778 | G711 | G637 | C568 | G502 | U427 |      | G281 | C201  | G148  |
| U1127 | U1056 | U999   | A937 | A864 | C779 | A712 | G638 | C569 | C503 | G428 |      | A282 | U208  |       |
|       | G1057 | A1000  | A938 | A865 | A760 | G713 |      | G570 | C504 | U429 |      | C283 | U209  |       |
| C1128 | G1058 | G1001  | G939 | C866 |      |      | C643 | A571 | G505 | A430 |      | G284 | U210  | A151  |
| C1129 |       | G1002  | C940 | C867 | C784 | G718 | G644 | A572 |      |      |      | G285 | G216  | C154  |
| A1130 | U1062 | G1003  | G941 | C868 | C785 | C719 | C645 | A573 | A510 | C433 |      | G286 | C217  | C155  |
| G1131 | C1063 | A1004  | G942 | C869 | A787 | C720 | U646 | A574 | C511 | U434 |      | U287 | C218  | G156  |
| C1132 | G1064 | A1005  | U943 | U788 | G721 | G721 | C647 | G575 | U512 | C435 |      | A288 | C219  | G157  |
| G1133 | U1065 | C1006  |      | U871 | A722 | A722 | A648 | G576 | C513 | C436 |      | G289 | G220  | G158  |
| C1134 | C1066 | C1007  | A946 | A872 | U723 | G723 | G649 | G577 | C514 | U437 |      |      | C221  | G159  |
| U1135 | A1067 | G1008  | G947 | A873 | A792 | G724 | G650 | G578 | G515 | G438 |      | U294 | U222  | A160  |
| U1136 | G1068 | G1009  | C948 | G874 | U793 | G725 | C651 | G579 | U516 | A439 |      |      | U223  | A161  |
| C1137 |       | G1010  | A949 | C875 | A794 | G726 | U652 | U580 | G517 |      |      | A298 | C224  | A162  |
| G1138 | G1071 | G1011  | U950 | C876 |      | G727 | A653 | G581 | C518 |      |      | G299 | C225  | A163  |
| G1139 | G1072 | U1012  | G951 | C877 | G797 | A728 |      |      | C519 | C444 |      | A300 | G226  | U164  |
| C1140 | U1073 | G1013  | U952 | G878 | A729 | G729 | C656 | G584 | A520 | G445 |      | G301 | G227  | C165  |
| C1141 | G1074 | C879   | G953 | C879 | U801 | A730 | G657 | G585 |      | G446 |      | G302 | C218  | G166  |
| C1142 | C1075 | A1015  | G954 | C880 | A802 | G731 | G658 | C586 | A523 | U447 |      | A303 | G229  | G167  |
| G1143 |       | A1016  | U955 | C881 | G803 | C732 | U659 | G587 |      | A448 |      |      | G230  | G168  |
| C1144 | U1078 | G1017  | U956 | C882 | U804 | G733 | G660 | G588 | C526 | C449 |      | G309 | G231  | C169  |
| C1145 | G1079 | C1018  | U957 | C883 | C805 | A734 | G661 | C589 | G527 | G450 |      | G310 | G232  | U170  |
| A1146 | A1080 | U1019  | U958 | U884 | C797 | C735 |      | C590 | C528 | A451 |      | G311 | C233  | A171  |
| C1147 | U1081 | G1020  | U959 | G885 | C811 | C736 | G664 | U591 | G529 | A452 |      | G312 | C234  | A172  |
| U1148 | G1082 |        | U960 |      | C812 | A737 | A665 | G592 | G530 | A453 |      | G313 | C235  | U173  |
| U1083 |       | G1023  | U961 |      | U813 | C738 | G666 | G593 | U531 | C454 |      | G314 | G236  | C174  |
| G1084 |       | U1024  | C962 | C893 | A814 | G739 | G667 | A532 | A532 | G455 |      | G315 | C237  | C175  |
| U1085 | U1025 | U1025  | G963 | G894 | A815 | U740 | G668 | A533 | A533 | C456 |      | G316 |       | C176  |
| U1086 | G1026 | C1027  | A964 | G895 | A816 | G741 | U669 | U534 | U534 | C457 |      | G317 | C242  | C177  |
| G1087 |       |        | A965 | C896 | C817 |      | G670 | U598 | A535 | C458 |      | G318 | C178  |       |
|       |       | C1028  | G966 | C897 | G818 | C744 |      | C599 | C536 | G464 |      | G319 | U244  |       |
| U1091 | U1091 | C1028A | C967 | C898 | A819 | C745 | G673 | C600 | G537 | A465 |      | G320 | C245  | U180  |
| A1092 | A1092 | C1028B | A968 | C899 | U820 | G746 | G674 | C601 | G538 | C466 |      | G321 | A246  | G181  |
| A1093 | G1029 | G1029  | A969 | A900 | G821 | A747 | A675 | A602 | A539 | G467 |      | C322 | G247  | U182  |
| G1094 |       | C1030  | C970 |      | C822 | C748 | A676 | U603 | G540 | A468 |      | U323 |       |       |
| U1095 | U1095 | A1031  | G971 | G903 | G823 | G749 | U677 | G604 | G541 | G474 |      | G324 | A250  | C186  |
| G1096 | C1096 | G1032  | C972 | C904 | G824 | G750 |      | U605 | G542 | G475 |      | A325 | G251  |       |
| C1097 | C1097 | G1032A | G973 | G825 | G825 | U751 | C681 | G606 |      | C476 |      | G326 |       |       |
| G1098 |       | G1032B | A974 | A909 | C826 | G752 | G682 | A607 | C545 | G477 |      | A327 | G255  | G186C |
| C1099 | G1099 | G1033  | A975 | C910 | U827 | A753 | G683 | A608 | G546 | A478 |      | G328 | U256  | C186D |
| G1100 |       | G1034  | G976 |      | A828 | C754 | A684 |      | A547 | C479 |      | A329 | G257  | C186E |
| A1101 | A1101 | A1035  | G977 | A913 | G829 | G755 | G685 | G616 | G548 | U490 |      | C330 | G258  | G186F |
| U1157 | A1102 | G1036  | A978 | A914 | G830 | C756 | G686 | G617 | C549 | G481 |      | G331 | G259  | U188  |
| A1169 | C1103 | C1037  | C979 | A915 | U831 | U757 | A687 | C618 | C550 | A482 |      | G332 | G260  | U189  |
| U1170 | G1104 | G1038  | C980 | G916 | U832 | G758 | G688 | U619 | U551 | C483 |      | G333 | U261  | G190  |
| G1171 |       | C1039  | U981 | C917 | C832 |      | C689 |      | U552 | G484 |      | G334 | A262  | G191A |
| C1172 |       | U1040  | U982 | A918 | G838 | G763 | G690 | A622 | A553 | G485 |      | C335 | A263  | G191B |
| G1173 | A1041 | G1041  | A983 | A919 | U841 | C764 |      | C623 | C554 | U486 |      |      | U264  | G191C |
| G1174 |       | G1042  | C984 | U920 | C842 | G765 | G693 | C624 | C555 | A487 |      | A338 | G265  | U191D |
|       | A1111 | C1043  | C985 | U921 | U843 | A766 | A694 | G625 | C556 | C488 |      |      | G266  | G191E |



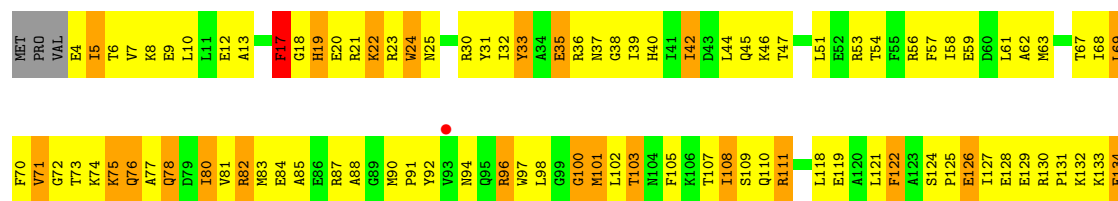
• Molecule 2: 30S ribosomal protein S2

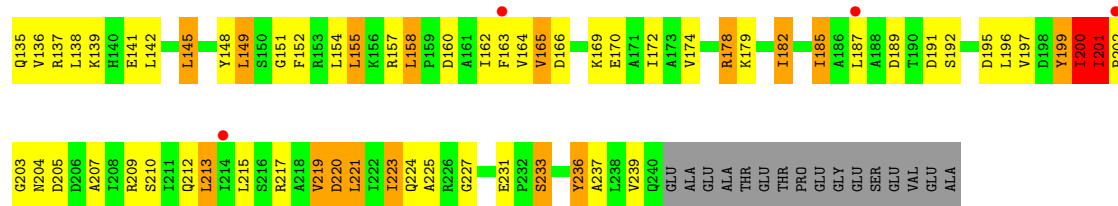
Chain 1E: 37% 38% 16% 7%



• Molecule 2: 30S ribosomal protein S2

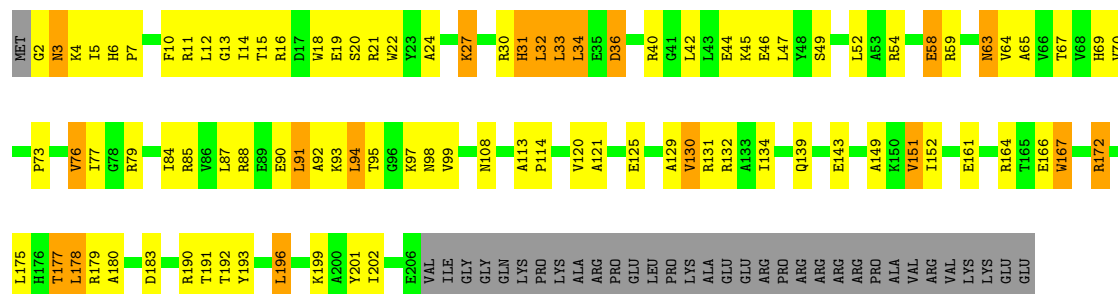
Chain 12: 2% 31% 45% 15% 7%





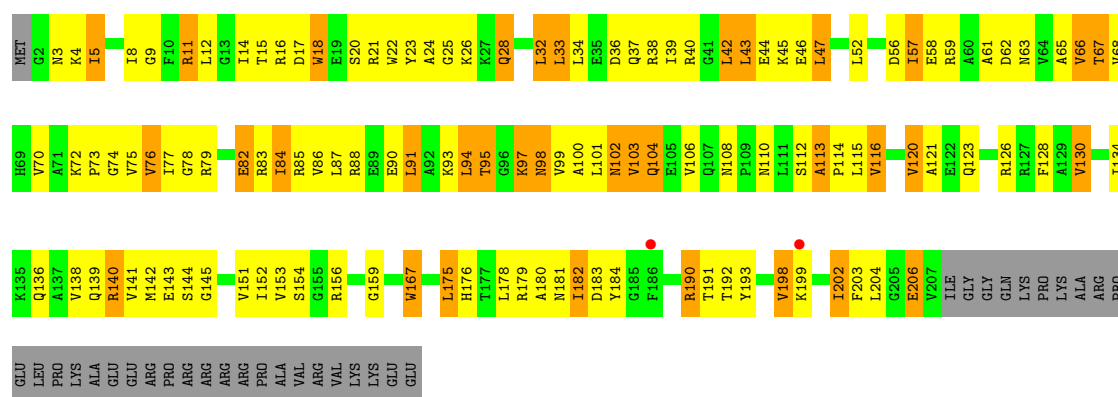
• Molecule 3: 30S ribosomal protein S3

Chain 2E: 46% 32% 8% 14%



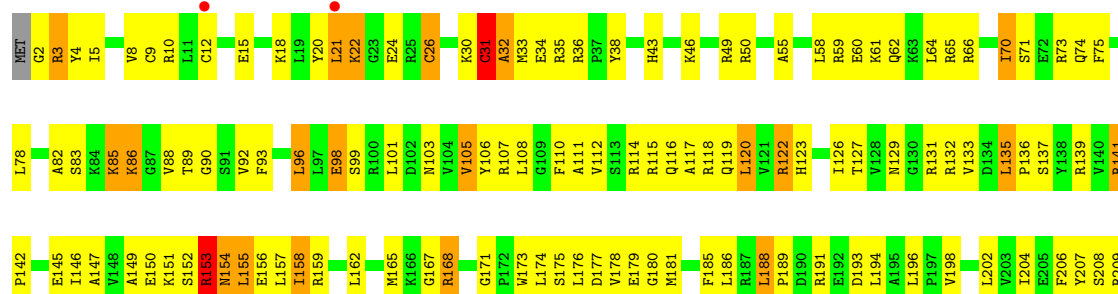
• Molecule 3: 30S ribosomal protein S3

Chain 22: 34% 38% 15% 14%

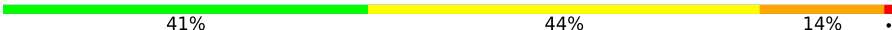


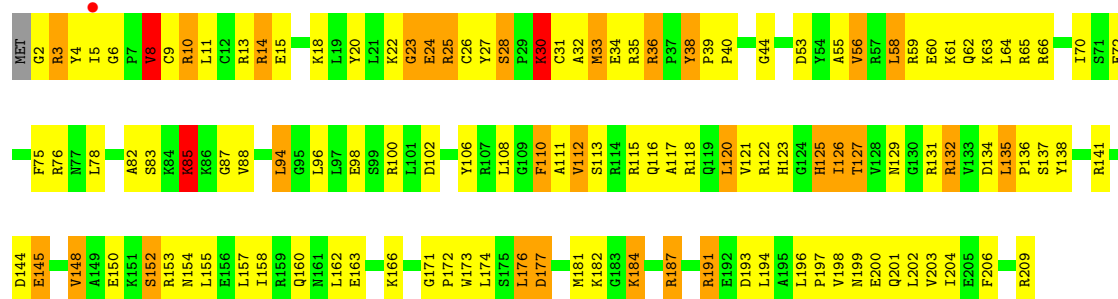
• Molecule 4: 30S ribosomal protein S4

Chain 3E: 39% 50% 10%



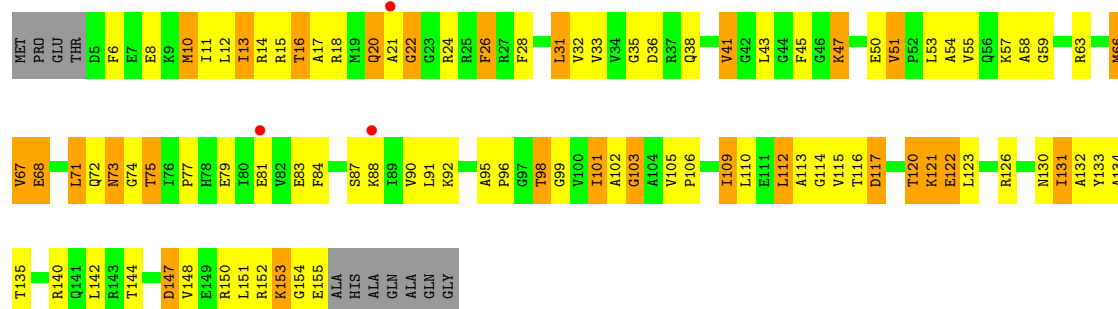
- Molecule 4: 30S ribosomal protein S4

Chain 32:  41% 44% 14%

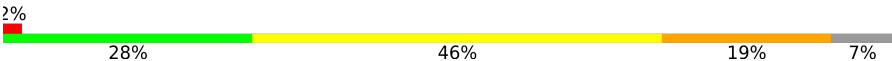


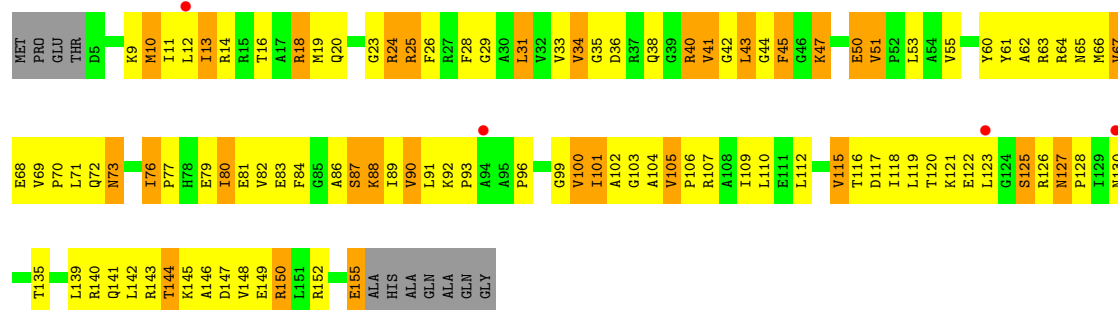
- Molecule 5: 30S ribosomal protein S5

Chain 4E:  36% 40% 17% 7%

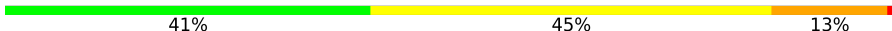


- Molecule 5: 30S ribosomal protein S5

Chain 42:  28% 46% 19% 7%



- Molecule 6: 30S ribosomal protein S6

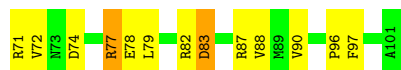
Chain 5E:  41% 45% 13%





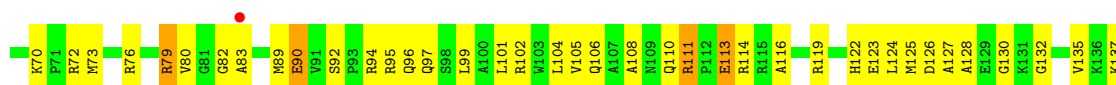
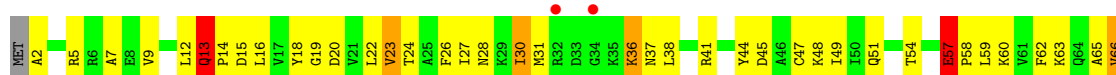
• Molecule 6: 30S ribosomal protein S6

Chain 52: 50% 40% 10% .



• Molecule 7: 30S ribosomal protein S7

Chain 6E: 2% 45% 47% 6% ..



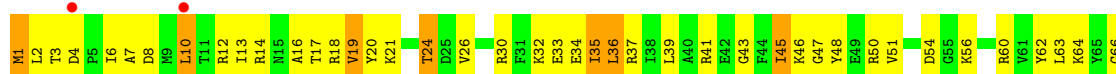
• Molecule 7: 30S ribosomal protein S7

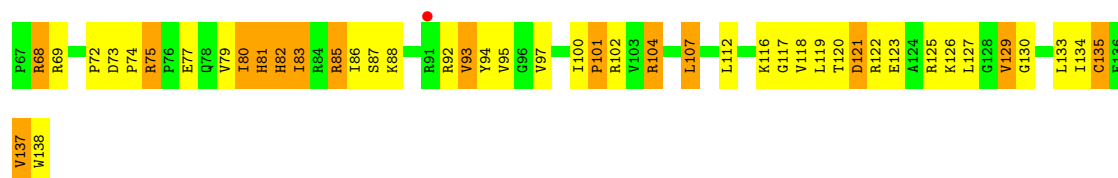
Chain 62: % 42% 42% 10% 6%



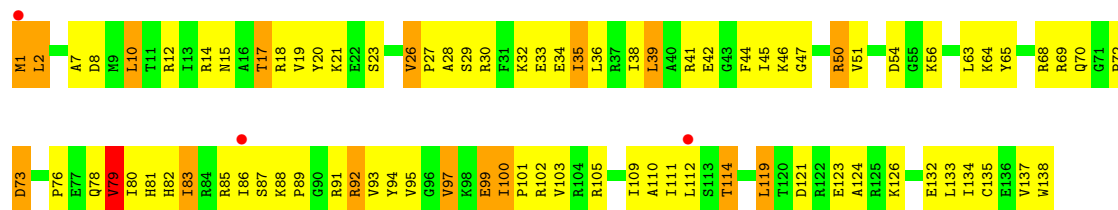
• Molecule 8: 30S ribosomal protein S8

Chain 7E: 2% 37% 47% 16%

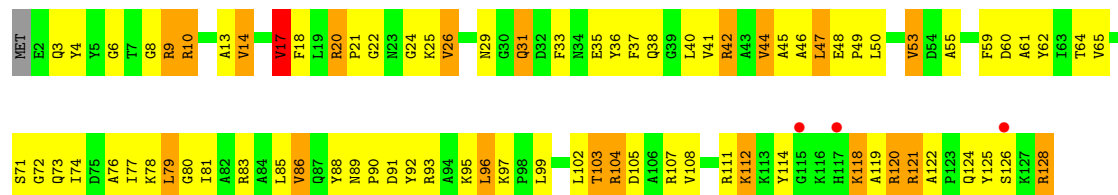




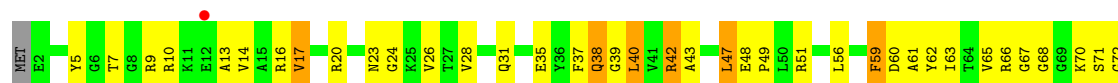
- Molecule 8: 30S ribosomal protein S8



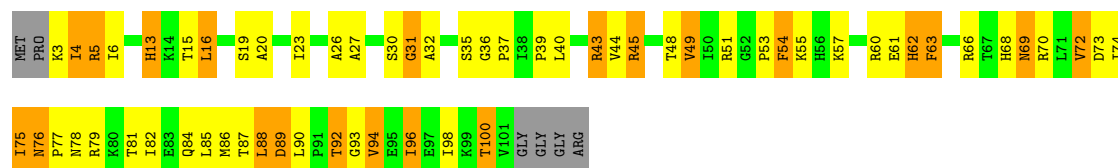
- Molecule 9: 30S ribosomal protein S9



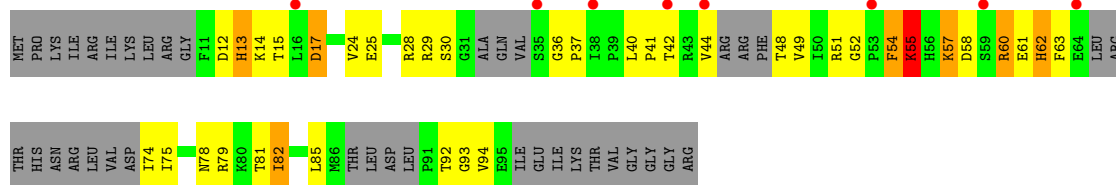
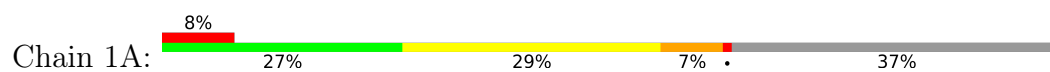
- Molecule 9: 30S ribosomal protein S9



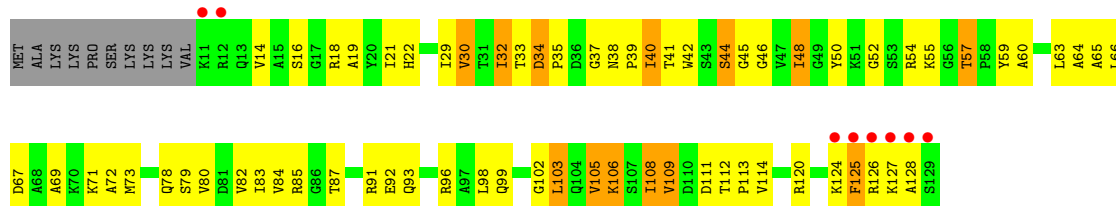
- Molecule 10: 30S ribosomal protein S10



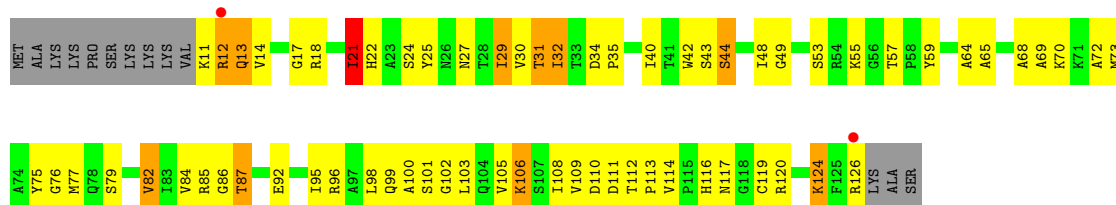
- Molecule 10: 30S ribosomal protein S10



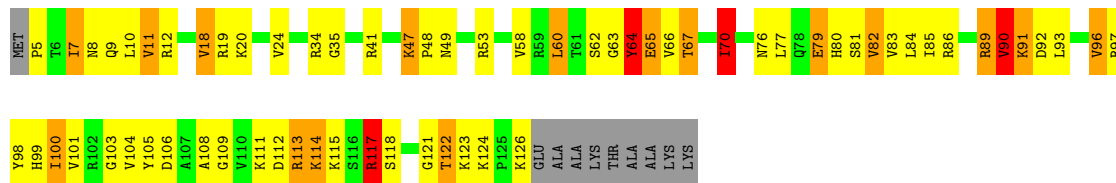
- Molecule 11: 30S ribosomal protein S11



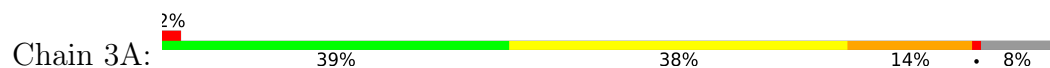
- Molecule 11: 30S ribosomal protein S11

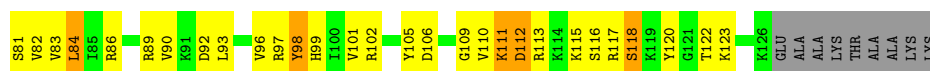


- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

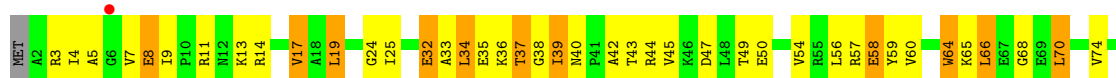




• Molecule 13: 30S ribosomal protein S13



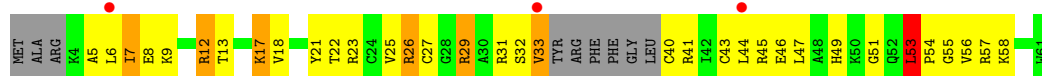
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z



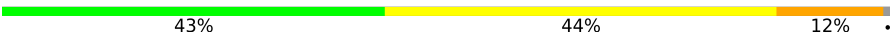
• Molecule 14: 30S ribosomal protein S14 type Z

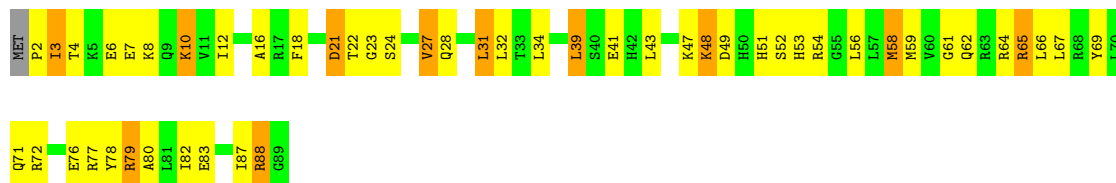


• Molecule 15: 30S ribosomal protein S15



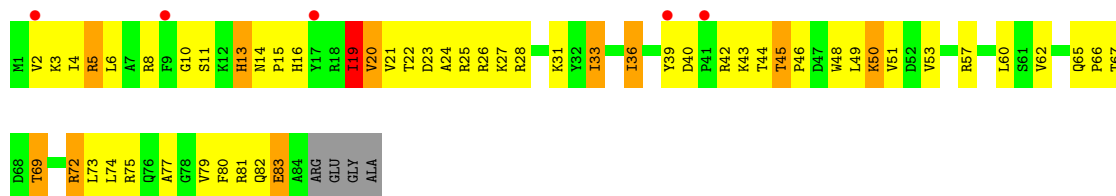
- Molecule 15: 30S ribosomal protein S15

Chain 6A: 

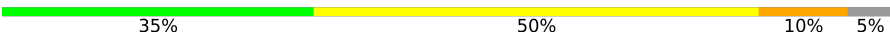


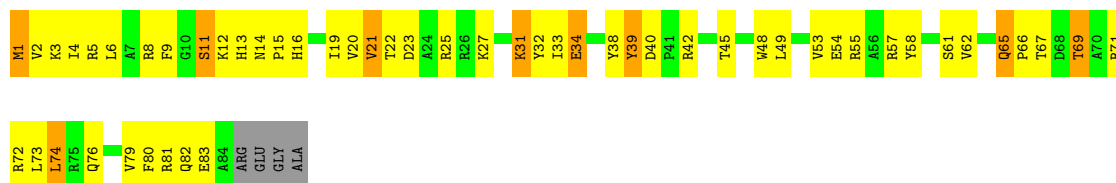
- Molecule 16: 30S ribosomal protein S16

Chain 7I: 

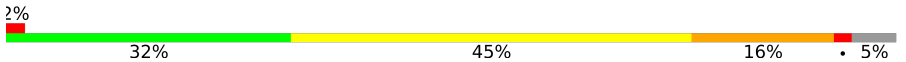


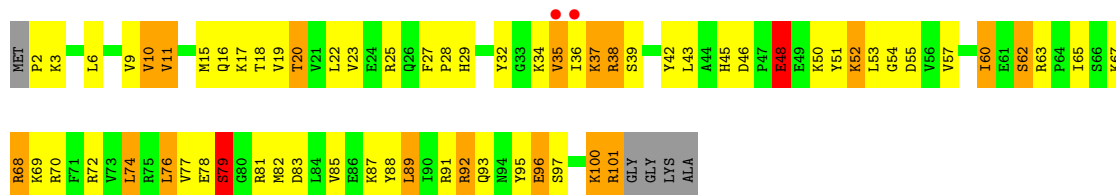
- Molecule 16: 30S ribosomal protein S16

Chain 7A: 



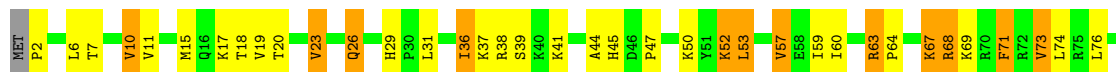
- Molecule 17: 30S ribosomal protein S17

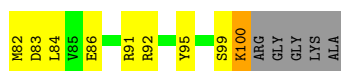
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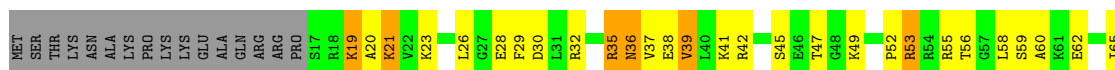
- Molecule 17: 30S ribosomal protein S17

Chain 8A: 





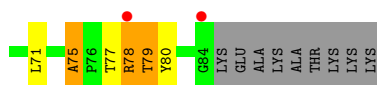
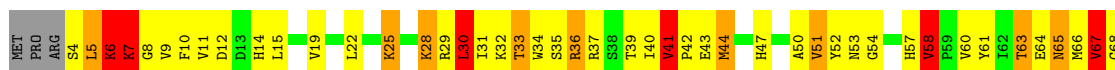
• Molecule 18: 30S ribosomal protein S18



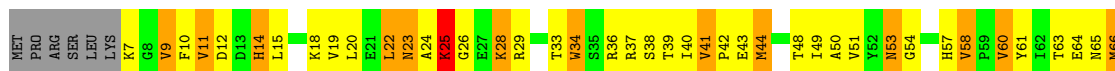
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19

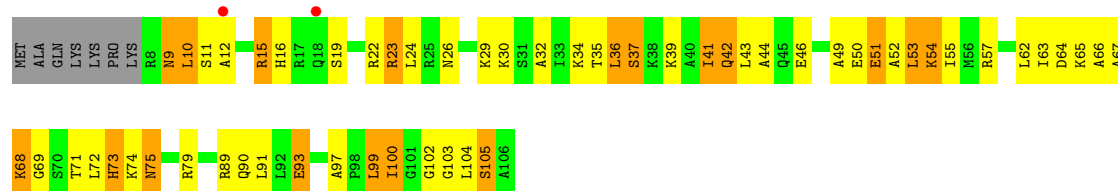


• Molecule 19: 30S ribosomal protein S19

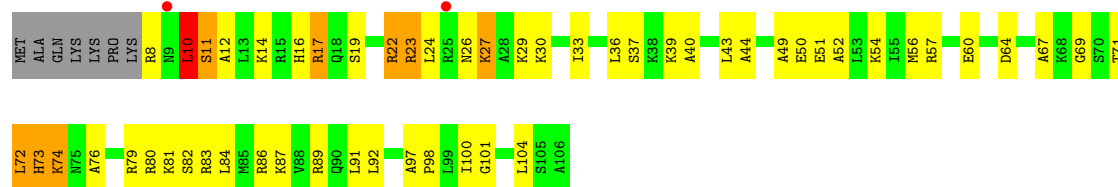
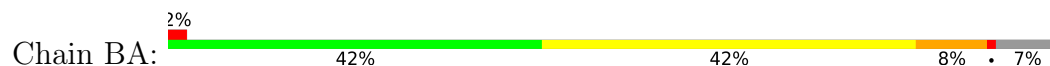


• Molecule 20: 30S ribosomal protein S20





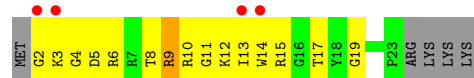
- Molecule 20: 30S ribosomal protein S20



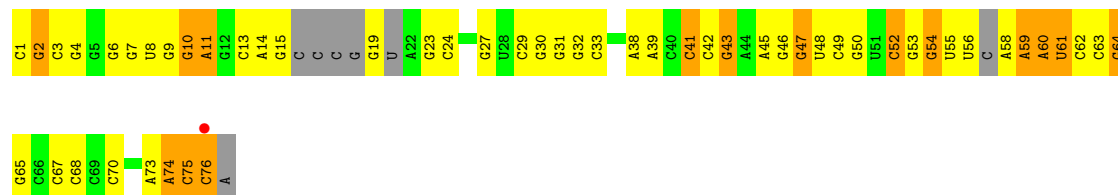
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA-fMet

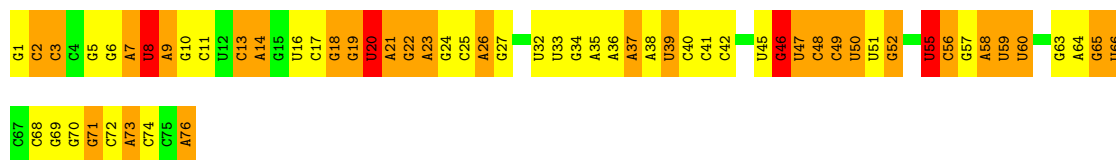


- Molecule 23: tRNA-fMet



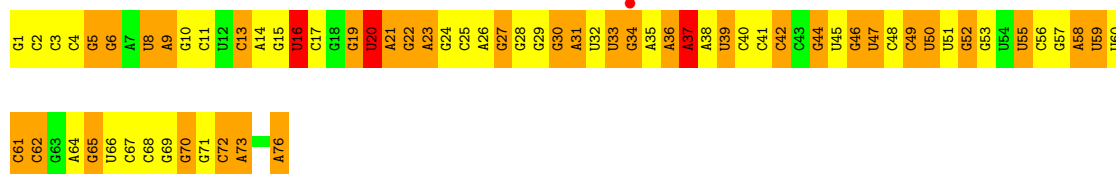
- Molecule 24: tRNA-Phe

Chain 3K: 20% 38% 37% 5%



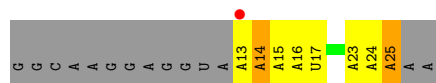
• Molecule 24: tRNA-Phe

Chain 3L: 11% 42% 43% .



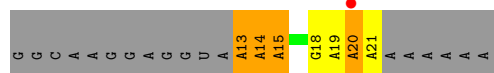
• Molecule 25: mRNA

Chain 4K: 4% 19% 22% 7% 52%



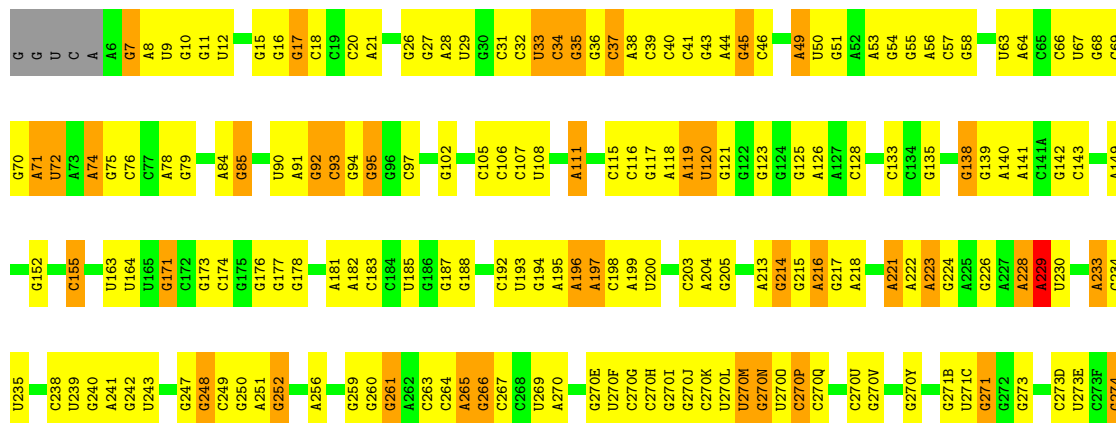
• Molecule 25: mRNA

Chain 4L: 4% 7% 11% 15% 67%



• Molecule 26: 23S ribosomal RNA

Chain 1H: 32% 51% 16% .



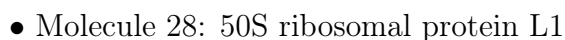
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| G1239 | G1240  | A1095 | U1033 | C888 | C814 | G743 | C664 | C618A | A547 | U475 | C404 | C343  | G275 |
| U1240 | A1241  | A1096 | G1034 | C889 | C815 |      | C665 | G619  | A548 |      | U405 | G344  | A276 |
| A1242 | G1170  | U1097 | U1035 | A890 | C816 | U747 | G666 | G620  | G549 | A478 | G406 | A345  | C277 |
| G1243 | G1171  |       | G1036 | C892 | C817 | G748 | U667 | A621  | G550 | A479 | G407 | A346  | A278 |
| G1244 |        | C1100 | G1037 | C893 | C818 | C749 | G668 | G622  | G551 |      | G408 | A347  | C279 |
|       | U1175  | U1101 | C1038 | C894 |      | A750 | G669 | G623  |      | G481 | C409 | G348  | C280 |
| G1248 | G1176  | C1102 | G1039 | U895 | A821 | A751 |      | C624  | G556 | A482 | G410 | C349  | G281 |
| A1177 | C1178  | C1040 | C971  | A896 | U822 | A752 | C873 | G625  | U557 | A483 | G411 | U350  | A282 |
| U1249 | C1179  | C1041 | G972  | C897 | G823 | C753 | G674 | U626  | G558 | A484 | A112 | G351  | A283 |
| G1250 | U1105  | C1042 | A973  | C898 | A824 | C754 | G675 | A627  | G559 | C485 | C413 | G352  | U284 |
| C1251 | G1106  | G974  | C974  | A899 |      |      | A676 | G628  |      | C486 | C414 | G353  | C285 |
| G1252 | C1181  | U107  | A1045 | A900 | U827 | C758 |      | G629  | G563 |      | A415 | G354  | C286 |
| A1263 | U1108  | G975  | A1046 | A901 | U828 | G759 | C683 | G630  | G564 | G491 | C416 | G355  | C287 |
| A1264 | C1109  |       | G1047 | C902 |      | G760 | G684 | A631  | C565 | A492 |      | G356  | C288 |
| A1265 | G1110  | A983  | U1048 | C903 | G831 | A761 | A685 |       | U566 | G493 | C419 | A357  | A289 |
| U1266 | A1111  | A984  | C1049 |      | U832 | U762 | G686 |       | G567 | G494 | C420 | U358  |      |
| G1267 | U1188  | C1257 | A1050 | U907 | U833 | G763 | C687 | G636  | U568 | G495 |      | A359  | G295 |
| G1268 | U1189  | U1113 | G1051 | C908 | U836 | A764 | U688 | A637  | U569 |      | G424 | G360  | G298 |
| G1269 | G1190  | G1114 | C1052 | A909 | C837 | G765 |      | U639  | G570 |      | G425 | G361  | A299 |
| G1270 | G1191  |       | C1053 | A910 |      | G771 | G695 | C640  | A572 | G500 | G426 | U362  | A300 |
| G1271 | C1119  |       | A1054 | C914 | A841 | A774 | G696 | A643  | A573 | A501 | U427 | G363  | G301 |
| U1205 | U1120  |       | G1055 | C915 | C842 | G775 | C698 | A644  | G574 | A502 |      | G364  | C302 |
| U1206 | C1121  |       | G1056 | G916 | C843 | G776 | G700 | C645  | A575 | A503 | A432 | G365  | U303 |
| A1266 | A1126  |       | A1057 | A917 | C844 | G777 | G701 | A646  |      |      | C433 | G366  | G304 |
| G1267 | A1129  |       | U1060 | A918 | C845 | A778 |      | G647  | G579 |      | U434 | U367E | U306 |
| A1268 | U1130  |       | U1061 | A919 | C846 | G779 | A705 | G648  | C580 | G508 | G438 | A363F | G307 |
| A1269 | C1131  |       | G1062 | G920 | U847 | U779 | G780 | G649  | G582 | C509 | C439 | C364  |      |
| G1270 | G1135  |       | G1063 | C921 | C848 | G780 |      | G650  | G583 | C510 |      | C365  |      |
| A1204 | G1136  |       | C1064 | C850 | U849 | A781 | G710 | G651  |      | U511 | G442 | G370  | A311 |
| U1205 | G1137  |       | U1065 |      | C850 | A782 | G711 |       |      | G512 | G443 | G371  | G312 |
| A1272 | G1138  |       | U1066 | C924 |      | A783 | U714 | A654  | A586 |      | C444 | A372  | G315 |
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| A1274 | U1140  |       | G1068 | A926 | C856 | G785 |      |       | U588 |      | C446 | C376  | G317 |
| A1275 | U1141  |       | A1069 | G928 | C857 | C786 | A716 |       | C589 | C516 |      | G377  | C318 |
| G1276 | U1142  |       | C1070 | G929 | U858 | U787 | G717 | G654D | A590 | C517 | A447 | G378  | C319 |
| A1210 | A1142A |       | G1071 | C931 | C859 | A788 | C719 | G654E | C591 | G518 | U448 | G379  | A320 |
| A1213 | A1143  |       | C1072 | G932 | A861 | A789 | C720 | G654F | G592 | U519 | A449 | U380  | G321 |
| G1216 | G1144  |       |       | A933 | C862 | C790 | C721 | C654H | G593 | G520 | G450 | G381  | A322 |
| G1219 | C1145  |       | C1075 | G934 | C863 | G792 | A722 | C654I | U594 |      | C452 | G382  | G323 |
| C1221 | G1149  |       | C1076 | C935 | C864 | A793 | G723 | A654J |      |      | C453 | U383  | A324 |
| C1222 | C1150  |       | U1077 | C936 | C865 | G794 | G724 | G654K | G598 | U524 | U454 | G325  | G326 |
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| A1227 | U1080  |       | C1079 | G938 | C869 | C796 | G726 | C654M | G600 | C527 | C456 | G386  | U329 |
| G1229 | U1081  |       | U1082 | A941 | A870 | C797 | A727 | G654N | G601 | A528 | A457 | U387  | A330 |
| G1230 | U1082  |       | U1083 | U942 | C876 | A800 | G732 | G654P | G604 | G530 | U459 | G388  | A331 |
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| C1295 | G1160  |       | G1021 | C951 | C882 | U807 | G738 | G659  | G615 |      | G469 | G396  | G338 |
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| C1297 | U1162  |       | G1023 | C953 | C884 | U810 | U740 | G661  | G545 |      | A472 | G398  | A340 |
| G1298 | G1163  |       | U1024 | C954 | C885 | U811 | G662 | G662  | G617 | G546 | G473 | G400  | G342 |
| C1299 | U1164  |       | A1027 | C955 | C886 | U812 |      | G663  |      |      | G474 |       |      |
| U1300 | U1165  |       | U1028 | C956 | C887 | U813 |      |       |      |      |      |       |      |
| A1301 | C1236  |       | G1092 | U957 | C888 |      |      |       |      |      |      |       |      |
| A1302 | U1166  |       | U1029 | U958 | C889 |      |      |       |      |      |      |       |      |
| G1238 | G1238  |       | U1094 | A959 | A887 |      |      |       |      |      |      |       |      |

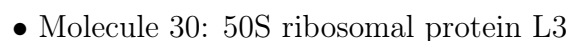
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| A2241 | G1377 | G1440  | C1509 | A1571  | A1640 | G1726 | G1799 | G1878 | U1983 | C2043 | C2105 | G2166 | A2241 |
| C2242 | A1378 | G1441  | C1509 | A1572  | G1642 | G1727 | C1801 | C1879 | G1984 | C2044 | C2106 | U2167 | C2242 |
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| U2244 | G1380 | G1443  | G1512 | G1574  | C1644 | G1728 | A1805 | G1884 | A1966 | U2046 | U2108 | A2169 | U2244 |
| U2245 | G1381 | G1444  | C1513 | C1574  | C1645 | A1729 | U1806 | A1884 | C1967 | U2047 | G2109 | U2170 | U2245 |
| G2246 | G1382 | A1444A | U1514 | C1577  | G1647 | U1730 | U1807 | C1887 | G1968 | G2048 | G2110 | G2171 | G2246 |
| A2247 | G1383 | U1316  | C1515 | U1578  | C1648 | G1731 | U1808 | C1888 | A1969 | G2049 | C2111 | U2172 | A2247 |
| C2248 | A1384 | G1448  | U1516 | A1579  | C1649 | G1732 | U1809 | G1888 | U1970 | C2050 | G2112 | A2173 | C2248 |
| U2249 | G1385 | G1449  | G1517 | A1580  | G1651 | G1733 | A1809 | A1889 | A1971 | A2051 | A2113 | C2174 | U2249 |
| G2250 | G1386 | G1449A | C1518 | G1581  | A1652 | C1734 | A1810 | A1890 | A1972 | G2052 | A2114 | G2175 | G2250 |
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| C2255 | U1390 | G1455  | U1523 | A1587  | C1657 | G1746 | A1815 | G1999 | U1977 | A2057 | A2119 | U2180 | C2255 |
| G2256 | U1391 | C1458  | U1524 | C1588  | G1658 | G1747 | A1816 | G1999 | U1978 | U2057 | G2120 | G2181 | G2256 |
| U2257 | A1392 | G1459  | G1525 | C1589  | U1659 | G1748 | G1817 | A1900 | A1981 | A2059 | G2121 | G2182 | U2257 |
| C2258 | A1393 | A1460  | G1526 | U1590  | C1662 | A1749 | U1818 | A1901 | C1982 | A2060 | U2122 | C2183 | C2258 |
| G2259 | U1394 | A1461  | G1527 | G1591  | C1663 | C1756 | U1819 | C1902 | C1983 | G2061 | G2123 | C2184 | G2259 |
| C2260 | A1395 | C1462  | U1528 | C1592  | C1664 | G1757 | U1820 | G1906 | U1987 | A2062 | G2124 | G2186 | C2260 |
| C2261 | U1397 | U1466  | A1529 | G1593  | C1665 | U1757 | U1821 | G1906 | C1988 | C2063 | G2125 | G2187 | C2261 |
| U2262 | A1398 | G1466  | G1530 | G1594  | G1666 | G1758 | A1822 | U1914 | G1989 | C2064 | A2126 | C2188 | U2262 |
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| G2264 | G1400 | C1467  | C1532 | C1596  | C1668 | A1760 | G1827 | C1914 | U1991 | U2068 | C2128 | G2190 | C2264 |
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| A1342 | A1412 | G1479  | C1542 | A1608  | C1680 | U1772 | G1836 | G1930 | U2000 | C2077 | C2138 | C2207 | C2277 |
| G1343 | A1413 | U1483  | C1543 | A1609  | C1681 | U1773 | G1837 | G1931 | A2005 | C2078 | C2139 | G2208 | G2278 |
| G1344 | G1413 | C1483  | C1544 | A1610  | C1682 | U1774 | G1839 | U1931 | A2013 | U2079 | C2140 | U2208 | G2279 |
| G1345 | U1416 | G1484  | A1545 | C1613  | C1684 | U1775 | G1840 | G1935 | A2014 | G2080 | C2143 | C2209 | C2280 |
| G1346 | G1417 | G1485  | A1546 | G1614  | C1689 | G1776 | C1841 | G1936 | A2015 | C2081 | C2144 | G2210 | C2281 |
| G1347 | G1418 | A1486  | C1547 | A1614  | A1689 | U1777 | C1842 | G1937 | U2016 | C2082 | U2144 | G2211 | C2282 |
| A1349 | A1419 | G1487  | C1548 | C1617  | A1690 | U1778 | C1843 | A1936 | U2017 | G2083 | C2145 | A2212 | C2283 |
| U1352 | U1420 | G1488  | C1549 | C1618  | C1691 | U1779 | G1844 | A1937 | U2018 | C2084 | C2146 | U2213 | C2284 |
| U1357 | G1421 | U1489  | C1550 | A1618  | U1692 | A1780 | G1845 | A1938 | G2023 | C2085 | G2147 | G2215 | A2287 |
| G1358 | G1422 | A1490  | C1551 | G1619  | U1693 | C1781 | A1846 | U1939 | C2024 | U2086 | G2148 | G2216 | A2288 |
| A1359 | G1423 | G1491  | G1552 | G1622  | C1694 | C1782 | A1847 | U1940 | C2025 | G2087 | G2149 | C2217 | G2289 |
| A1360 | G1424 | C1492  | A1553 | G1626  | C1695 | C1783 | G1848 | G1945 | C2026 | G2088 | U2150 | A2225 | G2290 |
| U1364 | U1427 | C1498  | A1554 | G1630A | G1696 | U1784 | A1849 | G1946 | G2027 | U2089 | G2151 | C2226 | U2291 |
| A1365 | C1428 | U1497  | G1555 | A1631  | G1697 | A1785 | C1850 | U1947 | U2028 | G2090 | G2152 | A2227 | C2292 |
| G1368 | C1430 | C1498  | C1556 | A1632  | G1699 | U1786 | G1851 | C1948 | U2029 | U2091 | G2153 | G2228 | C2293 |
| G1369 | U1431 | C1499  | G1557 | G1633  | G1705 | A1787 | A1852 | G1949 | A2030 | U2092 | G2154 | C2229 | C2294 |
| C1370 | U1433 | C1499  | G1560 | A1634  | G1706 | C1788 | A1853 | C1949 | A2031 | C2093 | G2155 | G2230 | C2295 |
| G1371 | U1434 | C1500  | G1561 | G1635  | U1707 | U1789 | A1854 | G1950 | A2032 | U2096 | G2156 | C2231 | U2296 |
| U1372 | G1435 | U1503  | A1566 | C1636  | G1708 | C1790 | G1858 | G1951 | A2033 | U2097 | G2157 | U2232 | C2297 |
| A1373 | G1436 | C1504  | A1567 | A1637  | C1709 | G1791 | A1859 | U1952 | U2034 | C2098 | G2158 | U2233 | A2298 |
| G1374 | C1437 | C1506  | G1568 | C1638  | C1708 | G1792 | G1860 | A1952 | U2035 | U2099 | G2159 | G2234 | C2299 |
| C1375 | U1438 | A1507  | A1569 | C1639  | U1716 | C1793 | G1861 | U1955 | C2036 | U2099 | G2160 | G2235 | C2300 |
|       |       |        |       |        |       | U1794 | U1864 | U1956 | G2037 | U2099 | C2161 | C2236 | G2302 |
|       |       |        |       |        |       | U1795 | G1869 | U1957 | G2038 | U2101 | G2162 | G2237 | G2303 |
|       |       |        |       |        |       | U1796 | A1870 | C1957 | G2039 | U2102 | C2163 | G2238 | G2304 |
|       |       |        |       |        |       | C1797 | A1871 | A1960 | C2103 | C2103 | C2164 | G2239 | C2305 |
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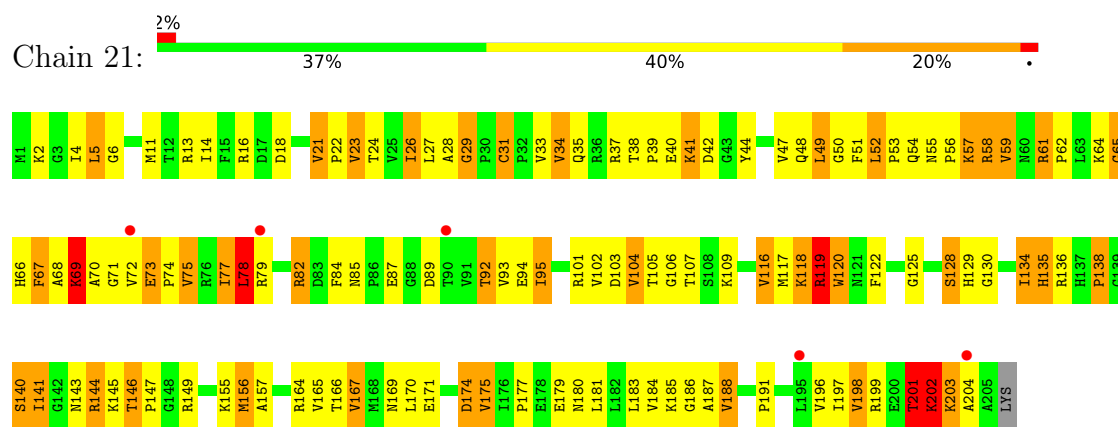


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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|
| A1274 | A1275 | A1276 | A1277 | A1278 | G1279 | G1280 | G1281 |       | G1285 | A1286 | A1287 | U1288 | C1289 | C1290 | C1291 | U1292 | C1293 | U1294 | C1295  | G1296 | C1297 | C1298 | C1299 | U1300 | A1301 | A1302 |       | C1306 |       | U1312 | U1313 | C1314 | C1315 | U1316 | A1317 | G1318 | C1319 | C1320 | A1321 | A1322 | U1323 | G1324 |       | C1327 | G1328 | U1329 | C1330 | A1331 | G1332 | C1333 |       | A1336 | G1337 | G1338 | G1339 | U1340 | U1341 | A1342 | G1343 |        |       |
| A1143 | G1144 | A1145 | C1146 | C1147 | A1148 | G1149 | C1150 | G1151 | C1152 | C1153 | G1154 | A1155 | A1156 |       | U1159 | G1160 | C1161 | G1162 | G1163  | G1164 | U1165 | C1166 | U1167 | G1168 | G1169 | G1170 | G1171 | G1172 | G1173 | A1174 | U1175 | G1176 | A1177 | C1178 | C1179 | C1180 | U1181 | A1182 | G1183 |       | G1187 | U1188 | A1189 | G1190 |       | A1194 | G1195 | C1196 | G1197 | U1198 | U1199 |       | C1200 | C1201 |       | A1204 | U1205 | G1206 | G1207 | C1208  | G1209 |
| A1210 | U1211 | A1212 | A1213 | A1214 |       | C1217 | G1218 | G1219 | A1220 | C1221 | G1222 | C1223 | G1224 | G1225 | G1226 | A1227 | G1228 | G1229 | G1229A | C1230 |       | U1234 | G1235 | G1236 | A1237 | G1238 | G1239 | U1240 | U1241 |       |       | G1244 | G1245 | A1246 | G1247 | G1248 | U1249 | G1250 | C1251 | A1252 | A1253 |       | G1256 | C1257 | G1258 | G1259 | G1260 | C1261 | A1262 | U1263 | G1264 | A1265 | U1266 | U1267 | A1268 | A1269 | G1270 | G1271 | A1272 | U1273  |       |
| C1076 | A     | U     | C     | U     | A     | U     | U     | U     | A     | A     | A     | G     | A     | G     | U1090 | G1091 | C1092 | G1093 | U1094  | A1095 | A1096 | U1097 | A1098 | G1099 | C1100 | U1101 | C1102 | A1103 | C1104 | U1105 |       | C1109 | G1110 | A1111 | G1112 | U1113 | G1114 | G1115 | C1116 | G1117 |       | G1122 |       | G1125 |       | A1128 | U1129 | U1130 | G1131 | A1132 | U1133 | C1135 | G1136 | G1137 | U1138 | G1139 | C1140 | U1141 | U1142 | A1142A |       |
| G954  | C955  | G956  | A957  | U958  | U959  | A960  | C961  | C962  | G963  | C964  |       | G968  | U969  | C970  | C971  | G972  | A973  | G974  | C974A  | G975  | C976  | G977  | G978  | G979  | A980  | A981  | G982  | A983  | A984  | C985  | G986  | G987  | A988  | G989  | A990  | C991  | C992  | G993  | C994  | C995  | A996  | G997  | C998  | U999  | A1000 | A1001 | G1002 | G1003 | C1004 | C1005 | C1006 | C1007 | A1008 | A1009 | A1010 | G1011 | U1012 | C1013 | U1014 |        |       |
| C889  | A890  | G892  | C893  | U894  | U895  | A896  | C897  | C898  | A899  | A900  | A901  | C902  | C903  | C904  | U905  | G906  | U907  | C908  | A909   | A910  | C911  | C912  | U913  | C914  | C915  | G916  | G917  | C918  | A918  | G919  | C920  | C921  | U922  | C923  | C924  | C925  | A926  | G928  | G929  |       | G932  | A933  | G934  | C935  | C936  | U937  | G938  | G939  | G940  | A941  | C942  | U943  | G944  | A945  | C1008 | G946  | G947  |       | G950  | C951   |       |
| A824  | C825  | U826  | U827  | U828  | A829  | G830  | G831  | G832  | U833  |       | G836  | C837  | C838  | C839  | C840  |       | G843  | C844  | G845   | C846  | U847  | G848  | A849  | C850  | U851  | G852  | G853  | G854  | C855  | C856  | C857  | U858  | G859  | U860  | A861  | G862  | A863  | G864  | C865  |       | U868  | G869  | A870  | U871  | A872  | G873  |       | U877  | G878  | G879  | G880  | G881  | G882  | G883  | C885  | C886  | A887  | C888  |       |        |       |
| G1015 | G1016 | G1017 | C1018 | A1019 | A1020 | A1021 | G1022 | U1023 | G1024 | G1025 | U1026 | A1027 | A1028 |       | G1030 | G1031 | G1032 | U1033 | G1034  | U1035 | G1036 | G1037 |       | G1040 | C1041 | G1042 | C1043 | G1044 | A1045 | G1046 | G1047 | A1048 | C1049 | G1050 | G1051 | C1052 | G1053 | A1054 | G1055 | G1056 | A1057 | U1058 | G1059 | U1060 | G1061 | G1062 | C1063 | U1064 | U1065 | U1066 | A1067 | G1068 | A1069 | G1070 | G1071 | C1072 | A1073 | G1074 | C1075 |        |       |
| A1143 | G1144 | A1145 | C1146 | C1147 | A1148 | G1149 | C1150 | G1151 | C1152 | C1153 | G1154 | A1155 | A1156 |       | U1159 | G1160 | C1161 | G1162 | G1163  | G1164 | U1165 | C1166 | U1167 | G1168 | G1169 | G1170 | G1171 | G1172 | G1173 | A1174 | U1175 | G1176 | A1177 | C1178 | C1179 | C1180 | U1181 | A1182 | G1183 |       | G1187 | U1188 | A1189 | G1190 |       | A1194 | G1195 | C1196 | G1197 | U1198 | U1199 |       | C1200 | C1201 |       | A1204 | U1205 | G1206 | G1207 | C1208  | G1209 |
| A1210 | U1211 | A1212 | A1213 | A1214 |       | C1217 | G1218 | G1219 | A1220 | C1221 | G1222 | C1223 | G1224 | G1225 | G1226 | A1227 | G1228 | G1229 | G1229A | C1230 |       | U1234 | G1235 | G1236 | A1237 | G1238 | G1239 | U1240 | U1241 |       |       | G1244 | G1245 | A1246 | G1247 | G1248 | U1249 | G1250 | C1251 | A1252 | A1253 |       | G1256 | C1257 | G1258 | G1259 | G1260 | C1261 | A1262 | U1263 | G1264 | A1265 | U1266 | U1267 | A1268 | A1269 | G1270 | G1271 | A1272 | U1273  |       |

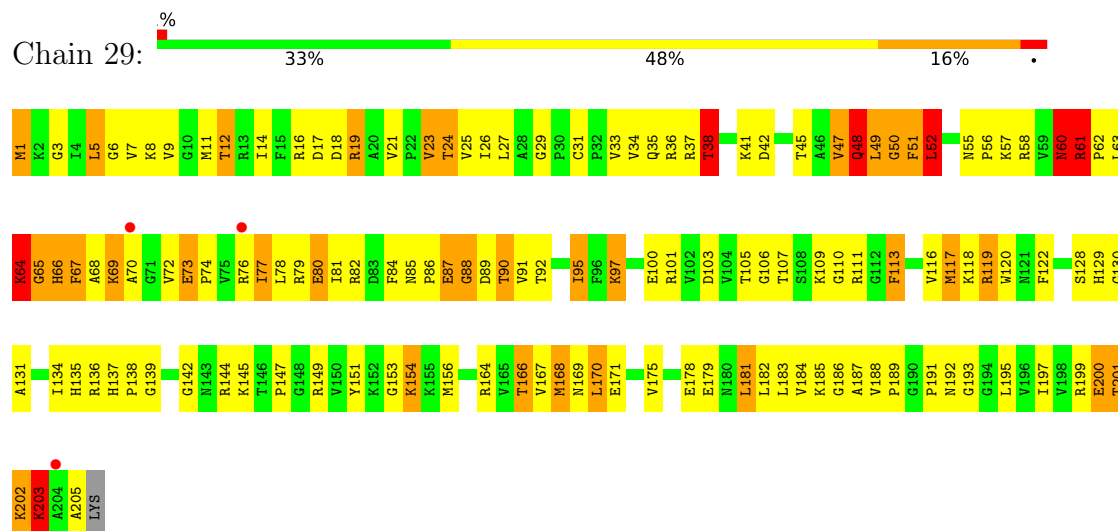
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK







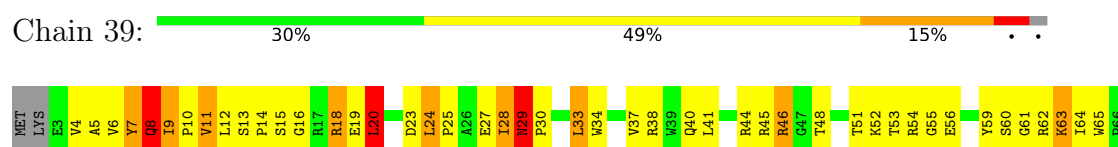
- Molecule 30: 50S ribosomal protein L3

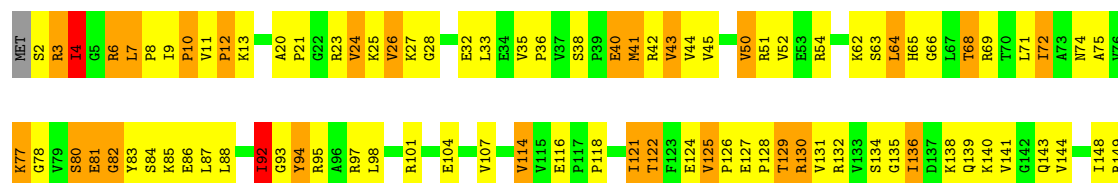


- Molecule 31: 50S ribosomal protein L4

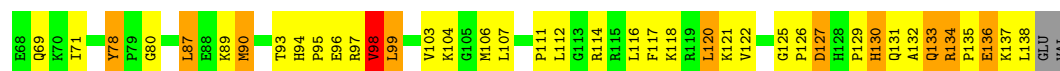


- Molecule 31: 50S ribosomal protein L4

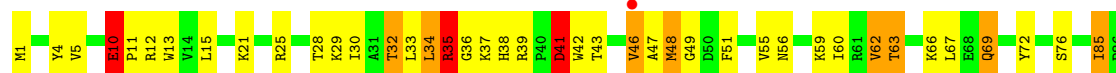
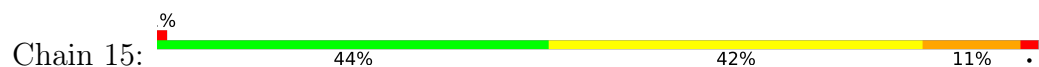




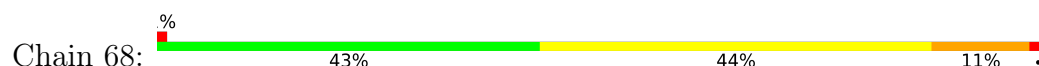




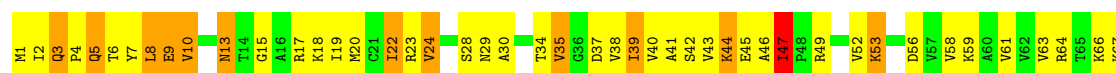
• Molecule 35: 50S ribosomal protein L13



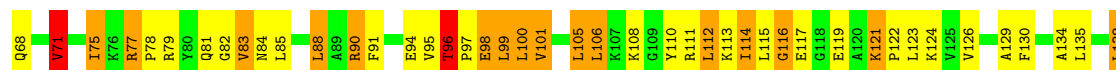
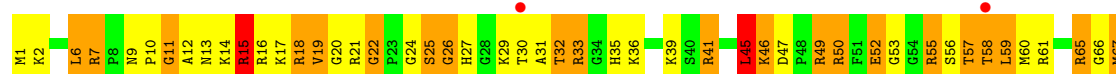
• Molecule 36: 50S ribosomal protein L14



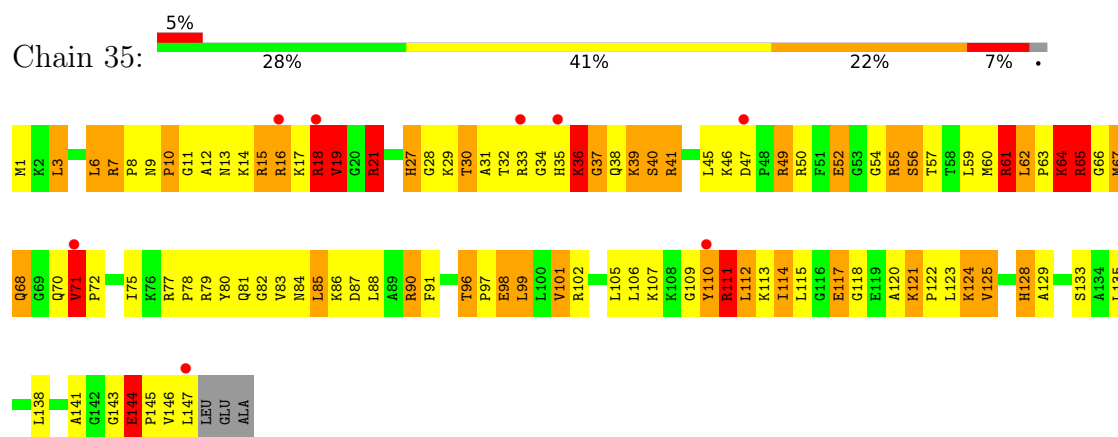
• Molecule 36: 50S ribosomal protein L14



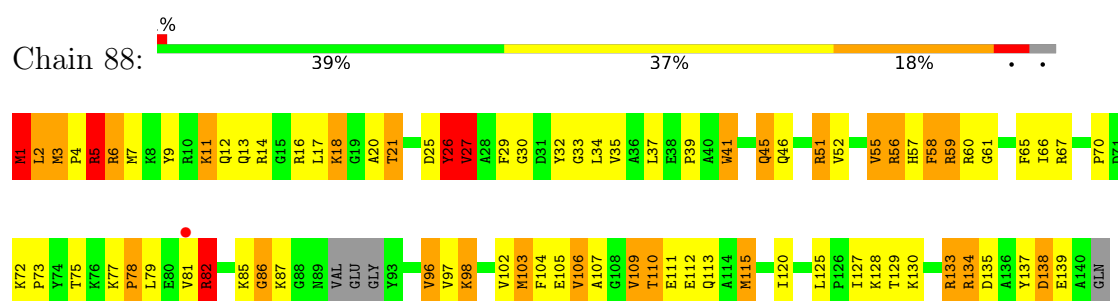
• Molecule 37: 50S ribosomal protein L15



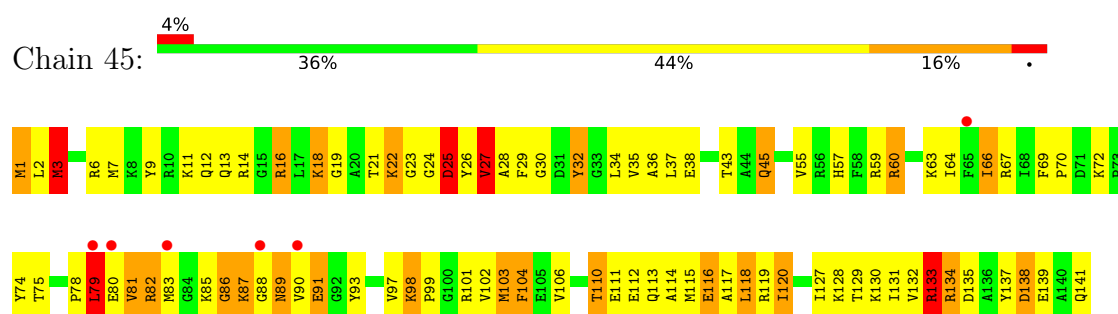
• Molecule 37: 50S ribosomal protein L15



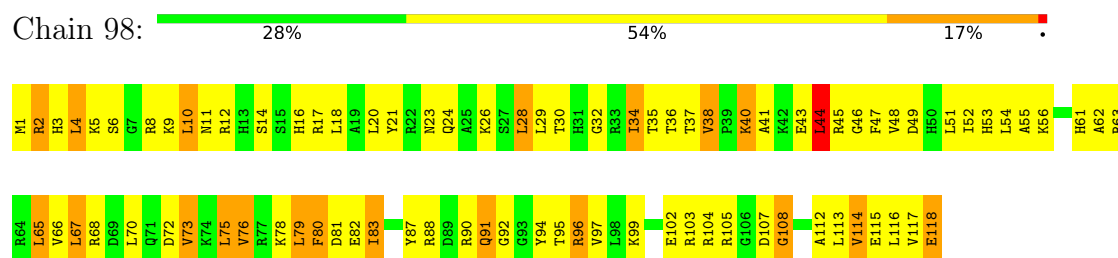
• Molecule 38: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L16

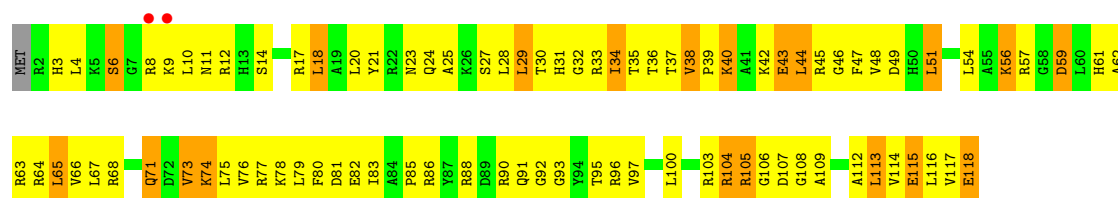


• Molecule 39: 50S ribosomal protein L17



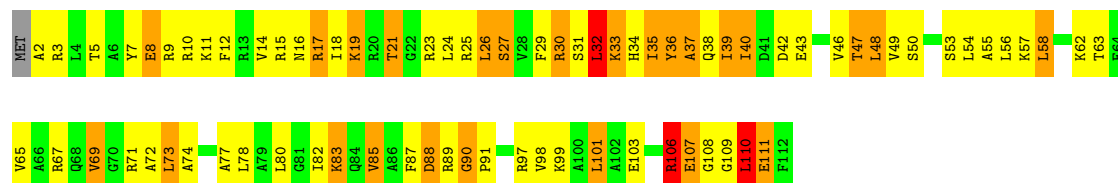
• Molecule 39: 50S ribosomal protein L17





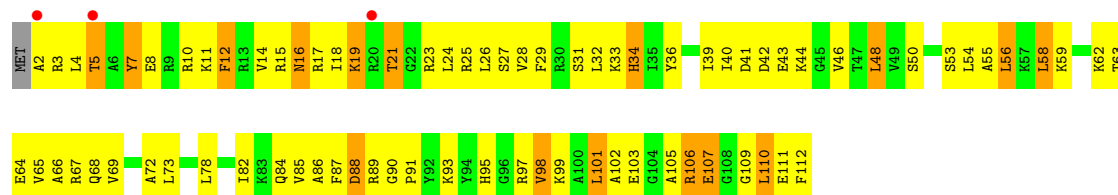
• Molecule 40: 50S ribosomal protein L18

Chain A8: 30% 44% 22% . .



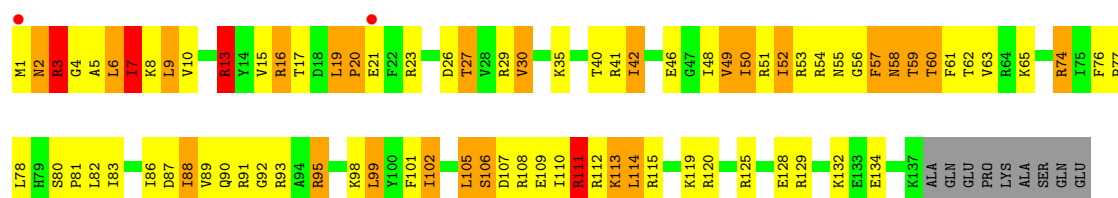
• Molecule 40: 50S ribosomal protein L18

Chain 65: 3% 29% 55% 14% .



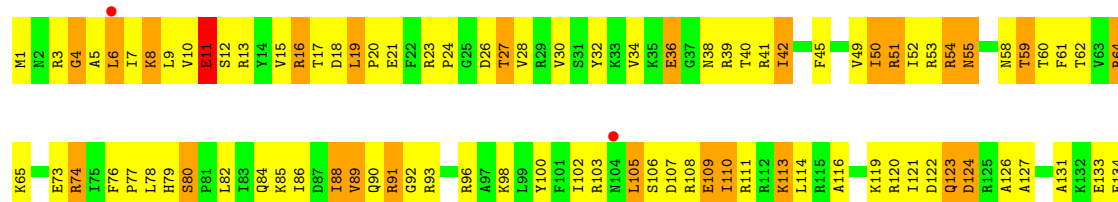
• Molecule 41: 50S ribosomal protein L19

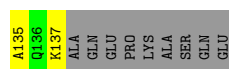
Chain B8: % 37% 37% 17% 6%



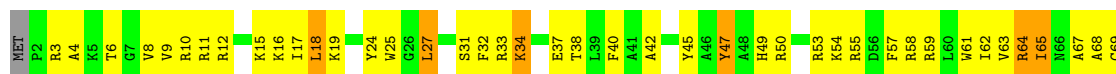
• Molecule 41: 50S ribosomal protein L19

Chain 75: % 30% 46% 17% 6%

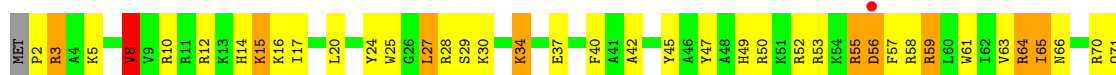




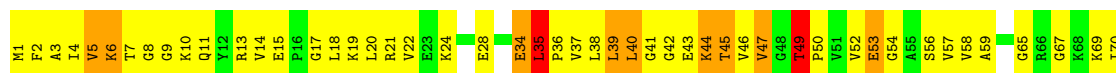
- Molecule 42: 50S ribosomal protein L20



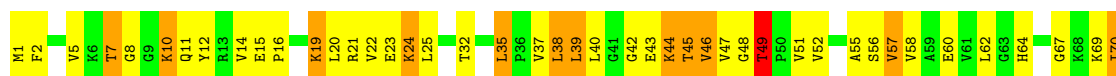
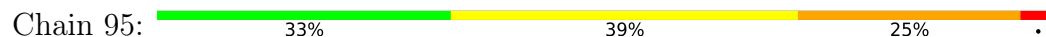
- Molecule 42: 50S ribosomal protein L20



- Molecule 43: 50S ribosomal protein L21

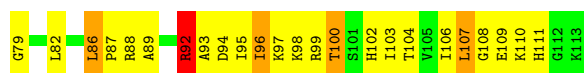


- Molecule 43: 50S ribosomal protein L21



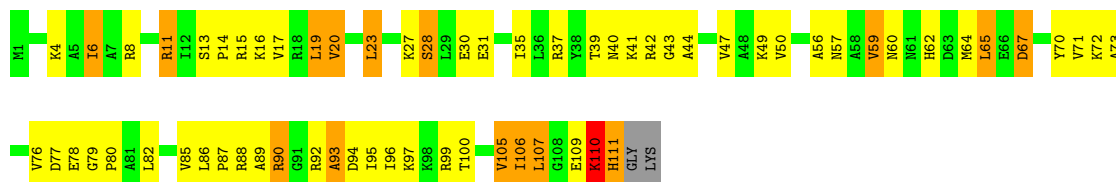
- Molecule 44: 50S ribosomal protein L22





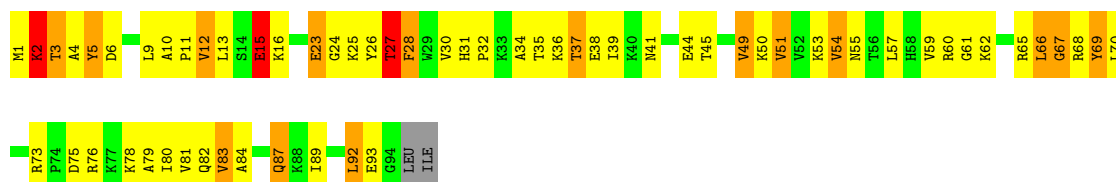
- Molecule 44: 50S ribosomal protein L22

Chain A5: 41% 43% 13% ..



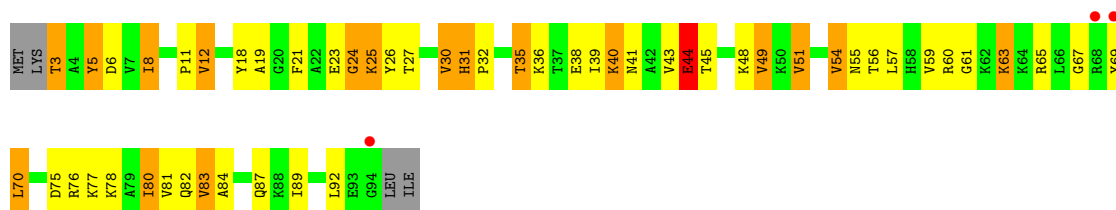
- Molecule 45: 50S ribosomal protein L23

Chain F8: 33% 46% 16% ..



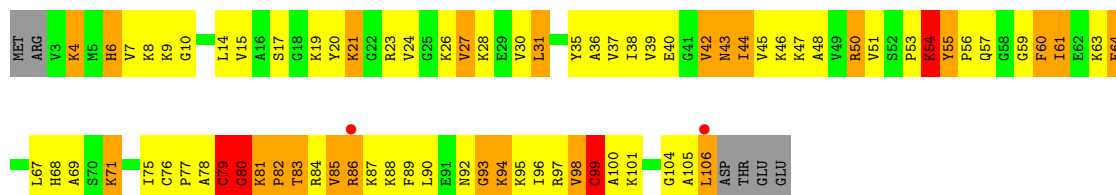
- Molecule 45: 50S ribosomal protein L23

Chain B5: 3% 41% 36% 18% ..



- Molecule 46: 50S ribosomal protein L24

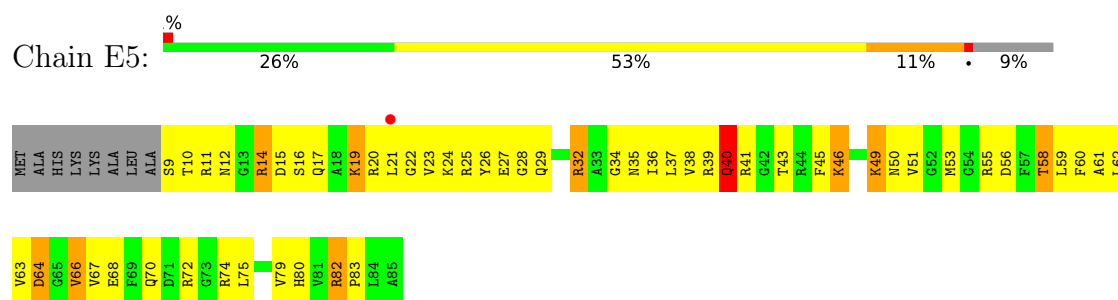
Chain G8: 2% 25% 45% 21% 5%



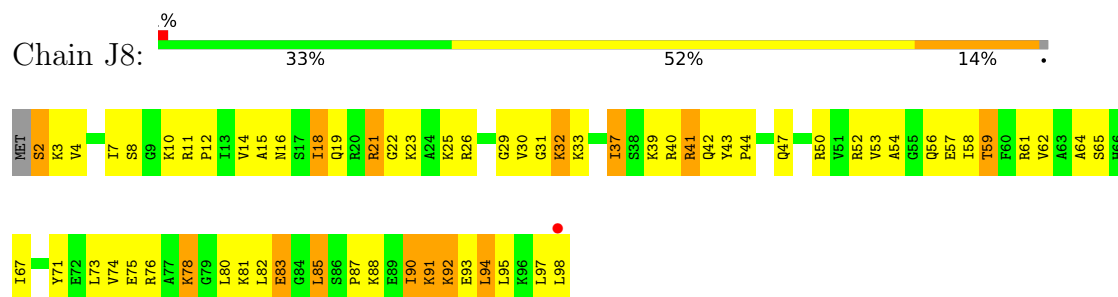
- Molecule 46: 50S ribosomal protein L24

Chain C5: 4% 28% 42% 23% 5%

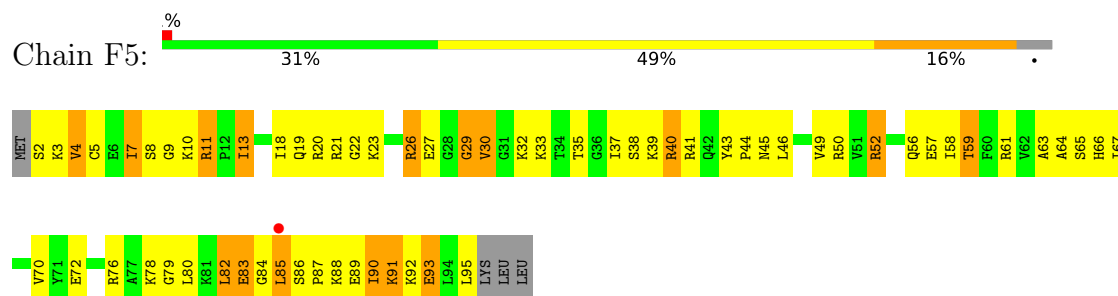




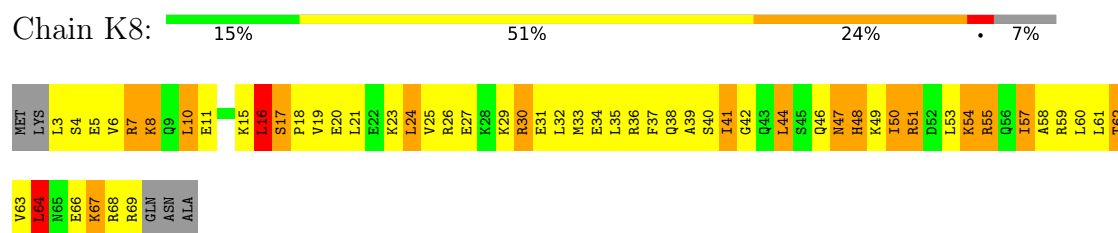
- Molecule 49: 50S ribosomal protein L28



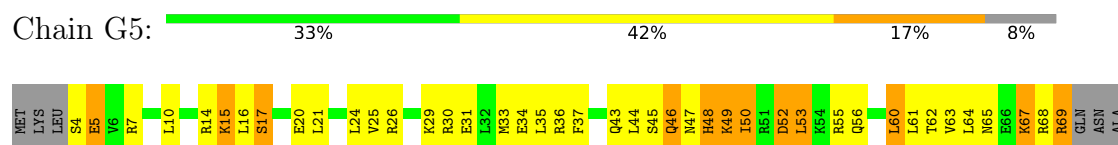
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29

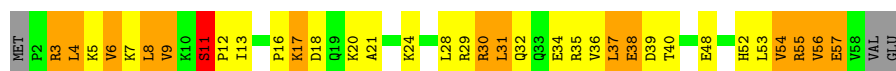


- Molecule 50: 50S ribosomal protein L29



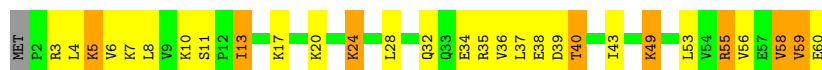
- Molecule 51: 50S ribosomal protein L30





- Molecule 51: 50S ribosomal protein L30

Chain H5: 50% 35% 13%



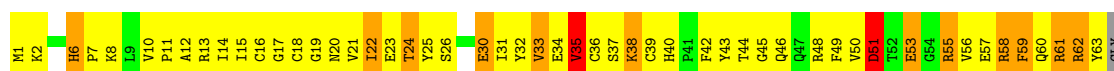
- Molecule 52: 50S ribosomal protein L31

Chain M8: 28% 42% 20% 7%



- Molecule 52: 50S ribosomal protein L31

Chain I5: 15% 54% 17% 11%



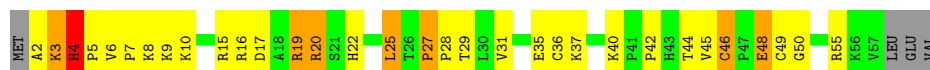
- Molecule 53: 50S ribosomal protein L32

Chain N8: 47% 25% 13% 5% 10%



- Molecule 53: 50S ribosomal protein L32

Chain J5: 40% 40% 12% 7%

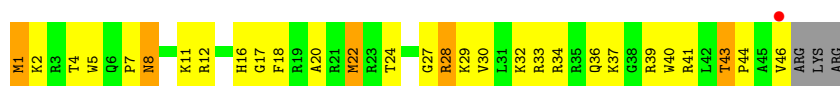


- Molecule 54: 50S ribosomal protein L34

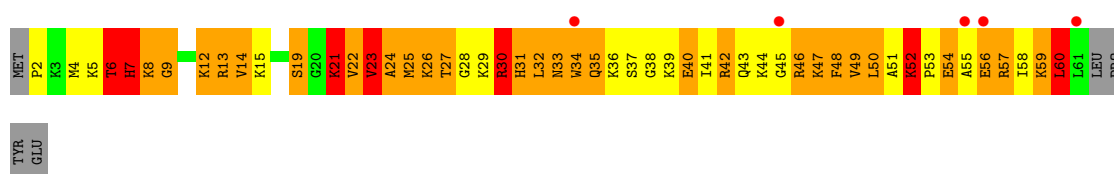
Chain P8: 47% 39% 10%



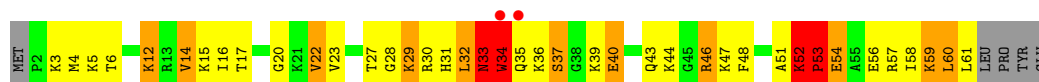
## • Molecule 54: 50S ribosomal protein L34



## • Molecule 55: 50S ribosomal protein L35



## • Molecule 55: 50S ribosomal protein L35



## • Molecule 56: tRNA-fMet



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.20Å 448.80Å 621.00Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 153.41 – 3.30<br>153.41 – 3.30                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (153.41-3.30)<br>92.6 (153.41-3.30)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.46                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.96 (at 3.33Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.191 , 0.258<br>(Not available) , 0.230                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (0.23%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 96.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.268                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 79.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 295920                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 115.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: OMC, PSU, MIA, ZN, 5MU, 4SU, MG, 7MG

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   | 13    | 0.45         | 0/36028      | 0.69        | 11/56231 (0.0%) |
| 1   | 1G    | 0.41         | 0/36025      | 0.64        | 5/56227 (0.0%)  |
| 2   | 12    | 0.59         | 0/1959       | 1.15        | 16/2642 (0.6%)  |
| 2   | 1E    | 0.60         | 0/1959       | 1.13        | 15/2642 (0.6%)  |
| 3   | 22    | 0.57         | 0/1636       | 1.07        | 8/2205 (0.4%)   |
| 3   | 2E    | 0.69         | 0/1629       | 1.12        | 4/2195 (0.2%)   |
| 4   | 32    | 0.62         | 0/1732       | 1.22        | 18/2318 (0.8%)  |
| 4   | 3E    | 0.69         | 0/1732       | 1.20        | 11/2318 (0.5%)  |
| 5   | 42    | 0.68         | 0/1171       | 1.18        | 6/1576 (0.4%)   |
| 5   | 4E    | 0.73         | 0/1171       | 1.11        | 6/1576 (0.4%)   |
| 6   | 52    | 0.68         | 0/855        | 1.10        | 3/1154 (0.3%)   |
| 6   | 5E    | 0.71         | 0/855        | 1.07        | 2/1154 (0.2%)   |
| 7   | 62    | 0.61         | 0/1211       | 1.07        | 3/1622 (0.2%)   |
| 7   | 6E    | 0.68         | 0/1275       | 1.04        | 6/1709 (0.4%)   |
| 8   | 72    | 0.61         | 0/1135       | 1.13        | 6/1527 (0.4%)   |
| 8   | 7E    | 0.69         | 0/1135       | 1.31        | 15/1527 (1.0%)  |
| 9   | 82    | 0.55         | 0/1028       | 1.06        | 3/1379 (0.2%)   |
| 9   | 8E    | 0.62         | 0/1028       | 1.08        | 1/1379 (0.1%)   |
| 10  | 1A    | 0.64         | 0/529        | 1.11        | 2/706 (0.3%)    |
| 10  | 1I    | 0.66         | 0/814        | 1.16        | 6/1095 (0.5%)   |
| 11  | 2A    | 0.66         | 0/879        | 1.17        | 6/1187 (0.5%)   |
| 11  | 2I    | 0.83         | 1/899 (0.1%) | 1.30        | 7/1213 (0.6%)   |
| 12  | 3A    | 0.77         | 0/972        | 1.19        | 7/1301 (0.5%)   |
| 12  | 3I    | 0.86         | 0/972        | 1.31        | 10/1301 (0.8%)  |
| 13  | 4A    | 0.56         | 0/943        | 1.05        | 5/1265 (0.4%)   |
| 13  | 4I    | 0.69         | 0/943        | 1.11        | 4/1265 (0.3%)   |
| 14  | 5A    | 0.62         | 0/423        | 1.08        | 2/560 (0.4%)    |
| 14  | 5I    | 0.79         | 0/500        | 1.07        | 3/664 (0.5%)    |
| 15  | 6A    | 0.69         | 0/744        | 1.00        | 1/992 (0.1%)    |
| 15  | 6I    | 0.80         | 0/744        | 1.15        | 4/992 (0.4%)    |
| 16  | 7A    | 0.64         | 0/721        | 1.10        | 1/970 (0.1%)    |
| 16  | 7I    | 0.63         | 0/721        | 1.14        | 9/970 (0.9%)    |

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5          |
| 17  | 8A    | 0.63         | 0/836         | 1.12        | 6/1117 (0.5%)    |
| 17  | 8I    | 0.71         | 0/847         | 1.15        | 5/1131 (0.4%)    |
| 18  | 9A    | 0.62         | 0/595         | 1.04        | 1/790 (0.1%)     |
| 18  | 9I    | 0.76         | 0/595         | 1.13        | 3/790 (0.4%)     |
| 19  | AA    | 0.61         | 0/638         | 1.16        | 10/860 (1.2%)    |
| 19  | AI    | 0.72         | 1/661 (0.2%)  | 1.34        | 9/890 (1.0%)     |
| 20  | BA    | 0.65         | 0/764         | 1.20        | 6/1007 (0.6%)    |
| 20  | BI    | 0.60         | 0/764         | 1.06        | 2/1007 (0.2%)    |
| 21  | 1B    | 0.71         | 0/192         | 0.99        | 0/252            |
| 21  | 1F    | 0.57         | 0/221         | 1.14        | 0/288            |
| 22  | 1K    | 0.40         | 0/1623        | 0.61        | 0/2521           |
| 23  | 2K    | 0.61         | 1/1721 (0.1%) | 0.73        | 0/2682           |
| 24  | 3K    | 0.49         | 2/1669 (0.1%) | 0.57        | 0/2599           |
| 24  | 3L    | 0.50         | 3/1669 (0.2%) | 0.56        | 0/2599           |
| 25  | 4K    | 0.51         | 0/322         | 0.70        | 0/500            |
| 25  | 4L    | 0.56         | 0/222         | 0.73        | 0/344            |
| 26  | 14    | 0.53         | 0/69405       | 0.77        | 10/108348 (0.0%) |
| 26  | 1H    | 0.64         | 0/69998       | 0.85        | 21/109276 (0.0%) |
| 27  | 16    | 0.52         | 0/2928        | 0.80        | 0/4568           |
| 27  | 1J    | 0.43         | 0/2928        | 0.72        | 0/4568           |
| 28  | 71    | 1.00         | 0/749         | 1.27        | 7/1004 (0.7%)    |
| 29  | 11    | 1.10         | 4/2165 (0.2%) | 1.43        | 27/2919 (0.9%)   |
| 29  | 19    | 0.96         | 1/2170 (0.0%) | 1.46        | 37/2926 (1.3%)   |
| 30  | 21    | 0.90         | 0/1601        | 1.59        | 33/2160 (1.5%)   |
| 30  | 29    | 0.91         | 1/1601 (0.1%) | 1.53        | 26/2160 (1.2%)   |
| 31  | 31    | 0.99         | 2/1620 (0.1%) | 1.34        | 18/2194 (0.8%)   |
| 31  | 39    | 0.86         | 1/1645 (0.1%) | 1.45        | 24/2228 (1.1%)   |
| 32  | 41    | 0.75         | 0/1498        | 1.17        | 9/2016 (0.4%)    |
| 32  | 49    | 0.57         | 0/1498        | 1.19        | 13/2016 (0.6%)   |
| 33  | 51    | 0.82         | 0/1362        | 1.44        | 22/1841 (1.2%)   |
| 33  | 59    | 0.71         | 1/1332 (0.1%) | 1.44        | 29/1802 (1.6%)   |
| 34  | 61    | 0.79         | 0/1151        | 1.27        | 11/1558 (0.7%)   |
| 34  | 69    | 0.67         | 0/1151        | 1.20        | 15/1558 (1.0%)   |
| 35  | 15    | 0.75         | 0/1131        | 1.27        | 10/1525 (0.7%)   |
| 35  | 58    | 0.89         | 0/1131        | 1.38        | 16/1525 (1.0%)   |
| 36  | 25    | 0.85         | 0/942         | 1.23        | 6/1269 (0.5%)    |
| 36  | 68    | 0.94         | 0/942         | 1.26        | 12/1269 (0.9%)   |
| 37  | 35    | 0.87         | 2/1139 (0.2%) | 1.48        | 21/1514 (1.4%)   |
| 37  | 78    | 0.94         | 0/1161        | 1.54        | 22/1544 (1.4%)   |
| 38  | 45    | 0.90         | 2/1142 (0.2%) | 1.35        | 18/1527 (1.2%)   |
| 38  | 88    | 1.08         | 2/1097 (0.2%) | 1.64        | 25/1466 (1.7%)   |
| 39  | 55    | 0.89         | 1/973 (0.1%)  | 1.23        | 4/1302 (0.3%)    |
| 39  | 98    | 0.88         | 1/981 (0.1%)  | 1.29        | 9/1312 (0.7%)    |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 40  | 65    | 0.74         | 1/891 (0.1%)     | 1.29        | 9/1187 (0.8%)     |
| 40  | A8    | 0.89         | 0/891            | 1.33        | 9/1187 (0.8%)     |
| 41  | 75    | 0.81         | 0/1155           | 1.19        | 9/1542 (0.6%)     |
| 41  | B8    | 0.91         | 0/1155           | 1.43        | 13/1542 (0.8%)    |
| 42  | 85    | 0.78         | 0/981            | 1.16        | 4/1306 (0.3%)     |
| 42  | C8    | 1.02         | 2/981 (0.2%)     | 1.26        | 8/1306 (0.6%)     |
| 43  | 95    | 0.83         | 1/789 (0.1%)     | 1.33        | 9/1057 (0.9%)     |
| 43  | D8    | 0.88         | 0/789            | 1.50        | 8/1057 (0.8%)     |
| 44  | A5    | 0.94         | 0/897            | 1.16        | 4/1204 (0.3%)     |
| 44  | E8    | 0.97         | 0/910            | 1.32        | 10/1220 (0.8%)    |
| 45  | B5    | 0.92         | 0/739            | 1.30        | 7/993 (0.7%)      |
| 45  | F8    | 1.05         | 0/756            | 1.43        | 13/1014 (1.3%)    |
| 46  | C5    | 0.95         | 2/807 (0.2%)     | 1.57        | 12/1076 (1.1%)    |
| 46  | G8    | 0.98         | 1/804 (0.1%)     | 1.52        | 13/1073 (1.2%)    |
| 47  | D5    | 0.61         | 0/1151           | 1.39        | 22/1557 (1.4%)    |
| 47  | H8    | 0.82         | 3/1135 (0.3%)    | 1.43        | 18/1535 (1.2%)    |
| 48  | E5    | 0.85         | 0/620            | 1.27        | 8/827 (1.0%)      |
| 48  | I8    | 0.98         | 0/634            | 1.36        | 5/847 (0.6%)      |
| 49  | F5    | 0.81         | 0/744            | 1.35        | 7/989 (0.7%)      |
| 49  | J8    | 1.01         | 0/769            | 1.40        | 8/1022 (0.8%)     |
| 50  | G5    | 0.73         | 0/560            | 1.18        | 3/741 (0.4%)      |
| 50  | K8    | 0.97         | 0/565            | 1.51        | 8/748 (1.1%)      |
| 51  | H5    | 0.76         | 0/473            | 1.28        | 6/635 (0.9%)      |
| 51  | L8    | 0.97         | 0/457            | 1.57        | 6/613 (1.0%)      |
| 52  | I5    | 0.73         | 0/527            | 1.34        | 7/709 (1.0%)      |
| 52  | M8    | 0.76         | 0/545            | 1.37        | 6/733 (0.8%)      |
| 53  | J5    | 0.89         | 0/448            | 1.50        | 7/606 (1.2%)      |
| 53  | N8    | 0.83         | 0/436            | 1.58        | 9/589 (1.5%)      |
| 54  | L5    | 0.97         | 0/406            | 1.29        | 0/536             |
| 54  | P8    | 1.12         | 0/417            | 1.45        | 6/550 (1.1%)      |
| 55  | M5    | 1.17         | 2/483 (0.4%)     | 1.57        | 12/634 (1.9%)     |
| 55  | Q8    | 1.59         | 6/486 (1.2%)     | 2.29        | 22/638 (3.4%)     |
| 56  | 2L    | 0.61         | 5/1742 (0.3%)    | 0.69        | 0/2712            |
| All | All   | 0.63         | 49/318291 (0.0%) | 0.93        | 981/476619 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | 12    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | 1E    | 0                   | 2                   |
| 4   | 32    | 0                   | 3                   |
| 4   | 3E    | 0                   | 1                   |
| 6   | 5E    | 0                   | 1                   |
| 9   | 82    | 0                   | 1                   |
| 10  | 1A    | 0                   | 1                   |
| 11  | 2A    | 0                   | 1                   |
| 12  | 3A    | 0                   | 1                   |
| 13  | 4A    | 0                   | 1                   |
| 13  | 4I    | 0                   | 1                   |
| 14  | 5A    | 0                   | 1                   |
| 19  | AI    | 0                   | 2                   |
| 20  | BA    | 0                   | 3                   |
| 29  | 11    | 0                   | 2                   |
| 29  | 19    | 0                   | 5                   |
| 30  | 21    | 0                   | 4                   |
| 30  | 29    | 0                   | 5                   |
| 31  | 31    | 0                   | 1                   |
| 31  | 39    | 0                   | 4                   |
| 32  | 41    | 0                   | 1                   |
| 32  | 49    | 0                   | 1                   |
| 33  | 59    | 0                   | 1                   |
| 34  | 61    | 0                   | 4                   |
| 34  | 69    | 0                   | 1                   |
| 35  | 15    | 0                   | 1                   |
| 36  | 25    | 0                   | 1                   |
| 37  | 35    | 0                   | 3                   |
| 37  | 78    | 0                   | 2                   |
| 38  | 45    | 0                   | 5                   |
| 38  | 88    | 0                   | 3                   |
| 39  | 98    | 0                   | 1                   |
| 40  | 65    | 0                   | 1                   |
| 40  | A8    | 0                   | 2                   |
| 41  | 75    | 0                   | 2                   |
| 41  | B8    | 0                   | 2                   |
| 42  | 85    | 0                   | 3                   |
| 42  | C8    | 0                   | 2                   |
| 43  | 95    | 0                   | 1                   |
| 44  | A5    | 0                   | 2                   |
| 45  | B5    | 0                   | 2                   |
| 46  | C5    | 0                   | 3                   |
| 46  | G8    | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 47  | D5    | 0                   | 2                   |
| 47  | H8    | 0                   | 3                   |
| 48  | E5    | 0                   | 1                   |
| 48  | I8    | 0                   | 2                   |
| 49  | J8    | 0                   | 1                   |
| 50  | G5    | 0                   | 2                   |
| 50  | K8    | 0                   | 3                   |
| 52  | I5    | 0                   | 2                   |
| 52  | M8    | 0                   | 1                   |
| 53  | N8    | 0                   | 1                   |
| 55  | M5    | 0                   | 2                   |
| 55  | Q8    | 0                   | 7                   |
| All | All   | 0                   | 116                 |

The worst 5 of 49 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 56  | 2L    | 55  | U    | N1-C2 | 10.08 | 1.58        | 1.38     |
| 55  | Q8    | 6   | THR  | CA-CB | 8.64  | 1.66        | 1.53     |
| 23  | 2K    | 21  | U    | C5-C6 | 8.46  | 1.51        | 1.34     |
| 56  | 2L    | 21  | U    | C5-C6 | 8.25  | 1.50        | 1.34     |
| 24  | 3L    | 20  | U    | C5-C6 | 7.87  | 1.49        | 1.34     |

The worst 5 of 981 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 30  | 21    | 52  | LEU  | CA-C-N | 18.03 | 137.49      | 119.82   |
| 30  | 21    | 52  | LEU  | C-N-CA | 18.03 | 137.49      | 119.82   |
| 50  | K8    | 17  | SER  | N-CA-C | 17.39 | 123.78      | 108.13   |
| 29  | 19    | 235 | GLY  | N-CA-C | 16.73 | 129.10      | 112.04   |
| 51  | L8    | 11  | SER  | CA-C-N | 15.04 | 135.51      | 119.87   |

There are no chirality outliers.

5 of 116 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | 1E    | 15  | VAL  | Peptide |
| 2   | 1E    | 237 | ALA  | Peptide |
| 4   | 3E    | 31  | CYS  | Peptide |
| 13  | 4I    | 107 | ALA  | Peptide |
| 6   | 5E    | 41  | 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   | 13    | 32185 | 0        | 16244    | 1067    | 0            |
| 1   | 1G    | 32182 | 0        | 16244    | 1088    | 0            |
| 2   | 12    | 1924  | 0        | 1975     | 116     | 0            |
| 2   | 1E    | 1924  | 0        | 1975     | 131     | 0            |
| 3   | 22    | 1612  | 0        | 1677     | 114     | 0            |
| 3   | 2E    | 1605  | 0        | 1668     | 62      | 0            |
| 4   | 32    | 1702  | 0        | 1763     | 115     | 0            |
| 4   | 3E    | 1702  | 0        | 1762     | 112     | 0            |
| 5   | 42    | 1155  | 0        | 1213     | 85      | 0            |
| 5   | 4E    | 1155  | 0        | 1213     | 72      | 0            |
| 6   | 52    | 842   | 0        | 857      | 37      | 0            |
| 6   | 5E    | 842   | 0        | 857      | 49      | 0            |
| 7   | 62    | 1194  | 0        | 1234     | 59      | 0            |
| 7   | 6E    | 1256  | 0        | 1296     | 64      | 0            |
| 8   | 72    | 1115  | 0        | 1177     | 61      | 0            |
| 8   | 7E    | 1115  | 0        | 1177     | 69      | 0            |
| 9   | 82    | 1009  | 0        | 1037     | 79      | 0            |
| 9   | 8E    | 1009  | 0        | 1037     | 76      | 0            |
| 10  | 1A    | 522   | 0        | 530      | 32      | 0            |
| 10  | 1I    | 801   | 0        | 849      | 55      | 0            |
| 11  | 2A    | 864   | 0        | 881      | 53      | 0            |
| 11  | 2I    | 884   | 0        | 904      | 47      | 0            |
| 12  | 3A    | 956   | 0        | 1046     | 57      | 0            |
| 12  | 3I    | 956   | 0        | 1046     | 49      | 0            |
| 13  | 4A    | 933   | 0        | 992      | 61      | 0            |
| 13  | 4I    | 933   | 0        | 992      | 64      | 0            |
| 14  | 5A    | 418   | 0        | 456      | 35      | 0            |
| 14  | 5I    | 491   | 0        | 529      | 43      | 0            |
| 15  | 6A    | 733   | 0        | 771      | 41      | 0            |
| 15  | 6I    | 733   | 0        | 771      | 47      | 0            |
| 16  | 7A    | 705   | 0        | 725      | 36      | 0            |
| 16  | 7I    | 705   | 0        | 725      | 59      | 0            |
| 17  | 8A    | 823   | 0        | 891      | 28      | 0            |
| 17  | 8I    | 834   | 0        | 904      | 65      | 0            |
| 18  | 9A    | 590   | 0        | 662      | 28      | 0            |
| 18  | 9I    | 590   | 0        | 662      | 32      | 0            |
| 19  | AA    | 624   | 0        | 636      | 55      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | AI    | 647   | 0        | 665      | 50      | 0            |
| 20  | BA    | 762   | 0        | 861      | 44      | 0            |
| 20  | BI    | 762   | 0        | 861      | 52      | 0            |
| 21  | 1B    | 188   | 0        | 195      | 16      | 0            |
| 21  | 1F    | 217   | 0        | 234      | 10      | 0            |
| 22  | 1K    | 1497  | 0        | 770      | 36      | 0            |
| 23  | 2K    | 1646  | 0        | 845      | 36      | 0            |
| 24  | 3K    | 1627  | 0        | 838      | 64      | 0            |
| 24  | 3L    | 1627  | 0        | 838      | 79      | 0            |
| 25  | 4K    | 285   | 0        | 143      | 16      | 0            |
| 25  | 4L    | 197   | 0        | 99       | 6       | 0            |
| 26  | 14    | 61968 | 0        | 31239    | 1916    | 0            |
| 26  | 1H    | 62497 | 0        | 31504    | 1944    | 2            |
| 27  | 16    | 2617  | 0        | 1328     | 94      | 0            |
| 27  | 1J    | 2617  | 0        | 1328     | 123     | 0            |
| 28  | 71    | 737   | 0        | 743      | 65      | 0            |
| 29  | 11    | 2115  | 0        | 2195     | 131     | 0            |
| 29  | 19    | 2120  | 0        | 2197     | 129     | 0            |
| 30  | 21    | 1568  | 0        | 1634     | 111     | 0            |
| 30  | 29    | 1568  | 0        | 1634     | 139     | 0            |
| 31  | 31    | 1585  | 0        | 1632     | 115     | 0            |
| 31  | 39    | 1610  | 0        | 1655     | 146     | 0            |
| 32  | 41    | 1473  | 0        | 1535     | 109     | 0            |
| 32  | 49    | 1473  | 0        | 1535     | 102     | 0            |
| 33  | 51    | 1336  | 0        | 1418     | 98      | 0            |
| 33  | 59    | 1307  | 0        | 1382     | 96      | 0            |
| 34  | 61    | 1136  | 0        | 1223     | 72      | 0            |
| 34  | 69    | 1136  | 0        | 1223     | 61      | 0            |
| 35  | 15    | 1104  | 0        | 1180     | 57      | 0            |
| 35  | 58    | 1104  | 0        | 1180     | 80      | 0            |
| 36  | 25    | 932   | 0        | 996      | 64      | 0            |
| 36  | 68    | 932   | 0        | 996      | 49      | 0            |
| 37  | 35    | 1122  | 0        | 1206     | 129     | 0            |
| 37  | 78    | 1144  | 0        | 1228     | 119     | 0            |
| 38  | 45    | 1121  | 0        | 1179     | 95      | 0            |
| 38  | 88    | 1077  | 0        | 1121     | 82      | 0            |
| 39  | 55    | 959   | 0        | 1021     | 72      | 0            |
| 39  | 98    | 967   | 0        | 1033     | 78      | 0            |
| 40  | 65    | 881   | 0        | 943      | 76      | 0            |
| 40  | A8    | 881   | 0        | 943      | 72      | 0            |
| 41  | 75    | 1141  | 0        | 1202     | 71      | 0            |
| 41  | B8    | 1141  | 0        | 1202     | 81      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 42  | 85    | 963   | 0        | 1022     | 72      | 0            |
| 42  | C8    | 963   | 0        | 1022     | 68      | 0            |
| 43  | 95    | 778   | 0        | 852      | 84      | 0            |
| 43  | D8    | 778   | 0        | 852      | 60      | 0            |
| 44  | A5    | 886   | 0        | 948      | 43      | 0            |
| 44  | E8    | 899   | 0        | 964      | 51      | 0            |
| 45  | B5    | 725   | 0        | 778      | 34      | 0            |
| 45  | F8    | 742   | 0        | 803      | 49      | 0            |
| 46  | C5    | 794   | 0        | 884      | 70      | 0            |
| 46  | G8    | 791   | 0        | 881      | 65      | 0            |
| 47  | D5    | 1126  | 0        | 1154     | 94      | 0            |
| 47  | H8    | 1110  | 0        | 1141     | 76      | 0            |
| 48  | E5    | 612   | 0        | 633      | 44      | 0            |
| 48  | I8    | 626   | 0        | 642      | 43      | 0            |
| 49  | F5    | 737   | 0        | 813      | 39      | 0            |
| 49  | J8    | 762   | 0        | 848      | 43      | 0            |
| 50  | G5    | 558   | 0        | 610      | 27      | 1            |
| 50  | K8    | 563   | 0        | 612      | 55      | 0            |
| 51  | H5    | 468   | 0        | 518      | 15      | 1            |
| 51  | L8    | 452   | 0        | 503      | 29      | 0            |
| 52  | I5    | 515   | 0        | 514      | 64      | 0            |
| 52  | M8    | 533   | 0        | 526      | 52      | 0            |
| 53  | J5    | 434   | 0        | 454      | 32      | 0            |
| 53  | N8    | 422   | 0        | 440      | 28      | 0            |
| 54  | L5    | 398   | 0        | 441      | 27      | 0            |
| 54  | P8    | 409   | 0        | 454      | 15      | 0            |
| 55  | M5    | 477   | 0        | 540      | 50      | 0            |
| 55  | Q8    | 480   | 0        | 549      | 106     | 0            |
| 56  | 2L    | 1645  | 0        | 843      | 40      | 0            |
| 57  | 11    | 3     | 0        | 0        | 0       | 0            |
| 57  | 13    | 99    | 0        | 0        | 0       | 0            |
| 57  | 14    | 327   | 0        | 0        | 0       | 0            |
| 57  | 16    | 11    | 0        | 0        | 0       | 0            |
| 57  | 1G    | 72    | 0        | 0        | 0       | 0            |
| 57  | 1H    | 444   | 0        | 0        | 0       | 0            |
| 57  | 1J    | 3     | 0        | 0        | 0       | 0            |
| 57  | 25    | 1     | 0        | 0        | 0       | 0            |
| 57  | 29    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2K    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2L    | 2     | 0        | 0        | 0       | 0            |
| 57  | 35    | 1     | 0        | 0        | 0       | 0            |
| 57  | 3E    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | 3L    | 2     | 0        | 0        | 0       | 0            |
| 57  | 4I    | 2     | 0        | 0        | 0       | 0            |
| 57  | 45    | 1     | 0        | 0        | 0       | 0            |
| 57  | 4E    | 1     | 0        | 0        | 0       | 0            |
| 57  | 4I    | 1     | 0        | 0        | 0       | 0            |
| 57  | 55    | 1     | 0        | 0        | 0       | 0            |
| 57  | 68    | 2     | 0        | 0        | 0       | 0            |
| 57  | 78    | 2     | 0        | 0        | 0       | 0            |
| 57  | 88    | 1     | 0        | 0        | 0       | 0            |
| 57  | 98    | 1     | 0        | 0        | 0       | 0            |
| 57  | I8    | 2     | 0        | 0        | 0       | 0            |
| 57  | J8    | 2     | 0        | 0        | 0       | 0            |
| 57  | L8    | 1     | 0        | 0        | 0       | 0            |
| 57  | M5    | 1     | 0        | 0        | 0       | 0            |
| 57  | P8    | 1     | 0        | 0        | 0       | 0            |
| 58  | 32    | 1     | 0        | 0        | 0       | 0            |
| 58  | 3E    | 1     | 0        | 0        | 0       | 0            |
| 58  | 5A    | 1     | 0        | 0        | 0       | 0            |
| 58  | 5I    | 1     | 0        | 0        | 0       | 0            |
| 58  | C5    | 1     | 0        | 0        | 0       | 0            |
| 58  | G8    | 1     | 0        | 0        | 0       | 0            |
| 59  | 11    | 11    | 0        | 0        | 1       | 0            |
| 59  | 13    | 144   | 0        | 0        | 29      | 0            |
| 59  | 14    | 592   | 0        | 0        | 151     | 0            |
| 59  | 16    | 22    | 0        | 0        | 0       | 0            |
| 59  | 19    | 8     | 0        | 0        | 1       | 0            |
| 59  | 1G    | 48    | 0        | 0        | 9       | 0            |
| 59  | 1H    | 933   | 0        | 0        | 316     | 0            |
| 59  | 1I    | 1     | 0        | 0        | 0       | 0            |
| 59  | 21    | 3     | 0        | 0        | 1       | 0            |
| 59  | 25    | 6     | 0        | 0        | 1       | 0            |
| 59  | 29    | 5     | 0        | 0        | 2       | 0            |
| 59  | 2K    | 6     | 0        | 0        | 0       | 0            |
| 59  | 31    | 9     | 0        | 0        | 0       | 0            |
| 59  | 35    | 2     | 0        | 0        | 0       | 0            |
| 59  | 39    | 4     | 0        | 0        | 0       | 0            |
| 59  | 3E    | 2     | 0        | 0        | 1       | 0            |
| 59  | 3I    | 2     | 0        | 0        | 0       | 0            |
| 59  | 4K    | 2     | 0        | 0        | 0       | 0            |
| 59  | 55    | 3     | 0        | 0        | 2       | 0            |
| 59  | 5I    | 2     | 0        | 0        | 0       | 0            |
| 59  | 75    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 59  | 78    | 6      | 0        | 0        | 2       | 0            |
| 59  | A5    | 1      | 0        | 0        | 0       | 0            |
| 59  | D8    | 1      | 0        | 0        | 0       | 0            |
| 59  | F8    | 2      | 0        | 0        | 0       | 0            |
| 59  | G8    | 2      | 0        | 0        | 0       | 0            |
| 59  | H5    | 2      | 0        | 0        | 1       | 0            |
| 59  | I8    | 5      | 0        | 0        | 2       | 0            |
| 59  | J8    | 1      | 0        | 0        | 0       | 0            |
| 59  | L5    | 1      | 0        | 0        | 0       | 0            |
| 59  | L8    | 1      | 0        | 0        | 1       | 0            |
| 59  | M5    | 1      | 0        | 0        | 0       | 0            |
| 59  | P8    | 2      | 0        | 0        | 0       | 0            |
| 59  | Q8    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 295920 | 0        | 197803   | 11433   | 2            |

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 24.

The worst 5 of 11433 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) |
|-------------------|------------------|--------------------------|-------------------|
| 26:1H:270(L):U:H3 | 34:61:50:ARG:HG2 | 1.19                     | 1.06              |
| 26:1H:2714:G:OP2  | 59:1H:3574:HOH:O | 1.71                     | 1.06              |
| 26:1H:2781:A:H5'  | 26:1H:2782:G:H5' | 1.35                     | 1.06              |
| 26:1H:741:G:OP1   | 59:1H:3910:HOH:O | 1.74                     | 1.05              |
| 5:4E:99:GLY:H     | 5:4E:117:ASP:HB3 | 1.21                     | 1.04              |

All (2) 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) |
|--------------------|-------------------------|--------------------------|-------------------|
| 26:1H:654(H):G:O2' | 51:H5:55:ARG:NH2[2_464] | 2.11                     | 0.09              |
| 26:1H:277:C:O2'    | 50:G5:49:LYS:NZ[2_564]  | 2.16                     | 0.04              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | 12    | 205/220 (93%)  | 152 (74%) | 53 (26%) | 0           | 2  |
| 2   | 1E    | 205/220 (93%)  | 153 (75%) | 52 (25%) | 0           | 3  |
| 3   | 22    | 160/188 (85%)  | 122 (76%) | 38 (24%) | 1           | 4  |
| 3   | 2E    | 159/188 (85%)  | 124 (78%) | 35 (22%) | 1           | 5  |
| 4   | 32    | 180/181 (99%)  | 142 (79%) | 38 (21%) | 1           | 5  |
| 4   | 3E    | 180/181 (99%)  | 148 (82%) | 32 (18%) | 2           | 8  |
| 5   | 42    | 116/123 (94%)  | 76 (66%)  | 40 (34%) | 0           | 1  |
| 5   | 4E    | 116/123 (94%)  | 78 (67%)  | 38 (33%) | 0           | 1  |
| 6   | 52    | 90/90 (100%)   | 72 (80%)  | 18 (20%) | 1           | 6  |
| 6   | 5E    | 90/90 (100%)   | 70 (78%)  | 20 (22%) | 1           | 5  |
| 7   | 62    | 121/127 (95%)  | 93 (77%)  | 28 (23%) | 1           | 4  |
| 7   | 6E    | 126/127 (99%)  | 99 (79%)  | 27 (21%) | 1           | 5  |
| 8   | 72    | 119/119 (100%) | 89 (75%)  | 30 (25%) | 0           | 3  |
| 8   | 7E    | 119/119 (100%) | 91 (76%)  | 28 (24%) | 1           | 4  |
| 9   | 82    | 98/99 (99%)    | 82 (84%)  | 16 (16%) | 2           | 11 |
| 9   | 8E    | 98/99 (99%)    | 69 (70%)  | 29 (30%) | 0           | 1  |
| 10  | 1A    | 58/92 (63%)    | 44 (76%)  | 14 (24%) | 1           | 3  |
| 10  | 1I    | 89/92 (97%)    | 65 (73%)  | 24 (27%) | 0           | 2  |
| 11  | 2A    | 88/99 (89%)    | 69 (78%)  | 19 (22%) | 1           | 5  |
| 11  | 2I    | 90/99 (91%)    | 73 (81%)  | 17 (19%) | 1           | 7  |
| 12  | 3A    | 103/109 (94%)  | 75 (73%)  | 28 (27%) | 0           | 2  |
| 12  | 3I    | 103/109 (94%)  | 75 (73%)  | 28 (27%) | 0           | 2  |
| 13  | 4A    | 94/101 (93%)   | 61 (65%)  | 33 (35%) | 0           | 1  |
| 13  | 4I    | 94/101 (93%)   | 69 (73%)  | 25 (27%) | 0           | 2  |
| 14  | 5A    | 43/50 (86%)    | 33 (77%)  | 10 (23%) | 1           | 4  |
| 14  | 5I    | 49/50 (98%)    | 42 (86%)  | 7 (14%)  | 3           | 14 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 15  | 6A    | 79/80 (99%)    | 61 (77%)  | 18 (23%) | 1           | 4  |
| 15  | 6I    | 79/80 (99%)    | 68 (86%)  | 11 (14%) | 3           | 15 |
| 16  | 7A    | 72/74 (97%)    | 53 (74%)  | 19 (26%) | 0           | 2  |
| 16  | 7I    | 72/74 (97%)    | 57 (79%)  | 15 (21%) | 1           | 6  |
| 17  | 8A    | 94/97 (97%)    | 75 (80%)  | 19 (20%) | 1           | 6  |
| 17  | 8I    | 95/97 (98%)    | 71 (75%)  | 24 (25%) | 0           | 3  |
| 18  | 9A    | 63/77 (82%)    | 46 (73%)  | 17 (27%) | 0           | 2  |
| 18  | 9I    | 63/77 (82%)    | 49 (78%)  | 14 (22%) | 1           | 5  |
| 19  | AA    | 67/80 (84%)    | 52 (78%)  | 15 (22%) | 1           | 5  |
| 19  | AI    | 70/80 (88%)    | 42 (60%)  | 28 (40%) | 0           | 0  |
| 20  | BA    | 76/82 (93%)    | 64 (84%)  | 12 (16%) | 2           | 12 |
| 20  | BI    | 76/82 (93%)    | 54 (71%)  | 22 (29%) | 0           | 2  |
| 21  | 1B    | 17/22 (77%)    | 16 (94%)  | 1 (6%)   | 18          | 46 |
| 21  | 1F    | 20/22 (91%)    | 19 (95%)  | 1 (5%)   | 22          | 50 |
| 28  | 7I    | 77/181 (42%)   | 56 (73%)  | 21 (27%) | 0           | 2  |
| 29  | 11    | 214/218 (98%)  | 159 (74%) | 55 (26%) | 0           | 2  |
| 29  | 19    | 214/218 (98%)  | 151 (71%) | 63 (29%) | 0           | 2  |
| 30  | 21    | 165/166 (99%)  | 121 (73%) | 44 (27%) | 0           | 2  |
| 30  | 29    | 165/166 (99%)  | 125 (76%) | 40 (24%) | 1           | 3  |
| 31  | 31    | 161/166 (97%)  | 115 (71%) | 46 (29%) | 0           | 2  |
| 31  | 39    | 163/166 (98%)  | 119 (73%) | 44 (27%) | 0           | 2  |
| 32  | 41    | 155/156 (99%)  | 111 (72%) | 44 (28%) | 0           | 2  |
| 32  | 49    | 155/156 (99%)  | 111 (72%) | 44 (28%) | 0           | 2  |
| 33  | 51    | 145/148 (98%)  | 105 (72%) | 40 (28%) | 0           | 2  |
| 33  | 59    | 142/148 (96%)  | 104 (73%) | 38 (27%) | 0           | 2  |
| 34  | 61    | 122/124 (98%)  | 86 (70%)  | 36 (30%) | 0           | 2  |
| 34  | 69    | 122/124 (98%)  | 82 (67%)  | 40 (33%) | 0           | 1  |
| 35  | 15    | 117/119 (98%)  | 91 (78%)  | 26 (22%) | 1           | 5  |
| 35  | 58    | 117/119 (98%)  | 85 (73%)  | 32 (27%) | 0           | 2  |
| 36  | 25    | 100/100 (100%) | 67 (67%)  | 33 (33%) | 0           | 1  |
| 36  | 68    | 100/100 (100%) | 74 (74%)  | 26 (26%) | 0           | 2  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 37  | 35    | 114/116 (98%)  | 67 (59%)  | 47 (41%) | 0           | 0 |
| 37  | 78    | 116/116 (100%) | 74 (64%)  | 42 (36%) | 0           | 1 |
| 38  | 45    | 111/111 (100%) | 82 (74%)  | 29 (26%) | 0           | 2 |
| 38  | 88    | 103/111 (93%)  | 72 (70%)  | 31 (30%) | 0           | 1 |
| 39  | 55    | 100/101 (99%)  | 71 (71%)  | 29 (29%) | 0           | 2 |
| 39  | 98    | 101/101 (100%) | 74 (73%)  | 27 (27%) | 0           | 2 |
| 40  | 65    | 87/88 (99%)    | 67 (77%)  | 20 (23%) | 1           | 4 |
| 40  | A8    | 87/88 (99%)    | 58 (67%)  | 29 (33%) | 0           | 1 |
| 41  | 75    | 120/127 (94%)  | 81 (68%)  | 39 (32%) | 0           | 1 |
| 41  | B8    | 120/127 (94%)  | 82 (68%)  | 38 (32%) | 0           | 1 |
| 42  | 85    | 93/94 (99%)    | 69 (74%)  | 24 (26%) | 0           | 2 |
| 42  | C8    | 93/94 (99%)    | 74 (80%)  | 19 (20%) | 1           | 6 |
| 43  | 95    | 82/82 (100%)   | 52 (63%)  | 30 (37%) | 0           | 1 |
| 43  | D8    | 82/82 (100%)   | 58 (71%)  | 24 (29%) | 0           | 2 |
| 44  | A5    | 91/92 (99%)    | 61 (67%)  | 30 (33%) | 0           | 1 |
| 44  | E8    | 92/92 (100%)   | 64 (70%)  | 28 (30%) | 0           | 1 |
| 45  | B5    | 74/78 (95%)    | 52 (70%)  | 22 (30%) | 0           | 1 |
| 45  | F8    | 76/78 (97%)    | 50 (66%)  | 26 (34%) | 0           | 1 |
| 46  | C5    | 85/91 (93%)    | 60 (71%)  | 25 (29%) | 0           | 2 |
| 46  | G8    | 85/91 (93%)    | 55 (65%)  | 30 (35%) | 0           | 1 |
| 47  | D5    | 126/179 (70%)  | 94 (75%)  | 32 (25%) | 0           | 3 |
| 47  | H8    | 124/179 (69%)  | 93 (75%)  | 31 (25%) | 0           | 3 |
| 48  | E5    | 62/67 (92%)    | 45 (73%)  | 17 (27%) | 0           | 2 |
| 48  | I8    | 61/67 (91%)    | 41 (67%)  | 20 (33%) | 0           | 1 |
| 49  | F5    | 79/83 (95%)    | 52 (66%)  | 27 (34%) | 0           | 1 |
| 49  | J8    | 82/83 (99%)    | 57 (70%)  | 25 (30%) | 0           | 1 |
| 50  | G5    | 62/67 (92%)    | 40 (64%)  | 22 (36%) | 0           | 1 |
| 50  | K8    | 62/67 (92%)    | 42 (68%)  | 20 (32%) | 0           | 1 |
| 51  | H5    | 51/52 (98%)    | 36 (71%)  | 15 (29%) | 0           | 2 |
| 51  | L8    | 49/52 (94%)    | 31 (63%)  | 18 (37%) | 0           | 1 |
| 52  | I5    | 57/63 (90%)    | 42 (74%)  | 15 (26%) | 0           | 2 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|------------------|------------|------------|-------------|---|
| 52  | M8    | 59/63 (94%)      | 41 (70%)   | 18 (30%)   | 0           | 1 |
| 53  | J5    | 48/52 (92%)      | 35 (73%)   | 13 (27%)   | 0           | 2 |
| 53  | N8    | 47/52 (90%)      | 34 (72%)   | 13 (28%)   | 0           | 2 |
| 54  | L5    | 39/42 (93%)      | 27 (69%)   | 12 (31%)   | 0           | 1 |
| 54  | P8    | 40/42 (95%)      | 32 (80%)   | 8 (20%)    | 1           | 6 |
| 55  | M5    | 49/55 (89%)      | 33 (67%)   | 16 (33%)   | 0           | 1 |
| 55  | Q8    | 50/55 (91%)      | 31 (62%)   | 19 (38%)   | 0           | 0 |
| All | All   | 9429/10075 (94%) | 6884 (73%) | 2545 (27%) | 0           | 2 |

5 of 2545 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | 29    | 200 | GLU  |
| 43  | 95    | 83  | ARG  |
| 32  | 49    | 34  | LEU  |
| 30  | 29    | 188 | VAL  |
| 36  | 25    | 117 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 69    | 104 | GLN  |
| 45  | B5    | 41  | ASN  |
| 35  | 15    | 56  | ASN  |
| 38  | 45    | 45  | GLN  |
| 53  | J5    | 23  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 13    | 1495/1522 (98%) | 397 (26%)         | 38 (2%)         |
| 1   | 1G    | 1495/1522 (98%) | 398 (26%)         | 36 (2%)         |
| 22  | 1K    | 65/77 (84%)     | 28 (43%)          | 3 (4%)          |
| 23  | 2K    | 76/77 (98%)     | 16 (21%)          | 1 (1%)          |
| 24  | 3K    | 76/76 (100%)    | 35 (46%)          | 6 (7%)          |
| 24  | 3L    | 75/76 (98%)     | 39 (52%)          | 2 (2%)          |
| 25  | 4K    | 12/27 (44%)     | 2 (16%)           | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 25  | 4L    | 9/27 (33%)      | 4 (44%)           | 1 (11%)         |
| 26  | 14    | 2874/2917 (98%) | 805 (28%)         | 48 (1%)         |
| 26  | 1H    | 2901/2917 (99%) | 739 (25%)         | 52 (1%)         |
| 27  | 16    | 121/122 (99%)   | 25 (20%)          | 0               |
| 27  | 1J    | 121/122 (99%)   | 39 (32%)          | 1 (0%)          |
| 56  | 2L    | 76/77 (98%)     | 22 (28%)          | 3 (3%)          |
| All | All   | 9396/9559 (98%) | 2549 (27%)        | 191 (2%)        |

5 of 2549 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 13    | 5   | U    |
| 1   | 13    | 6   | G    |
| 1   | 13    | 7   | G    |
| 1   | 13    | 8   | A    |
| 1   | 13    | 9   | G    |

5 of 191 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1G    | 632  | A    |
| 26  | 14    | 49   | A    |
| 1   | 1G    | 913  | A    |
| 1   | 1G    | 1300 | G    |
| 26  | 14    | 573  | G    |

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

23 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 | $\# Z  > 2$ |
| 24  | MIA  | 3L    | 37  | 24   | 28,31,32     | 2.56 | 4 (14%)     | 38,44,47    | 3.16 | 17 (44%)    |
| 24  | 7MG  | 3K    | 46  | 24   | 23,26,27     | 2.96 | 7 (30%)     | 27,39,42    | 2.92 | 9 (33%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | 4SU  | 3L    | 8   | 24   | 18,21,22     | 1.97 | 4 (22%)  | 25,30,33    | 2.02 | 5 (20%)  |
| 24  | 7MG  | 3L    | 46  | 24   | 23,26,27     | 3.20 | 8 (34%)  | 27,39,42    | 2.82 | 9 (33%)  |
| 24  | 4SU  | 3K    | 8   | 24   | 18,21,22     | 1.92 | 3 (16%)  | 25,30,33    | 2.51 | 5 (20%)  |
| 23  | OMC  | 2K    | 33  | 23   | 19,22,23     | 1.82 | 3 (15%)  | 25,31,34    | 0.94 | 1 (4%)   |
| 24  | PSU  | 3L    | 32  | 24   | 18,21,22     | 1.31 | 1 (5%)   | 21,30,33    | 1.58 | 2 (9%)   |
| 23  | 5MU  | 2K    | 55  | 23   | 19,22,23     | 3.82 | 5 (26%)  | 27,32,35    | 3.18 | 10 (37%) |
| 56  | OMC  | 2L    | 33  | 56   | 19,22,23     | 1.76 | 3 (15%)  | 25,31,34    | 1.12 | 3 (12%)  |
| 24  | PSU  | 3L    | 39  | 24   | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.76 | 4 (19%)  |
| 24  | PSU  | 3K    | 32  | 24   | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.76 | 4 (19%)  |
| 22  | OMC  | 1K    | 33  | 22   | 19,22,23     | 1.71 | 3 (15%)  | 25,31,34    | 0.77 | 0        |
| 22  | 5MU  | 1K    | 55  | 22   | 19,22,23     | 3.91 | 5 (26%)  | 27,32,35    | 3.31 | 10 (37%) |
| 24  | PSU  | 3K    | 39  | 24   | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.84 | 4 (19%)  |
| 24  | MIA  | 3K    | 37  | 24   | 28,31,32     | 2.33 | 4 (14%)  | 38,44,47    | 3.33 | 13 (34%) |
| 56  | 4SU  | 2L    | 8   | 56   | 18,21,22     | 1.98 | 5 (27%)  | 25,30,33    | 2.74 | 6 (24%)  |
| 24  | PSU  | 3L    | 55  | 24   | 18,21,22     | 1.19 | 1 (5%)   | 21,30,33    | 1.75 | 3 (14%)  |
| 23  | 4SU  | 2K    | 8   | 23   | 18,21,22     | 1.70 | 4 (22%)  | 25,30,33    | 3.22 | 5 (20%)  |
| 24  | PSU  | 3K    | 55  | 24   | 18,21,22     | 1.18 | 1 (5%)   | 21,30,33    | 2.15 | 7 (33%)  |
| 56  | 7MG  | 2L    | 47  | 56   | 23,26,27     | 2.96 | 8 (34%)  | 27,39,42    | 2.90 | 9 (33%)  |
| 56  | PSU  | 2L    | 56  | 56   | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 1.85 | 4 (19%)  |
| 23  | PSU  | 2K    | 56  | 23   | 18,21,22     | 1.28 | 2 (11%)  | 21,30,33    | 2.36 | 5 (23%)  |
| 23  | 7MG  | 2K    | 47  | 23   | 23,26,27     | 2.88 | 8 (34%)  | 27,39,42    | 2.94 | 9 (33%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 24  | MIA  | 3L    | 37  | 24   | -       | 7/15/33/34 | 0/3/3/3 |
| 24  | 7MG  | 3K    | 46  | 24   | -       | 2/7/37/38  | 0/3/3/3 |
| 24  | 4SU  | 3L    | 8   | 24   | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | 7MG  | 3L    | 46  | 24   | -       | 2/7/37/38  | 0/3/3/3 |
| 24  | 4SU  | 3K    | 8   | 24   | -       | 5/7/25/26  | 0/2/2/2 |
| 23  | OMC  | 2K    | 33  | 23   | -       | 1/9/27/28  | 0/2/2/2 |
| 24  | PSU  | 3L    | 32  | 24   | -       | 1/7/25/26  | 0/2/2/2 |
| 23  | 5MU  | 2K    | 55  | 23   | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | OMC  | 2L    | 33  | 56   | -       | 0/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 24  | PSU  | 3L    | 39  | 24   | -       | 2/7/25/26  | 0/2/2/2 |
| 24  | PSU  | 3K    | 32  | 24   | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | OMC  | 1K    | 33  | 22   | -       | 0/9/27/28  | 0/2/2/2 |
| 22  | 5MU  | 1K    | 55  | 22   | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | PSU  | 3K    | 39  | 24   | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | MIA  | 3K    | 37  | 24   | -       | 6/15/33/34 | 0/3/3/3 |
| 56  | 4SU  | 2L    | 8   | 56   | -       | 2/7/25/26  | 0/2/2/2 |
| 24  | PSU  | 3L    | 55  | 24   | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | 4SU  | 2K    | 8   | 23   | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | PSU  | 3K    | 55  | 24   | -       | 3/7/25/26  | 0/2/2/2 |
| 56  | 7MG  | 2L    | 47  | 56   | -       | 3/7/37/38  | 0/3/3/3 |
| 56  | PSU  | 2L    | 56  | 56   | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | PSU  | 2K    | 56  | 23   | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | 7MG  | 2K    | 47  | 23   | -       | 2/7/37/38  | 0/3/3/3 |

The worst 5 of 84 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 1K    | 55  | 5MU  | C2-N1   | 12.61 | 1.58        | 1.38     |
| 23  | 2K    | 55  | 5MU  | C2-N1   | 12.01 | 1.57        | 1.38     |
| 24  | 3L    | 46  | 7MG  | C5-N7   | 8.67  | 1.46        | 1.35     |
| 24  | 3K    | 37  | MIA  | C13-C14 | 8.33  | 1.57        | 1.32     |
| 24  | 3L    | 37  | MIA  | C13-C14 | 8.30  | 1.57        | 1.32     |

The worst 5 of 144 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 22  | 1K    | 55  | 5MU  | C5-C4-N3    | 11.44  | 125.26      | 115.32   |
| 24  | 3K    | 37  | MIA  | C11-S10-C2  | 11.35  | 110.77      | 102.25   |
| 23  | 2K    | 8   | 4SU  | C4-N3-C2    | -10.09 | 117.64      | 127.31   |
| 24  | 3K    | 37  | MIA  | C12-C13-C14 | -10.07 | 108.93      | 127.01   |
| 23  | 2K    | 8   | 4SU  | C5-C4-N3    | 9.49   | 123.58      | 114.75   |

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | 2K    | 33  | OMC  | C1'-C2'-O2'-CM2 |
| 24  | 3K    | 8   | 4SU  | C2'-C1'-N1-C2   |
| 24  | 3K    | 8   | 4SU  | C2'-C1'-N1-C6   |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 24  | 3K    | 37  | MIA  | C5-C6-N6-C12  |
| 24  | 3K    | 37  | MIA  | N1-C2-S10-C11 |

There are no ring outliers.

15 monomers are involved in 29 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | 3L    | 37  | MIA  | 2       | 0            |
| 24  | 3K    | 46  | 7MG  | 2       | 0            |
| 24  | 3L    | 8   | 4SU  | 5       | 0            |
| 24  | 3K    | 8   | 4SU  | 1       | 0            |
| 23  | 2K    | 33  | OMC  | 2       | 0            |
| 56  | 2L    | 33  | OMC  | 1       | 0            |
| 24  | 3K    | 39  | PSU  | 2       | 0            |
| 24  | 3K    | 37  | MIA  | 2       | 0            |
| 56  | 2L    | 8   | 4SU  | 1       | 0            |
| 24  | 3L    | 55  | PSU  | 1       | 0            |
| 23  | 2K    | 8   | 4SU  | 1       | 0            |
| 24  | 3K    | 55  | PSU  | 2       | 0            |
| 56  | 2L    | 47  | 7MG  | 2       | 0            |
| 56  | 2L    | 56  | PSU  | 2       | 0            |
| 23  | 2K    | 47  | 7MG  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 995 ligands modelled in this entry, 995 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 22  | 1K    | 1                |
| 56  | 2L    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 1K    | 69:C      | O3'    | 70:C      | P      | 5.53         |
| 1     | 2L    | 54:G      | O3'    | 55:U      | P      | 2.94         |

## 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   | 13    | 1497/1522 (98%) | -0.59  | 3 (0%) 91 86 | 70, 114, 187, 287     | 0     |
| 1   | 1G    | 1497/1522 (98%) | -0.55  | 3 (0%) 91 86 | 79, 129, 197, 297     | 0     |
| 2   | 12    | 237/256 (92%)   | 0.10   | 5 (2%) 63 44 | 143, 175, 203, 210    | 0     |
| 2   | 1E    | 237/256 (92%)   | -0.11  | 1 (0%) 88 79 | 124, 155, 178, 191    | 0     |
| 3   | 22    | 206/239 (86%)   | -0.12  | 2 (0%) 79 63 | 132, 155, 182, 195    | 0     |
| 3   | 2E    | 205/239 (85%)   | -0.19  | 0 100 100    | 101, 124, 154, 164    | 0     |
| 4   | 32    | 208/209 (99%)   | 0.06   | 1 (0%) 87 76 | 118, 137, 157, 163    | 0     |
| 4   | 3E    | 208/209 (99%)   | -0.06  | 2 (0%) 79 63 | 100, 127, 145, 153    | 0     |
| 5   | 42    | 151/162 (93%)   | 0.00   | 4 (2%) 57 38 | 115, 132, 153, 171    | 0     |
| 5   | 4E    | 151/162 (93%)   | -0.01  | 3 (1%) 65 46 | 93, 117, 136, 166     | 0     |
| 6   | 52    | 101/101 (100%)  | -0.59  | 0 100 100    | 102, 116, 134, 144    | 0     |
| 6   | 5E    | 101/101 (100%)  | -0.44  | 0 100 100    | 89, 112, 132, 144     | 0     |
| 7   | 62    | 147/156 (94%)   | -0.29  | 1 (0%) 84 70 | 122, 138, 151, 165    | 0     |
| 7   | 6E    | 155/156 (99%)   | -0.20  | 3 (1%) 66 48 | 108, 123, 152, 169    | 0     |
| 8   | 72    | 138/138 (100%)  | 0.08   | 3 (2%) 62 43 | 111, 137, 150, 157    | 0     |
| 8   | 7E    | 138/138 (100%)  | -0.11  | 3 (2%) 62 43 | 107, 122, 136, 144    | 0     |
| 9   | 82    | 127/128 (99%)   | 0.31   | 7 (5%) 30 21 | 125, 161, 179, 186    | 0     |
| 9   | 8E    | 127/128 (99%)   | 0.05   | 3 (2%) 59 40 | 98, 142, 161, 174     | 0     |
| 10  | 1A    | 66/105 (62%)    | 0.70   | 8 (12%) 8 7  | 130, 158, 176, 188    | 0     |
| 10  | 1I    | 99/105 (94%)    | -0.01  | 0 100 100    | 98, 147, 178, 183     | 0     |
| 11  | 2A    | 116/129 (89%)   | -0.17  | 2 (1%) 69 50 | 103, 124, 142, 169    | 0     |
| 11  | 2I    | 119/129 (92%)   | 0.04   | 8 (6%) 24 16 | 85, 112, 156, 180     | 0     |
| 12  | 3A    | 122/132 (92%)   | -0.11  | 2 (1%) 70 52 | 97, 113, 129, 145     | 0     |
| 12  | 3I    | 122/132 (92%)   | -0.26  | 0 100 100    | 83, 93, 119, 143      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------|-----|-----|-----------------------|-------|
| 13  | 4A    | 117/126 (92%)   | -0.03  | 6 (5%)  | 33  | 22  | 125, 155, 178, 192    | 0     |
| 13  | 4I    | 117/126 (92%)   | 0.10   | 5 (4%)  | 40  | 25  | 95, 131, 145, 162     | 0     |
| 14  | 5A    | 52/61 (85%)     | 0.72   | 3 (5%)  | 29  | 19  | 138, 151, 163, 167    | 0     |
| 14  | 5I    | 60/61 (98%)     | 0.02   | 0       | 100 | 100 | 101, 113, 127, 134    | 0     |
| 15  | 6A    | 88/89 (98%)     | -0.23  | 0       | 100 | 100 | 99, 120, 141, 148     | 0     |
| 15  | 6I    | 88/89 (98%)     | -0.17  | 0       | 100 | 100 | 87, 110, 128, 134     | 0     |
| 16  | 7A    | 84/88 (95%)     | -0.16  | 0       | 100 | 100 | 108, 123, 139, 168    | 0     |
| 16  | 7I    | 84/88 (95%)     | 0.47   | 5 (5%)  | 27  | 19  | 113, 127, 155, 174    | 0     |
| 17  | 8A    | 99/105 (94%)    | -0.26  | 0       | 100 | 100 | 101, 116, 131, 136    | 0     |
| 17  | 8I    | 100/105 (95%)   | -0.13  | 2 (2%)  | 65  | 46  | 100, 117, 127, 131    | 0     |
| 18  | 9A    | 72/88 (81%)     | -0.54  | 0       | 100 | 100 | 109, 130, 167, 194    | 0     |
| 18  | 9I    | 72/88 (81%)     | -0.39  | 0       | 100 | 100 | 96, 115, 152, 185     | 0     |
| 19  | AA    | 78/93 (83%)     | 0.09   | 3 (3%)  | 44  | 30  | 137, 178, 195, 198    | 0     |
| 19  | AI    | 81/93 (87%)     | -0.01  | 2 (2%)  | 58  | 39  | 107, 129, 146, 157    | 0     |
| 20  | BA    | 99/106 (93%)    | -0.10  | 2 (2%)  | 65  | 46  | 104, 122, 141, 156    | 0     |
| 20  | BI    | 99/106 (93%)    | 0.07   | 2 (2%)  | 65  | 46  | 120, 135, 156, 164    | 0     |
| 21  | 1B    | 22/27 (81%)     | 1.17   | 4 (18%) | 3   | 3   | 122, 142, 149, 152    | 0     |
| 21  | 1F    | 25/27 (92%)     | 0.40   | 1 (4%)  | 42  | 28  | 106, 118, 135, 147    | 0     |
| 22  | 1K    | 68/77 (88%)     | -0.37  | 1 (1%)  | 72  | 53  | 117, 196, 214, 216    | 0     |
| 23  | 2K    | 72/77 (93%)     | -0.79  | 0       | 100 | 100 | 80, 108, 138, 146     | 0     |
| 24  | 3K    | 70/76 (92%)     | -0.32  | 0       | 100 | 100 | 83, 231, 262, 266     | 0     |
| 24  | 3L    | 70/76 (92%)     | -0.13  | 1 (1%)  | 73  | 55  | 96, 239, 268, 279     | 0     |
| 25  | 4K    | 13/27 (48%)     | -0.02  | 1 (7%)  | 19  | 14  | 83, 115, 170, 170     | 0     |
| 25  | 4L    | 9/27 (33%)      | 0.65   | 1 (11%) | 10  | 9   | 100, 136, 151, 157    | 0     |
| 26  | 14    | 2877/2917 (98%) | -0.78  | 2 (0%)  | 92  | 90  | 62, 96, 237, 329      | 0     |
| 26  | 1H    | 2902/2917 (99%) | -0.90  | 1 (0%)  | 100 | 100 | 50, 81, 226, 314      | 0     |
| 27  | 16    | 122/122 (100%)  | -0.93  | 0       | 100 | 100 | 76, 99, 116, 199      | 0     |
| 27  | 1J    | 122/122 (100%)  | -0.43  | 1 (0%)  | 82  | 68  | 98, 136, 162, 199     | 0     |
| 28  | 7I    | 93/229 (40%)    | 0.13   | 1 (1%)  | 78  | 60  | 109, 115, 131, 143    | 0     |
| 29  | 11    | 272/276 (98%)   | -0.24  | 1 (0%)  | 88  | 79  | 52, 71, 87, 95        | 0     |
| 29  | 19    | 273/276 (98%)   | -0.21  | 4 (1%)  | 72  | 53  | 60, 83, 100, 111      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 30  | 21    | 205/206 (99%)  | -0.07  | 5 (2%) 59 40  | 59, 95, 137, 152      | 0     |
| 30  | 29    | 205/206 (99%)  | -0.09  | 3 (1%) 72 53  | 70, 104, 144, 178     | 0     |
| 31  | 31    | 202/210 (96%)  | -0.41  | 0 100 100     | 55, 84, 120, 142      | 0     |
| 31  | 39    | 206/210 (98%)  | -0.23  | 0 100 100     | 70, 110, 163, 190     | 0     |
| 32  | 41    | 181/182 (99%)  | -0.09  | 5 (2%) 55 36  | 85, 110, 141, 149     | 0     |
| 32  | 49    | 181/182 (99%)  | 0.10   | 6 (3%) 49 33  | 133, 152, 174, 187    | 0     |
| 33  | 51    | 174/180 (96%)  | -0.24  | 1 (0%) 85 73  | 88, 108, 123, 136     | 0     |
| 33  | 59    | 170/180 (94%)  | 0.35   | 12 (7%) 22 15 | 131, 193, 221, 241    | 0     |
| 34  | 61    | 146/148 (98%)  | -0.28  | 0 100 100     | 81, 135, 151, 154     | 0     |
| 34  | 69    | 146/148 (98%)  | 0.04   | 5 (3%) 48 32  | 97, 138, 155, 163     | 0     |
| 35  | 15    | 138/140 (98%)  | 0.10   | 2 (1%) 73 55  | 87, 114, 146, 168     | 0     |
| 35  | 58    | 138/140 (98%)  | -0.22  | 0 100 100     | 73, 95, 129, 147      | 0     |
| 36  | 25    | 122/122 (100%) | -0.36  | 0 100 100     | 75, 96, 112, 124      | 0     |
| 36  | 68    | 122/122 (100%) | -0.39  | 1 (0%) 82 68  | 65, 85, 103, 115      | 0     |
| 37  | 35    | 147/150 (98%)  | 0.07   | 8 (5%) 31 21  | 70, 114, 145, 159     | 0     |
| 37  | 78    | 150/150 (100%) | -0.12  | 2 (1%) 75 56  | 57, 85, 111, 159      | 0     |
| 38  | 45    | 141/141 (100%) | 0.05   | 6 (4%) 40 25  | 80, 111, 139, 153     | 0     |
| 38  | 88    | 137/141 (97%)  | -0.23  | 1 (0%) 84 70  | 63, 84, 103, 146      | 0     |
| 39  | 55    | 117/118 (99%)  | -0.27  | 2 (1%) 69 50  | 69, 88, 105, 121      | 0     |
| 39  | 98    | 118/118 (100%) | -0.20  | 0 100 100     | 70, 91, 111, 121      | 0     |
| 40  | 65    | 111/112 (99%)  | 0.08   | 3 (2%) 56 37  | 104, 128, 140, 146    | 0     |
| 40  | A8    | 111/112 (99%)  | -0.23  | 0 100 100     | 81, 95, 120, 129      | 0     |
| 41  | 75    | 137/146 (93%)  | -0.15  | 2 (1%) 72 53  | 86, 104, 164, 200     | 0     |
| 41  | B8    | 137/146 (93%)  | -0.21  | 2 (1%) 72 53  | 80, 99, 151, 186      | 0     |
| 42  | 85    | 117/118 (99%)  | -0.01  | 1 (0%) 81 65  | 76, 103, 142, 163     | 0     |
| 42  | C8    | 117/118 (99%)  | -0.02  | 2 (1%) 69 50  | 63, 83, 117, 136      | 0     |
| 43  | 95    | 101/101 (100%) | -0.02  | 0 100 100     | 72, 129, 143, 161     | 0     |
| 43  | D8    | 101/101 (100%) | -0.15  | 0 100 100     | 63, 108, 131, 145     | 0     |
| 44  | A5    | 111/113 (98%)  | -0.27  | 0 100 100     | 69, 83, 117, 151      | 0     |
| 44  | E8    | 113/113 (100%) | -0.20  | 0 100 100     | 66, 80, 116, 158      | 0     |
| 45  | B5    | 92/96 (95%)    | -0.14  | 3 (3%) 49 33  | 78, 94, 113, 133      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 45  | F8    | 94/96 (97%)       | -0.34  | 0 100 100      | 65, 77, 101, 118      | 0     |
| 46  | C5    | 104/110 (94%)     | 0.16   | 4 (3%) 44 30   | 98, 120, 152, 163     | 0     |
| 46  | G8    | 104/110 (94%)     | 0.04   | 2 (1%) 66 48   | 76, 98, 132, 143      | 0     |
| 47  | D5    | 137/206 (66%)     | -0.18  | 2 (1%) 72 53   | 118, 147, 190, 205    | 0     |
| 47  | H8    | 135/206 (65%)     | -0.28  | 0 100 100      | 89, 115, 161, 182     | 0     |
| 48  | E5    | 77/85 (90%)       | 0.20   | 1 (1%) 75 56   | 81, 97, 115, 148      | 0     |
| 48  | I8    | 80/85 (94%)       | -0.14  | 2 (2%) 58 39   | 66, 78, 106, 122      | 0     |
| 49  | F5    | 94/98 (95%)       | 0.09   | 1 (1%) 78 60   | 72, 94, 135, 145      | 0     |
| 49  | J8    | 97/98 (98%)       | -0.32  | 1 (1%) 79 63   | 60, 79, 122, 155      | 0     |
| 50  | G5    | 66/72 (91%)       | -0.15  | 0 100 100      | 95, 113, 128, 155     | 0     |
| 50  | K8    | 67/72 (93%)       | -0.34  | 0 100 100      | 70, 89, 107, 139      | 0     |
| 51  | H5    | 59/60 (98%)       | -0.31  | 0 100 100      | 87, 104, 146, 161     | 0     |
| 51  | L8    | 57/60 (95%)       | -0.57  | 0 100 100      | 70, 86, 105, 121      | 0     |
| 52  | I5    | 63/71 (88%)       | -0.27  | 0 100 100      | 163, 192, 207, 213    | 0     |
| 52  | M8    | 66/71 (92%)       | 0.18   | 1 (1%) 72 53   | 120, 156, 195, 205    | 0     |
| 53  | J5    | 56/60 (93%)       | -0.13  | 0 100 100      | 69, 94, 139, 149      | 0     |
| 53  | N8    | 54/60 (90%)       | -0.13  | 0 100 100      | 62, 100, 155, 165     | 0     |
| 54  | L5    | 46/49 (93%)       | -0.41  | 1 (2%) 62 43   | 61, 71, 82, 95        | 0     |
| 54  | P8    | 47/49 (95%)       | -0.40  | 0 100 100      | 53, 60, 76, 85        | 0     |
| 55  | M5    | 60/65 (92%)       | 0.29   | 2 (3%) 49 33   | 78, 90, 114, 129      | 0     |
| 55  | Q8    | 60/65 (92%)       | 0.61   | 5 (8%) 17 13   | 64, 77, 102, 113      | 0     |
| 56  | 2L    | 73/77 (94%)       | -0.85  | 0 100 100      | 91, 123, 156, 173     | 0     |
| All | All   | 20765/21734 (95%) | -0.38  | 207 (0%) 79 63 | 50, 110, 186, 329     | 0     |

The worst 5 of 207 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 41  | B8    | 1   | MET  | 6.5  |
| 11  | 2I    | 127 | LYS  | 6.1  |
| 24  | 3L    | 34  | G    | 5.7  |
| 32  | 41    | 26  | GLN  | 5.4  |
| 11  | 2I    | 129 | SER  | 5.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 24  | PSU  | 3L    | 55  | 20/21 | 0.42 | 0.09 | 244,253,256,256            | 0     |
| 24  | PSU  | 3K    | 55  | 20/21 | 0.59 | 0.08 | 233,248,253,253            | 0     |
| 24  | 7MG  | 3K    | 46  | 24/25 | 0.59 | 0.09 | 234,242,250,254            | 0     |
| 24  | 7MG  | 3L    | 46  | 24/25 | 0.60 | 0.10 | 242,245,250,252            | 0     |
| 24  | 4SU  | 3K    | 8   | 20/21 | 0.64 | 0.10 | 240,248,252,254            | 0     |
| 24  | PSU  | 3L    | 32  | 20/21 | 0.66 | 0.14 | 165,176,183,185            | 0     |
| 24  | PSU  | 3L    | 39  | 20/21 | 0.76 | 0.10 | 156,173,181,188            | 0     |
| 22  | 5MU  | 1K    | 55  | 21/22 | 0.79 | 0.09 | 147,158,168,170            | 0     |
| 24  | 4SU  | 3L    | 8   | 20/21 | 0.83 | 0.07 | 239,245,250,250            | 0     |
| 24  | MIA  | 3L    | 37  | 29/30 | 0.84 | 0.14 | 158,185,200,208            | 0     |
| 24  | PSU  | 3K    | 39  | 20/21 | 0.85 | 0.08 | 126,143,151,159            | 0     |
| 24  | MIA  | 3K    | 37  | 29/30 | 0.85 | 0.13 | 139,155,160,161            | 0     |
| 24  | PSU  | 3K    | 32  | 20/21 | 0.88 | 0.09 | 149,154,157,159            | 0     |
| 56  | 7MG  | 2L    | 47  | 24/25 | 0.88 | 0.06 | 137,143,153,157            | 0     |
| 56  | 4SU  | 2L    | 8   | 20/21 | 0.89 | 0.08 | 127,132,138,139            | 0     |
| 23  | 7MG  | 2K    | 47  | 24/25 | 0.90 | 0.07 | 113,121,127,130            | 0     |
| 56  | PSU  | 2L    | 56  | 20/21 | 0.90 | 0.07 | 116,124,129,135            | 0     |
| 23  | 5MU  | 2K    | 55  | 21/22 | 0.91 | 0.06 | 96,109,114,116             | 0     |
| 22  | OMC  | 1K    | 33  | 21/22 | 0.94 | 0.11 | 114,132,138,141            | 0     |
| 23  | 4SU  | 2K    | 8   | 20/21 | 0.94 | 0.06 | 101,110,114,119            | 0     |
| 23  | PSU  | 2K    | 56  | 20/21 | 0.94 | 0.06 | 95,103,113,113             | 0     |
| 56  | OMC  | 2L    | 33  | 21/22 | 0.95 | 0.08 | 105,114,117,119            | 0     |
| 23  | OMC  | 2K    | 33  | 21/22 | 0.96 | 0.08 | 84,91,99,106               | 0     |

## 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1G    | 1641 | 1/1   | 0.40 | 0.49 | 113,113,113,113             | 0     |
| 57  | MG   | 13    | 1667 | 1/1   | 0.47 | 0.25 | 119,119,119,119             | 0     |
| 57  | MG   | 1G    | 1646 | 1/1   | 0.53 | 0.34 | 117,117,117,117             | 0     |
| 57  | MG   | 1H    | 3252 | 1/1   | 0.59 | 0.38 | 92,92,92,92                 | 0     |
| 57  | MG   | 1G    | 1631 | 1/1   | 0.59 | 0.34 | 97,97,97,97                 | 0     |
| 57  | MG   | 1J    | 203  | 1/1   | 0.59 | 0.37 | 90,90,90,90                 | 0     |
| 57  | MG   | 1G    | 1658 | 1/1   | 0.61 | 0.19 | 132,132,132,132             | 0     |
| 57  | MG   | 13    | 1659 | 1/1   | 0.61 | 0.36 | 100,100,100,100             | 0     |
| 57  | MG   | 45    | 201  | 1/1   | 0.62 | 0.20 | 98,98,98,98                 | 0     |
| 57  | MG   | 1H    | 3191 | 1/1   | 0.63 | 0.41 | 102,102,102,102             | 0     |
| 57  | MG   | 1G    | 1660 | 1/1   | 0.63 | 0.20 | 124,124,124,124             | 0     |
| 57  | MG   | 13    | 1664 | 1/1   | 0.64 | 0.33 | 95,95,95,95                 | 0     |
| 57  | MG   | 1H    | 3184 | 1/1   | 0.64 | 0.25 | 86,86,86,86                 | 0     |
| 57  | MG   | 1H    | 3190 | 1/1   | 0.64 | 0.26 | 94,94,94,94                 | 0     |
| 57  | MG   | 3L    | 101  | 1/1   | 0.65 | 0.16 | 156,156,156,156             | 0     |
| 57  | MG   | 14    | 3180 | 1/1   | 0.65 | 0.25 | 112,112,112,112             | 0     |
| 57  | MG   | 1G    | 1648 | 1/1   | 0.65 | 0.36 | 99,99,99,99                 | 0     |
| 57  | MG   | 1G    | 1651 | 1/1   | 0.65 | 0.36 | 94,94,94,94                 | 0     |
| 57  | MG   | 1H    | 3168 | 1/1   | 0.66 | 0.28 | 100,100,100,100             | 0     |
| 57  | MG   | 13    | 1655 | 1/1   | 0.67 | 0.17 | 81,81,81,81                 | 0     |
| 57  | MG   | 2L    | 102  | 1/1   | 0.67 | 0.26 | 96,96,96,96                 | 0     |
| 57  | MG   | 13    | 1657 | 1/1   | 0.67 | 0.21 | 129,129,129,129             | 0     |
| 57  | MG   | 1H    | 3240 | 1/1   | 0.68 | 0.20 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3174 | 1/1   | 0.68 | 0.26 | 88,88,88,88                 | 0     |
| 57  | MG   | 1H    | 3254 | 1/1   | 0.68 | 0.30 | 94,94,94,94                 | 0     |
| 57  | MG   | 13    | 1634 | 1/1   | 0.68 | 0.22 | 110,110,110,110             | 0     |
| 57  | MG   | 1H    | 3232 | 1/1   | 0.68 | 0.25 | 102,102,102,102             | 0     |
| 57  | MG   | 13    | 1661 | 1/1   | 0.69 | 0.32 | 89,89,89,89                 | 0     |
| 57  | MG   | 14    | 3211 | 1/1   | 0.69 | 0.30 | 101,101,101,101             | 0     |
| 57  | MG   | 14    | 3128 | 1/1   | 0.69 | 0.20 | 98,98,98,98                 | 0     |
| 57  | MG   | 14    | 3179 | 1/1   | 0.69 | 0.33 | 100,100,100,100             | 0     |
| 57  | MG   | 14    | 3212 | 1/1   | 0.70 | 0.34 | 86,86,86,86                 | 0     |
| 57  | MG   | 1G    | 1663 | 1/1   | 0.70 | 0.20 | 89,89,89,89                 | 0     |
| 57  | MG   | 14    | 3098 | 1/1   | 0.70 | 0.20 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3236 | 1/1   | 0.71 | 0.23 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3099 | 1/1   | 0.71 | 0.16 | 88,88,88,88                 | 0     |
| 57  | MG   | 1G    | 1654 | 1/1   | 0.71 | 0.29 | 92,92,92,92                 | 0     |
| 57  | MG   | 1H    | 3257 | 1/1   | 0.71 | 0.38 | 90,90,90,90                 | 0     |
| 57  | MG   | 1G    | 1612 | 1/1   | 0.72 | 0.23 | 99,99,99,99                 | 0     |
| 57  | MG   | 1H    | 3098 | 1/1   | 0.72 | 0.25 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3248 | 1/1   | 0.73 | 0.31 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3269 | 1/1   | 0.73 | 0.30 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3048 | 1/1   | 0.74 | 0.22 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3129 | 1/1   | 0.74 | 0.26 | 90,90,90,90                 | 0     |
| 57  | MG   | 13    | 1650 | 1/1   | 0.74 | 0.27 | 88,88,88,88                 | 0     |
| 57  | MG   | 1G    | 1621 | 1/1   | 0.74 | 0.31 | 92,92,92,92                 | 0     |
| 57  | MG   | 13    | 1662 | 1/1   | 0.74 | 0.32 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3027 | 1/1   | 0.74 | 0.28 | 94,94,94,94                 | 0     |
| 57  | MG   | 1H    | 3109 | 1/1   | 0.74 | 0.22 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3127 | 1/1   | 0.74 | 0.27 | 77,77,77,77                 | 0     |
| 57  | MG   | 13    | 1666 | 1/1   | 0.75 | 0.19 | 116,116,116,116             | 0     |
| 57  | MG   | 1G    | 1642 | 1/1   | 0.75 | 0.28 | 93,93,93,93                 | 0     |
| 57  | MG   | 13    | 1615 | 1/1   | 0.75 | 0.26 | 85,85,85,85                 | 0     |
| 57  | MG   | 14    | 3142 | 1/1   | 0.75 | 0.19 | 86,86,86,86                 | 0     |
| 57  | MG   | 1G    | 1616 | 1/1   | 0.75 | 0.19 | 105,105,105,105             | 0     |
| 57  | MG   | 1H    | 3114 | 1/1   | 0.75 | 0.23 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3022 | 1/1   | 0.75 | 0.27 | 89,89,89,89                 | 0     |
| 57  | MG   | 1H    | 3267 | 1/1   | 0.75 | 0.27 | 106,106,106,106             | 0     |
| 57  | MG   | 1G    | 1655 | 1/1   | 0.75 | 0.30 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3111 | 1/1   | 0.75 | 0.36 | 89,89,89,89                 | 0     |
| 57  | MG   | 13    | 1611 | 1/1   | 0.76 | 0.29 | 107,107,107,107             | 0     |
| 57  | MG   | 14    | 3156 | 1/1   | 0.76 | 0.17 | 107,107,107,107             | 0     |
| 57  | MG   | 14    | 3100 | 1/1   | 0.76 | 0.22 | 82,82,82,82                 | 0     |
| 57  | MG   | 4I    | 201  | 1/1   | 0.76 | 0.14 | 97,97,97,97                 | 0     |
| 57  | MG   | 14    | 3199 | 1/1   | 0.76 | 0.32 | 95,95,95,95                 | 0     |
| 57  | MG   | 14    | 3124 | 1/1   | 0.76 | 0.27 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3238 | 1/1   | 0.76 | 0.25 | 101,101,101,101             | 0     |
| 57  | MG   | 1H    | 3207 | 1/1   | 0.76 | 0.24 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3069 | 1/1   | 0.76 | 0.35 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3171 | 1/1   | 0.77 | 0.29 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3160 | 1/1   | 0.77 | 0.14 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3069 | 1/1   | 0.77 | 0.26 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3277 | 1/1   | 0.77 | 0.17 | 89,89,89,89                 | 0     |
| 57  | MG   | 14    | 3188 | 1/1   | 0.77 | 0.23 | 87,87,87,87                 | 0     |
| 57  | MG   | 16    | 205  | 1/1   | 0.77 | 0.23 | 90,90,90,90                 | 0     |
| 57  | MG   | 14    | 3201 | 1/1   | 0.77 | 0.37 | 78,78,78,78                 | 0     |
| 57  | MG   | 41    | 202  | 1/1   | 0.77 | 0.23 | 93,93,93,93                 | 0     |
| 57  | MG   | 13    | 1612 | 1/1   | 0.77 | 0.28 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3215 | 1/1   | 0.77 | 0.31 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3221 | 1/1   | 0.77 | 0.31 | 79,79,79,79                 | 0     |
| 57  | MG   | 1H    | 3266 | 1/1   | 0.77 | 0.19 | 85,85,85,85                 | 0     |
| 57  | MG   | 13    | 1652 | 1/1   | 0.78 | 0.19 | 104,104,104,104             | 0     |
| 57  | MG   | 3L    | 102  | 1/1   | 0.78 | 0.11 | 165,165,165,165             | 0     |
| 57  | MG   | 16    | 207  | 1/1   | 0.78 | 0.18 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3025 | 1/1   | 0.78 | 0.24 | 95,95,95,95                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3173 | 1/1   | 0.78 | 0.20 | 99,99,99,99                 | 0     |
| 57  | MG   | 1G    | 1610 | 1/1   | 0.78 | 0.22 | 111,111,111,111             | 0     |
| 57  | MG   | 1H    | 3043 | 1/1   | 0.78 | 0.17 | 75,75,75,75                 | 0     |
| 57  | MG   | 13    | 1610 | 1/1   | 0.78 | 0.27 | 72,72,72,72                 | 0     |
| 57  | MG   | 14    | 3203 | 1/1   | 0.78 | 0.19 | 83,83,83,83                 | 0     |
| 57  | MG   | 1G    | 1656 | 1/1   | 0.78 | 0.26 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3188 | 1/1   | 0.78 | 0.18 | 82,82,82,82                 | 0     |
| 57  | MG   | 1H    | 3050 | 1/1   | 0.78 | 0.12 | 68,68,68,68                 | 0     |
| 57  | MG   | 1J    | 201  | 1/1   | 0.78 | 0.40 | 88,88,88,88                 | 0     |
| 57  | MG   | 1G    | 1635 | 1/1   | 0.78 | 0.22 | 79,79,79,79                 | 0     |
| 57  | MG   | 13    | 1630 | 1/1   | 0.78 | 0.22 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3151 | 1/1   | 0.79 | 0.34 | 71,71,71,71                 | 0     |
| 57  | MG   | 1G    | 1645 | 1/1   | 0.79 | 0.24 | 107,107,107,107             | 0     |
| 57  | MG   | 13    | 1607 | 1/1   | 0.79 | 0.31 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3174 | 1/1   | 0.79 | 0.38 | 87,87,87,87                 | 0     |
| 57  | MG   | 14    | 3060 | 1/1   | 0.79 | 0.24 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3255 | 1/1   | 0.79 | 0.26 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3107 | 1/1   | 0.79 | 0.30 | 81,81,81,81                 | 0     |
| 57  | MG   | 1G    | 1653 | 1/1   | 0.79 | 0.28 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3118 | 1/1   | 0.80 | 0.19 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3075 | 1/1   | 0.80 | 0.22 | 103,103,103,103             | 0     |
| 57  | MG   | 1H    | 3120 | 1/1   | 0.80 | 0.26 | 56,56,56,56                 | 0     |
| 57  | MG   | 13    | 1629 | 1/1   | 0.80 | 0.30 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3100 | 1/1   | 0.80 | 0.16 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3119 | 1/1   | 0.80 | 0.19 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3122 | 1/1   | 0.80 | 0.16 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3087 | 1/1   | 0.80 | 0.30 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3096 | 1/1   | 0.80 | 0.14 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3210 | 1/1   | 0.80 | 0.33 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3178 | 1/1   | 0.80 | 0.27 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3181 | 1/1   | 0.80 | 0.15 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3141 | 1/1   | 0.80 | 0.27 | 67,67,67,67                 | 0     |
| 57  | MG   | 1G    | 1634 | 1/1   | 0.80 | 0.20 | 93,93,93,93                 | 0     |
| 57  | MG   | 14    | 3148 | 1/1   | 0.80 | 0.16 | 93,93,93,93                 | 0     |
| 57  | MG   | 13    | 1671 | 1/1   | 0.80 | 0.28 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3244 | 1/1   | 0.81 | 0.36 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3153 | 1/1   | 0.81 | 0.38 | 87,87,87,87                 | 0     |
| 57  | MG   | 1H    | 3146 | 1/1   | 0.81 | 0.32 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3147 | 1/1   | 0.81 | 0.25 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3053 | 1/1   | 0.81 | 0.33 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3022 | 1/1   | 0.81 | 0.29 | 64,64,64,64                 | 0     |
| 57  | MG   | 1G    | 1659 | 1/1   | 0.81 | 0.18 | 101,101,101,101             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3219 | 1/1   | 0.81 | 0.23 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3070 | 1/1   | 0.81 | 0.25 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3225 | 1/1   | 0.81 | 0.29 | 95,95,95,95                 | 0     |
| 57  | MG   | 13    | 1663 | 1/1   | 0.81 | 0.40 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3095 | 1/1   | 0.81 | 0.37 | 74,74,74,74                 | 0     |
| 57  | MG   | 13    | 1638 | 1/1   | 0.81 | 0.24 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3134 | 1/1   | 0.81 | 0.20 | 72,72,72,72                 | 0     |
| 57  | MG   | 14    | 3138 | 1/1   | 0.81 | 0.17 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3218 | 1/1   | 0.81 | 0.28 | 74,74,74,74                 | 0     |
| 57  | MG   | 13    | 1616 | 1/1   | 0.81 | 0.28 | 93,93,93,93                 | 0     |
| 57  | MG   | 1H    | 3242 | 1/1   | 0.81 | 0.40 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3032 | 1/1   | 0.81 | 0.21 | 98,98,98,98                 | 0     |
| 57  | MG   | 1G    | 1636 | 1/1   | 0.82 | 0.31 | 96,96,96,96                 | 0     |
| 57  | MG   | 13    | 1645 | 1/1   | 0.82 | 0.17 | 89,89,89,89                 | 0     |
| 57  | MG   | 14    | 3166 | 1/1   | 0.82 | 0.33 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3169 | 1/1   | 0.82 | 0.27 | 59,59,59,59                 | 0     |
| 57  | MG   | 1G    | 1601 | 1/1   | 0.82 | 0.23 | 90,90,90,90                 | 0     |
| 57  | MG   | 1G    | 1602 | 1/1   | 0.82 | 0.32 | 79,79,79,79                 | 0     |
| 57  | MG   | 13    | 1621 | 1/1   | 0.82 | 0.21 | 88,88,88,88                 | 0     |
| 57  | MG   | 1H    | 3199 | 1/1   | 0.82 | 0.17 | 98,98,98,98                 | 0     |
| 57  | MG   | 14    | 3007 | 1/1   | 0.82 | 0.19 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3200 | 1/1   | 0.82 | 0.28 | 90,90,90,90                 | 0     |
| 57  | MG   | 1G    | 1650 | 1/1   | 0.82 | 0.31 | 86,86,86,86                 | 0     |
| 57  | MG   | 1H    | 3270 | 1/1   | 0.82 | 0.23 | 102,102,102,102             | 0     |
| 57  | MG   | 14    | 3205 | 1/1   | 0.82 | 0.24 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3226 | 1/1   | 0.82 | 0.24 | 70,70,70,70                 | 0     |
| 57  | MG   | 16    | 201  | 1/1   | 0.82 | 0.20 | 90,90,90,90                 | 0     |
| 57  | MG   | 14    | 3040 | 1/1   | 0.82 | 0.20 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3213 | 1/1   | 0.82 | 0.27 | 102,102,102,102             | 0     |
| 57  | MG   | 14    | 3058 | 1/1   | 0.82 | 0.25 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3144 | 1/1   | 0.82 | 0.21 | 72,72,72,72                 | 0     |
| 57  | MG   | 1G    | 1632 | 1/1   | 0.82 | 0.24 | 131,131,131,131             | 0     |
| 57  | MG   | 1H    | 3256 | 1/1   | 0.82 | 0.29 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3097 | 1/1   | 0.82 | 0.22 | 93,93,93,93                 | 0     |
| 57  | MG   | 55    | 201  | 1/1   | 0.82 | 0.19 | 57,57,57,57                 | 0     |
| 57  | MG   | 1H    | 3115 | 1/1   | 0.83 | 0.20 | 63,63,63,63                 | 0     |
| 57  | MG   | 1G    | 1644 | 1/1   | 0.83 | 0.31 | 90,90,90,90                 | 0     |
| 57  | MG   | 1H    | 3020 | 1/1   | 0.83 | 0.26 | 70,70,70,70                 | 0     |
| 57  | MG   | 13    | 1626 | 1/1   | 0.83 | 0.24 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3197 | 1/1   | 0.83 | 0.28 | 78,78,78,78                 | 0     |
| 57  | MG   | 14    | 3008 | 1/1   | 0.83 | 0.24 | 59,59,59,59                 | 0     |
| 57  | MG   | 14    | 3018 | 1/1   | 0.83 | 0.45 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3218 | 1/1   | 0.83 | 0.28 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3030 | 1/1   | 0.83 | 0.27 | 79,79,79,79                 | 0     |
| 57  | MG   | 1G    | 1619 | 1/1   | 0.83 | 0.19 | 103,103,103,103             | 0     |
| 57  | MG   | 1H    | 3042 | 1/1   | 0.83 | 0.20 | 77,77,77,77                 | 0     |
| 57  | MG   | 1G    | 1628 | 1/1   | 0.83 | 0.21 | 108,108,108,108             | 0     |
| 57  | MG   | 1H    | 3150 | 1/1   | 0.83 | 0.26 | 65,65,65,65                 | 0     |
| 57  | MG   | 16    | 203  | 1/1   | 0.83 | 0.15 | 98,98,98,98                 | 0     |
| 57  | MG   | 1H    | 3153 | 1/1   | 0.83 | 0.25 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3230 | 1/1   | 0.83 | 0.36 | 97,97,97,97                 | 0     |
| 57  | MG   | 13    | 1643 | 1/1   | 0.83 | 0.20 | 91,91,91,91                 | 0     |
| 57  | MG   | 68    | 202  | 1/1   | 0.83 | 0.28 | 91,91,91,91                 | 0     |
| 57  | MG   | 14    | 3106 | 1/1   | 0.83 | 0.25 | 86,86,86,86                 | 0     |
| 57  | MG   | 14    | 3108 | 1/1   | 0.83 | 0.26 | 77,77,77,77                 | 0     |
| 57  | MG   | M5    | 101  | 1/1   | 0.83 | 0.30 | 85,85,85,85                 | 0     |
| 57  | MG   | 1H    | 3129 | 1/1   | 0.84 | 0.21 | 93,93,93,93                 | 0     |
| 57  | MG   | 14    | 3170 | 1/1   | 0.84 | 0.50 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3016 | 1/1   | 0.84 | 0.24 | 71,71,71,71                 | 0     |
| 57  | MG   | 14    | 3176 | 1/1   | 0.84 | 0.48 | 85,85,85,85                 | 0     |
| 57  | MG   | 1H    | 3074 | 1/1   | 0.84 | 0.22 | 63,63,63,63                 | 0     |
| 57  | MG   | 14    | 3114 | 1/1   | 0.84 | 0.21 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3182 | 1/1   | 0.84 | 0.33 | 84,84,84,84                 | 0     |
| 57  | MG   | 13    | 1636 | 1/1   | 0.84 | 0.20 | 103,103,103,103             | 0     |
| 57  | MG   | 14    | 3194 | 1/1   | 0.84 | 0.23 | 79,79,79,79                 | 0     |
| 57  | MG   | 1H    | 3090 | 1/1   | 0.84 | 0.35 | 47,47,47,47                 | 0     |
| 57  | MG   | 1H    | 3259 | 1/1   | 0.84 | 0.20 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3262 | 1/1   | 0.84 | 0.24 | 75,75,75,75                 | 0     |
| 57  | MG   | 13    | 1670 | 1/1   | 0.84 | 0.25 | 101,101,101,101             | 0     |
| 57  | MG   | 1H    | 3198 | 1/1   | 0.84 | 0.19 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3268 | 1/1   | 0.84 | 0.23 | 96,96,96,96                 | 0     |
| 57  | MG   | 14    | 3207 | 1/1   | 0.84 | 0.16 | 70,70,70,70                 | 0     |
| 57  | MG   | 13    | 1632 | 1/1   | 0.84 | 0.20 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3172 | 1/1   | 0.84 | 0.26 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3062 | 1/1   | 0.84 | 0.28 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3245 | 1/1   | 0.84 | 0.25 | 96,96,96,96                 | 0     |
| 57  | MG   | 13    | 1640 | 1/1   | 0.84 | 0.20 | 141,141,141,141             | 0     |
| 57  | MG   | 14    | 3088 | 1/1   | 0.84 | 0.21 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3152 | 1/1   | 0.84 | 0.15 | 93,93,93,93                 | 0     |
| 57  | MG   | 14    | 3095 | 1/1   | 0.84 | 0.24 | 83,83,83,83                 | 0     |
| 57  | MG   | 1G    | 1662 | 1/1   | 0.84 | 0.33 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3251 | 1/1   | 0.84 | 0.30 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3103 | 1/1   | 0.84 | 0.24 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3228 | 1/1   | 0.85 | 0.27 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3039 | 1/1   | 0.85 | 0.26 | 69,69,69,69                 | 0     |
| 57  | MG   | 14    | 3086 | 1/1   | 0.85 | 0.22 | 82,82,82,82                 | 0     |
| 57  | MG   | 1G    | 1649 | 1/1   | 0.85 | 0.32 | 70,70,70,70                 | 0     |
| 57  | MG   | 1H    | 3011 | 1/1   | 0.85 | 0.33 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3234 | 1/1   | 0.85 | 0.30 | 86,86,86,86                 | 0     |
| 57  | MG   | 13    | 1624 | 1/1   | 0.85 | 0.16 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3126 | 1/1   | 0.85 | 0.21 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3018 | 1/1   | 0.85 | 0.13 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3143 | 1/1   | 0.85 | 0.30 | 64,64,64,64                 | 0     |
| 57  | MG   | 14    | 3109 | 1/1   | 0.85 | 0.17 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3164 | 1/1   | 0.85 | 0.22 | 94,94,94,94                 | 0     |
| 57  | MG   | 13    | 1641 | 1/1   | 0.85 | 0.27 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3029 | 1/1   | 0.85 | 0.21 | 78,78,78,78                 | 0     |
| 57  | MG   | 4E    | 201  | 1/1   | 0.85 | 0.25 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3034 | 1/1   | 0.85 | 0.23 | 82,82,82,82                 | 0     |
| 57  | MG   | 1J    | 202  | 1/1   | 0.85 | 0.23 | 74,74,74,74                 | 0     |
| 57  | MG   | 13    | 1614 | 1/1   | 0.85 | 0.23 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3043 | 1/1   | 0.85 | 0.24 | 71,71,71,71                 | 0     |
| 57  | MG   | 1G    | 1661 | 1/1   | 0.85 | 0.15 | 109,109,109,109             | 0     |
| 57  | MG   | 1H    | 3152 | 1/1   | 0.85 | 0.28 | 92,92,92,92                 | 0     |
| 57  | MG   | 1H    | 3089 | 1/1   | 0.86 | 0.15 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3132 | 1/1   | 0.86 | 0.19 | 81,81,81,81                 | 0     |
| 57  | MG   | 1G    | 1647 | 1/1   | 0.86 | 0.32 | 101,101,101,101             | 0     |
| 57  | MG   | 1H    | 3014 | 1/1   | 0.86 | 0.18 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3237 | 1/1   | 0.86 | 0.30 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3073 | 1/1   | 0.86 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | 14    | 3102 | 1/1   | 0.86 | 0.30 | 81,81,81,81                 | 0     |
| 57  | MG   | 1G    | 1608 | 1/1   | 0.86 | 0.28 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3105 | 1/1   | 0.86 | 0.14 | 89,89,89,89                 | 0     |
| 57  | MG   | 14    | 3204 | 1/1   | 0.86 | 0.17 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3179 | 1/1   | 0.86 | 0.31 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3064 | 1/1   | 0.86 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 14    | 3045 | 1/1   | 0.86 | 0.21 | 66,66,66,66                 | 0     |
| 57  | MG   | 14    | 3051 | 1/1   | 0.86 | 0.32 | 74,74,74,74                 | 0     |
| 57  | MG   | 13    | 1639 | 1/1   | 0.86 | 0.28 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3165 | 1/1   | 0.86 | 0.32 | 86,86,86,86                 | 0     |
| 57  | MG   | 14    | 3214 | 1/1   | 0.86 | 0.16 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3215 | 1/1   | 0.86 | 0.26 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3167 | 1/1   | 0.86 | 0.25 | 91,91,91,91                 | 0     |
| 57  | MG   | 14    | 3063 | 1/1   | 0.86 | 0.20 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3012 | 1/1   | 0.86 | 0.26 | 60,60,60,60                 | 0     |
| 57  | MG   | 14    | 3171 | 1/1   | 0.86 | 0.26 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3125 | 1/1   | 0.86 | 0.31 | 68,68,68,68                 | 0     |
| 57  | MG   | 14    | 3073 | 1/1   | 0.86 | 0.29 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3216 | 1/1   | 0.86 | 0.22 | 75,75,75,75                 | 0     |
| 57  | MG   | 11    | 301  | 1/1   | 0.87 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3015 | 1/1   | 0.87 | 0.24 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3249 | 1/1   | 0.87 | 0.28 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3019 | 1/1   | 0.87 | 0.24 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3020 | 1/1   | 0.87 | 0.35 | 76,76,76,76                 | 0     |
| 57  | MG   | 13    | 1628 | 1/1   | 0.87 | 0.33 | 90,90,90,90                 | 0     |
| 57  | MG   | 78    | 201  | 1/1   | 0.87 | 0.23 | 60,60,60,60                 | 0     |
| 57  | MG   | 14    | 3117 | 1/1   | 0.87 | 0.19 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3181 | 1/1   | 0.87 | 0.32 | 85,85,85,85                 | 0     |
| 57  | MG   | 1H    | 3031 | 1/1   | 0.87 | 0.18 | 87,87,87,87                 | 0     |
| 57  | MG   | 1H    | 3180 | 1/1   | 0.87 | 0.17 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3148 | 1/1   | 0.87 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3032 | 1/1   | 0.87 | 0.22 | 75,75,75,75                 | 0     |
| 57  | MG   | 13    | 1646 | 1/1   | 0.87 | 0.19 | 102,102,102,102             | 0     |
| 57  | MG   | 1H    | 3021 | 1/1   | 0.87 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3233 | 1/1   | 0.87 | 0.29 | 86,86,86,86                 | 0     |
| 57  | MG   | 1G    | 1657 | 1/1   | 0.87 | 0.30 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3162 | 1/1   | 0.87 | 0.23 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3166 | 1/1   | 0.87 | 0.31 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3139 | 1/1   | 0.87 | 0.14 | 93,93,93,93                 | 0     |
| 57  | MG   | 1H    | 3122 | 1/1   | 0.87 | 0.47 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3202 | 1/1   | 0.87 | 0.19 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3203 | 1/1   | 0.87 | 0.23 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3147 | 1/1   | 0.87 | 0.24 | 79,79,79,79                 | 0     |
| 57  | MG   | 13    | 1648 | 1/1   | 0.87 | 0.22 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3080 | 1/1   | 0.87 | 0.24 | 89,89,89,89                 | 0     |
| 57  | MG   | 14    | 3084 | 1/1   | 0.87 | 0.18 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3220 | 1/1   | 0.87 | 0.17 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3291 | 1/1   | 0.87 | 0.08 | 126,126,126,126             | 0     |
| 57  | MG   | 1H    | 3103 | 1/1   | 0.87 | 0.17 | 80,80,80,80                 | 0     |
| 57  | MG   | 1G    | 1637 | 1/1   | 0.87 | 0.38 | 85,85,85,85                 | 0     |
| 57  | MG   | 1H    | 3091 | 1/1   | 0.87 | 0.16 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3247 | 1/1   | 0.87 | 0.16 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3144 | 1/1   | 0.87 | 0.13 | 95,95,95,95                 | 0     |
| 57  | MG   | 14    | 3010 | 1/1   | 0.87 | 0.20 | 58,58,58,58                 | 0     |
| 58  | ZN   | C5    | 201  | 1/1   | 0.87 | 0.12 | 187,187,187,187             | 0     |
| 57  | MG   | 1H    | 3158 | 1/1   | 0.88 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | 14    | 3191 | 1/1   | 0.88 | 0.32 | 72,72,72,72                 | 0     |
| 57  | MG   | 14    | 3101 | 1/1   | 0.88 | 0.18 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3196 | 1/1   | 0.88 | 0.21 | 86,86,86,86                 | 0     |
| 57  | MG   | 13    | 1604 | 1/1   | 0.88 | 0.19 | 79,79,79,79                 | 0     |
| 57  | MG   | 1H    | 3229 | 1/1   | 0.88 | 0.16 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3164 | 1/1   | 0.88 | 0.22 | 66,66,66,66                 | 0     |
| 57  | MG   | 1H    | 3001 | 1/1   | 0.88 | 0.31 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3202 | 1/1   | 0.88 | 0.16 | 88,88,88,88                 | 0     |
| 57  | MG   | 1H    | 3019 | 1/1   | 0.88 | 0.17 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3131 | 1/1   | 0.88 | 0.21 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3049 | 1/1   | 0.88 | 0.26 | 63,63,63,63                 | 0     |
| 57  | MG   | 14    | 3157 | 1/1   | 0.88 | 0.21 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3112 | 1/1   | 0.88 | 0.24 | 78,78,78,78                 | 0     |
| 57  | MG   | 14    | 3161 | 1/1   | 0.88 | 0.20 | 88,88,88,88                 | 0     |
| 57  | MG   | 1H    | 3105 | 1/1   | 0.88 | 0.24 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3204 | 1/1   | 0.88 | 0.22 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3010 | 1/1   | 0.88 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | 13    | 1637 | 1/1   | 0.88 | 0.12 | 105,105,105,105             | 0     |
| 57  | MG   | 14    | 3217 | 1/1   | 0.88 | 0.10 | 83,83,83,83                 | 0     |
| 57  | MG   | 1G    | 1611 | 1/1   | 0.88 | 0.09 | 98,98,98,98                 | 0     |
| 57  | MG   | 1H    | 3110 | 1/1   | 0.88 | 0.31 | 84,84,84,84                 | 0     |
| 57  | MG   | 1G    | 1613 | 1/1   | 0.88 | 0.18 | 89,89,89,89                 | 0     |
| 57  | MG   | 13    | 1603 | 1/1   | 0.88 | 0.20 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3071 | 1/1   | 0.88 | 0.21 | 66,66,66,66                 | 0     |
| 57  | MG   | 14    | 3178 | 1/1   | 0.88 | 0.18 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3072 | 1/1   | 0.88 | 0.29 | 66,66,66,66                 | 0     |
| 57  | MG   | 1G    | 1622 | 1/1   | 0.88 | 0.26 | 80,80,80,80                 | 0     |
| 57  | MG   | 1G    | 1627 | 1/1   | 0.88 | 0.20 | 103,103,103,103             | 0     |
| 57  | MG   | 1H    | 3024 | 1/1   | 0.88 | 0.11 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3140 | 1/1   | 0.89 | 0.21 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3175 | 1/1   | 0.89 | 0.36 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3030 | 1/1   | 0.89 | 0.25 | 64,64,64,64                 | 0     |
| 57  | MG   | 1G    | 1615 | 1/1   | 0.89 | 0.30 | 90,90,90,90                 | 0     |
| 57  | MG   | 14    | 3115 | 1/1   | 0.89 | 0.20 | 71,71,71,71                 | 0     |
| 57  | MG   | 13    | 1672 | 1/1   | 0.89 | 0.20 | 84,84,84,84                 | 0     |
| 57  | MG   | 1G    | 1618 | 1/1   | 0.89 | 0.16 | 100,100,100,100             | 0     |
| 57  | MG   | 1H    | 3211 | 1/1   | 0.89 | 0.15 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3275 | 1/1   | 0.89 | 0.24 | 63,63,63,63                 | 0     |
| 57  | MG   | 13    | 1673 | 1/1   | 0.89 | 0.28 | 87,87,87,87                 | 0     |
| 57  | MG   | 14    | 3192 | 1/1   | 0.89 | 0.31 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3012 | 1/1   | 0.89 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3047 | 1/1   | 0.89 | 0.25 | 61,61,61,61                 | 0     |
| 57  | MG   | 13    | 1693 | 1/1   | 0.89 | 0.08 | 118,118,118,118             | 0     |
| 57  | MG   | 14    | 3062 | 1/1   | 0.89 | 0.21 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 16    | 206  | 1/1   | 0.89 | 0.16 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3067 | 1/1   | 0.89 | 0.23 | 71,71,71,71                 | 0     |
| 57  | MG   | 14    | 3068 | 1/1   | 0.89 | 0.17 | 81,81,81,81                 | 0     |
| 57  | MG   | 1G    | 1633 | 1/1   | 0.89 | 0.17 | 141,141,141,141             | 0     |
| 57  | MG   | 1H    | 3116 | 1/1   | 0.89 | 0.11 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3143 | 1/1   | 0.89 | 0.15 | 92,92,92,92                 | 0     |
| 57  | MG   | 14    | 3074 | 1/1   | 0.89 | 0.30 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3208 | 1/1   | 0.89 | 0.19 | 77,77,77,77                 | 0     |
| 57  | MG   | 13    | 1647 | 1/1   | 0.89 | 0.15 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3182 | 1/1   | 0.89 | 0.22 | 78,78,78,78                 | 0     |
| 57  | MG   | 13    | 1625 | 1/1   | 0.89 | 0.18 | 80,80,80,80                 | 0     |
| 57  | MG   | 1G    | 1639 | 1/1   | 0.89 | 0.21 | 90,90,90,90                 | 0     |
| 57  | MG   | 1H    | 3157 | 1/1   | 0.89 | 0.24 | 89,89,89,89                 | 0     |
| 57  | MG   | L8    | 101  | 1/1   | 0.89 | 0.14 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3013 | 1/1   | 0.89 | 0.27 | 55,55,55,55                 | 0     |
| 57  | MG   | 14    | 3159 | 1/1   | 0.89 | 0.17 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3099 | 1/1   | 0.89 | 0.16 | 108,108,108,108             | 0     |
| 57  | MG   | 1H    | 3076 | 1/1   | 0.89 | 0.23 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3054 | 1/1   | 0.89 | 0.23 | 41,41,41,41                 | 0     |
| 57  | MG   | 1G    | 1605 | 1/1   | 0.89 | 0.28 | 104,104,104,104             | 0     |
| 57  | MG   | 1H    | 3104 | 1/1   | 0.89 | 0.13 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3130 | 1/1   | 0.89 | 0.31 | 81,81,81,81                 | 0     |
| 57  | MG   | 14    | 3024 | 1/1   | 0.89 | 0.33 | 78,78,78,78                 | 0     |
| 57  | MG   | 13    | 1613 | 1/1   | 0.89 | 0.20 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3170 | 1/1   | 0.89 | 0.21 | 88,88,88,88                 | 0     |
| 57  | MG   | 14    | 3039 | 1/1   | 0.90 | 0.21 | 75,75,75,75                 | 0     |
| 57  | MG   | 1H    | 3239 | 1/1   | 0.90 | 0.24 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3271 | 1/1   | 0.90 | 0.32 | 90,90,90,90                 | 0     |
| 57  | MG   | 1H    | 3078 | 1/1   | 0.90 | 0.11 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3120 | 1/1   | 0.90 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | 1H    | 3212 | 1/1   | 0.90 | 0.42 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3279 | 1/1   | 0.90 | 0.18 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3280 | 1/1   | 0.90 | 0.38 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3151 | 1/1   | 0.90 | 0.32 | 75,75,75,75                 | 0     |
| 57  | MG   | 16    | 202  | 1/1   | 0.90 | 0.24 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3193 | 1/1   | 0.90 | 0.23 | 78,78,78,78                 | 0     |
| 57  | MG   | 1G    | 1630 | 1/1   | 0.90 | 0.19 | 102,102,102,102             | 0     |
| 57  | MG   | 14    | 3066 | 1/1   | 0.90 | 0.25 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3085 | 1/1   | 0.90 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 14    | 3137 | 1/1   | 0.90 | 0.13 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3065 | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 1H    | 3006 | 1/1   | 0.90 | 0.20 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3001 | 1/1   | 0.90 | 0.21 | 58,58,58,58                 | 0     |
| 57  | MG   | 14    | 3002 | 1/1   | 0.90 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3049 | 1/1   | 0.90 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | 1H    | 3222 | 1/1   | 0.90 | 0.25 | 81,81,81,81                 | 0     |
| 57  | MG   | 14    | 3081 | 1/1   | 0.90 | 0.14 | 94,94,94,94                 | 0     |
| 57  | MG   | 13    | 1623 | 1/1   | 0.90 | 0.16 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3209 | 1/1   | 0.90 | 0.17 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3253 | 1/1   | 0.90 | 0.22 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3017 | 1/1   | 0.90 | 0.18 | 81,81,81,81                 | 0     |
| 57  | MG   | 78    | 202  | 1/1   | 0.90 | 0.24 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3142 | 1/1   | 0.90 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 1H    | 3167 | 1/1   | 0.90 | 0.33 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3158 | 1/1   | 0.90 | 0.15 | 94,94,94,94                 | 0     |
| 57  | MG   | 14    | 3216 | 1/1   | 0.90 | 0.35 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3196 | 1/1   | 0.90 | 0.12 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3112 | 1/1   | 0.90 | 0.21 | 76,76,76,76                 | 0     |
| 57  | MG   | 1G    | 1606 | 1/1   | 0.90 | 0.15 | 92,92,92,92                 | 0     |
| 57  | MG   | 1H    | 3169 | 1/1   | 0.90 | 0.36 | 72,72,72,72                 | 0     |
| 57  | MG   | 1G    | 1609 | 1/1   | 0.90 | 0.12 | 106,106,106,106             | 0     |
| 57  | MG   | 13    | 1618 | 1/1   | 0.90 | 0.18 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3027 | 1/1   | 0.90 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | 1H    | 3075 | 1/1   | 0.90 | 0.31 | 59,59,59,59                 | 0     |
| 57  | MG   | 14    | 3110 | 1/1   | 0.90 | 0.15 | 82,82,82,82                 | 0     |
| 57  | MG   | 3E    | 301  | 1/1   | 0.90 | 0.12 | 127,127,127,127             | 0     |
| 58  | ZN   | G8    | 201  | 1/1   | 0.90 | 0.15 | 176,176,176,176             | 0     |
| 57  | MG   | 14    | 3035 | 1/1   | 0.90 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 1H    | 3121 | 1/1   | 0.91 | 0.24 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3042 | 1/1   | 0.91 | 0.16 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3113 | 1/1   | 0.91 | 0.17 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3177 | 1/1   | 0.91 | 0.19 | 65,65,65,65                 | 0     |
| 57  | MG   | 1G    | 1620 | 1/1   | 0.91 | 0.22 | 71,71,71,71                 | 0     |
| 57  | MG   | 14    | 3044 | 1/1   | 0.91 | 0.32 | 82,82,82,82                 | 0     |
| 57  | MG   | 1H    | 3165 | 1/1   | 0.91 | 0.14 | 96,96,96,96                 | 0     |
| 57  | MG   | 14    | 3048 | 1/1   | 0.91 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | 1H    | 3314 | 1/1   | 0.91 | 0.07 | 86,86,86,86                 | 0     |
| 57  | MG   | 14    | 3186 | 1/1   | 0.91 | 0.51 | 75,75,75,75                 | 0     |
| 57  | MG   | 1H    | 3063 | 1/1   | 0.91 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 14    | 3189 | 1/1   | 0.91 | 0.22 | 69,69,69,69                 | 0     |
| 57  | MG   | 14    | 3053 | 1/1   | 0.91 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | 13    | 1665 | 1/1   | 0.91 | 0.24 | 86,86,86,86                 | 0     |
| 57  | MG   | 1G    | 1629 | 1/1   | 0.91 | 0.24 | 96,96,96,96                 | 0     |
| 57  | MG   | 1H    | 3036 | 1/1   | 0.91 | 0.17 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3067 | 1/1   | 0.91 | 0.20 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3131 | 1/1   | 0.91 | 0.20 | 76,76,76,76                 | 0     |
| 57  | MG   | 13    | 1601 | 1/1   | 0.91 | 0.15 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3133 | 1/1   | 0.91 | 0.25 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3137 | 1/1   | 0.91 | 0.21 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3217 | 1/1   | 0.91 | 0.34 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3040 | 1/1   | 0.91 | 0.14 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3101 | 1/1   | 0.91 | 0.25 | 70,70,70,70                 | 0     |
| 57  | MG   | 13    | 1631 | 1/1   | 0.91 | 0.12 | 83,83,83,83                 | 0     |
| 57  | MG   | 13    | 1627 | 1/1   | 0.91 | 0.23 | 84,84,84,84                 | 0     |
| 57  | MG   | 1G    | 1640 | 1/1   | 0.91 | 0.10 | 107,107,107,107             | 0     |
| 57  | MG   | 1H    | 3145 | 1/1   | 0.91 | 0.36 | 66,66,66,66                 | 0     |
| 57  | MG   | 14    | 3083 | 1/1   | 0.91 | 0.32 | 57,57,57,57                 | 0     |
| 57  | MG   | 14    | 3016 | 1/1   | 0.91 | 0.14 | 86,86,86,86                 | 0     |
| 57  | MG   | 14    | 3085 | 1/1   | 0.91 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3044 | 1/1   | 0.91 | 0.18 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3258 | 1/1   | 0.91 | 0.28 | 86,86,86,86                 | 0     |
| 57  | MG   | 1H    | 3023 | 1/1   | 0.91 | 0.18 | 68,68,68,68                 | 0     |
| 57  | MG   | 14    | 3097 | 1/1   | 0.91 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3021 | 1/1   | 0.91 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 13    | 1633 | 1/1   | 0.91 | 0.22 | 90,90,90,90                 | 0     |
| 57  | MG   | 1H    | 3264 | 1/1   | 0.91 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3025 | 1/1   | 0.91 | 0.14 | 66,66,66,66                 | 0     |
| 57  | MG   | 2K    | 102  | 1/1   | 0.91 | 0.08 | 111,111,111,111             | 0     |
| 57  | MG   | 1H    | 3052 | 1/1   | 0.91 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1H    | 3028 | 1/1   | 0.91 | 0.20 | 71,71,71,71                 | 0     |
| 57  | MG   | 29    | 302  | 1/1   | 0.91 | 0.13 | 68,68,68,68                 | 0     |
| 57  | MG   | 1H    | 3235 | 1/1   | 0.91 | 0.19 | 69,69,69,69                 | 0     |
| 57  | MG   | 14    | 3168 | 1/1   | 0.91 | 0.20 | 51,51,51,51                 | 0     |
| 57  | MG   | 13    | 1658 | 1/1   | 0.91 | 0.20 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3060 | 1/1   | 0.91 | 0.29 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3002 | 1/1   | 0.91 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1H    | 3092 | 1/1   | 0.92 | 0.30 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3009 | 1/1   | 0.92 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | 14    | 3183 | 1/1   | 0.92 | 0.24 | 77,77,77,77                 | 0     |
| 57  | MG   | 98    | 201  | 1/1   | 0.92 | 0.25 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3187 | 1/1   | 0.92 | 0.19 | 81,81,81,81                 | 0     |
| 57  | MG   | J8    | 101  | 1/1   | 0.92 | 0.17 | 62,62,62,62                 | 0     |
| 57  | MG   | 1G    | 1638 | 1/1   | 0.92 | 0.14 | 83,83,83,83                 | 0     |
| 57  | MG   | J8    | 102  | 1/1   | 0.92 | 0.17 | 68,68,68,68                 | 0     |
| 57  | MG   | 1H    | 3260 | 1/1   | 0.92 | 0.28 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3111 | 1/1   | 0.92 | 0.34 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3200 | 1/1   | 0.92 | 0.26 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3195 | 1/1   | 0.92 | 0.24 | 88,88,88,88                 | 0     |
| 57  | MG   | 1G    | 1603 | 1/1   | 0.92 | 0.19 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3141 | 1/1   | 0.92 | 0.23 | 81,81,81,81                 | 0     |
| 57  | MG   | 14    | 3087 | 1/1   | 0.92 | 0.26 | 76,76,76,76                 | 0     |
| 57  | MG   | 13    | 1668 | 1/1   | 0.92 | 0.12 | 119,119,119,119             | 0     |
| 57  | MG   | 13    | 1602 | 1/1   | 0.92 | 0.17 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3096 | 1/1   | 0.92 | 0.14 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3149 | 1/1   | 0.92 | 0.16 | 96,96,96,96                 | 0     |
| 57  | MG   | 13    | 1656 | 1/1   | 0.92 | 0.12 | 96,96,96,96                 | 0     |
| 57  | MG   | 13    | 1617 | 1/1   | 0.92 | 0.24 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3206 | 1/1   | 0.92 | 0.26 | 78,78,78,78                 | 0     |
| 57  | MG   | 13    | 1642 | 1/1   | 0.92 | 0.16 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3155 | 1/1   | 0.92 | 0.16 | 70,70,70,70                 | 0     |
| 57  | MG   | 1H    | 3080 | 1/1   | 0.92 | 0.17 | 81,81,81,81                 | 0     |
| 57  | MG   | 1G    | 1652 | 1/1   | 0.92 | 0.27 | 82,82,82,82                 | 0     |
| 57  | MG   | 1H    | 3084 | 1/1   | 0.92 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1H    | 3246 | 1/1   | 0.92 | 0.30 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3068 | 1/1   | 0.92 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3125 | 1/1   | 0.92 | 0.23 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3041 | 1/1   | 0.92 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3003 | 1/1   | 0.92 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1H    | 3250 | 1/1   | 0.92 | 0.20 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3127 | 1/1   | 0.92 | 0.21 | 63,63,63,63                 | 0     |
| 57  | MG   | 14    | 3219 | 1/1   | 0.92 | 0.34 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3128 | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 1G    | 1625 | 1/1   | 0.92 | 0.21 | 81,81,81,81                 | 0     |
| 57  | MG   | 13    | 1622 | 1/1   | 0.92 | 0.22 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3161 | 1/1   | 0.92 | 0.13 | 71,71,71,71                 | 0     |
| 57  | MG   | 13    | 1635 | 1/1   | 0.92 | 0.16 | 92,92,92,92                 | 0     |
| 57  | MG   | 29    | 301  | 1/1   | 0.92 | 0.23 | 67,67,67,67                 | 0     |
| 57  | MG   | 11    | 303  | 1/1   | 0.92 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1H    | 3163 | 1/1   | 0.92 | 0.28 | 65,65,65,65                 | 0     |
| 57  | MG   | 68    | 201  | 1/1   | 0.92 | 0.11 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3192 | 1/1   | 0.92 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 14    | 3005 | 1/1   | 0.92 | 0.20 | 61,61,61,61                 | 0     |
| 57  | MG   | 1H    | 3061 | 1/1   | 0.92 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 14    | 3052 | 1/1   | 0.93 | 0.15 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3041 | 1/1   | 0.93 | 0.17 | 68,68,68,68                 | 0     |
| 57  | MG   | 14    | 3057 | 1/1   | 0.93 | 0.12 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3051 | 1/1   | 0.93 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 14    | 3123 | 1/1   | 0.93 | 0.30 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3231 | 1/1   | 0.93 | 0.30 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3061 | 1/1   | 0.93 | 0.31 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3184 | 1/1   | 0.93 | 0.25 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3185 | 1/1   | 0.93 | 0.28 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3077 | 1/1   | 0.93 | 0.28 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3197 | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | P8    | 101  | 1/1   | 0.93 | 0.20 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3066 | 1/1   | 0.93 | 0.18 | 59,59,59,59                 | 0     |
| 57  | MG   | 14    | 3011 | 1/1   | 0.93 | 0.29 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3005 | 1/1   | 0.93 | 0.22 | 51,51,51,51                 | 0     |
| 57  | MG   | 14    | 3070 | 1/1   | 0.93 | 0.20 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3135 | 1/1   | 0.93 | 0.28 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3081 | 1/1   | 0.93 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1H    | 3201 | 1/1   | 0.93 | 0.21 | 68,68,68,68                 | 0     |
| 57  | MG   | 1H    | 3083 | 1/1   | 0.93 | 0.24 | 61,61,61,61                 | 0     |
| 57  | MG   | 14    | 3076 | 1/1   | 0.93 | 0.13 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3017 | 1/1   | 0.93 | 0.10 | 75,75,75,75                 | 0     |
| 57  | MG   | 1H    | 3102 | 1/1   | 0.93 | 0.07 | 82,82,82,82                 | 0     |
| 57  | MG   | 13    | 1669 | 1/1   | 0.93 | 0.26 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3145 | 1/1   | 0.93 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 14    | 3146 | 1/1   | 0.93 | 0.19 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3241 | 1/1   | 0.93 | 0.35 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3008 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 1H    | 3208 | 1/1   | 0.93 | 0.21 | 48,48,48,48                 | 0     |
| 57  | MG   | 14    | 3150 | 1/1   | 0.93 | 0.24 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3023 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | 1H    | 3210 | 1/1   | 0.93 | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | 1G    | 1614 | 1/1   | 0.93 | 0.32 | 72,72,72,72                 | 0     |
| 57  | MG   | 14    | 3154 | 1/1   | 0.93 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | 1H    | 3059 | 1/1   | 0.93 | 0.15 | 75,75,75,75                 | 0     |
| 57  | MG   | 1H    | 3175 | 1/1   | 0.93 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3046 | 1/1   | 0.93 | 0.30 | 75,75,75,75                 | 0     |
| 57  | MG   | 16    | 204  | 1/1   | 0.93 | 0.10 | 78,78,78,78                 | 0     |
| 57  | MG   | 14    | 3033 | 1/1   | 0.93 | 0.12 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3156 | 1/1   | 0.93 | 0.28 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3037 | 1/1   | 0.93 | 0.32 | 55,55,55,55                 | 0     |
| 57  | MG   | 14    | 3162 | 1/1   | 0.93 | 0.15 | 102,102,102,102             | 0     |
| 57  | MG   | 14    | 3258 | 1/1   | 0.93 | 0.09 | 80,80,80,80                 | 0     |
| 57  | MG   | 2K    | 101  | 1/1   | 0.93 | 0.20 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3304 | 1/1   | 0.93 | 0.07 | 103,103,103,103             | 0     |
| 57  | MG   | 1G    | 1624 | 1/1   | 0.93 | 0.23 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3159 | 1/1   | 0.93 | 0.23 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 11    | 302  | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1H    | 3183 | 1/1   | 0.93 | 0.30 | 87,87,87,87                 | 0     |
| 57  | MG   | 13    | 1644 | 1/1   | 0.93 | 0.16 | 78,78,78,78                 | 0     |
| 57  | MG   | 1G    | 1664 | 1/1   | 0.93 | 0.30 | 87,87,87,87                 | 0     |
| 57  | MG   | 1H    | 3186 | 1/1   | 0.93 | 0.14 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3138 | 1/1   | 0.93 | 0.10 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3050 | 1/1   | 0.93 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3093 | 1/1   | 0.93 | 0.16 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3220 | 1/1   | 0.94 | 0.23 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3054 | 1/1   | 0.94 | 0.24 | 53,53,53,53                 | 0     |
| 57  | MG   | 1H    | 3057 | 1/1   | 0.94 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | 1G    | 1607 | 1/1   | 0.94 | 0.13 | 98,98,98,98                 | 0     |
| 57  | MG   | 14    | 3107 | 1/1   | 0.94 | 0.18 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3059 | 1/1   | 0.94 | 0.40 | 45,45,45,45                 | 0     |
| 57  | MG   | 13    | 1649 | 1/1   | 0.94 | 0.06 | 97,97,97,97                 | 0     |
| 57  | MG   | 1H    | 3224 | 1/1   | 0.94 | 0.26 | 66,66,66,66                 | 0     |
| 57  | MG   | 16    | 208  | 1/1   | 0.94 | 0.06 | 102,102,102,102             | 0     |
| 57  | MG   | 1H    | 3265 | 1/1   | 0.94 | 0.10 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3064 | 1/1   | 0.94 | 0.18 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3065 | 1/1   | 0.94 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 1H    | 3136 | 1/1   | 0.94 | 0.08 | 55,55,55,55                 | 0     |
| 57  | MG   | 14    | 3116 | 1/1   | 0.94 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3082 | 1/1   | 0.94 | 0.22 | 60,60,60,60                 | 0     |
| 57  | MG   | 14    | 3118 | 1/1   | 0.94 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | 14    | 3026 | 1/1   | 0.94 | 0.10 | 83,83,83,83                 | 0     |
| 57  | MG   | 1G    | 1668 | 1/1   | 0.94 | 0.07 | 120,120,120,120             | 0     |
| 57  | MG   | 14    | 3121 | 1/1   | 0.94 | 0.07 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3028 | 1/1   | 0.94 | 0.19 | 67,67,67,67                 | 0     |
| 57  | MG   | 2L    | 101  | 1/1   | 0.94 | 0.10 | 80,80,80,80                 | 0     |
| 57  | MG   | 41    | 201  | 1/1   | 0.94 | 0.12 | 82,82,82,82                 | 0     |
| 57  | MG   | 1H    | 3013 | 1/1   | 0.94 | 0.16 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3045 | 1/1   | 0.94 | 0.21 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3172 | 1/1   | 0.94 | 0.20 | 68,68,68,68                 | 0     |
| 57  | MG   | 1G    | 1617 | 1/1   | 0.94 | 0.16 | 88,88,88,88                 | 0     |
| 57  | MG   | 1H    | 3209 | 1/1   | 0.94 | 0.22 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3004 | 1/1   | 0.94 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | 13    | 1653 | 1/1   | 0.94 | 0.09 | 92,92,92,92                 | 0     |
| 57  | MG   | 14    | 3244 | 1/1   | 0.94 | 0.07 | 93,93,93,93                 | 0     |
| 57  | MG   | 14    | 3006 | 1/1   | 0.94 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 1H    | 3274 | 1/1   | 0.94 | 0.29 | 86,86,86,86                 | 0     |
| 57  | MG   | 14    | 3293 | 1/1   | 0.94 | 0.12 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3302 | 1/1   | 0.94 | 0.11 | 106,106,106,106             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3124 | 1/1   | 0.94 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 14    | 3307 | 1/1   | 0.94 | 0.14 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3034 | 1/1   | 0.94 | 0.11 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3094 | 1/1   | 0.94 | 0.27 | 94,94,94,94                 | 0     |
| 57  | MG   | 1H    | 3213 | 1/1   | 0.94 | 0.34 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3046 | 1/1   | 0.94 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | 1H    | 3160 | 1/1   | 0.94 | 0.18 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3088 | 1/1   | 0.94 | 0.20 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3015 | 1/1   | 0.94 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 1H    | 3113 | 1/1   | 0.94 | 0.20 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3079 | 1/1   | 0.94 | 0.21 | 66,66,66,66                 | 0     |
| 57  | MG   | 14    | 3190 | 1/1   | 0.94 | 0.23 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3149 | 1/1   | 0.95 | 0.07 | 61,61,61,61                 | 0     |
| 57  | MG   | 1H    | 3058 | 1/1   | 0.95 | 0.06 | 71,71,71,71                 | 0     |
| 57  | MG   | 14    | 3071 | 1/1   | 0.95 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | 1H    | 3272 | 1/1   | 0.95 | 0.18 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3273 | 1/1   | 0.95 | 0.29 | 85,85,85,85                 | 0     |
| 57  | MG   | 13    | 1698 | 1/1   | 0.95 | 0.09 | 105,105,105,105             | 0     |
| 57  | MG   | 13    | 1606 | 1/1   | 0.95 | 0.14 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3163 | 1/1   | 0.95 | 0.23 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3187 | 1/1   | 0.95 | 0.33 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3278 | 1/1   | 0.95 | 0.34 | 68,68,68,68                 | 0     |
| 57  | MG   | 1H    | 3135 | 1/1   | 0.95 | 0.30 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3189 | 1/1   | 0.95 | 0.17 | 70,70,70,70                 | 0     |
| 57  | MG   | 1H    | 3205 | 1/1   | 0.95 | 0.18 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3126 | 1/1   | 0.95 | 0.27 | 66,66,66,66                 | 0     |
| 57  | MG   | 1G    | 1626 | 1/1   | 0.95 | 0.15 | 81,81,81,81                 | 0     |
| 57  | MG   | 14    | 3047 | 1/1   | 0.95 | 0.28 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3363 | 1/1   | 0.95 | 0.10 | 69,69,69,69                 | 0     |
| 57  | MG   | 14    | 3091 | 1/1   | 0.95 | 0.16 | 69,69,69,69                 | 0     |
| 57  | MG   | 14    | 3092 | 1/1   | 0.95 | 0.33 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3093 | 1/1   | 0.95 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3392 | 1/1   | 0.95 | 0.13 | 96,96,96,96                 | 0     |
| 57  | MG   | 1H    | 3425 | 1/1   | 0.95 | 0.07 | 110,110,110,110             | 0     |
| 57  | MG   | 1H    | 3154 | 1/1   | 0.95 | 0.23 | 101,101,101,101             | 0     |
| 57  | MG   | 14    | 3228 | 1/1   | 0.95 | 0.05 | 69,69,69,69                 | 0     |
| 57  | MG   | 1G    | 1604 | 1/1   | 0.95 | 0.13 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3007 | 1/1   | 0.95 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 14    | 3281 | 1/1   | 0.95 | 0.07 | 95,95,95,95                 | 0     |
| 57  | MG   | 1H    | 3261 | 1/1   | 0.95 | 0.32 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3056 | 1/1   | 0.95 | 0.11 | 65,65,65,65                 | 0     |
| 57  | MG   | 13    | 1608 | 1/1   | 0.95 | 0.12 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3227 | 1/1   | 0.95 | 0.20 | 66,66,66,66                 | 0     |
| 57  | MG   | 1H    | 3193 | 1/1   | 0.95 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3310 | 1/1   | 0.95 | 0.07 | 102,102,102,102             | 0     |
| 57  | MG   | 14    | 3318 | 1/1   | 0.95 | 0.06 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3325 | 1/1   | 0.95 | 0.12 | 104,104,104,104             | 0     |
| 57  | MG   | 14    | 3104 | 1/1   | 0.95 | 0.23 | 68,68,68,68                 | 0     |
| 57  | MG   | 1H    | 3195 | 1/1   | 0.95 | 0.23 | 70,70,70,70                 | 0     |
| 57  | MG   | 1G    | 1665 | 1/1   | 0.95 | 0.05 | 117,117,117,117             | 0     |
| 57  | MG   | 1H    | 3094 | 1/1   | 0.95 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | 1G    | 1669 | 1/1   | 0.95 | 0.06 | 129,129,129,129             | 0     |
| 57  | MG   | 35    | 201  | 1/1   | 0.95 | 0.10 | 77,77,77,77                 | 0     |
| 57  | MG   | 1G    | 1670 | 1/1   | 0.95 | 0.07 | 129,129,129,129             | 0     |
| 57  | MG   | 1G    | 1671 | 1/1   | 0.95 | 0.06 | 117,117,117,117             | 0     |
| 57  | MG   | 1H    | 3004 | 1/1   | 0.95 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3214 | 1/1   | 0.95 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 14    | 3031 | 1/1   | 0.95 | 0.18 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3082 | 1/1   | 0.96 | 0.09 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3035 | 1/1   | 0.96 | 0.11 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3132 | 1/1   | 0.96 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 1H    | 3119 | 1/1   | 0.96 | 0.26 | 62,62,62,62                 | 0     |
| 57  | MG   | 13    | 1620 | 1/1   | 0.96 | 0.06 | 61,61,61,61                 | 0     |
| 57  | MG   | 1H    | 3108 | 1/1   | 0.96 | 0.26 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3055 | 1/1   | 0.96 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 14    | 3089 | 1/1   | 0.96 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 14    | 3090 | 1/1   | 0.96 | 0.15 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3139 | 1/1   | 0.96 | 0.19 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3130 | 1/1   | 0.96 | 0.10 | 84,84,84,84                 | 0     |
| 57  | MG   | 1H    | 3123 | 1/1   | 0.96 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 1H    | 3223 | 1/1   | 0.96 | 0.29 | 63,63,63,63                 | 0     |
| 57  | MG   | 1G    | 1623 | 1/1   | 0.96 | 0.25 | 66,66,66,66                 | 0     |
| 57  | MG   | 13    | 1651 | 1/1   | 0.96 | 0.06 | 110,110,110,110             | 0     |
| 57  | MG   | 1H    | 3038 | 1/1   | 0.96 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1H    | 3287 | 1/1   | 0.96 | 0.06 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3312 | 1/1   | 0.96 | 0.14 | 93,93,93,93                 | 0     |
| 57  | MG   | 1H    | 3243 | 1/1   | 0.96 | 0.24 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3234 | 1/1   | 0.96 | 0.07 | 86,86,86,86                 | 0     |
| 57  | MG   | 14    | 3237 | 1/1   | 0.96 | 0.09 | 69,69,69,69                 | 0     |
| 57  | MG   | 14    | 3140 | 1/1   | 0.96 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | 14    | 3248 | 1/1   | 0.96 | 0.07 | 103,103,103,103             | 0     |
| 57  | MG   | 14    | 3254 | 1/1   | 0.96 | 0.07 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3320 | 1/1   | 0.96 | 0.06 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3260 | 1/1   | 0.96 | 0.06 | 86,86,86,86                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3263 | 1/1   | 0.96 | 0.06 | 99,99,99,99                 | 0     |
| 57  | MG   | 14    | 3278 | 1/1   | 0.96 | 0.04 | 109,109,109,109             | 0     |
| 57  | MG   | 14    | 3280 | 1/1   | 0.96 | 0.10 | 75,75,75,75                 | 0     |
| 57  | MG   | 1H    | 3326 | 1/1   | 0.96 | 0.08 | 105,105,105,105             | 0     |
| 57  | MG   | 14    | 3288 | 1/1   | 0.96 | 0.06 | 108,108,108,108             | 0     |
| 57  | MG   | 1H    | 3335 | 1/1   | 0.96 | 0.08 | 74,74,74,74                 | 0     |
| 57  | MG   | 13    | 1609 | 1/1   | 0.96 | 0.21 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3294 | 1/1   | 0.96 | 0.07 | 107,107,107,107             | 0     |
| 57  | MG   | 14    | 3296 | 1/1   | 0.96 | 0.06 | 110,110,110,110             | 0     |
| 57  | MG   | 1H    | 3376 | 1/1   | 0.96 | 0.07 | 90,90,90,90                 | 0     |
| 57  | MG   | 1H    | 3377 | 1/1   | 0.96 | 0.06 | 103,103,103,103             | 0     |
| 57  | MG   | 1H    | 3263 | 1/1   | 0.96 | 0.39 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3308 | 1/1   | 0.96 | 0.07 | 106,106,106,106             | 0     |
| 57  | MG   | 1H    | 3400 | 1/1   | 0.96 | 0.10 | 85,85,85,85                 | 0     |
| 57  | MG   | 1H    | 3404 | 1/1   | 0.96 | 0.05 | 110,110,110,110             | 0     |
| 57  | MG   | 13    | 1678 | 1/1   | 0.96 | 0.06 | 106,106,106,106             | 0     |
| 57  | MG   | 14    | 3327 | 1/1   | 0.96 | 0.07 | 108,108,108,108             | 0     |
| 57  | MG   | 1H    | 3427 | 1/1   | 0.96 | 0.05 | 122,122,122,122             | 0     |
| 57  | MG   | 1H    | 3439 | 1/1   | 0.96 | 0.08 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3444 | 1/1   | 0.96 | 0.08 | 96,96,96,96                 | 0     |
| 57  | MG   | 14    | 3037 | 1/1   | 0.96 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 14    | 3038 | 1/1   | 0.96 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 1H    | 3194 | 1/1   | 0.96 | 0.10 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3198 | 1/1   | 0.96 | 0.23 | 86,86,86,86                 | 0     |
| 57  | MG   | 13    | 1605 | 1/1   | 0.96 | 0.12 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3079 | 1/1   | 0.96 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | 13    | 1694 | 1/1   | 0.96 | 0.06 | 111,111,111,111             | 0     |
| 57  | MG   | 13    | 1654 | 1/1   | 0.96 | 0.07 | 133,133,133,133             | 0     |
| 57  | MG   | 1H    | 3418 | 1/1   | 0.97 | 0.10 | 82,82,82,82                 | 0     |
| 57  | MG   | 13    | 1675 | 1/1   | 0.97 | 0.05 | 70,70,70,70                 | 0     |
| 57  | MG   | 1H    | 3426 | 1/1   | 0.97 | 0.06 | 97,97,97,97                 | 0     |
| 57  | MG   | 13    | 1619 | 1/1   | 0.97 | 0.15 | 72,72,72,72                 | 0     |
| 57  | MG   | 14    | 3232 | 1/1   | 0.97 | 0.08 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3428 | 1/1   | 0.97 | 0.07 | 103,103,103,103             | 0     |
| 57  | MG   | 1H    | 3435 | 1/1   | 0.97 | 0.11 | 90,90,90,90                 | 0     |
| 57  | MG   | 14    | 3238 | 1/1   | 0.97 | 0.08 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3241 | 1/1   | 0.97 | 0.10 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3281 | 1/1   | 0.97 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | 1G    | 1672 | 1/1   | 0.97 | 0.05 | 117,117,117,117             | 0     |
| 57  | MG   | 1H    | 3086 | 1/1   | 0.97 | 0.25 | 48,48,48,48                 | 0     |
| 57  | MG   | 1H    | 3301 | 1/1   | 0.97 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | 1H    | 3033 | 1/1   | 0.97 | 0.08 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3072 | 1/1   | 0.97 | 0.09 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3268 | 1/1   | 0.97 | 0.05 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3271 | 1/1   | 0.97 | 0.07 | 92,92,92,92                 | 0     |
| 57  | MG   | 14    | 3276 | 1/1   | 0.97 | 0.07 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3313 | 1/1   | 0.97 | 0.05 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3036 | 1/1   | 0.97 | 0.29 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3106 | 1/1   | 0.97 | 0.33 | 69,69,69,69                 | 0     |
| 57  | MG   | 1G    | 1643 | 1/1   | 0.97 | 0.10 | 97,97,97,97                 | 0     |
| 57  | MG   | 14    | 3078 | 1/1   | 0.97 | 0.07 | 70,70,70,70                 | 0     |
| 57  | MG   | 14    | 3003 | 1/1   | 0.97 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1H    | 3117 | 1/1   | 0.97 | 0.17 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3321 | 1/1   | 0.97 | 0.07 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3322 | 1/1   | 0.97 | 0.08 | 74,74,74,74                 | 0     |
| 57  | MG   | 13    | 1699 | 1/1   | 0.97 | 0.04 | 119,119,119,119             | 0     |
| 57  | MG   | 16    | 211  | 1/1   | 0.97 | 0.07 | 99,99,99,99                 | 0     |
| 57  | MG   | 1H    | 3056 | 1/1   | 0.97 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 1H    | 3336 | 1/1   | 0.97 | 0.05 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3312 | 1/1   | 0.97 | 0.03 | 115,115,115,115             | 0     |
| 57  | MG   | 14    | 3315 | 1/1   | 0.97 | 0.06 | 80,80,80,80                 | 0     |
| 57  | MG   | 14    | 3316 | 1/1   | 0.97 | 0.06 | 88,88,88,88                 | 0     |
| 57  | MG   | 1H    | 3344 | 1/1   | 0.97 | 0.08 | 57,57,57,57                 | 0     |
| 57  | MG   | 13    | 1686 | 1/1   | 0.97 | 0.05 | 89,89,89,89                 | 0     |
| 57  | MG   | 1H    | 3029 | 1/1   | 0.97 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 14    | 3014 | 1/1   | 0.97 | 0.12 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3133 | 1/1   | 0.97 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 1H    | 3379 | 1/1   | 0.97 | 0.05 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3134 | 1/1   | 0.97 | 0.27 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3394 | 1/1   | 0.97 | 0.07 | 83,83,83,83                 | 0     |
| 57  | MG   | 13    | 1674 | 1/1   | 0.97 | 0.04 | 83,83,83,83                 | 0     |
| 57  | MG   | I8    | 101  | 1/1   | 0.97 | 0.08 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3177 | 1/1   | 0.97 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | 14    | 3136 | 1/1   | 0.97 | 0.12 | 66,66,66,66                 | 0     |
| 57  | MG   | 1H    | 3408 | 1/1   | 0.97 | 0.12 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3410 | 1/1   | 0.97 | 0.08 | 102,102,102,102             | 0     |
| 57  | MG   | 1H    | 3440 | 1/1   | 0.98 | 0.04 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3441 | 1/1   | 0.98 | 0.06 | 70,70,70,70                 | 0     |
| 57  | MG   | 1H    | 3443 | 1/1   | 0.98 | 0.04 | 100,100,100,100             | 0     |
| 57  | MG   | 1H    | 3026 | 1/1   | 0.98 | 0.08 | 62,62,62,62                 | 0     |
| 57  | MG   | 13    | 1687 | 1/1   | 0.98 | 0.06 | 103,103,103,103             | 0     |
| 57  | MG   | 1H    | 3315 | 1/1   | 0.98 | 0.15 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3317 | 1/1   | 0.98 | 0.05 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3318 | 1/1   | 0.98 | 0.04 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3185 | 1/1   | 0.98 | 0.05 | 121,121,121,121             | 0     |
| 57  | MG   | 13    | 1688 | 1/1   | 0.98 | 0.09 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3155 | 1/1   | 0.98 | 0.12 | 68,68,68,68                 | 0     |
| 57  | MG   | 13    | 1689 | 1/1   | 0.98 | 0.04 | 115,115,115,115             | 0     |
| 57  | MG   | 1H    | 3327 | 1/1   | 0.98 | 0.13 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3328 | 1/1   | 0.98 | 0.04 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3329 | 1/1   | 0.98 | 0.11 | 80,80,80,80                 | 0     |
| 57  | MG   | 13    | 1677 | 1/1   | 0.98 | 0.08 | 98,98,98,98                 | 0     |
| 57  | MG   | 1H    | 3206 | 1/1   | 0.98 | 0.18 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3340 | 1/1   | 0.98 | 0.04 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3342 | 1/1   | 0.98 | 0.06 | 63,63,63,63                 | 0     |
| 57  | MG   | 13    | 1660 | 1/1   | 0.98 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | 1H    | 3348 | 1/1   | 0.98 | 0.14 | 90,90,90,90                 | 0     |
| 57  | MG   | 1H    | 3349 | 1/1   | 0.98 | 0.04 | 68,68,68,68                 | 0     |
| 57  | MG   | 1G    | 1666 | 1/1   | 0.98 | 0.05 | 89,89,89,89                 | 0     |
| 57  | MG   | 88    | 201  | 1/1   | 0.98 | 0.08 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3351 | 1/1   | 0.98 | 0.07 | 79,79,79,79                 | 0     |
| 57  | MG   | 1H    | 3354 | 1/1   | 0.98 | 0.06 | 66,66,66,66                 | 0     |
| 57  | MG   | 1H    | 3356 | 1/1   | 0.98 | 0.07 | 81,81,81,81                 | 0     |
| 57  | MG   | 1H    | 3357 | 1/1   | 0.98 | 0.06 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3276 | 1/1   | 0.98 | 0.21 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3225 | 1/1   | 0.98 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | 1H    | 3367 | 1/1   | 0.98 | 0.04 | 90,90,90,90                 | 0     |
| 57  | MG   | 14    | 3229 | 1/1   | 0.98 | 0.04 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3231 | 1/1   | 0.98 | 0.05 | 66,66,66,66                 | 0     |
| 57  | MG   | 1H    | 3371 | 1/1   | 0.98 | 0.04 | 66,66,66,66                 | 0     |
| 57  | MG   | 14    | 3233 | 1/1   | 0.98 | 0.05 | 82,82,82,82                 | 0     |
| 57  | MG   | 13    | 1696 | 1/1   | 0.98 | 0.03 | 101,101,101,101             | 0     |
| 57  | MG   | 13    | 1680 | 1/1   | 0.98 | 0.04 | 91,91,91,91                 | 0     |
| 57  | MG   | 13    | 1681 | 1/1   | 0.98 | 0.05 | 71,71,71,71                 | 0     |
| 57  | MG   | 14    | 3239 | 1/1   | 0.98 | 0.07 | 92,92,92,92                 | 0     |
| 57  | MG   | 14    | 3077 | 1/1   | 0.98 | 0.07 | 61,61,61,61                 | 0     |
| 57  | MG   | 1H    | 3381 | 1/1   | 0.98 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 1H    | 3382 | 1/1   | 0.98 | 0.07 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3250 | 1/1   | 0.98 | 0.05 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3385 | 1/1   | 0.98 | 0.07 | 112,112,112,112             | 0     |
| 57  | MG   | 14    | 3255 | 1/1   | 0.98 | 0.05 | 72,72,72,72                 | 0     |
| 57  | MG   | 14    | 3257 | 1/1   | 0.98 | 0.05 | 89,89,89,89                 | 0     |
| 57  | MG   | 1H    | 3388 | 1/1   | 0.98 | 0.04 | 75,75,75,75                 | 0     |
| 57  | MG   | 1H    | 3389 | 1/1   | 0.98 | 0.04 | 87,87,87,87                 | 0     |
| 57  | MG   | 1H    | 3390 | 1/1   | 0.98 | 0.08 | 99,99,99,99                 | 0     |
| 57  | MG   | 14    | 3264 | 1/1   | 0.98 | 0.06 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3266 | 1/1   | 0.98 | 0.07 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3391 | 1/1   | 0.98 | 0.05 | 91,91,91,91                 | 0     |
| 57  | MG   | 14    | 3269 | 1/1   | 0.98 | 0.05 | 108,108,108,108             | 0     |
| 57  | MG   | 14    | 3270 | 1/1   | 0.98 | 0.04 | 97,97,97,97                 | 0     |
| 57  | MG   | 13    | 1682 | 1/1   | 0.98 | 0.14 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3273 | 1/1   | 0.98 | 0.06 | 69,69,69,69                 | 0     |
| 57  | MG   | 14    | 3274 | 1/1   | 0.98 | 0.06 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3275 | 1/1   | 0.98 | 0.04 | 90,90,90,90                 | 0     |
| 57  | MG   | 1H    | 3009 | 1/1   | 0.98 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 14    | 3277 | 1/1   | 0.98 | 0.04 | 98,98,98,98                 | 0     |
| 57  | MG   | 1H    | 3396 | 1/1   | 0.98 | 0.06 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3398 | 1/1   | 0.98 | 0.03 | 98,98,98,98                 | 0     |
| 57  | MG   | 1H    | 3399 | 1/1   | 0.98 | 0.03 | 111,111,111,111             | 0     |
| 57  | MG   | 14    | 3283 | 1/1   | 0.98 | 0.04 | 74,74,74,74                 | 0     |
| 57  | MG   | 14    | 3284 | 1/1   | 0.98 | 0.06 | 84,84,84,84                 | 0     |
| 57  | MG   | 14    | 3287 | 1/1   | 0.98 | 0.05 | 101,101,101,101             | 0     |
| 57  | MG   | 1H    | 3282 | 1/1   | 0.98 | 0.05 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3290 | 1/1   | 0.98 | 0.04 | 114,114,114,114             | 0     |
| 57  | MG   | 1H    | 3401 | 1/1   | 0.98 | 0.08 | 80,80,80,80                 | 0     |
| 57  | MG   | 1H    | 3402 | 1/1   | 0.98 | 0.04 | 88,88,88,88                 | 0     |
| 57  | MG   | 13    | 1683 | 1/1   | 0.98 | 0.04 | 96,96,96,96                 | 0     |
| 57  | MG   | 14    | 3295 | 1/1   | 0.98 | 0.05 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3407 | 1/1   | 0.98 | 0.07 | 77,77,77,77                 | 0     |
| 57  | MG   | 14    | 3297 | 1/1   | 0.98 | 0.05 | 92,92,92,92                 | 0     |
| 57  | MG   | 14    | 3299 | 1/1   | 0.98 | 0.03 | 114,114,114,114             | 0     |
| 57  | MG   | 1H    | 3295 | 1/1   | 0.98 | 0.05 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3409 | 1/1   | 0.98 | 0.04 | 99,99,99,99                 | 0     |
| 57  | MG   | 14    | 3305 | 1/1   | 0.98 | 0.09 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3296 | 1/1   | 0.98 | 0.06 | 51,51,51,51                 | 0     |
| 57  | MG   | 1H    | 3411 | 1/1   | 0.98 | 0.06 | 133,133,133,133             | 0     |
| 57  | MG   | 1H    | 3414 | 1/1   | 0.98 | 0.10 | 87,87,87,87                 | 0     |
| 57  | MG   | 14    | 3311 | 1/1   | 0.98 | 0.05 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3300 | 1/1   | 0.98 | 0.05 | 68,68,68,68                 | 0     |
| 57  | MG   | 14    | 3313 | 1/1   | 0.98 | 0.05 | 101,101,101,101             | 0     |
| 57  | MG   | 14    | 3314 | 1/1   | 0.98 | 0.03 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3419 | 1/1   | 0.98 | 0.07 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3421 | 1/1   | 0.98 | 0.03 | 104,104,104,104             | 0     |
| 57  | MG   | 1H    | 3422 | 1/1   | 0.98 | 0.07 | 86,86,86,86                 | 0     |
| 57  | MG   | 1H    | 3423 | 1/1   | 0.98 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | 13    | 1684 | 1/1   | 0.98 | 0.04 | 95,95,95,95                 | 0     |
| 57  | MG   | 1H    | 3302 | 1/1   | 0.98 | 0.05 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3303 | 1/1   | 0.98 | 0.06 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3308 | 1/1   | 0.98 | 0.06 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3429 | 1/1   | 0.98 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3431 | 1/1   | 0.98 | 0.05 | 66,66,66,66                 | 0     |
| 57  | MG   | 25    | 201  | 1/1   | 0.98 | 0.04 | 111,111,111,111             | 0     |
| 57  | MG   | 1H    | 3432 | 1/1   | 0.98 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3433 | 1/1   | 0.98 | 0.06 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3434 | 1/1   | 0.98 | 0.04 | 68,68,68,68                 | 0     |
| 57  | MG   | 1H    | 3310 | 1/1   | 0.98 | 0.04 | 91,91,91,91                 | 0     |
| 58  | ZN   | 3E    | 302  | 1/1   | 0.98 | 0.17 | 95,95,95,95                 | 0     |
| 57  | MG   | 1H    | 3437 | 1/1   | 0.98 | 0.05 | 64,64,64,64                 | 0     |
| 57  | MG   | 13    | 1676 | 1/1   | 0.98 | 0.04 | 110,110,110,110             | 0     |
| 57  | MG   | 1H    | 3286 | 1/1   | 0.99 | 0.03 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3368 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3055 | 1/1   | 0.99 | 0.07 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3369 | 1/1   | 0.99 | 0.04 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3370 | 1/1   | 0.99 | 0.05 | 60,60,60,60                 | 0     |
| 57  | MG   | 13    | 1679 | 1/1   | 0.99 | 0.04 | 100,100,100,100             | 0     |
| 57  | MG   | 1H    | 3372 | 1/1   | 0.99 | 0.11 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3221 | 1/1   | 0.99 | 0.04 | 67,67,67,67                 | 0     |
| 57  | MG   | 14    | 3223 | 1/1   | 0.99 | 0.03 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3224 | 1/1   | 0.99 | 0.05 | 55,55,55,55                 | 0     |
| 57  | MG   | 1H    | 3373 | 1/1   | 0.99 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 14    | 3227 | 1/1   | 0.99 | 0.04 | 64,64,64,64                 | 0     |
| 57  | MG   | 1H    | 3374 | 1/1   | 0.99 | 0.06 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3316 | 1/1   | 0.99 | 0.04 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3230 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 57  | MG   | 16    | 209  | 1/1   | 0.99 | 0.03 | 76,76,76,76                 | 0     |
| 57  | MG   | 16    | 210  | 1/1   | 0.99 | 0.05 | 88,88,88,88                 | 0     |
| 57  | MG   | 1H    | 3289 | 1/1   | 0.99 | 0.03 | 48,48,48,48                 | 0     |
| 57  | MG   | 1H    | 3378 | 1/1   | 0.99 | 0.04 | 59,59,59,59                 | 0     |
| 57  | MG   | 14    | 3235 | 1/1   | 0.99 | 0.03 | 66,66,66,66                 | 0     |
| 57  | MG   | 14    | 3236 | 1/1   | 0.99 | 0.05 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3291 | 1/1   | 0.99 | 0.04 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3380 | 1/1   | 0.99 | 0.07 | 57,57,57,57                 | 0     |
| 57  | MG   | 1H    | 3319 | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 57  | MG   | 14    | 3240 | 1/1   | 0.99 | 0.03 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3292 | 1/1   | 0.99 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 14    | 3242 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3243 | 1/1   | 0.99 | 0.04 | 74,74,74,74                 | 0     |
| 57  | MG   | 1G    | 1667 | 1/1   | 0.99 | 0.05 | 98,98,98,98                 | 0     |
| 57  | MG   | 14    | 3245 | 1/1   | 0.99 | 0.02 | 99,99,99,99                 | 0     |
| 57  | MG   | 14    | 3246 | 1/1   | 0.99 | 0.06 | 96,96,96,96                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 14    | 3247 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3383 | 1/1   | 0.99 | 0.12 | 82,82,82,82                 | 0     |
| 57  | MG   | 14    | 3249 | 1/1   | 0.99 | 0.04 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3384 | 1/1   | 0.99 | 0.05 | 68,68,68,68                 | 0     |
| 57  | MG   | 14    | 3252 | 1/1   | 0.99 | 0.03 | 71,71,71,71                 | 0     |
| 57  | MG   | 14    | 3253 | 1/1   | 0.99 | 0.03 | 66,66,66,66                 | 0     |
| 57  | MG   | 1H    | 3293 | 1/1   | 0.99 | 0.03 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3386 | 1/1   | 0.99 | 0.06 | 96,96,96,96                 | 0     |
| 57  | MG   | 14    | 3256 | 1/1   | 0.99 | 0.03 | 57,57,57,57                 | 0     |
| 57  | MG   | 1H    | 3387 | 1/1   | 0.99 | 0.05 | 82,82,82,82                 | 0     |
| 57  | MG   | 1H    | 3294 | 1/1   | 0.99 | 0.06 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3259 | 1/1   | 0.99 | 0.06 | 71,71,71,71                 | 0     |
| 57  | MG   | 1H    | 3323 | 1/1   | 0.99 | 0.05 | 83,83,83,83                 | 0     |
| 57  | MG   | 14    | 3262 | 1/1   | 0.99 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | I8    | 102  | 1/1   | 0.99 | 0.08 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3324 | 1/1   | 0.99 | 0.08 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3265 | 1/1   | 0.99 | 0.04 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3325 | 1/1   | 0.99 | 0.03 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3267 | 1/1   | 0.99 | 0.04 | 48,48,48,48                 | 0     |
| 57  | MG   | 13    | 1685 | 1/1   | 0.99 | 0.04 | 93,93,93,93                 | 0     |
| 57  | MG   | 1H    | 3393 | 1/1   | 0.99 | 0.03 | 58,58,58,58                 | 0     |
| 57  | MG   | 13    | 1695 | 1/1   | 0.99 | 0.03 | 87,87,87,87                 | 0     |
| 57  | MG   | 1H    | 3395 | 1/1   | 0.99 | 0.06 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3298 | 1/1   | 0.99 | 0.04 | 65,65,65,65                 | 0     |
| 57  | MG   | 1H    | 3397 | 1/1   | 0.99 | 0.03 | 76,76,76,76                 | 0     |
| 57  | MG   | 13    | 1690 | 1/1   | 0.99 | 0.03 | 83,83,83,83                 | 0     |
| 57  | MG   | 1H    | 3331 | 1/1   | 0.99 | 0.04 | 74,74,74,74                 | 0     |
| 57  | MG   | 1H    | 3332 | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 57  | MG   | 1H    | 3333 | 1/1   | 0.99 | 0.07 | 54,54,54,54                 | 0     |
| 57  | MG   | 14    | 3279 | 1/1   | 0.99 | 0.04 | 69,69,69,69                 | 0     |
| 57  | MG   | 1H    | 3334 | 1/1   | 0.99 | 0.05 | 54,54,54,54                 | 0     |
| 57  | MG   | 14    | 3173 | 1/1   | 0.99 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 14    | 3282 | 1/1   | 0.99 | 0.09 | 92,92,92,92                 | 0     |
| 57  | MG   | 1H    | 3403 | 1/1   | 0.99 | 0.04 | 76,76,76,76                 | 0     |
| 57  | MG   | 13    | 1697 | 1/1   | 0.99 | 0.04 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3286 | 1/1   | 0.99 | 0.10 | 91,91,91,91                 | 0     |
| 57  | MG   | 1H    | 3405 | 1/1   | 0.99 | 0.04 | 72,72,72,72                 | 0     |
| 57  | MG   | 1H    | 3406 | 1/1   | 0.99 | 0.05 | 106,106,106,106             | 0     |
| 57  | MG   | 14    | 3289 | 1/1   | 0.99 | 0.03 | 106,106,106,106             | 0     |
| 57  | MG   | 1H    | 3176 | 1/1   | 0.99 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1H    | 3337 | 1/1   | 0.99 | 0.04 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3292 | 1/1   | 0.99 | 0.04 | 91,91,91,91                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3338 | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 57  | MG   | 13    | 1691 | 1/1   | 0.99 | 0.05 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3341 | 1/1   | 0.99 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 1H    | 3412 | 1/1   | 0.99 | 0.07 | 94,94,94,94                 | 0     |
| 57  | MG   | 1H    | 3304 | 1/1   | 0.99 | 0.05 | 76,76,76,76                 | 0     |
| 57  | MG   | 14    | 3298 | 1/1   | 0.99 | 0.03 | 78,78,78,78                 | 0     |
| 57  | MG   | 1H    | 3415 | 1/1   | 0.99 | 0.03 | 105,105,105,105             | 0     |
| 57  | MG   | 14    | 3300 | 1/1   | 0.99 | 0.03 | 87,87,87,87                 | 0     |
| 57  | MG   | 14    | 3301 | 1/1   | 0.99 | 0.07 | 92,92,92,92                 | 0     |
| 57  | MG   | 1H    | 3416 | 1/1   | 0.99 | 0.09 | 81,81,81,81                 | 0     |
| 57  | MG   | 14    | 3303 | 1/1   | 0.99 | 0.10 | 85,85,85,85                 | 0     |
| 57  | MG   | 1H    | 3417 | 1/1   | 0.99 | 0.06 | 73,73,73,73                 | 0     |
| 57  | MG   | 1H    | 3343 | 1/1   | 0.99 | 0.06 | 57,57,57,57                 | 0     |
| 57  | MG   | 14    | 3306 | 1/1   | 0.99 | 0.06 | 82,82,82,82                 | 0     |
| 57  | MG   | 1H    | 3305 | 1/1   | 0.99 | 0.04 | 49,49,49,49                 | 0     |
| 57  | MG   | 1H    | 3420 | 1/1   | 0.99 | 0.04 | 60,60,60,60                 | 0     |
| 57  | MG   | 14    | 3309 | 1/1   | 0.99 | 0.04 | 86,86,86,86                 | 0     |
| 57  | MG   | 1H    | 3346 | 1/1   | 0.99 | 0.05 | 58,58,58,58                 | 0     |
| 57  | MG   | 1H    | 3306 | 1/1   | 0.99 | 0.04 | 70,70,70,70                 | 0     |
| 57  | MG   | 1H    | 3307 | 1/1   | 0.99 | 0.02 | 114,114,114,114             | 0     |
| 57  | MG   | 1H    | 3424 | 1/1   | 0.99 | 0.03 | 94,94,94,94                 | 0     |
| 57  | MG   | 1H    | 3350 | 1/1   | 0.99 | 0.03 | 74,74,74,74                 | 0     |
| 57  | MG   | 13    | 1692 | 1/1   | 0.99 | 0.03 | 100,100,100,100             | 0     |
| 57  | MG   | 1H    | 3352 | 1/1   | 0.99 | 0.09 | 68,68,68,68                 | 0     |
| 57  | MG   | 14    | 3317 | 1/1   | 0.99 | 0.07 | 76,76,76,76                 | 0     |
| 57  | MG   | 1H    | 3353 | 1/1   | 0.99 | 0.11 | 62,62,62,62                 | 0     |
| 57  | MG   | 14    | 3320 | 1/1   | 0.99 | 0.04 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3321 | 1/1   | 0.99 | 0.03 | 78,78,78,78                 | 0     |
| 57  | MG   | 14    | 3322 | 1/1   | 0.99 | 0.03 | 79,79,79,79                 | 0     |
| 57  | MG   | 14    | 3323 | 1/1   | 0.99 | 0.03 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3324 | 1/1   | 0.99 | 0.04 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3283 | 1/1   | 0.99 | 0.04 | 65,65,65,65                 | 0     |
| 57  | MG   | 14    | 3326 | 1/1   | 0.99 | 0.03 | 104,104,104,104             | 0     |
| 57  | MG   | 1H    | 3430 | 1/1   | 0.99 | 0.03 | 50,50,50,50                 | 0     |
| 57  | MG   | 1H    | 3311 | 1/1   | 0.99 | 0.04 | 70,70,70,70                 | 0     |
| 57  | MG   | 1H    | 3284 | 1/1   | 0.99 | 0.05 | 51,51,51,51                 | 0     |
| 57  | MG   | 1H    | 3359 | 1/1   | 0.99 | 0.03 | 79,79,79,79                 | 0     |
| 57  | MG   | 1H    | 3360 | 1/1   | 0.99 | 0.03 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3361 | 1/1   | 0.99 | 0.08 | 95,95,95,95                 | 0     |
| 57  | MG   | 1H    | 3436 | 1/1   | 0.99 | 0.05 | 50,50,50,50                 | 0     |
| 57  | MG   | 1H    | 3362 | 1/1   | 0.99 | 0.05 | 60,60,60,60                 | 0     |
| 57  | MG   | 1H    | 3438 | 1/1   | 0.99 | 0.06 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1H    | 3285 | 1/1   | 0.99 | 0.04 | 53,53,53,53                 | 0     |
| 57  | MG   | 1H    | 3364 | 1/1   | 0.99 | 0.03 | 93,93,93,93                 | 0     |
| 57  | MG   | 1H    | 3365 | 1/1   | 0.99 | 0.03 | 68,68,68,68                 | 0     |
| 58  | ZN   | 5I    | 101  | 1/1   | 0.99 | 0.03 | 100,100,100,100             | 0     |
| 57  | MG   | 1H    | 3442 | 1/1   | 0.99 | 0.06 | 73,73,73,73                 | 0     |
| 58  | ZN   | 32    | 301  | 1/1   | 0.99 | 0.17 | 117,117,117,117             | 0     |
| 58  | ZN   | 5A    | 101  | 1/1   | 0.99 | 0.03 | 139,139,139,139             | 0     |
| 57  | MG   | 1H    | 3366 | 1/1   | 0.99 | 0.03 | 75,75,75,75                 | 0     |
| 57  | MG   | 14    | 3285 | 1/1   | 1.00 | 0.03 | 87,87,87,87                 | 0     |
| 57  | MG   | 1H    | 3347 | 1/1   | 1.00 | 0.03 | 64,64,64,64                 | 0     |
| 57  | MG   | 14    | 3251 | 1/1   | 1.00 | 0.04 | 77,77,77,77                 | 0     |
| 57  | MG   | 1H    | 3358 | 1/1   | 1.00 | 0.03 | 73,73,73,73                 | 0     |
| 57  | MG   | 14    | 3222 | 1/1   | 1.00 | 0.03 | 62,62,62,62                 | 0     |
| 57  | MG   | 1H    | 3339 | 1/1   | 1.00 | 0.05 | 50,50,50,50                 | 0     |
| 57  | MG   | 14    | 3272 | 1/1   | 1.00 | 0.05 | 58,58,58,58                 | 0     |
| 57  | MG   | 1H    | 3299 | 1/1   | 1.00 | 0.04 | 49,49,49,49                 | 0     |
| 57  | MG   | 1H    | 3290 | 1/1   | 1.00 | 0.04 | 49,49,49,49                 | 0     |
| 57  | MG   | 14    | 3226 | 1/1   | 1.00 | 0.02 | 67,67,67,67                 | 0     |
| 57  | MG   | 1H    | 3309 | 1/1   | 1.00 | 0.02 | 66,66,66,66                 | 0     |
| 57  | MG   | 1H    | 3330 | 1/1   | 1.00 | 0.02 | 49,49,49,49                 | 0     |
| 57  | MG   | 1H    | 3375 | 1/1   | 1.00 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | 14    | 3261 | 1/1   | 1.00 | 0.04 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3297 | 1/1   | 1.00 | 0.01 | 47,47,47,47                 | 0     |
| 57  | MG   | 14    | 3319 | 1/1   | 1.00 | 0.04 | 63,63,63,63                 | 0     |
| 57  | MG   | 1H    | 3413 | 1/1   | 1.00 | 0.02 | 57,57,57,57                 | 0     |
| 57  | MG   | 1H    | 3345 | 1/1   | 1.00 | 0.02 | 53,53,53,53                 | 0     |
| 57  | MG   | 1H    | 3355 | 1/1   | 1.00 | 0.02 | 56,56,56,56                 | 0     |
| 57  | MG   | 1H    | 3288 | 1/1   | 1.00 | 0.04 | 55,55,55,55                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.