



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:39 pm BST

PDB ID : 5IBB
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and cognate tRNA^{Val} in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 2.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

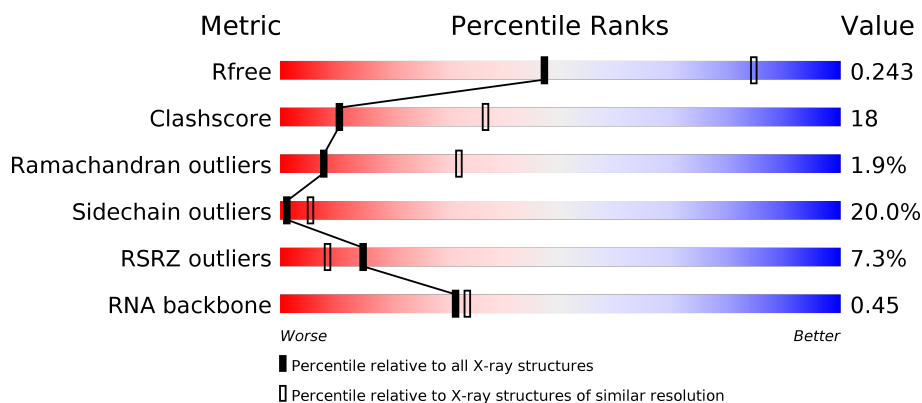
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 3104 (3.00-2.92) |
| Clashscore | 141614 | 3462 (3.00-2.92) |
| Ramachandran outliers | 138981 | 3340 (3.00-2.92) |
| Sidechain outliers | 138945 | 3343 (3.00-2.92) |
| RSRZ outliers | 127900 | 2986 (3.00-2.92) |
| RNA backbone | 3102 | 1065 (3.22-2.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 | |
| 1 | 1G | 1522 | |
| 2 | 12 | 256 | |
| 2 | 1E | 256 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | 22 | 239 | |
| 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 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | 6I | 89 | |
| 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 | 76 | |
| 23 | 2K | 77 | |
| 23 | 2L | 77 | |
| 24 | 3K | 76 | |
| 24 | 3L | 76 | |
| 25 | 4K | 30 | |
| 25 | 4L | 30 | |
| 26 | 14 | 2917 | |
| 26 | 1H | 2917 | |
| 27 | 16 | 122 | |
| 27 | 1J | 122 | |
| 28 | 7I | 229 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | 79 | 229 | |
| 29 | 11 | 276 | |
| 29 | 19 | 276 | |
| 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 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41 | 75 | 146 | |
| 41 | B8 | 146 | |
| 42 | 85 | 118 | |
| 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 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | N8 | 60 | |
| 54 | L5 | 49 | |
| 54 | P8 | 49 | |
| 55 | M5 | 65 | |
| 55 | Q8 | 65 | |
| 56 | 1L | 76 | |

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 | 13 | 1643 | - | - | - | X |
| 57 | MG | 13 | 1650 | - | - | - | X |
| 57 | MG | 13 | 1671 | - | - | - | X |
| 57 | MG | 13 | 1678 | - | - | - | X |
| 57 | MG | 13 | 1687 | - | - | - | X |
| 57 | MG | 13 | 1690 | - | - | - | X |
| 57 | MG | 14 | 3007 | - | - | - | X |
| 57 | MG | 14 | 3031 | - | - | - | X |
| 57 | MG | 14 | 3083 | - | - | - | X |
| 57 | MG | 14 | 3087 | - | - | - | X |
| 57 | MG | 14 | 3092 | - | - | - | X |
| 57 | MG | 14 | 3094 | - | - | - | X |
| 57 | MG | 14 | 3097 | - | - | - | X |
| 57 | MG | 14 | 3110 | - | - | - | X |
| 57 | MG | 14 | 3111 | - | - | - | X |
| 57 | MG | 14 | 3112 | - | - | - | X |
| 57 | MG | 14 | 3134 | - | - | - | X |
| 57 | MG | 14 | 3137 | - | - | - | X |
| 57 | MG | 14 | 3152 | - | - | - | X |
| 57 | MG | 14 | 3157 | - | - | - | X |
| 57 | MG | 14 | 3162 | - | - | - | X |
| 57 | MG | 14 | 3163 | - | - | - | X |
| 57 | MG | 14 | 3172 | - | - | - | X |
| 57 | MG | 14 | 3174 | - | - | - | X |
| 57 | MG | 14 | 3189 | - | - | - | X |
| 57 | MG | 14 | 3205 | - | - | - | X |
| 57 | MG | 14 | 3214 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | 14 | 3226 | - | - | - | X |
| 57 | MG | 1G | 1621 | - | - | - | X |
| 57 | MG | 1G | 1630 | - | - | - | X |
| 57 | MG | 1H | 3005 | - | - | - | X |
| 57 | MG | 1H | 3009 | - | - | - | X |
| 57 | MG | 1H | 3036 | - | - | - | X |
| 57 | MG | 1H | 3058 | - | - | - | X |
| 57 | MG | 1H | 3061 | - | - | - | X |
| 57 | MG | 1H | 3072 | - | - | - | X |
| 57 | MG | 1H | 3085 | - | - | - | X |
| 57 | MG | 1H | 3086 | - | - | - | X |
| 57 | MG | 1H | 3115 | - | - | - | X |
| 57 | MG | 1H | 3120 | - | - | - | X |
| 57 | MG | 1H | 3121 | - | - | - | X |
| 57 | MG | 1H | 3123 | - | - | - | X |
| 57 | MG | 1H | 3133 | - | - | - | X |
| 57 | MG | 1H | 3179 | - | - | - | X |
| 57 | MG | 1H | 3186 | - | - | - | X |
| 57 | MG | 1H | 3187 | - | - | - | X |
| 57 | MG | 1H | 3188 | - | - | - | X |
| 57 | MG | 1H | 3189 | - | - | - | X |
| 57 | MG | 1H | 3199 | - | - | - | X |
| 57 | MG | 1H | 3204 | - | - | - | X |
| 57 | MG | 1H | 3207 | - | - | - | X |
| 57 | MG | 1H | 3211 | - | - | - | X |
| 57 | MG | 1H | 3216 | - | - | - | X |
| 57 | MG | 1H | 3217 | - | - | - | X |
| 57 | MG | 1H | 3227 | - | - | - | X |
| 57 | MG | 1H | 3232 | - | - | - | X |
| 57 | MG | 1H | 3246 | - | - | - | X |
| 57 | MG | 1H | 3260 | - | - | - | X |
| 57 | MG | 1H | 3263 | - | - | - | X |
| 57 | MG | 1H | 3274 | - | - | - | X |
| 57 | MG | 1H | 3279 | - | - | - | X |
| 57 | MG | 1H | 3282 | - | - | - | X |
| 57 | MG | 1H | 3316 | - | - | - | X |
| 57 | MG | 1H | 3317 | - | - | - | X |
| 57 | MG | 1H | 3320 | - | - | - | X |
| 57 | MG | 2L | 102 | - | - | - | X |
| 57 | MG | 2L | 103 | - | - | - | X |
| 57 | MG | 4E | 201 | - | - | - | X |
| 59 | SF4 | 3E | 301 | - | - | X | - |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296743 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 | 1496 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32157 | 14313 | 5960 | 10388 | 1496 | | | |
| 1 | 1G | 1506 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32371 | 14409 | 6001 | 10456 | 1505 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| 13 | 1542 | G | U | conflict | GB 55771382 |
| 1G | 1542 | G | U | conflict | GB 55771382 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | 1E | 235 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1902 | 1215 | 340 | 342 | 5 | | | |
| 2 | 12 | 207 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1696 | 1083 | 306 | 303 | 4 | | | |

- 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 | 195 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1537 | 973 | 297 | 266 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | 3E | 207 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1698 | 1064 | 338 | 289 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 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 | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1142 | 722 | 216 | 200 | 4 | | | |
| 5 | 42 | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1139 | 721 | 216 | 198 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | 5E | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 837 | 528 | 154 | 152 | 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 | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1242 | 770 | 250 | 216 | 6 | | | |
| 7 | 62 | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1120 | 695 | 223 | 196 | 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 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1107 | 700 | 214 | 191 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | 8E | 126 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1000 | 634 | 196 | 170 | | | |
| 9 | 82 | 121 | Total | C | N | O | 0 | 0 | 0 |
| | | | 953 | 605 | 186 | 162 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | 1I | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 754 | 471 | 148 | 134 | 1 | | | |
| 10 | 1A | 80 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 646 | 403 | 129 | 114 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | 2I | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 512 | 154 | 154 | 3 | | | |
| 11 | 2A | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 835 | 520 | 156 | 156 | 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 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 942 | 582 | 194 | 164 | 2 | | | |
| 13 | 4A | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 893 | 552 | 183 | 156 | 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 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 486 | 309 | 103 | 70 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | 6I | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 146 | 124 | 2 | | | |
| 15 | 6A | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 146 | 124 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | 7I | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 700 | 443 | 139 | 117 | 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 | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 549 | 352 | 105 | 92 | | | |
| 18 | 9A | 67 | Total | C | N | O | 0 | 0 | 0 |
| | | | 544 | 349 | 104 | 91 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AI | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 661 | 422 | 123 | 114 | 2 | | | |
| 19 | AA | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 481 | 306 | 85 | 88 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | BI | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 746 | 461 | 157 | 126 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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 | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |
| 21 | 1B | 22 | Total | C | N | O | 0 | 0 | 0 |
| | | | 188 | 116 | 44 | 28 | | | |

- Molecule 22 is a RNA chain called tRNAVal.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | 1K | 72 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1540 | 688 | 274 | 506 | 72 | | | |

- Molecule 23 is a RNA chain called tRNAfMet.

| 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 | | | |
| 23 | 2L | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1626 | 726 | 296 | 527 | 76 | 1 | | | |

- Molecule 24 is a RNA chain called tRNAVal.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 24 | 3K | 70 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1491 | 665 | 268 | 488 | 70 | | | |
| 24 | 3L | 71 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1513 | 675 | 272 | 495 | 71 | | | |

- Molecule 25 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 25 | 4K | 21 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 462 | 207 | 96 | 138 | 21 | | | |
| 25 | 4L | 19 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 417 | 187 | 86 | 125 | 19 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26 | 1H | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61195 | 27234 | 11446 | 19674 | 2841 | | | |
| 26 | 14 | 2810 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60535 | 26940 | 11330 | 19455 | 2810 | | | |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| 1H | 161 | U | UNK | conflict | GB 55771382 |
| 1H | 654A | A | G | conflict | GB 55771382 |
| 1H | 654E | C | G | conflict | GB 55771382 |
| 1H | 654P | G | C | conflict | GB 55771382 |
| 1H | 654T | A | C | conflict | GB 55771382 |
| 1H | 1058 | U | G | conflict | GB 55771382 |
| 1H | 1080 | A | C | conflict | GB 55771382 |
| 14 | 158 | U | UNK | conflict | GB 55771382 |
| 14 | 654A | A | G | conflict | GB 55771382 |
| 14 | 654E | C | G | conflict | GB 55771382 |
| 14 | 654P | G | C | conflict | GB 55771382 |
| 14 | 654T | A | C | conflict | GB 55771382 |
| 14 | 1058 | U | G | conflict | GB 55771382 |
| 14 | 1080 | A | C | conflict | GB 55771382 |

- 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 | 133 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1033 | 651 | 194 | 187 | 1 | | | |
| 28 | 79 | 57 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 456 | 283 | 91 | 82 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | 11 | 273 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2120 | 1338 | 421 | 358 | 3 | | | |
| 29 | 19 | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2125 | 1341 | 422 | 359 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | 21 | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1505 | 951 | 281 | 267 | 6 | | | |
| 30 | 29 | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1563 | 988 | 299 | 270 | 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 | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1602 | 1022 | 299 | 279 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | 41 | 179 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1457 | 931 | 265 | 257 | 4 | | | |
| 32 | 49 | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1468 | 937 | 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 |
| | | | 1328 | 842 | 249 | 236 | 1 | | | |
| 33 | 59 | 167 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1283 | 815 | 239 | 228 | 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 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | 69 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 723 | 200 | 207 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | 58 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1096 | 706 | 205 | 181 | 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 | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 698 | 229 | 192 | 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 | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 712 | 211 | 187 | 7 | | | |
| 38 | 45 | 139 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 705 | 209 | 184 | 6 | | | |

- 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 | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 604 | 203 | 159 | 1 | | | |

- 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 | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 876 | 553 | 175 | 148 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | B8 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1124 | 700 | 231 | 192 | 1 | | | |
| 41 | 75 | 133 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1109 | 691 | 228 | 189 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | C8 | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 603 | 199 | 147 | 1 | | | |
| 42 | 85 | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | D8 | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 499 | 141 | 133 | 1 | | | |
| 43 | 95 | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 770 | 496 | 140 | 133 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | E8 | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 552 | 171 | 151 | 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 | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 743 | 482 | 134 | 126 | 1 | | | |
| 45 | B5 | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 735 | 477 | 133 | 125 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | G8 | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 777 | 501 | 145 | 126 | 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 | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1365 | 870 | 246 | 246 | 3 | | | |
| 47 | D5 | 133 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1079 | 694 | 194 | 189 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | I8 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 611 | 378 | 129 | 103 | 1 | | | |
| 48 | E5 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 603 | 372 | 128 | 102 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | J8 | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 737 | 463 | 146 | 127 | 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 | 68 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 358 | 116 | 100 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | G5 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 576 | 358 | 116 | 101 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 51 | L8 | 58 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 459 | 293 | 89 | 77 | | | | |
| 51 | H5 | 58 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 459 | 293 | 89 | 77 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | M8 | 61 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 299 | 86 | 89 | 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 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 437 | 275 | 87 | 70 | 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 |
| | | | 401 | 246 | 99 | 54 | 2 | | | |
| 54 | L5 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 401 | 246 | 99 | 54 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55 | Q8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 516 | 331 | 102 | 81 | 2 | | | |
| 55 | M5 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 516 | 331 | 102 | 81 | 2 | | | |

- Molecule 56 is a RNA chain called tRNAVal.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 56 | 1L | 69 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1469 | 656 | 262 | 482 | 69 | | | |

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57 | 45 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | 19 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | P8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | C5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | 13 | 148 | Total | Mg | 0 | 0 |
| | | | 148 | 148 | | |
| 57 | 1J | 7 | Total | Mg | 0 | 0 |
| | | | 7 | 7 | | |
| 57 | 5I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | 35 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | 4L | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | 16 | 11 | Total | Mg | 0 | 0 |
| | | | 11 | 11 | | |
| 57 | 42 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | B5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | 25 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | M5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | 21 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | 31 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | Q8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | L8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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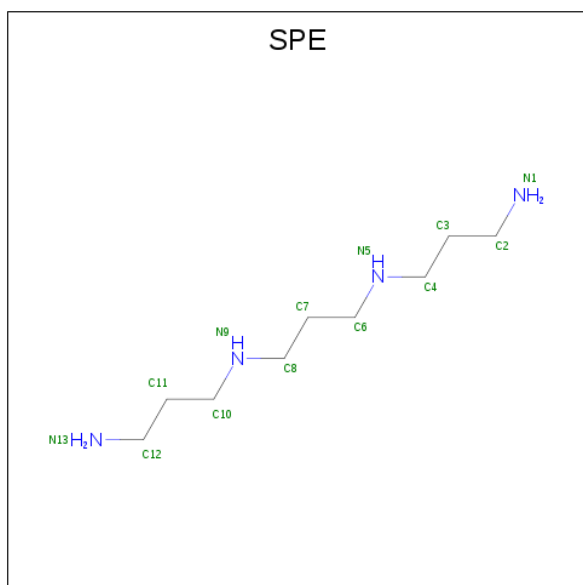
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | 9A | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 3I | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | I8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 68 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 29 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 2K | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | J8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 4A | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 39 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 1G | 133 | Total 133 | Mg 133 | 0 | 0 |
| 57 | 4E | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 11 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 1H | 548 | Total 548 | Mg 548 | 0 | 0 |
| 57 | E5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 88 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 5E | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 14 | 445 | Total 445 | Mg 445 | 0 | 0 |
| 57 | 78 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | F8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 4K | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 3A | 1 | Total 1 | Mg 1 | 0 | 0 |

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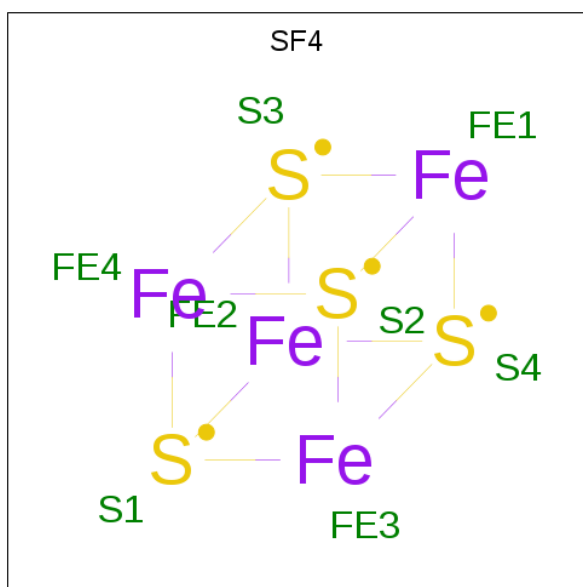
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57 | 41 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | 2L | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |

- Molecule 58 is THERMINE (three-letter code: SPE) (formula: C₉H₂₄N₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 58 | 13 | 1 | Total | C | N | 0 | 0 |
| | | | 13 | 9 | 4 | | |
| 58 | 1G | 1 | Total | C | N | 0 | 0 |
| | | | 13 | 9 | 4 | | |
| 58 | 14 | 1 | Total | C | N | 0 | 0 |
| | | | 13 | 9 | 4 | | |
| 58 | 14 | 1 | Total | C | N | 0 | 0 |
| | | | 13 | 9 | 4 | | |
| 58 | 1J | 1 | Total | C | N | 0 | 0 |
| | | | 13 | 9 | 4 | | |

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 59 | 3E | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 59 | 32 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60 | C5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | 5A | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | G8 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | 5I | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 61 | 13 | 304 | Total | O | 0 | 0 |
| | | | 304 | 304 | | |
| 61 | 3E | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 61 | 4E | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61 | 1I | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 2I | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 3I | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 5I | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 7I | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 1K | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 2K | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 3K | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 4K | 11 | Total 11 | O 11 | 0 | 0 |
| 61 | 1H | 1133 | Total 1133 | O 1133 | 0 | 0 |
| 61 | 16 | 15 | Total 15 | O 15 | 0 | 0 |
| 61 | 11 | 16 | Total 16 | O 16 | 0 | 0 |
| 61 | 21 | 8 | Total 8 | O 8 | 0 | 0 |
| 61 | 31 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | 58 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 78 | 11 | Total 11 | O 11 | 0 | 0 |
| 61 | 98 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | A8 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | B8 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | E8 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | F8 | 1 | Total 1 | O 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61 | I8 | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | K8 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | L8 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | P8 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | Q8 | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | 1G | 391 | Total 391 | O 391 | 0 | 0 |
| 61 | 22 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 42 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 52 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 3A | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 7A | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 9A | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BA | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 4L | 14 | Total 14 | O 14 | 0 | 0 |
| 61 | 14 | 1135 | Total 1135 | O 1135 | 0 | 0 |
| 61 | 1J | 18 | Total 18 | O 18 | 0 | 0 |
| 61 | 19 | 8 | Total 8 | O 8 | 0 | 0 |
| 61 | 29 | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 39 | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 25 | 11 | Total 11 | O 11 | 0 | 0 |
| 61 | 35 | 9 | Total 9 | O 9 | 0 | 0 |

Continued on next page...

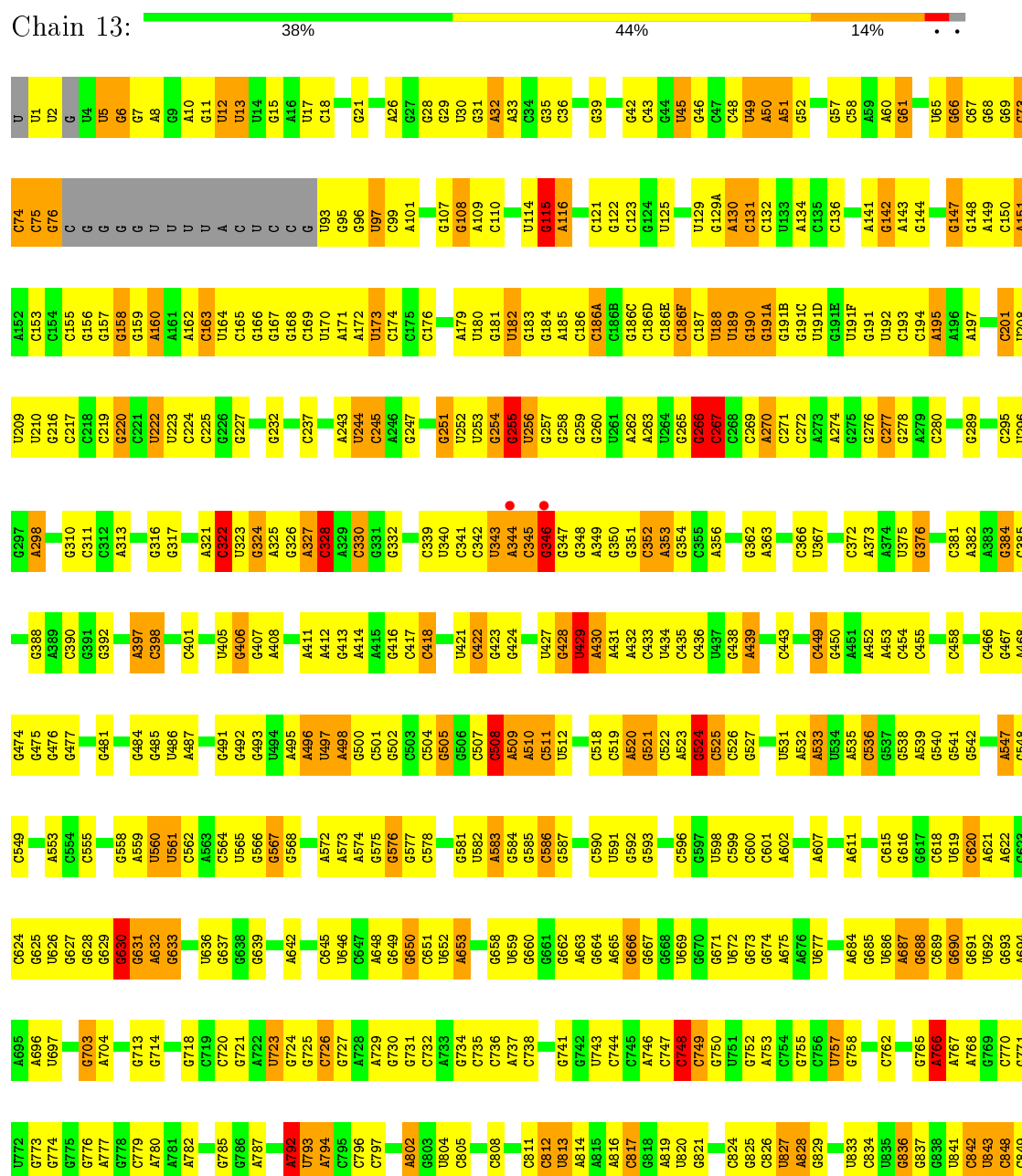
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 61 | 45 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 55 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 75 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 85 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | A5 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | C5 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | E5 | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | F5 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | H5 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | M5 | 7 | Total 7 | O 7 | 0 | 0 |

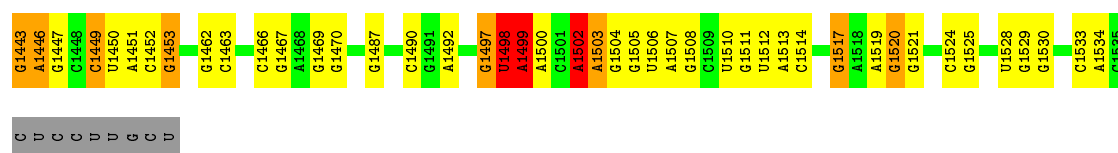
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

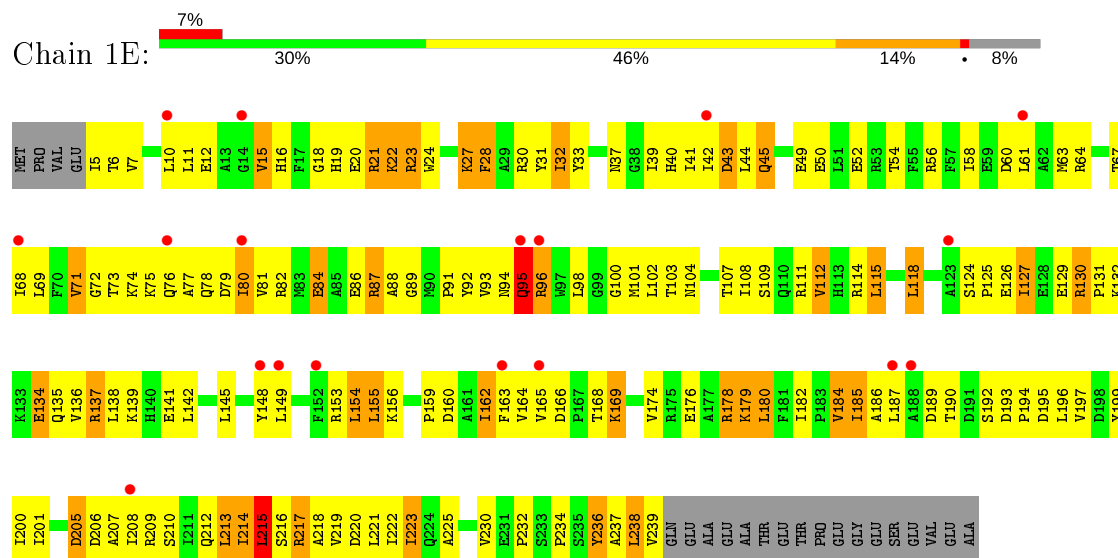
- Molecule 1: 16S ribosomal RNA



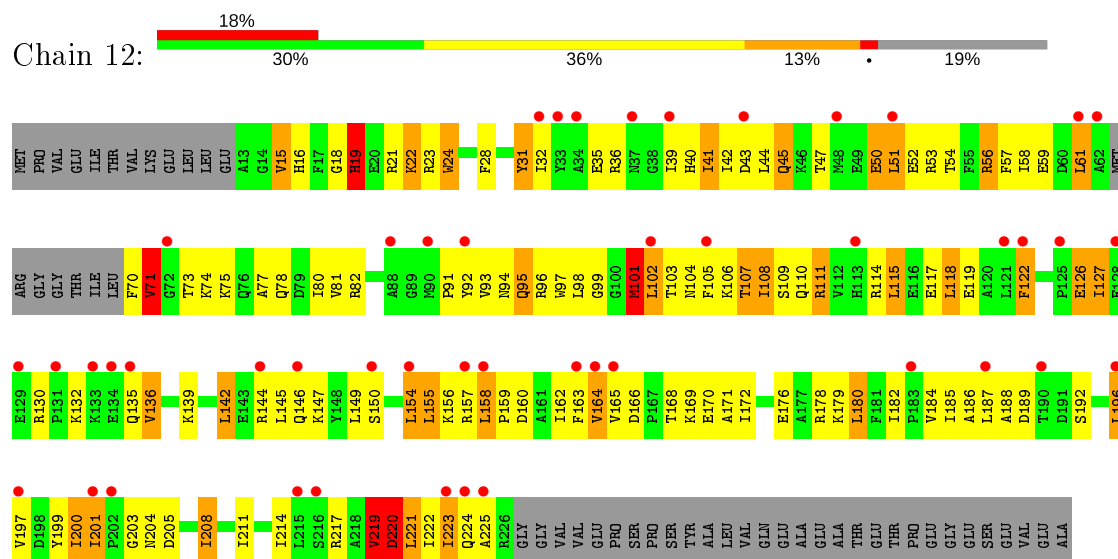
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|--------|-------|-------|-------|-------|--------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--|
| A1363 | A1364 | C1367 | C1368 | C1369 | C1370 | A1371 | A1372 | A1373 | A1374 | A1375 | A1376 | A1377 | G1386 | G1387 | G1388 | G1389 | G1390 | G1391 | G1392 | G1393 | G1394 | G1395 | G1396 | G1397 | G1398 | G1399 | G1400 | G1401 | G1402 | G1403 | G1404 | G1405 | G1406 | G1407 | A1408 | A1413 | A1414 | G1415 | G1416 | G1417 | A1418 | G1419 | G1422 | G1423 | C1424 | G1432 | G1435 | G1436 | G1437 | G1438 | G1439 | G1440 | G1441 | G1442 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1300 | G1301 | G1302 | G1303 | G1304 | G1305 | A1306 | G1307 | G1308 | G1309 | G1310 | G1311 | G1312 | G1313 | G1314 | G1315 | G1316 | G1317 | A1318 | A1319 | C1320 | C1321 | C1322 | G1323 | A1324 | G1325 | G1326 | G1327 | G1328 | G1329 | G1330 | G1331 | G1332 | G1333 | G1334 | G1335 | G1336 | G1337 | G1338 | A1339 | G1342 | G1343 | A1346 | G1347 | G1348 | A1349 | A1350 | G1351 | G1352 | G1353 | G1356 | A1357 | G1358 | G1359 | A1360 | G1362A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1222 | C1223 | G1224 | C1225 | C1226 | A1227 | C1228 | U1232 | U1233 | G1234 | U1235 | A1238 | A1239 | C1240 | G1241 | G1242 | A1245 | C1246 | C1249 | C1250 | C1251 | C1252 | C1253 | G1254 | A1255 | A1256 | U1257 | G1258 | G1259 | G1260 | G1261 | G1262 | G1263 | G1264 | G1265 | G1266 | G1267 | G1268 | G1269 | G1270 | G1271 | G1272 | G1273 | G1274 | G1275 | G1276 | G1277 | G1278 | G1279 | G1280 | G1281 | G1282 | G1283 | G1284 | G1285 | A1286 | A1287 | A1288 | A1289 | G1290 | G1291 | U1292 | C1296 | C1297 | C1298 | A1299 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C1158 | U1159 | C1160 | C1161 | C1162 | A1167 | A1169 | A1170 | G1171 | G1172 | G1173 | G1174 | G1175 | A1176 | G1177 | G1178 | A1179 | A1180 | G1181 | G1182 | G1183 | G1184 | G1185 | G1186 | G1187 | A1188 | G1189 | G1190 | A1191 | G1192 | G1193 | U1194 | C1195 | U1196 | G1197 | G1198 | U1199 | C1200 | G1201 | G1202 | G1203 | A1204 | U1205 | G1206 | G1207 | G1208 | C1209 | G1210 | U1211 | U1212 | A1213 | G1214 | G1215 | G1216 | G1217 | G1218 | U1219 | G1220 | G1221 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U1020 | G1021 | G1022 | G1023 | U1024 | U1025 | G1026 | C1027 | C1028 | A1028A | C1028B | G1029 | G1030 | G1031 | A1032 | G1032A | G1032B | G1033 | C1037 | C1038 | C1039 | U1040 | A1041 | G1042 | C1043 | A1046 | G1047 | G1048 | C1051 | U1052 | G1053 | C1054 | A1055 | U1056 | G1057 | G1058 | C1059 | C1060 | G1061 | U1062 | G1063 | G1064 | G1068 | C1069 | U1070 | G1071 | G1072 | U1073 | G1074 | G1077 | A1080 | G1081 | G1084 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U1085 | U1086 | G1087 | G1094 | U1095 | U1098 | C1099 | G1100 | A1101 | C1102 | A1105 | G1106 | C1107 | C1108 | C1109 | C1110 | C1111 | C1112 | G1117 | G1118 | C1119 | A1123 | G1124 | G1125 | U1126 | G1127 | G1128 | G1129 | A1130 | G1131 | G1132 | G1133 | G1134 | U1135 | U1136 | G1137 | G1138 | G1139 | C1140 | C1141 | G1142 | G1143 | G1144 | C1145 | A1146 | C1147 | U1148 | C1149 | U1150 | A1151 | A1152 | C1153 | G1154 | G1155 | A1157 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C1158 | U1159 | C1160 | C1161 | C1162 | A1167 | A1169 | A1170 | G1171 | G1172 | G1173 | G1174 | G1175 | A1176 | G1177 | G1178 | A1179 | A1180 | G1181 | G1182 | G1183 | G1184 | G1185 | G1186 | G1187 | A1188 | G1189 | G1190 | A1191 | G1192 | G1193 | U1194 | C1195 | U1196 | G1197 | G1198 | U1199 | C1200 | G1201 | G1202 | G1203 | A1204 | U1205 | G1206 | G1207 | G1208 | C1209 | G1210 | U1211 | U1212 | A1213 | G1214 | G1215 | G1216 | G1217 | G1218 | U1219 | G1220 | G1221 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1222 | C1223 | G1224 | C1225 | C1226 | A1227 | C1228 | U1232 | U1233 | G1234 | U1235 | A1238 | A1239 | C1240 | G1241 | G1242 | A1245 | C1246 | C1249 | C1250 | C1251 | C1252 | C1253 | G1254 | A1255 | A1256 | U1257 | G1258 | G1259 | G1260 | G1261 | G1262 | G1263 | G1264 | G1265 | G1266 | G1267 | G1268 | G1269 | G1270 | G1271 | G1272 | G1273 | G1274 | G1275 | G1276 | G1277 | G1278 | G1279 | G1280 | G1281 | G1282 | G1283 | G1284 | G1285 | A1286 | A1287 | A1288 | A1289 | G1290 | G1291 | U1292 | C1296 | C1297 | C1298 | A1299 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1300 | G1301 | G1302 | G1303 | G1304 | G1305 | A1306 | G1307 | G1308 | G1309 | G1310 | G1311 | G1312 | G1313 | G1314 | G1315 | G1316 | G1317 | A1318 | A1319 | C1320 | C1321 | C1322 | G1323 | A1324 | G1325 | G1326 | G1327 | G1328 | G1329 | G1330 | G1331 | G1332 | G1333 | G1334 | G1335 | G1336 | G1337 | G1338 | A1339 | G1342 | G1343 | A1346 | G1347 | G1348 | A1349 | A1350 | G1351 | G1352 | G1353 | G1356 | A1357 | G1358 | G1359 | A1360 | G1362A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1363 | A1364 | C1367 | C1368 | C1369 | C1370 | A1371 | A1372 | A1373 | A1374 | A1375 | A1376 | A1377 | G1386 | G1387 | G1388 | G1389 | G1390 | G1391 | G1392 | G1393 | G1394 | G1395 | G1396 | G1397 | G1398 | G1399 | G1400 | G1401 | G1402 | G1403 | G1404 | G1405 | G1406 | G1407 | A1408 | A1413 | A1414 | G1415 | G1416 | G1417 | A1418 | G1419 | G1422 | G1423 | C1424 | G1432 | G1435 | G1436 | G1437 | G1438 | G1439 | A1440 | G1441 | G1442 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G351 | G354 | G352 | C353 | U356 | G354 | G358 | G359 | G362 | G363 | G364 | G365 | G366 | G367 | G368 | G369 | G370 | G371 | G372 | G373 | G374 | G375 | G376 | G377 | G378 | G379 | G380 | G381 | G382 | G383 | G384 | G385 | G386 | G387 | G388 | G389 | G390 | G391 | G392 | G393 | G394 | G395 | G396 | G397 | G398 | G399 | A300 | G309 | G310 | A313 | C314 | A315 | G316 | A321 | C322 | C328 | A329 | C330 | G331 | G332 | G333 | G334 | G335 | G336 | G337 | A344 | C345 | G346 | G347 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U429 | A430 | U434 | U435 | U436 | U437 | U438 | A439 | A440 | C442 | G445 | G446 | G447 | G448 | G449 | G450 | G451 | G452 | A453 | C456 | A457 | C458 | G459 | G460 | G461 | G462 | G463 | G464 | G465 | G466 | G467 | G468 | G469 | G470 | G471 | G472 | G473 | G474 | G475 | G476 | G477 | G478 | G479 | G480 | G481 | G482 | G483 | G484 | G485 | U486 | C489 | U490 | G491 | A496 | U497 | G502 | C503 | C504 | G505 | G506 | G507 | G508 | G509 | A510 | C511 | U512 | C513 | U514 | U515 | U516 | U517 | U518 | U519 | U520 | U521 | U522 | U523 | U524 | U525 | U526 | U527 | U528 | U529 | U530 | U531 | A532 | U533 | U534 | U535 | U536 | U537 | U538 | U539 | U540 | U541 | U542 | U543 | U544 | U545 | U546 | U547 | U548 | U549 | U550 | U551 | U552 | U553 | U554 | U555 | U556 | U557 | U558 | U559 | U560 | U561 | U562 | U563 | U564 | U565 | U566 | U567 | U568 | U569 | U570 | U571 | U572 | U573 | U574 | U575 | U576 | U577 | U578 | U579 | U580 | U581 | U582 | U583 | U584 | U585 | U586 | U587 | U588 | U589 | U590 | U591 | U592 | U593 | U594 | U595 | U596 | U597 | U598 | U599 | U600 | U601 | U602 | U603 | U604 | U605 | U606 | U607 | U608 | U609 | U610 | U611 | U612 | U613 | U614 | U615 | U616 | U617 | U618 | U619 | U620 | U621 | U622 | U623 | U624 | U625 | U626 | U627 | U628 | U629 | U630 | U631 | U632 | U633 | U634 | U635 | U636 | U637 | U638 | U639 | U640 | U641 | U642 | U643 | U644 | U645 | U646 | U647 | U648 | U649 | U650 | U651 | U652 | U653 | U654 | U655 | U656 | U657 | U658 | U659 | U660 | U661 | U662 | U663 | U664 | U665 | U666 | U667 | U668 | U669 | U670 | U671 | U672 | U673 | U674 | U675 | U676 | U677 | U678 | U679 | U680 | U681 | U682 | U683 | U684 | U685 | U686 | U687 | U688 | U689 | U690 | U691 | U692 | U693 | U694 | U695 | U696 | U697 | U698 | U699 | U700 | U701 | U702 | U703 | U704 | U705 | U706 | U707 | U708 | U709 | U710 | U711 | U712 | U713 | U714 | U715 | U716 | U717 | U718 | U719 | U720 | U721 | U722 | U723 | U724 | U725 | U726 | U727 | U728 | U729 | U730 | U731 | U732 | U733 | U734 | U735 | U736 | U737 | U738 | U739 | U740 | U741 | U742 | U743 | U744 | U745 | U746 | U747 | U748 | U749 | U750 | U751 | U752 | U753 | U754 | U755 | U756 | U757 | U758 | U759 | U760 | U761 | U762 | U763 | U764 | U765 | U766 | U767 | U768 | U769 | U770 | U771 | U772 | U773 | U774 | U775 | U776 | U777 | U778 | U779 | U780 | U781 | U782 | U783 | U784 | U785 | U786 | U787 | U788 | U789 | U790 | U791 | U792 | U793 | U794 | U795 | U796 | U797 | U798 | U799 | U800 | U801 | U802 | U803 | U804 | U805 | U806 | U807 | U808 | U809 | U810 | U811 | U812 | U813 | U814 | U815 | U816 | U817 | U818 | U819 | U820 | U821 | U822 | U823 | U824 | U825 | U826 | U827 | U828 | U829 | U830 | U831 | U832 | U833 | U834 | U835 | U836 | U837 | U838 | U839 | U840 | U841 | U842 | U843 | U844 | U845 | U846 | U847 | U848 | U849 | U850 | U851 | U852 | U853 | U854 | U855 | U856 | U857 | U858 | U859 | U860 | U861 | U862 | U863 | U864 | U865 | U866 | U867 | U868 | U869 | U870 | U871 | U872 | U873 | U874 | U875 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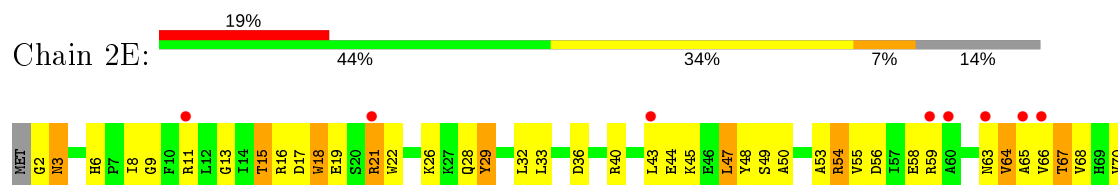
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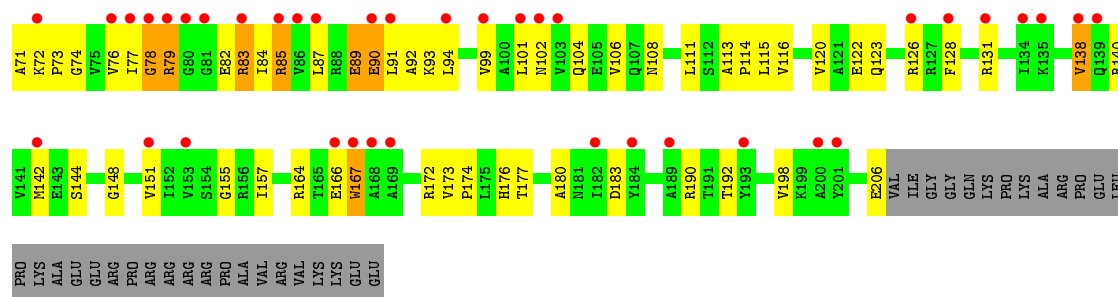


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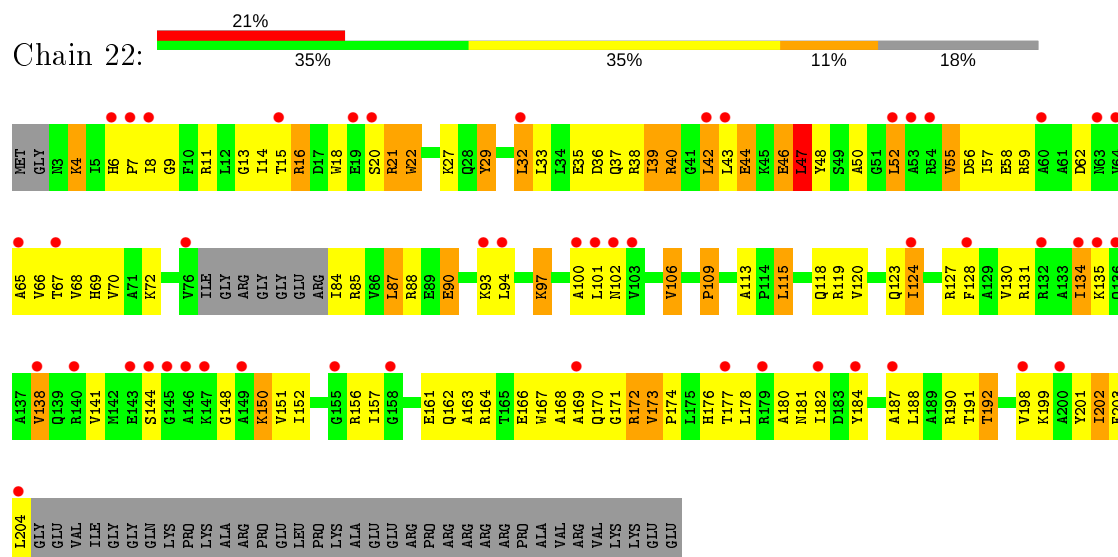


• Molecule 3: 30S ribosomal protein S3

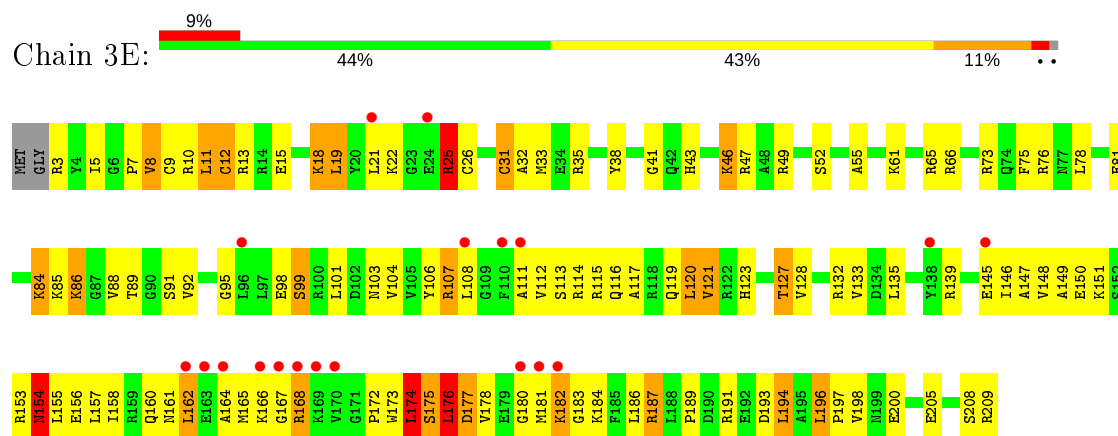




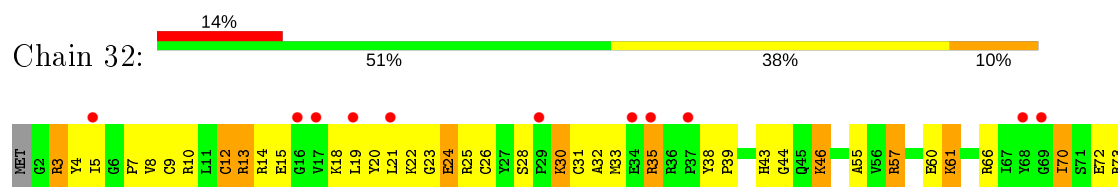
• Molecule 3: 30S ribosomal protein S3

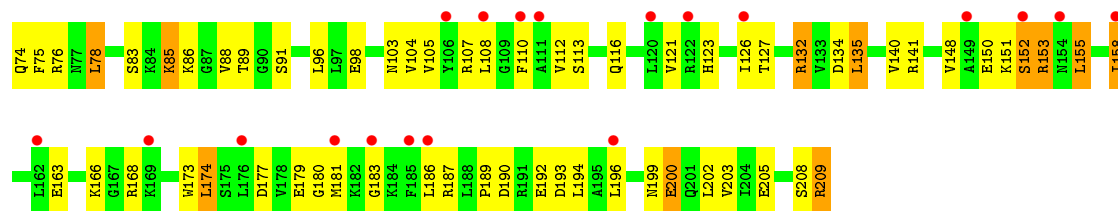


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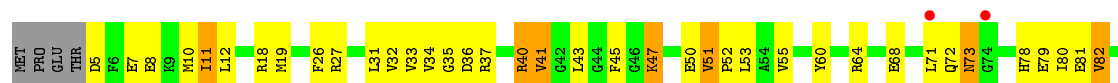


• Molecule 4: 30S ribosomal protein S4



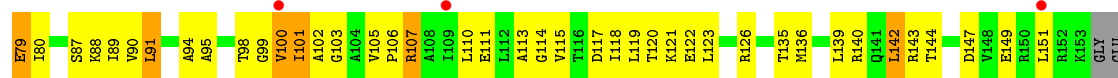


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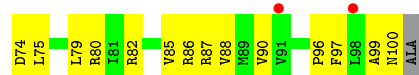
GLY

• Molecule 5: 30S ribosomal protein S5



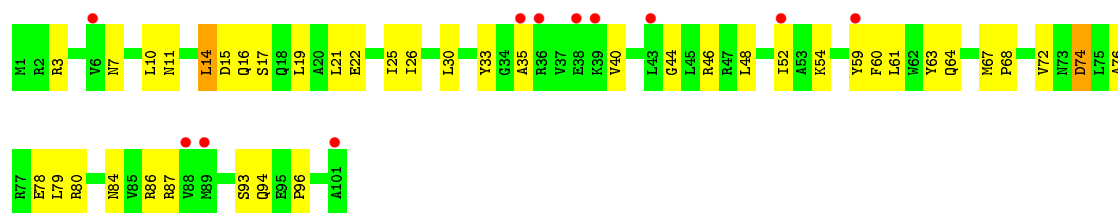
ALA
HIS
ALA
GLN
ALA
GLN
GLY

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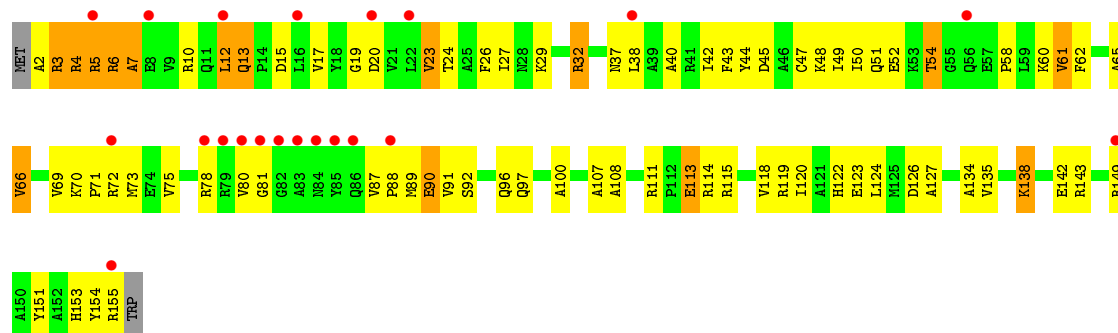


• Molecule 6: 30S ribosomal protein S6

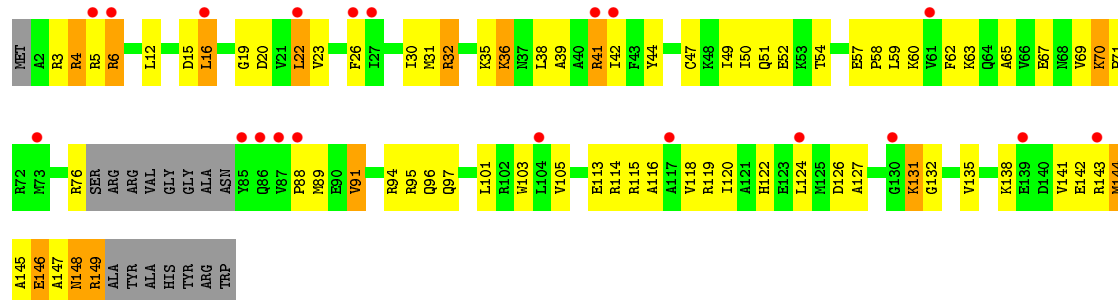
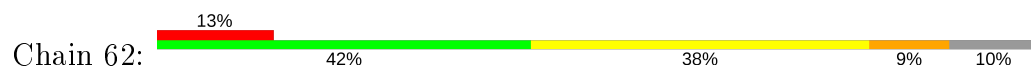




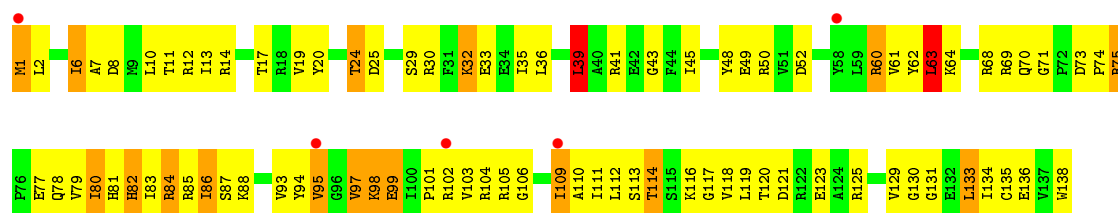
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

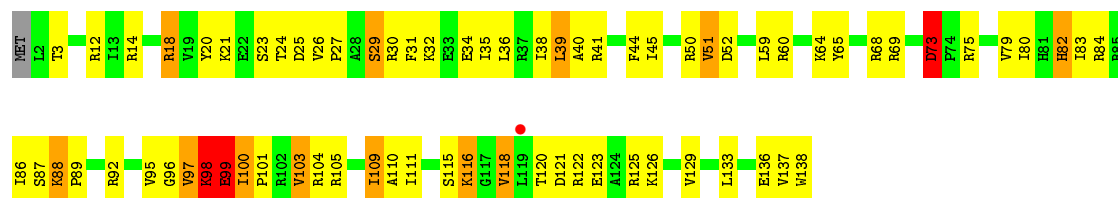


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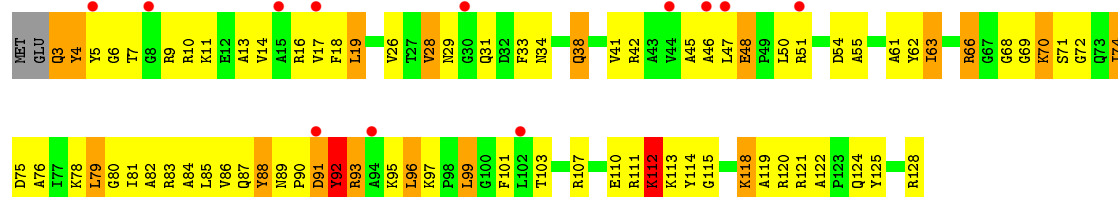


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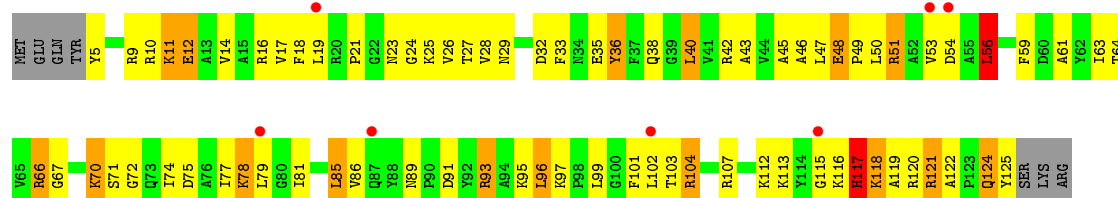




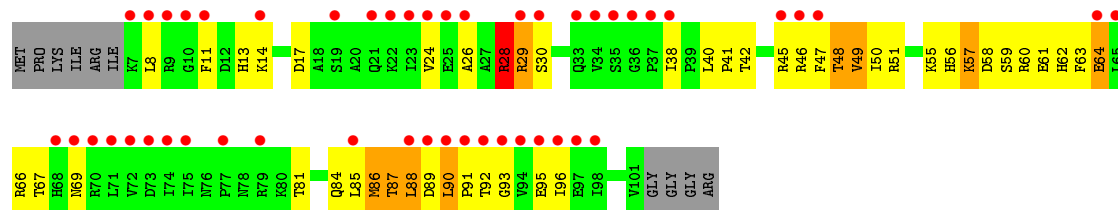
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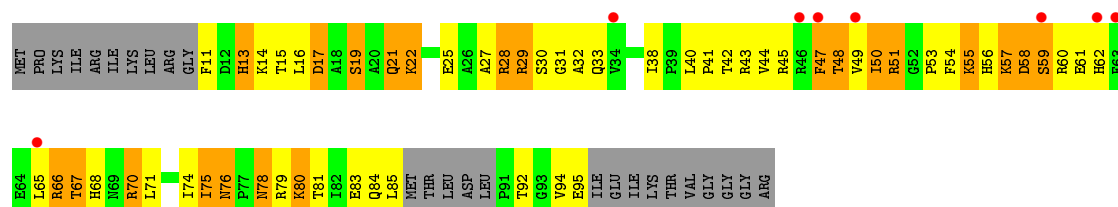
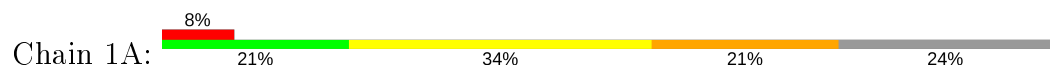
• Molecule 9: 30S ribosomal protein S9



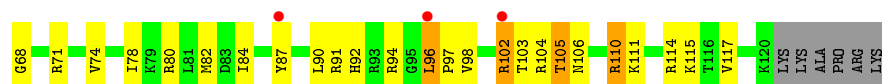
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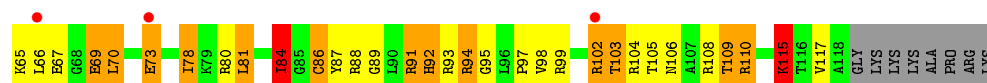
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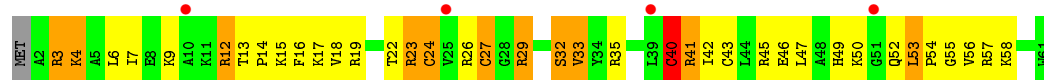
- Chain 4I:



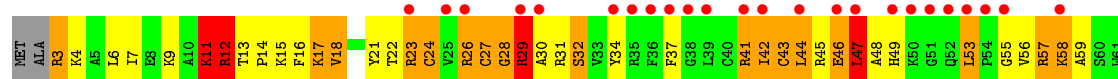
- Molecule 13: 30S ribosomal protein S13



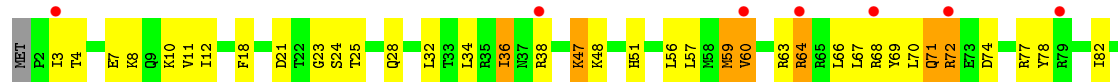
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



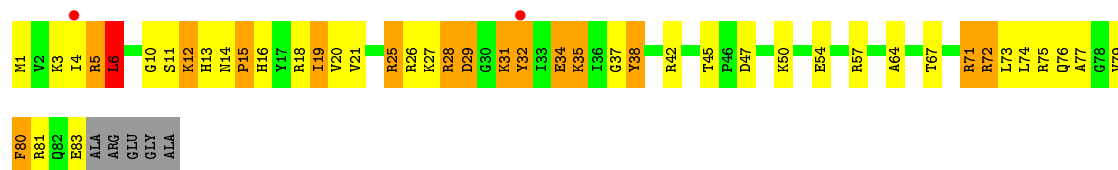
- Molecule 15: 30S ribosomal protein S15



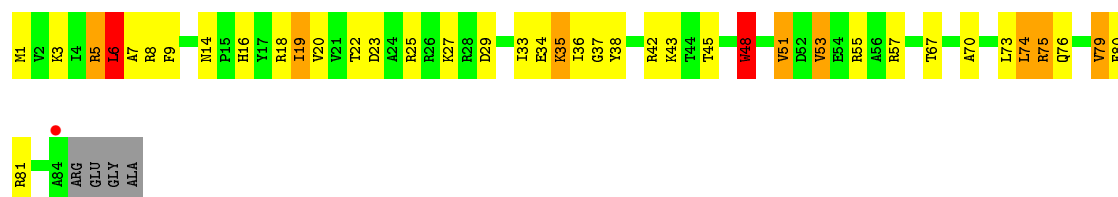
- Molecule 15: 30S ribosomal protein S15



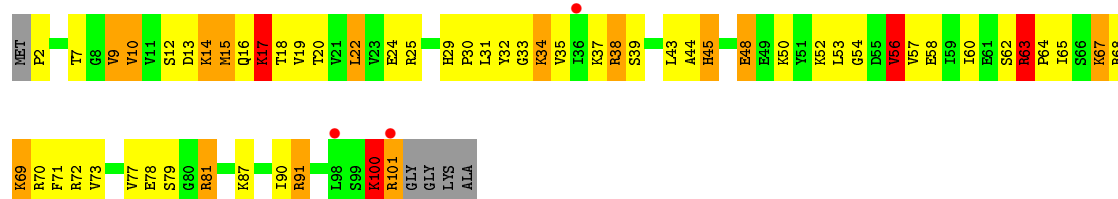
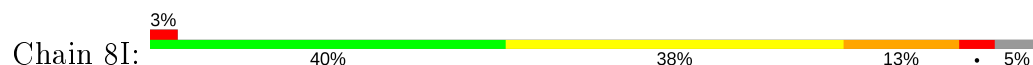
- Molecule 16: 30S ribosomal protein S16



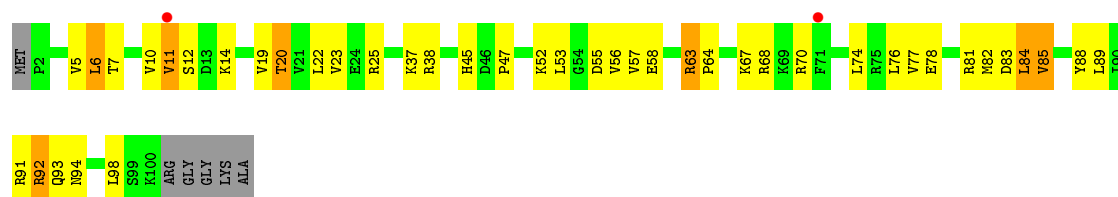
- Molecule 16: 30S ribosomal protein S16



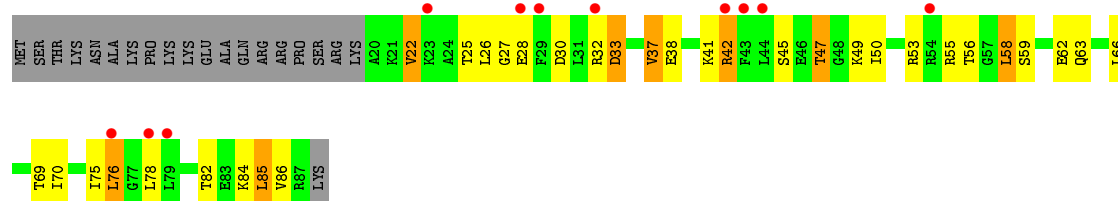
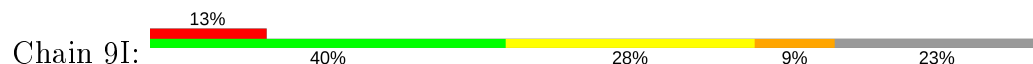
- Molecule 17: 30S ribosomal protein S17



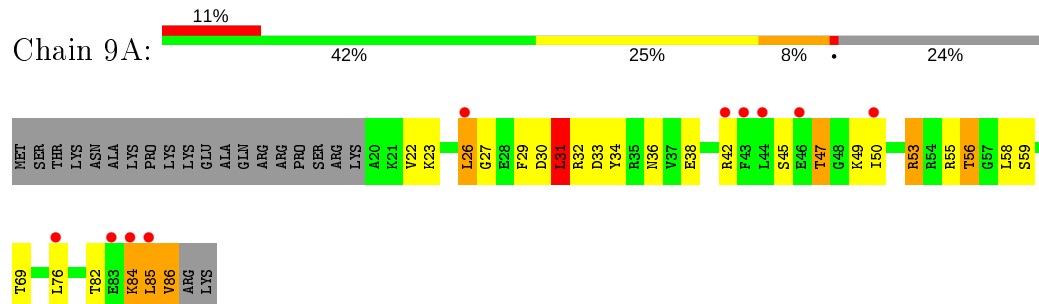
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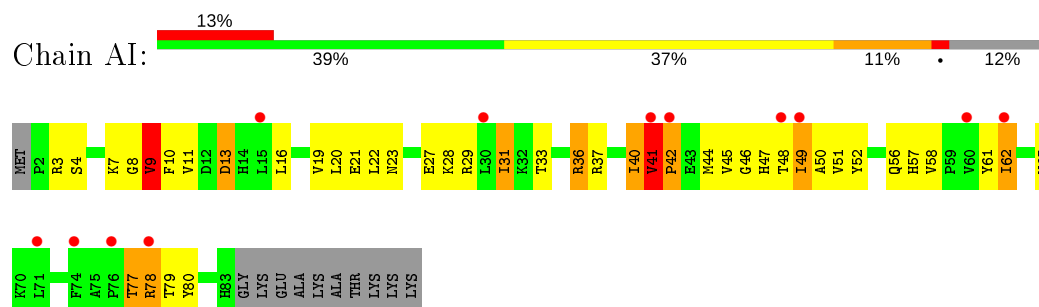
- Molecule 18: 30S ribosomal protein S18



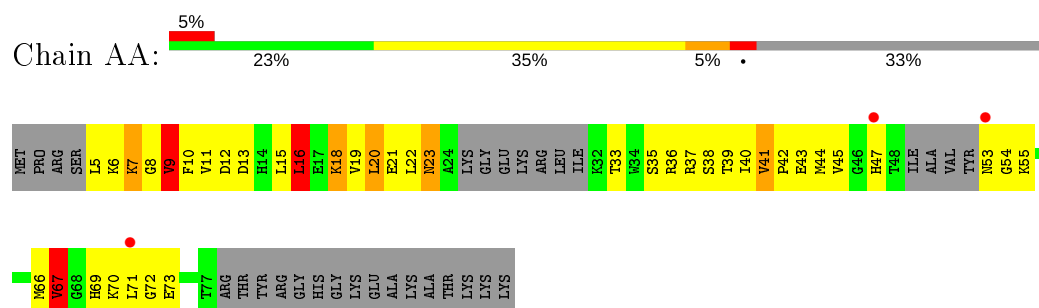
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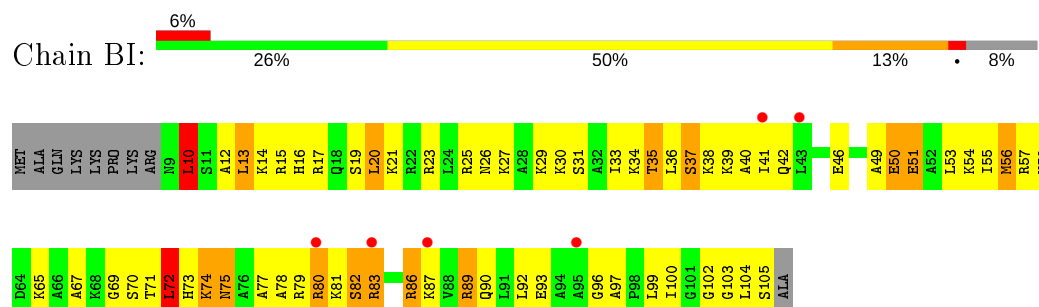
- Molecule 19: 30S ribosomal protein S19



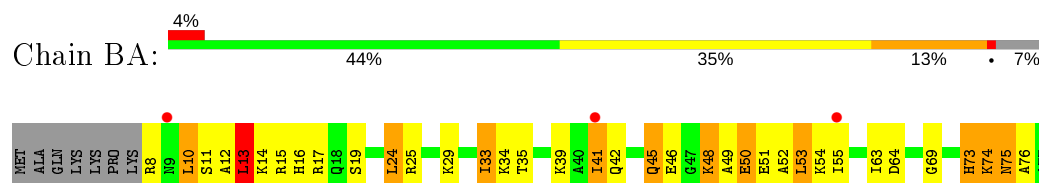
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

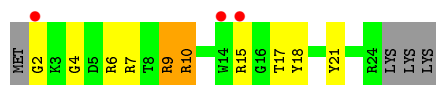


- Molecule 20: 30S ribosomal protein S20

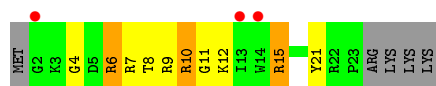




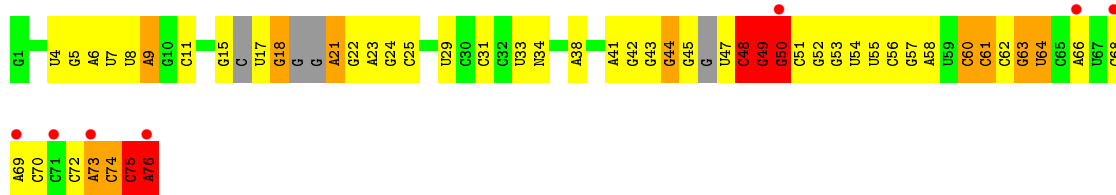
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



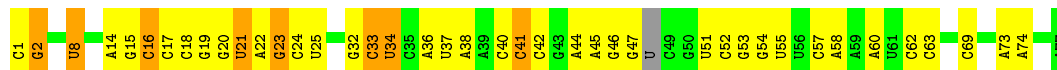
- Molecule 22: tRNAVal



- Molecule 23: tRNAfMet

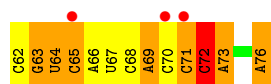


- Molecule 23: tRNAfMet

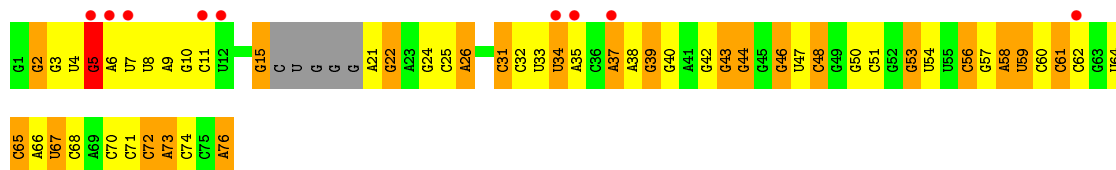
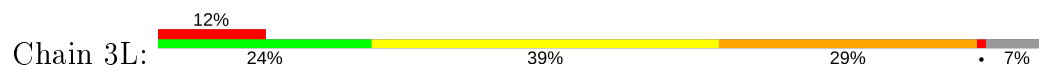


- Molecule 24: tRNAVal

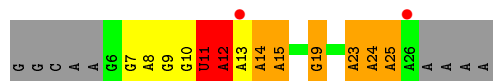
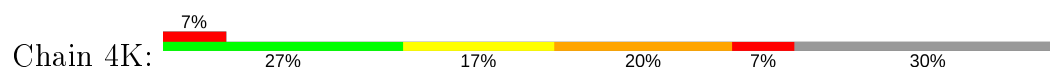




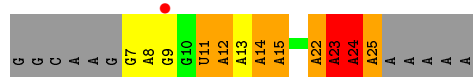
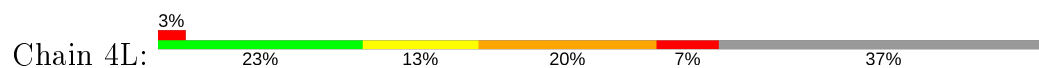
• Molecule 24: tRNAVal



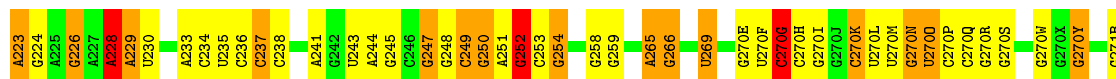
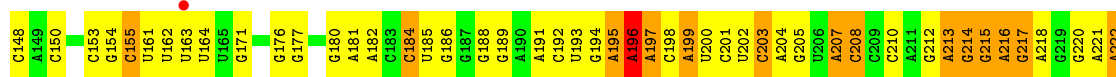
• Molecule 25: mRNA



• Molecule 25: mRNA

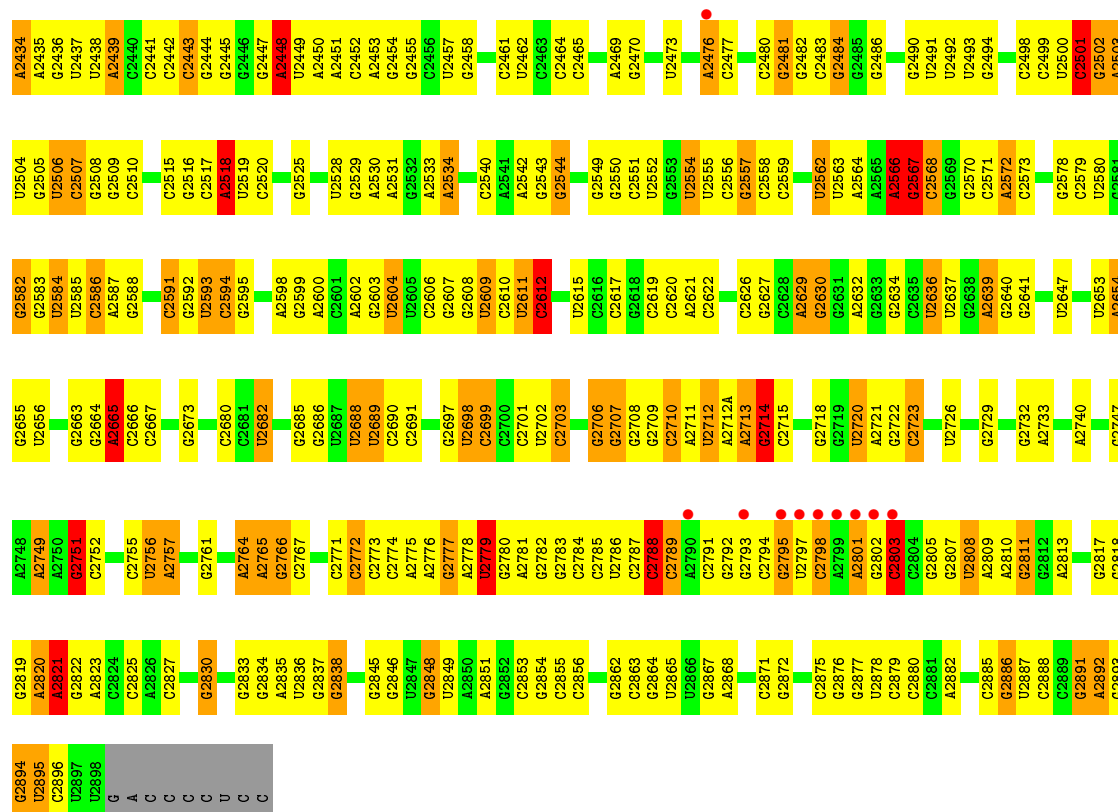


• Molecule 26: 23S ribosomal RNA

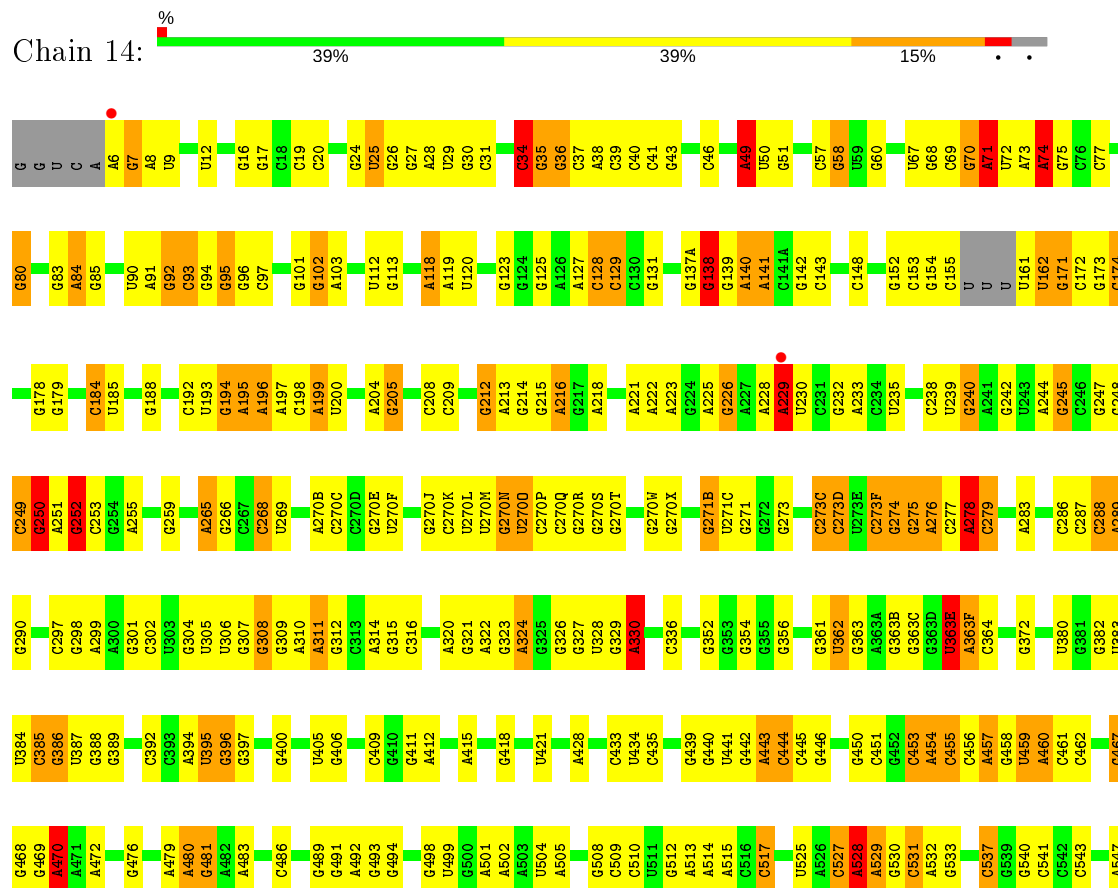


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| G1328 | G1329 | C1330 | A1331 | G1332 | A1336 | G1337 | G1338 | G1339 | U1340 | U1341 | A1342 | G1343 | U1344 | A1345 | G1346 | A1349 | U1352 | A1353 | A1354 | G1355 | G1356 | U1357 | G1358 | A1359 | A1360 | C1363 | G1364 | A1365 | G1371 | U1372 | A1373 | G1374 | C1375 | G1376 | G1377 | A1378 | A1379 | G1380 | G1381 | G1382 | G1385 | C1386 | C1387 | G1388 | G1389 | U1390 | U1391 | U1392 | A1393 | U1394 | U1395 | U1396 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1259 | G1260 | C1261 | A1262 | U1263 | G1264 | A1265 | G1266 | U1267 | A1268 | A1269 | G1270 | G1271 | A1272 | U1273 | A1274 | A1275 | A1276 | G1277 | A1278 | G1279 | G1280 | G1281 | U1282 | G1283 | A1284 | G1285 | U1286 | U1287 | U1288 | C1289 | G1290 | C1291 | U1292 | C1293 | G1297 | U1300 | A1301 | A1302 | C1303 | G1304 | A1307 | A1308 | U1312 | U1313 | C1314 | C1315 | U1316 | A1317 | U1321 | A1322 | U1323 | G1324 | U1325 | U1326 | C1327 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1194 | G1195 | C1196 | G1197 | U1198 | U1199 | C1200 | C1201 | C1202 | G1203 | A1204 | U1205 | G1206 | A1207 | C1208 | G1209 | A1210 | U1211 | G1212 | G1216 | C1217 | C1218 | G1219 | A1220 | C1221 | C1222 | G1225 | C1226 | A1227 | G1228 | C1230 | G1231 | G1232 | G1233 | U1234 | A1237 | G1238 | G1239 | U1240 | A1241 | A1242 | G1243 | G1244 | G1245 | A1246 | U1249 | G1250 | C1251 | G1252 | A1253 | A1254 | U1255 | G1256 | C1257 | G1258 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1123 | C1124 | G1125 | A1126 | A1127 | A1128 | A1129 | U1130 | G1131 | G1135 | G1136 | G1137 | G1138 | G1139 | A1140 | U1141 | U1142 | A1143 | C1147 | A1148 | G1149 | G1153 | G1154 | A1155 | A1156 | G1157 | G1161 | U1165 | C1166 | U1167 | G1168 | G1169 | G1170 | G1171 | G1172 | G1173 | A1174 | U1175 | G1176 | A1177 | C1178 | G1179 | G1180 | C1181 | A1182 | G1183 | G1186 | G1187 | A1188 | U1189 | A1190 | G1191 | G1192 | U1193 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1054 | G1055 | G | A | U | C | U | U | U | G | C | U | U | U | A | C | C | C | A | G | C | C | A | U | C | C | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C986 | G987 | A988 | G989 | A990 | G991 | G992 | G993 | C994 | C995 | A996 | G997 | C998 | U999 | A1000 | A1001 | G1002 | G1003 | C1004 | C1005 | C1006 | A1009 | A1010 | A1011 | A1012 | C1013 | G1017 | G1018 | U1019 | A1020 | A1021 | G1022 | C1023 | U1024 | G1025 | U1026 | A1027 | A1028 | A1029 | G1030 | A1031 | A1032 | U1033 | G1034 | U1035 | G1036 | C1040 | G1041 | G1042 | A1045 | A1046 | G1047 | A1048 | C1049 | A1050 | G1051 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A783 | A784 | G785 | C786 | G787 | A788 | A789 | C790 | G791 | C792 | A793 | C796 | C797 | G798 | C799 | G799 | A800 | G801 | A802 | U803 | A804 | A805 | U806 | U810 | U811 | C812 | U813 | C814 | C817 | G818 | A819 | A820 | A821 | U822 | G823 | A824 | C825 | U826 | U827 | U828 | A829 | G830 | G831 | U832 | U833 | C834 | A835 | G836 | C837 | C838 | U839 | C840 | G845 | C846 | U847 | G848 | A849 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G850 | U851 | G852 | G853 | G854 | G855 | G856 | C857 | U858 | G859 | U860 | A861 | G862 | A863 | G864 | C865 | A866 | G867 | U868 | G869 | A870 | U871 | A872 | G873 | G874 | A878 | G879 | G880 | G881 | G882 | C | C | C | C | A | G | C883 | C884 | C885 | G886 | A | C887 | C888 | C889 | A890 | A901 | C902 | C903 | C904 | U905 | G906 | U907 | C908 | A909 | A910 | U913 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C914 | C915 | G916 | A917 | A918 | G919 | G928 | G929 | U930 | C931 | G932 | A933 | G934 | C935 | C936 | A937 | G938 | G939 | G940 | G941 | A942 | G943 | G944 | A945 | G946 | G947 | G950 | G951 | G952 | A953 | G954 | C955 | U956 | A957 | U958 | A959 | A960 | C961 | U962 | U963 | G966 | C967 | G968 | U969 | G974 | C974A | G975 | G978 | G979 | A980 | A981 | C982 | C983 | A984 | C985 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C986 | G987 | A988 | G989 | A990 | G991 | G992 | G993 | C994 | C995 | A996 | G997 | C998 | U999 | A1000 | A1001 | G1002 | G1003 | C1004 | C1005 | C1006 | A1009 | A1010 | A1011 | A1012 | C1013 | G1017 | G1018 | U1019 | A1020 | A1021 | G1022 | C1023 | U1024 | G1025 | U1026 | A1027 | A1028 | A1029 | G1030 | A1031 | A1032 | U1033 | G1034 | U1035 | G1036 | C1040 | G1041 | G1042 | A1045 | A1046 | G1047 | A1048 | C1049 | A1050 | G1051 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1054 | G1055 | G | A | U | C | U | U | U | G | C | U | U | U | A | C | C | C | A | G | C | C | A | U | C | C | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | U | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C1123 | C1124 | G1125 | A1126 | A1127 | A1128 | A1129 | U1130 | G1131 | G1135 | G1136 | G1137 | G1138 | G1139 | A1140 | U1141 | U1142 | A1143 | C1147 | A1148 | G1149 | G1153 | G1154 | A1155 | A1156 | G1157 | G1161 | U1165 | C1166 | U1167 | G1168 | G1169 | G1170 | G1171 | G1172 | G1173 | A1174 | U1175 | G1176 | A1177 | C1178 | G1179 | G1180 | C1181 | A1182 | G1183 | G1186 | G1187 | A1188 | U1189 | A1190 | G1191 | G1192 | U1193 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1194 | G1195 | C1196 | G1197 | U1198 | U1199 | C1200 | C1201 | C1202 | G1203 | A1204 | U1205 | G1206 | A1207 | C1208 | G1209 | A1210 | U1211 | G1212 | G1216 | C1217 | C1218 | G1219 | A1220 | C1221 | C1222 | G1225 | C1226 | A1227 | G1228 | C1230 | G1231 | G1232 | G1233 | U1234 | A1237 | G1238 | G1239 | U1240 | A1241 | A1242 | G1243 | G1244 | G1245 | A1246 | U1249 | G1250 | C1251 | G1252 | A1253 | A1254 | U1255 | G1256 | C1257 | G1258 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1259 | G1260 | C1261 | A1262 | U1263 | G1264 | A1265 | G1266 | U1267 | A1268 | A1269 | G1270 | G1271 | A1272 | U1273 | A1274 | A1275 | A1276 | G1277 | A1278 | G1279 | G1280 | G1281 | U1282 | G1283 | A1284 | G1285 | U1286 | U1287 | U1288 | C1289 | G1290 | C1291 | U1292 | C1293 | G1297 | U1300 | A1301 | A1302 | C1303 | G1304 | A1307 | A1308 | U1312 | U1313 | C1314 | C1315 | U1316 | A1317 | U1321 | A1322 | U1323 | G1324 | U1325 | U1326 | C1327 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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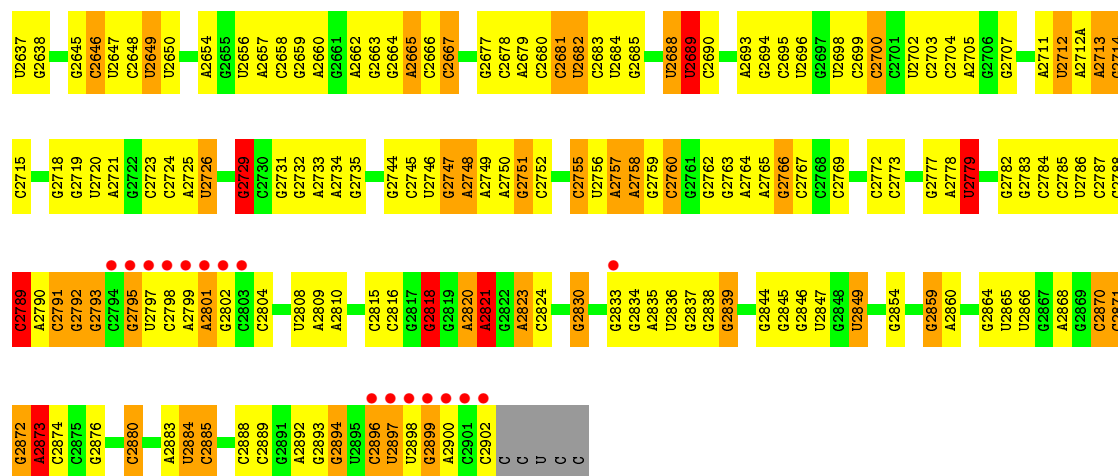


● Molecule 26: 23S ribosomal RNA

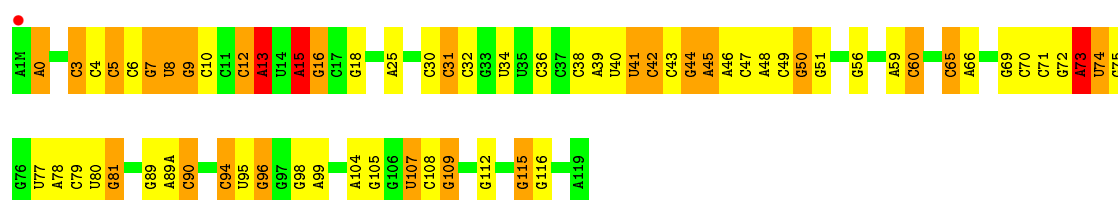


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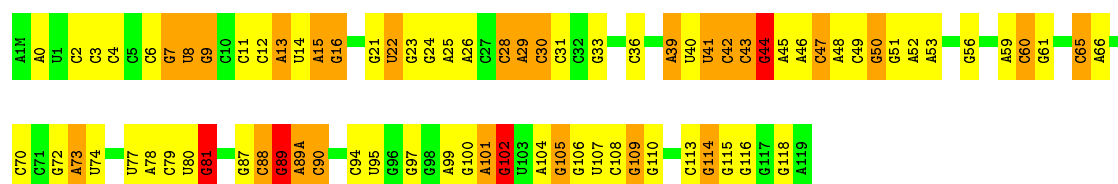
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| U2449 | C2379 | G2316 | G2379 | G2299 | G2250 | G2165 | C2085 | G2020 | U1939 | G1837 | G1769 | G1670 | G1595 |
| G2454 | C2380 | G2317 | C2380 | G2299 | G2251 | G2166 | G2104 | G2021 | C1942 | G1838 | G1770 | C1671 | C1598 |
| G2454 | C2381 | G2318 | C2381 | G2299 | G2252 | U2167 | G2105 | U2022 | U1943 | A1847 | G1771 | G1672 | C1599 |
| C2461 | G2382 | G2319 | G2382 | G2299 | G2253 | G2168 | C2107 | G2023 | U1946 | A1848 | U1772 | G1673 | G1600 |
| C2462 | C2383 | A2320 | G2383 | G2299 | G2254 | A | C2108 | G2024 | G1947 | U1851 | U1773 | G1674 | G1601 |
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| C2467 | A2388 | G2325 | A2388 | G2299 | G2259 | G2173 | G2112 | G2034 | A1952 | A1856 | U1778 | | G1606 |
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| | G2502 | G2360 | G2502 | G2299 | G2295 | G2211 | G2147 | | | A1892 | U1807 | G1648 | |
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| | U2506 | G2364 | U2506 | G2299 | G2299 | G2215 | G2151 | | | A1896 | U1811 | G1652 | |
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| | G2508 | A2435 | G2508 | G2299 | G2301 | G2217 | G2153 | | | A1898 | U1813 | G1654 | |
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| | C2524 | C2455 | C2524 | G2299 | U2251 | G2169 | G2169 | | | A1914 | U1829 | G1670 | |
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| | U2526 | A2457 | U2526 | G2299 | U2253 | G2171 | G2171 | | | A1916 | U1831 | G1672 | |
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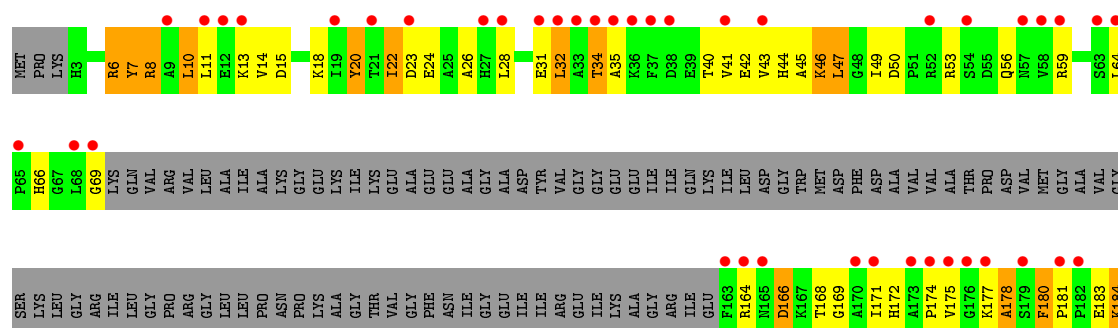
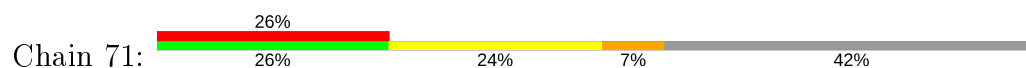
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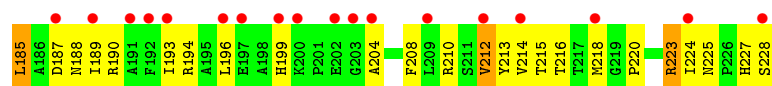


• Molecule 27: 5S ribosomal RNA

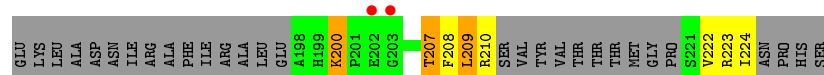
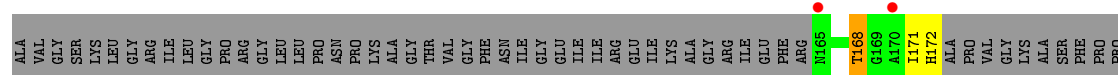
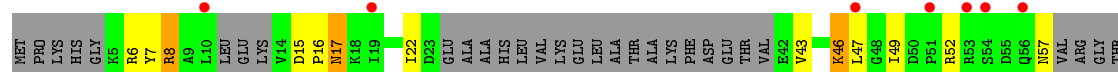


• Molecule 28: 50S ribosomal protein L1

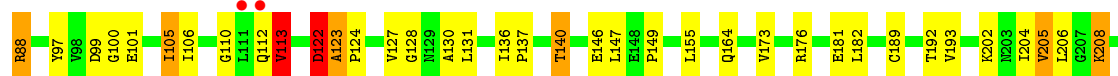
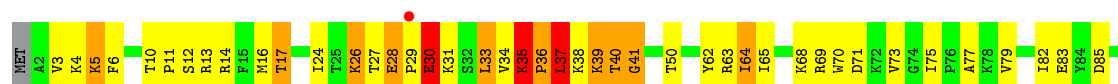




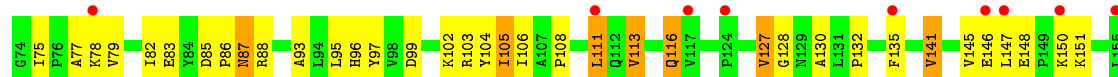
• Molecule 28: 50S ribosomal protein L1



• Molecule 29: 50S ribosomal protein L2

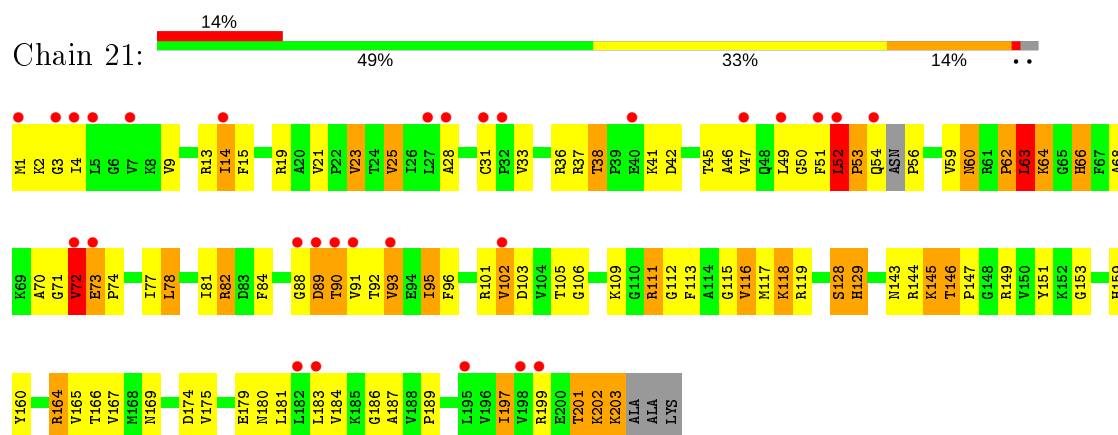


• Molecule 29: 50S ribosomal protein L2

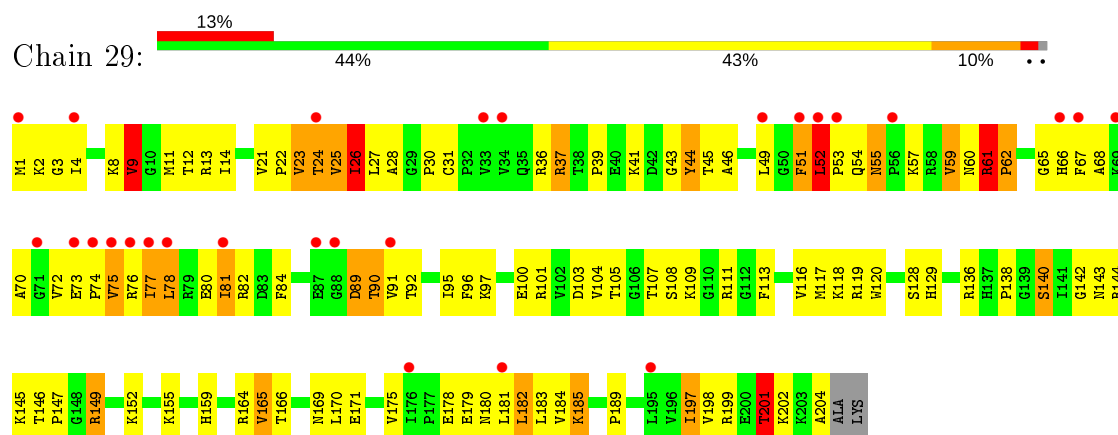




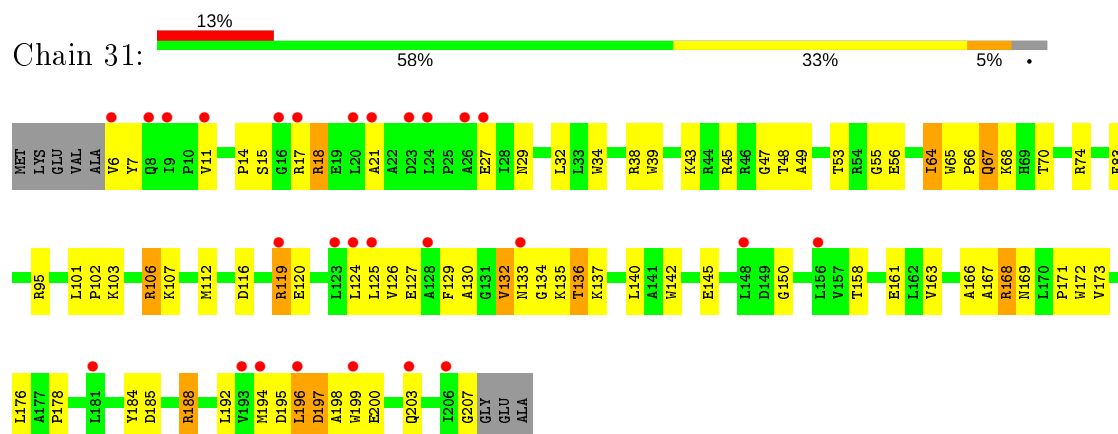
• Molecule 30: 50S ribosomal protein L3



• Molecule 30: 50S ribosomal protein L3

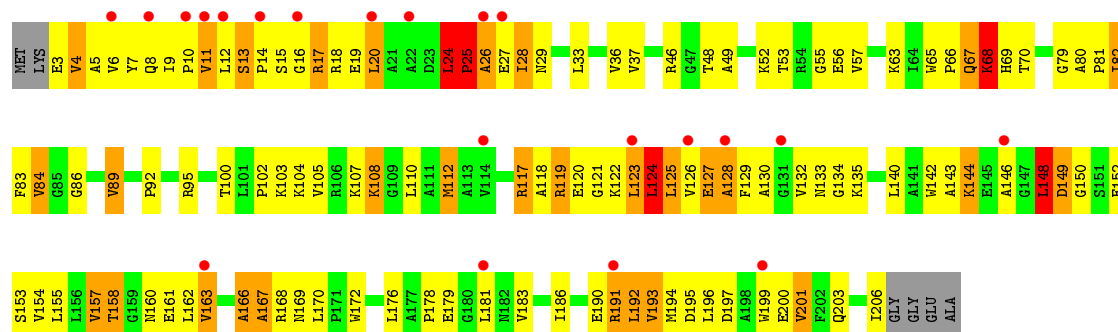


• Molecule 31: 50S ribosomal protein L4

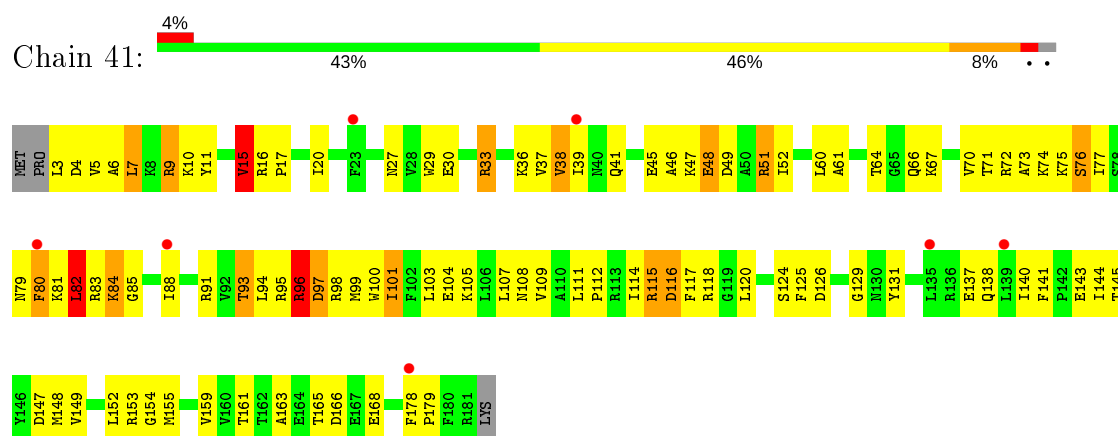


• Molecule 31: 50S ribosomal protein L4

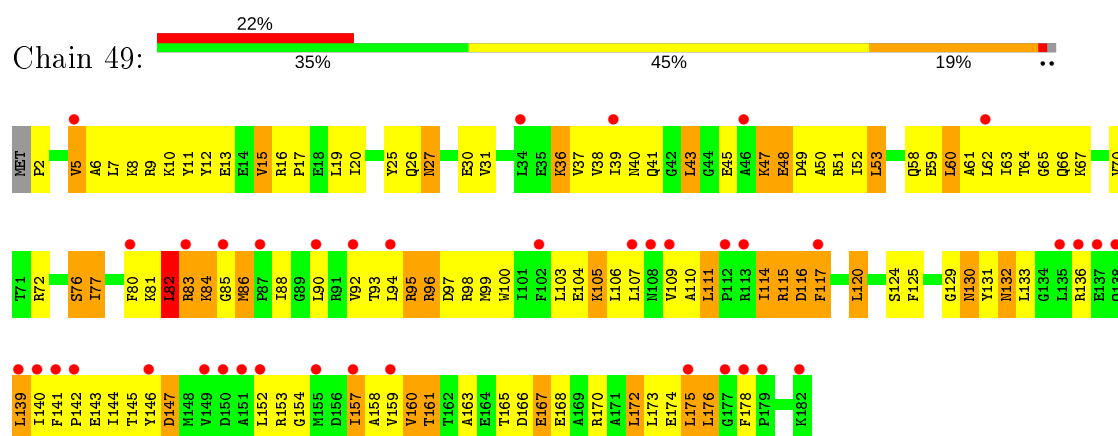




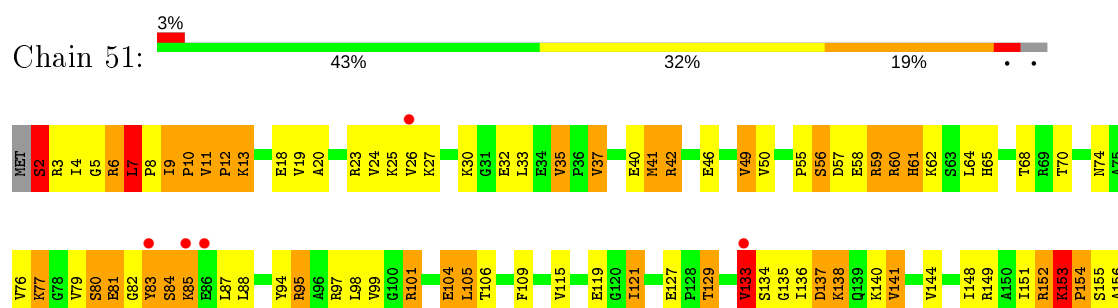
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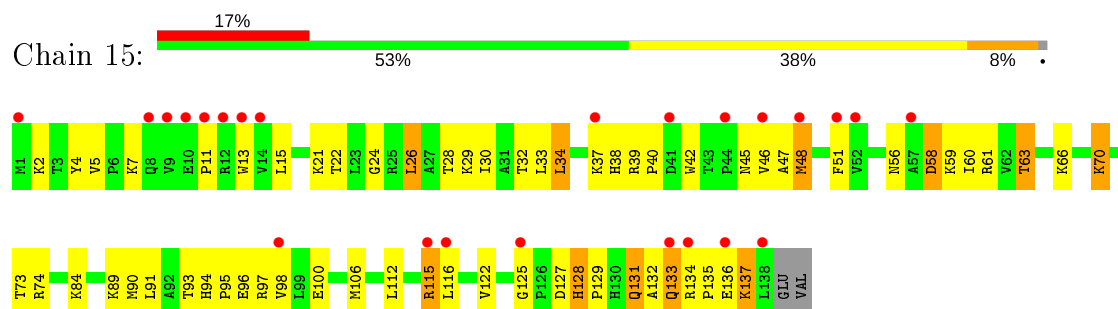
• Molecule 32: 50S ribosomal protein L5



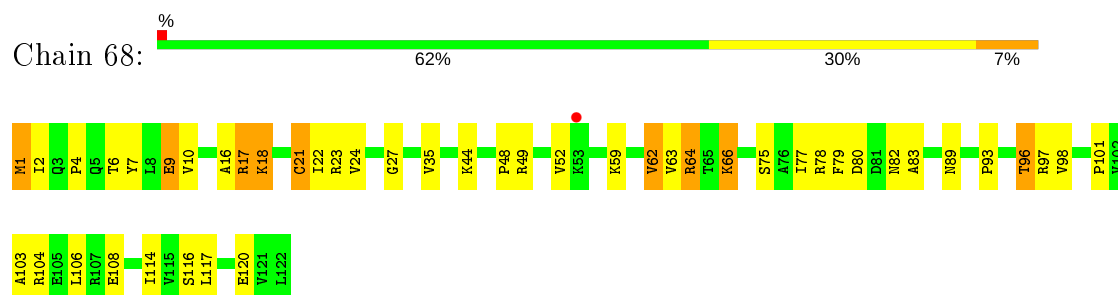
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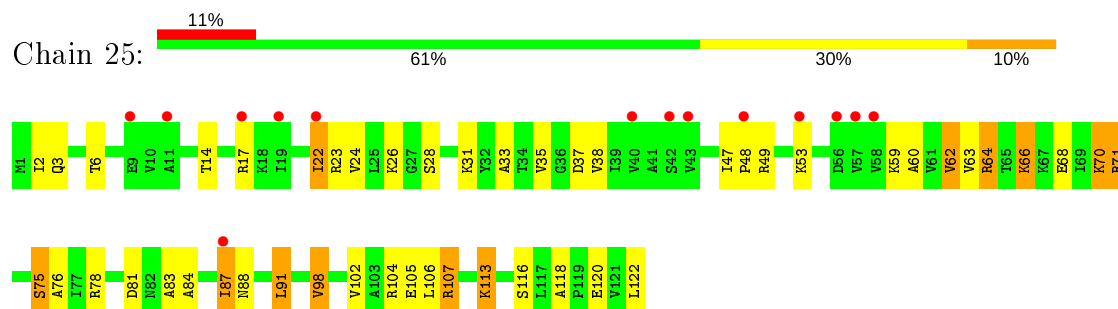
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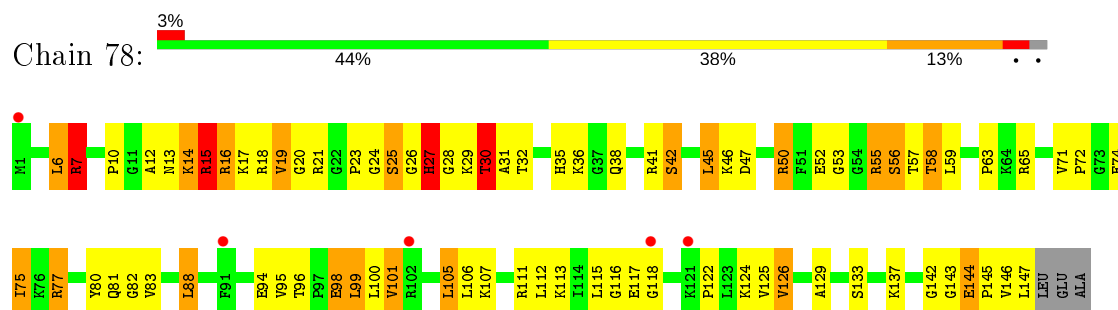
- Molecule 36: 50S ribosomal protein L14



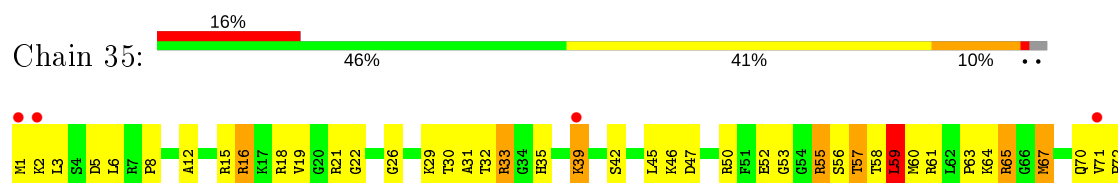
- Molecule 36: 50S ribosomal protein L14

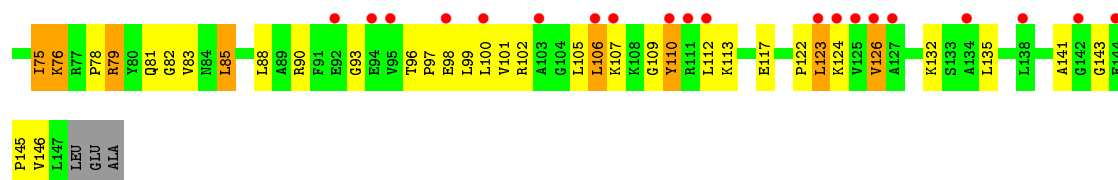


- Molecule 37: 50S ribosomal protein L15

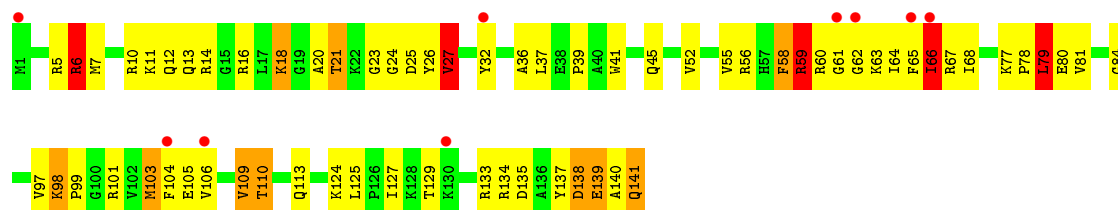


- Molecule 37: 50S ribosomal protein L15

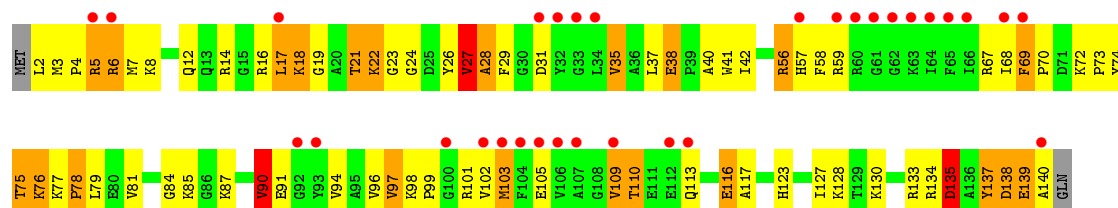




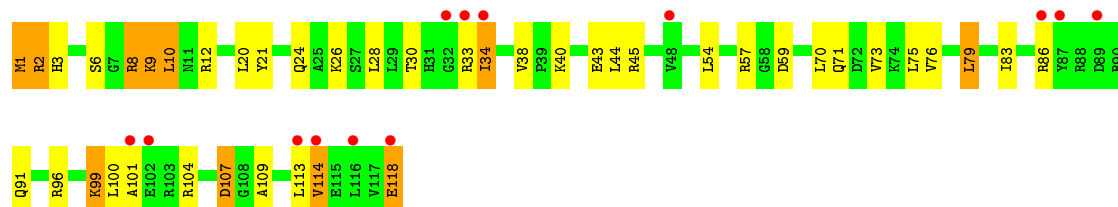
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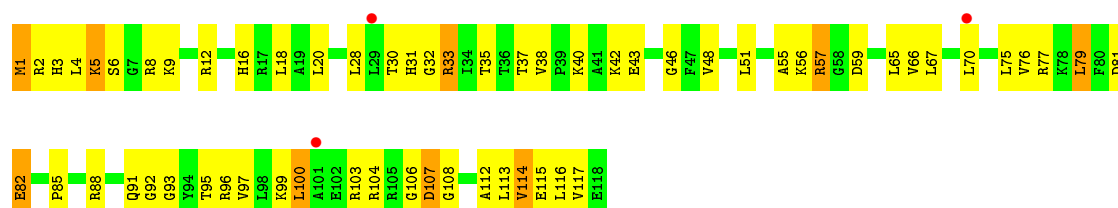
- Molecule 38: 50S ribosomal protein L16



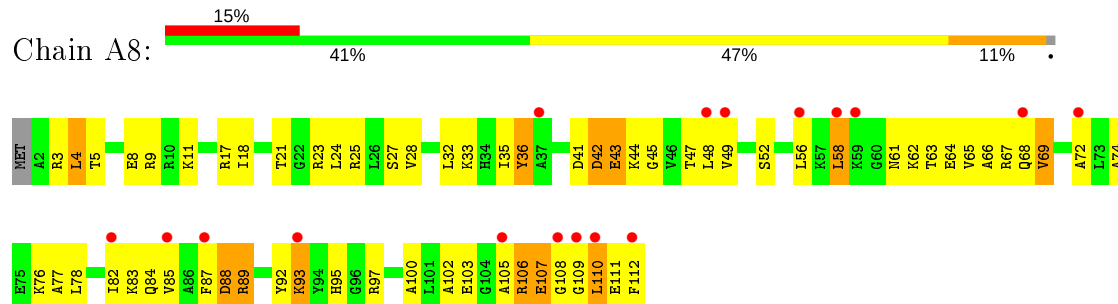
- Molecule 39: 50S ribosomal protein L17



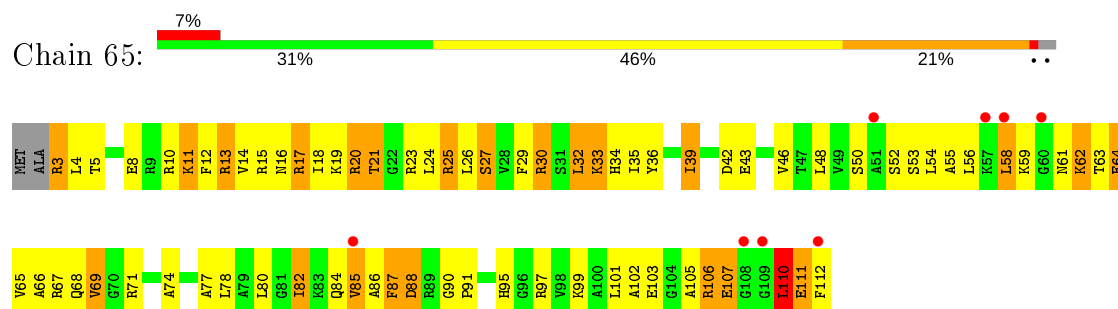
- Molecule 39: 50S ribosomal protein L17



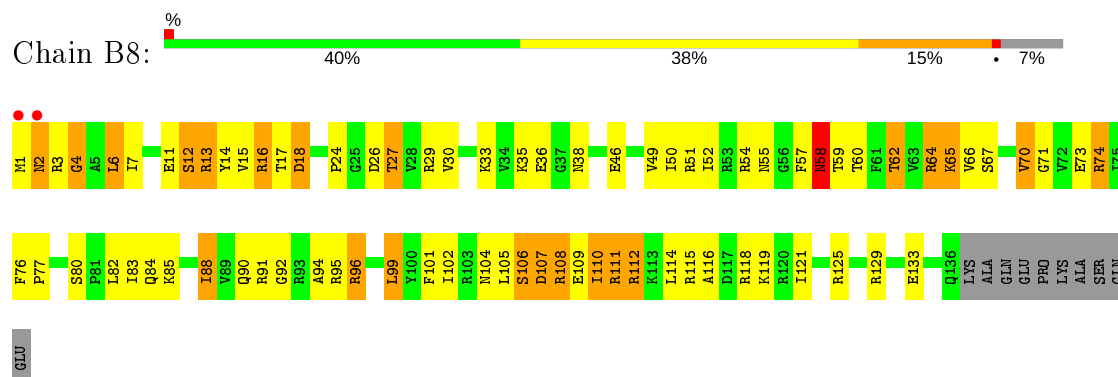
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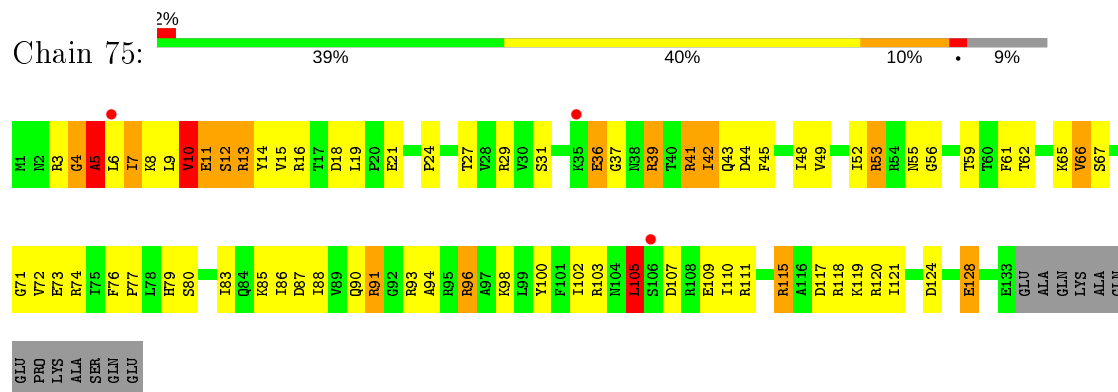
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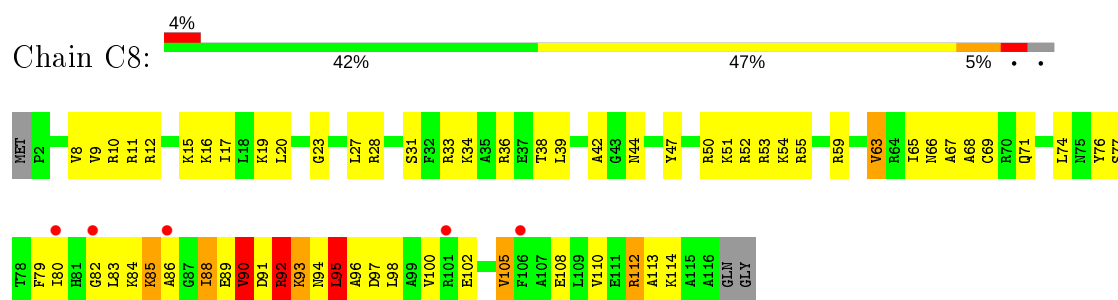
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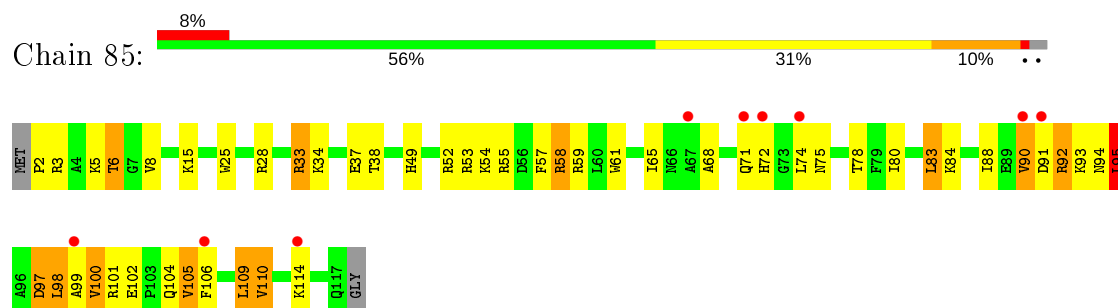
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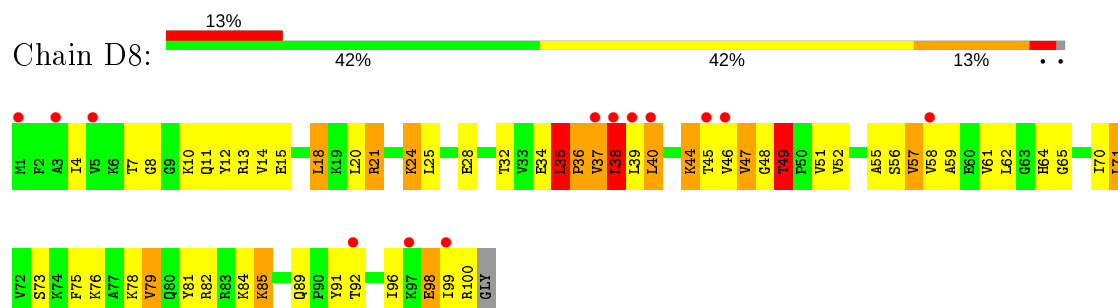
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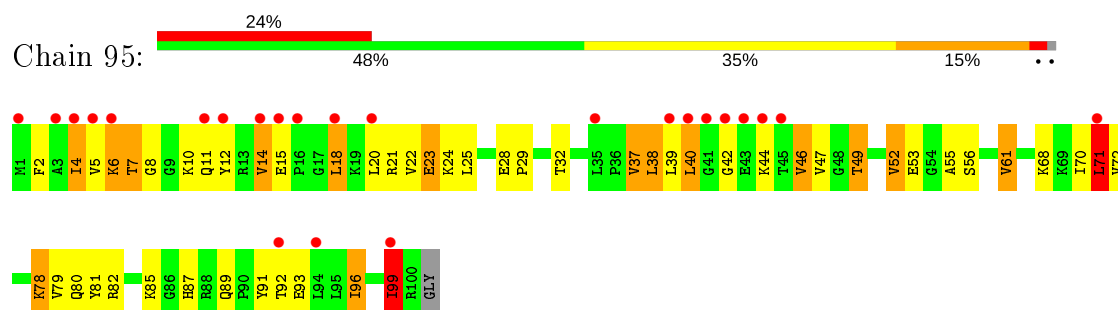
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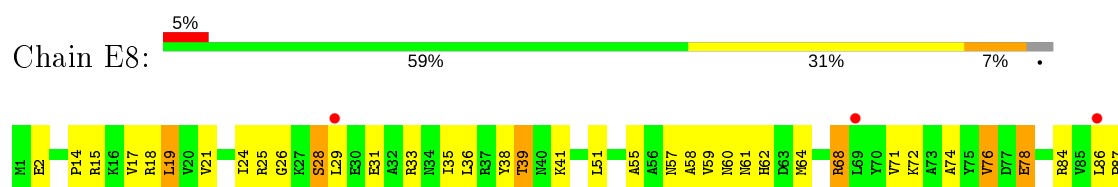
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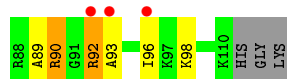


• Molecule 43: 50S ribosomal protein L21



• Molecule 44: 50S ribosomal protein L22

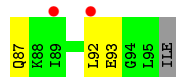
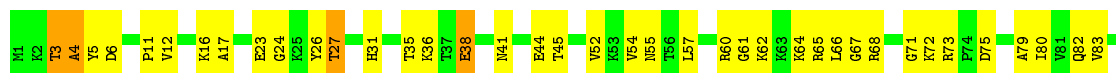




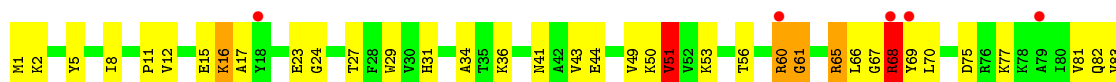
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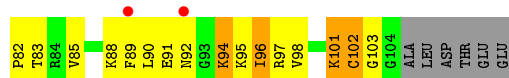
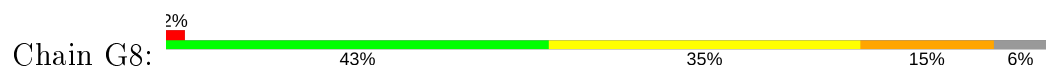
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- Molecule 45: 50S ribosomal protein L23

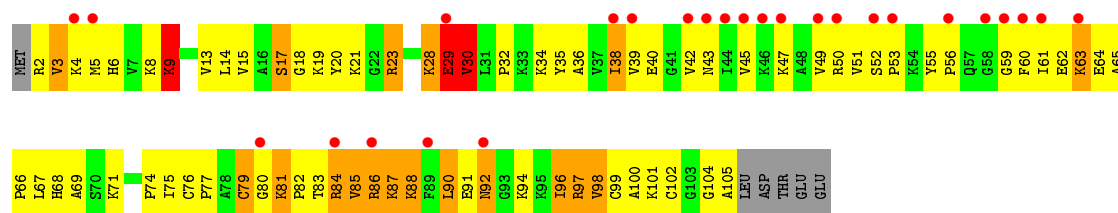


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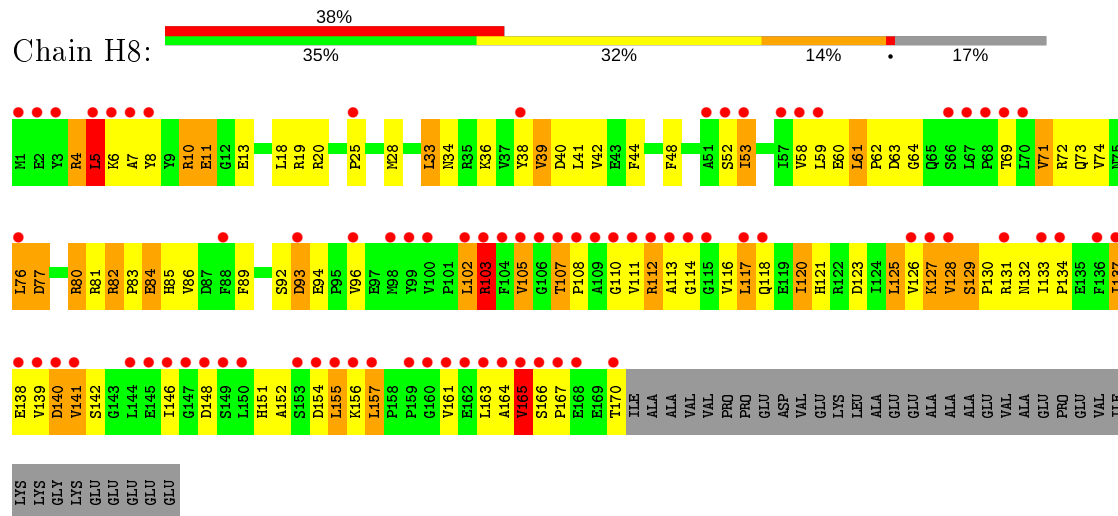


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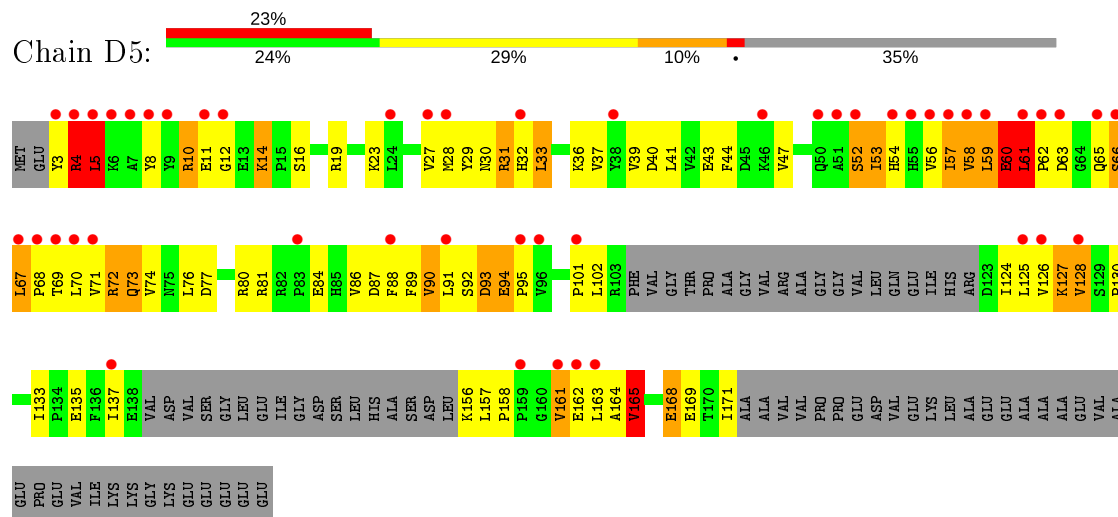




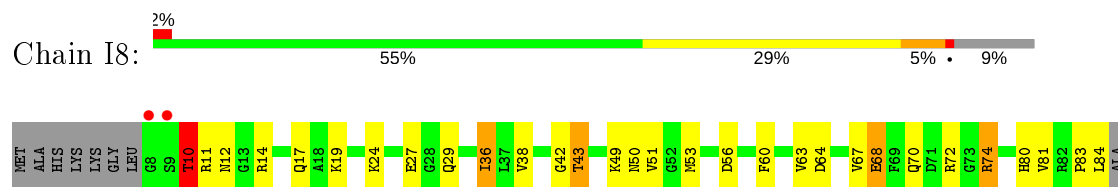
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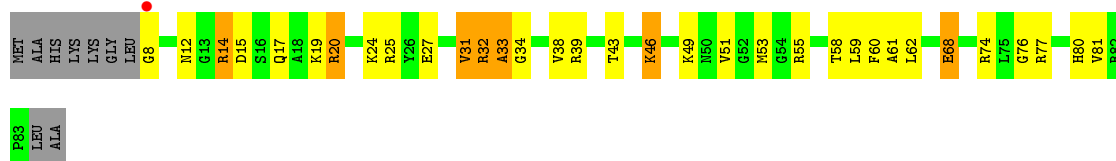
• Molecule 47: 50S ribosomal protein L25



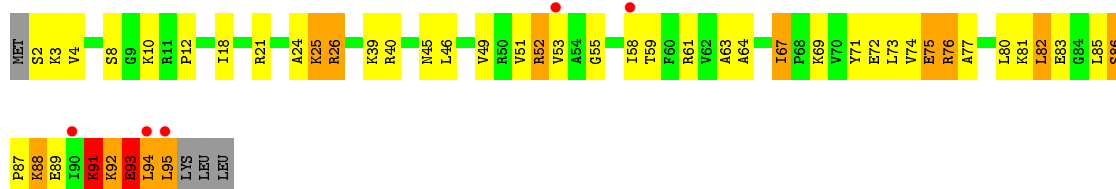
• Molecule 48: 50S ribosomal protein L27



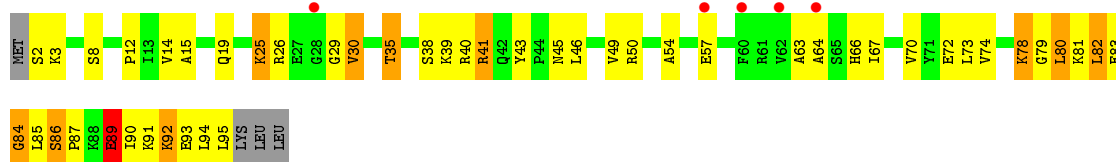
• Molecule 48: 50S ribosomal protein L27



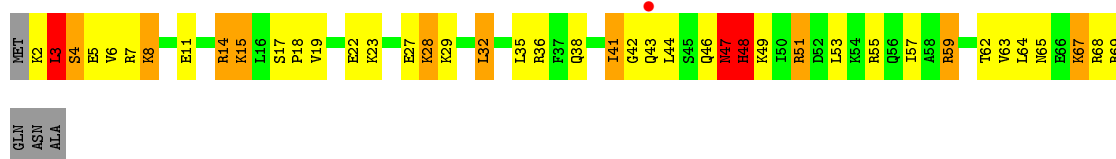
- Molecule 49: 50S ribosomal protein L28



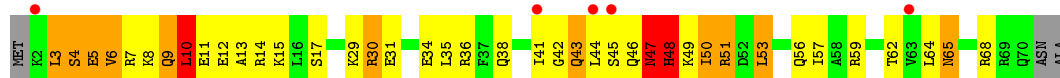
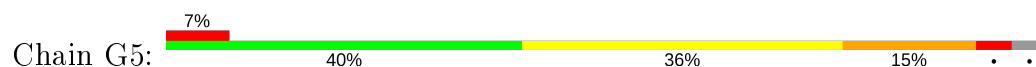
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29

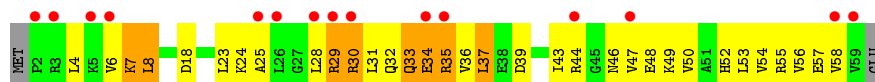
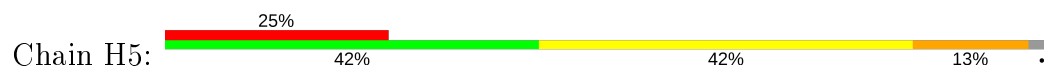


- Molecule 51: 50S ribosomal protein L30

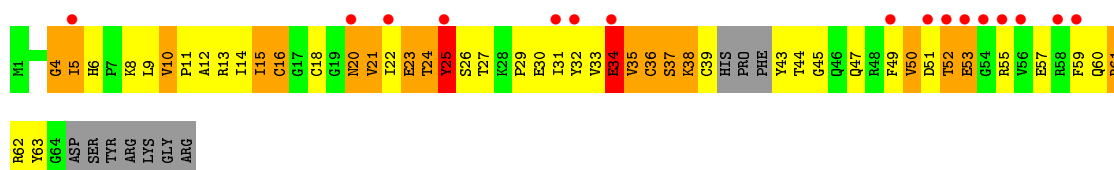
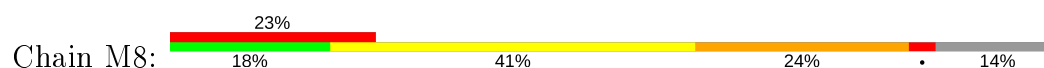




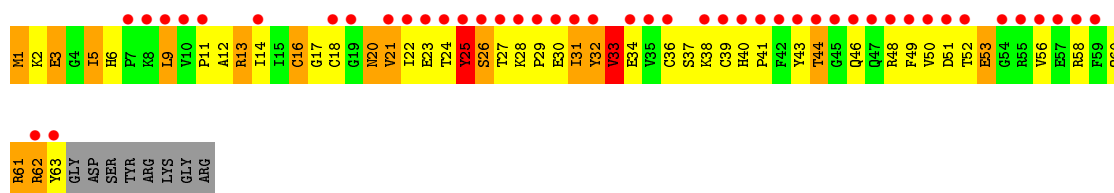
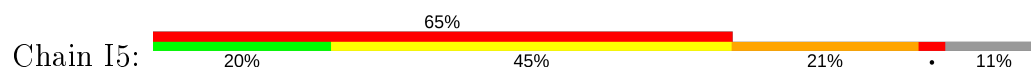
- Molecule 51: 50S ribosomal protein L30



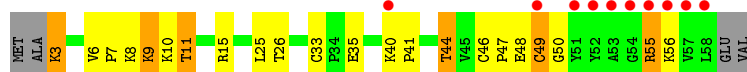
- Molecule 52: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L34

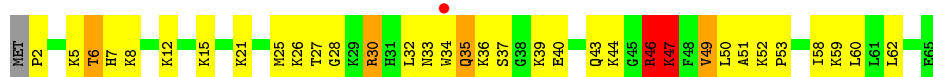




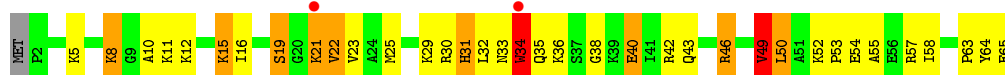
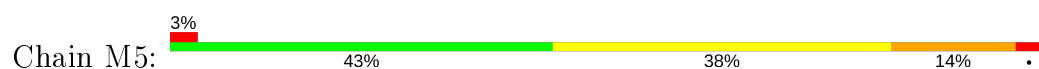
- Molecule 54: 50S ribosomal protein L34



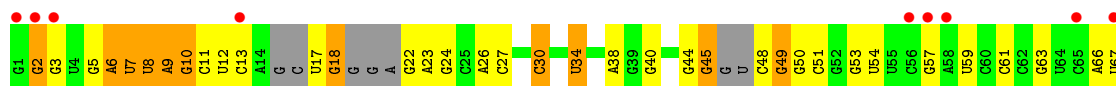
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNAVal



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.50 Å 448.90 Å 620.80 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 146.68 – 2.96 146.68 – 2.96 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (146.68-2.96) 89.3 (146.68-2.96) | Depositor EDS |
| R_{merge} | 0.44 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.84 (at 2.96 Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.201 , 0.243 0.201 , 0.243 | Depositor DCC |
| R_{free} test set | 2000 reflections (0.17%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 75.4 | Xtriage |
| Anisotropy | 0.336 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 67.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 296743 | wwPDB-VP |
| Average B, all atoms (Å ²) | 97.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, H2U, SF4, MG, CM0, 6MZ, 4SU, 7MG, SPE, PSU

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 | 0.67 | 6/35994 (0.0%) | 1.30 | 243/56171 (0.4%) |
| 1 | 1G | 0.61 | 1/36236 (0.0%) | 1.22 | 170/56555 (0.3%) |
| 2 | 12 | 0.39 | 0/1727 | 0.70 | 1/2326 (0.0%) |
| 2 | 1E | 0.40 | 0/1936 | 0.66 | 1/2611 (0.0%) |
| 3 | 22 | 0.62 | 1/1560 (0.1%) | 0.65 | 1/2104 (0.0%) |
| 3 | 2E | 0.49 | 1/1629 (0.1%) | 0.67 | 0/2195 |
| 4 | 32 | 0.45 | 0/1732 | 0.65 | 0/2318 |
| 4 | 3E | 0.48 | 0/1728 | 0.73 | 4/2313 (0.2%) |
| 5 | 42 | 0.46 | 0/1155 | 0.67 | 1/1555 (0.1%) |
| 5 | 4E | 0.46 | 0/1158 | 0.70 | 1/1559 (0.1%) |
| 6 | 52 | 0.47 | 0/855 | 0.63 | 0/1154 |
| 6 | 5E | 0.48 | 0/850 | 0.64 | 0/1147 |
| 7 | 62 | 0.42 | 0/1132 | 0.66 | 1/1514 (0.1%) |
| 7 | 6E | 0.45 | 0/1259 | 0.57 | 0/1686 |
| 8 | 72 | 0.41 | 0/1127 | 0.63 | 0/1517 |
| 8 | 7E | 0.43 | 0/1135 | 0.71 | 1/1527 (0.1%) |
| 9 | 82 | 0.41 | 0/971 | 0.74 | 1/1304 (0.1%) |
| 9 | 8E | 0.50 | 1/1019 (0.1%) | 0.76 | 1/1367 (0.1%) |
| 10 | 1A | 0.74 | 2/658 (0.3%) | 0.68 | 0/885 |
| 10 | 1I | 0.41 | 0/767 | 0.72 | 2/1034 (0.2%) |
| 11 | 2A | 0.46 | 0/850 | 0.66 | 0/1150 |
| 11 | 2I | 0.46 | 0/838 | 0.67 | 0/1133 |
| 12 | 3A | 0.56 | 0/972 | 0.73 | 1/1301 (0.1%) |
| 12 | 3I | 0.61 | 0/972 | 0.79 | 0/1301 |
| 13 | 4A | 0.42 | 0/903 | 0.69 | 1/1211 (0.1%) |
| 13 | 4I | 0.48 | 0/952 | 0.73 | 1/1277 (0.1%) |
| 14 | 5A | 0.46 | 0/495 | 0.89 | 2/657 (0.3%) |
| 14 | 5I | 0.63 | 2/500 (0.4%) | 0.90 | 3/664 (0.5%) |
| 15 | 6A | 0.47 | 0/740 | 0.63 | 0/987 |
| 15 | 6I | 0.47 | 0/740 | 0.70 | 0/987 |
| 16 | 7A | 0.45 | 0/721 | 0.74 | 1/970 (0.1%) |
| 16 | 7I | 0.47 | 0/716 | 0.76 | 1/963 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | 8A | 0.46 | 0/836 | 0.61 | 0/1117 |
| 17 | 8I | 0.55 | 1/847 (0.1%) | 0.77 | 1/1131 (0.1%) |
| 18 | 9A | 0.51 | 0/549 | 0.75 | 1/732 (0.1%) |
| 18 | 9I | 0.46 | 0/554 | 0.69 | 0/739 |
| 19 | AA | 0.43 | 0/490 | 0.75 | 2/662 (0.3%) |
| 19 | AI | 0.42 | 0/676 | 0.79 | 1/910 (0.1%) |
| 20 | BA | 0.40 | 0/764 | 0.71 | 0/1007 |
| 20 | BI | 0.56 | 1/748 (0.1%) | 0.81 | 2/986 (0.2%) |
| 21 | 1B | 0.44 | 0/192 | 0.65 | 0/252 |
| 21 | 1F | 0.44 | 0/203 | 0.67 | 0/266 |
| 22 | 1K | 0.64 | 0/1595 | 1.19 | 11/2475 (0.4%) |
| 23 | 2K | 0.77 | 0/1721 | 1.38 | 7/2682 (0.3%) |
| 23 | 2L | 0.67 | 0/1698 | 1.28 | 12/2644 (0.5%) |
| 24 | 3K | 0.54 | 0/1663 | 1.20 | 16/2585 (0.6%) |
| 24 | 3L | 0.56 | 0/1689 | 1.16 | 11/2628 (0.4%) |
| 25 | 4K | 0.72 | 0/520 | 1.23 | 3/808 (0.4%) |
| 25 | 4L | 0.64 | 0/470 | 1.23 | 4/732 (0.5%) |
| 26 | 14 | 0.81 | 39/67798 (0.1%) | 1.49 | 1064/105832 (1.0%) |
| 26 | 1H | 0.95 | 95/68537 (0.1%) | 1.67 | 1647/106989 (1.5%) |
| 27 | 16 | 0.79 | 0/2928 | 1.48 | 37/4568 (0.8%) |
| 27 | 1J | 0.73 | 0/2928 | 1.34 | 23/4568 (0.5%) |
| 28 | 71 | 0.32 | 0/1055 | 0.62 | 0/1425 |
| 28 | 79 | 0.31 | 0/459 | 0.58 | 0/608 |
| 29 | 11 | 0.68 | 1/2170 (0.0%) | 0.94 | 6/2926 (0.2%) |
| 29 | 19 | 0.61 | 0/2175 | 0.86 | 2/2933 (0.1%) |
| 30 | 21 | 0.58 | 0/1537 | 0.92 | 3/2081 (0.1%) |
| 30 | 29 | 0.53 | 0/1596 | 0.85 | 1/2153 (0.0%) |
| 31 | 31 | 0.58 | 0/1620 | 0.78 | 2/2194 (0.1%) |
| 31 | 39 | 0.54 | 1/1637 (0.1%) | 0.84 | 2/2218 (0.1%) |
| 32 | 41 | 0.51 | 1/1481 (0.1%) | 0.71 | 1/1994 (0.1%) |
| 32 | 49 | 0.42 | 0/1492 | 0.72 | 3/2008 (0.1%) |
| 33 | 51 | 0.54 | 0/1354 | 0.95 | 5/1833 (0.3%) |
| 33 | 59 | 0.36 | 0/1308 | 0.67 | 2/1771 (0.1%) |
| 34 | 61 | 0.46 | 0/1151 | 0.80 | 4/1558 (0.3%) |
| 34 | 69 | 0.45 | 0/1146 | 0.75 | 2/1551 (0.1%) |
| 35 | 15 | 0.47 | 1/1131 (0.1%) | 0.72 | 0/1525 |
| 35 | 58 | 0.52 | 0/1123 | 0.74 | 1/1514 (0.1%) |
| 36 | 25 | 0.51 | 0/942 | 0.70 | 0/1269 |
| 36 | 68 | 0.54 | 0/942 | 0.74 | 0/1269 |
| 37 | 35 | 0.55 | 0/1139 | 0.90 | 3/1514 (0.2%) |
| 37 | 78 | 0.64 | 0/1139 | 1.03 | 6/1514 (0.4%) |
| 38 | 45 | 0.65 | 2/1125 (0.2%) | 0.83 | 1/1505 (0.1%) |
| 38 | 88 | 0.71 | 0/1138 | 0.92 | 2/1523 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | 55 | 0.50 | 0/981 | 0.78 | 1/1312 (0.1%) |
| 39 | 98 | 0.51 | 0/981 | 0.78 | 0/1312 |
| 40 | 65 | 0.52 | 0/886 | 0.83 | 0/1180 |
| 40 | A8 | 0.56 | 0/891 | 0.78 | 0/1187 |
| 41 | 75 | 0.53 | 0/1123 | 0.83 | 4/1500 (0.3%) |
| 41 | B8 | 0.52 | 0/1138 | 0.82 | 1/1521 (0.1%) |
| 42 | 85 | 0.52 | 0/977 | 0.73 | 0/1301 |
| 42 | C8 | 0.57 | 0/968 | 0.85 | 4/1289 (0.3%) |
| 43 | 95 | 0.49 | 0/781 | 0.81 | 1/1048 (0.1%) |
| 43 | D8 | 0.54 | 0/785 | 0.86 | 2/1052 (0.2%) |
| 44 | A5 | 0.54 | 0/897 | 0.76 | 1/1204 (0.1%) |
| 44 | E8 | 0.58 | 0/886 | 0.81 | 1/1189 (0.1%) |
| 45 | B5 | 0.53 | 0/749 | 0.72 | 1/1007 (0.1%) |
| 45 | F8 | 0.59 | 0/757 | 0.77 | 1/1017 (0.1%) |
| 46 | C5 | 0.54 | 0/807 | 0.89 | 0/1076 |
| 46 | G8 | 0.64 | 0/790 | 0.93 | 3/1055 (0.3%) |
| 47 | D5 | 0.50 | 2/1103 (0.2%) | 0.80 | 2/1494 (0.1%) |
| 47 | H8 | 0.48 | 0/1395 | 0.77 | 2/1890 (0.1%) |
| 48 | E5 | 0.62 | 0/611 | 0.83 | 0/814 |
| 48 | I8 | 0.60 | 0/619 | 0.84 | 1/825 (0.1%) |
| 49 | F5 | 0.57 | 0/744 | 0.94 | 4/989 (0.4%) |
| 49 | J8 | 0.61 | 0/744 | 0.89 | 1/989 (0.1%) |
| 50 | G5 | 0.51 | 0/578 | 0.81 | 1/766 (0.1%) |
| 50 | K8 | 0.65 | 0/577 | 0.88 | 1/763 (0.1%) |
| 51 | H5 | 0.49 | 0/464 | 0.66 | 0/623 |
| 51 | L8 | 0.49 | 0/464 | 0.73 | 0/623 |
| 52 | I5 | 0.41 | 0/527 | 0.84 | 0/709 |
| 52 | M8 | 0.54 | 0/486 | 0.87 | 2/652 (0.3%) |
| 53 | J5 | 0.51 | 0/448 | 0.83 | 1/606 (0.2%) |
| 53 | N8 | 0.58 | 0/451 | 0.75 | 0/610 |
| 54 | L5 | 0.61 | 0/409 | 0.75 | 0/540 |
| 54 | P8 | 0.78 | 0/409 | 0.96 | 3/540 (0.6%) |
| 55 | M5 | 0.61 | 1/524 (0.2%) | 0.91 | 1/691 (0.1%) |
| 55 | Q8 | 0.67 | 0/524 | 0.96 | 2/691 (0.3%) |
| 56 | 1L | 0.53 | 0/1592 | 1.05 | 1/2472 (0.0%) |
| All | All | 0.73 | 159/317359 (0.1%) | 1.32 | 3368/475179 (0.7%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | 12 | 0 | 5 |
| 2 | 1E | 0 | 3 |
| 3 | 22 | 0 | 1 |
| 3 | 2E | 0 | 1 |
| 4 | 32 | 0 | 2 |
| 4 | 3E | 0 | 2 |
| 7 | 6E | 0 | 1 |
| 8 | 72 | 0 | 2 |
| 8 | 7E | 0 | 1 |
| 9 | 82 | 0 | 1 |
| 9 | 8E | 0 | 2 |
| 10 | 1I | 0 | 2 |
| 11 | 2A | 0 | 2 |
| 12 | 3I | 0 | 6 |
| 13 | 4A | 0 | 4 |
| 13 | 4I | 0 | 2 |
| 14 | 5A | 0 | 5 |
| 14 | 5I | 0 | 1 |
| 16 | 7I | 0 | 1 |
| 17 | 8I | 0 | 1 |
| 18 | 9I | 0 | 1 |
| 19 | AA | 0 | 1 |
| 19 | AI | 0 | 1 |
| 20 | BA | 0 | 2 |
| 28 | 71 | 0 | 1 |
| 29 | 11 | 0 | 3 |
| 29 | 19 | 0 | 4 |
| 30 | 21 | 0 | 5 |
| 30 | 29 | 0 | 3 |
| 31 | 31 | 0 | 1 |
| 31 | 39 | 0 | 9 |
| 32 | 41 | 0 | 3 |
| 32 | 49 | 0 | 3 |
| 33 | 51 | 0 | 7 |
| 33 | 59 | 0 | 2 |
| 34 | 61 | 0 | 3 |
| 34 | 69 | 0 | 5 |
| 35 | 58 | 0 | 1 |
| 36 | 68 | 0 | 1 |
| 37 | 35 | 0 | 5 |
| 37 | 78 | 0 | 4 |
| 38 | 45 | 0 | 3 |
| 38 | 88 | 0 | 4 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 39 | 55 | 0 | 1 |
| 39 | 98 | 0 | 2 |
| 40 | 65 | 0 | 1 |
| 40 | A8 | 0 | 3 |
| 41 | 75 | 0 | 3 |
| 41 | B8 | 0 | 4 |
| 42 | 85 | 0 | 4 |
| 42 | C8 | 0 | 3 |
| 43 | 95 | 0 | 3 |
| 43 | D8 | 0 | 3 |
| 44 | A5 | 0 | 1 |
| 45 | B5 | 0 | 1 |
| 45 | F8 | 0 | 1 |
| 46 | C5 | 0 | 2 |
| 46 | G8 | 0 | 4 |
| 47 | D5 | 0 | 3 |
| 47 | H8 | 0 | 3 |
| 49 | F5 | 0 | 2 |
| 49 | J8 | 0 | 4 |
| 50 | G5 | 0 | 2 |
| 50 | K8 | 0 | 2 |
| 52 | I5 | 0 | 3 |
| 52 | M8 | 0 | 4 |
| 54 | P8 | 0 | 1 |
| 55 | M5 | 0 | 1 |
| 55 | Q8 | 0 | 2 |
| All | All | 0 | 180 |

The worst 5 of 159 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 3 | 22 | 173 | VAL | C-N | 19.50 | 1.71 | 1.34 |
| 10 | 1A | 38 | ILE | C-N | 14.98 | 1.62 | 1.34 |
| 26 | 1H | 1698 | A | N9-C4 | -11.67 | 1.30 | 1.37 |
| 26 | 1H | 783 | A | N3-C4 | -10.65 | 1.28 | 1.34 |
| 20 | BI | 97 | ALA | C-N | 10.36 | 1.53 | 1.34 |

The worst 5 of 3368 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 26 | 1H | 1899 | G | N3-C4-N9 | -25.58 | 110.65 | 126.00 |
| 26 | 1H | 945 | A | N1-C6-N6 | 24.24 | 133.14 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 26 | 1H | 945 | A | C6-C5-N7 | -23.79 | 115.65 | 132.30 |
| 26 | 1H | 945 | A | C5-N7-C8 | -20.19 | 93.80 | 103.90 |
| 26 | 1H | 1899 | G | N3-C4-C5 | 19.48 | 138.34 | 128.60 |

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | 1E | 15 | VAL | Peptide |
| 2 | 1E | 236 | TYR | Peptide |
| 2 | 1E | 95 | GLN | Peptide |
| 3 | 2E | 78 | GLY | Peptide |
| 4 | 3E | 154 | ASN | 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 | 32157 | 0 | 16234 | 739 | 0 |
| 1 | 1G | 32371 | 0 | 16342 | 719 | 0 |
| 2 | 12 | 1696 | 0 | 1730 | 124 | 0 |
| 2 | 1E | 1902 | 0 | 1949 | 157 | 0 |
| 3 | 22 | 1537 | 0 | 1603 | 116 | 0 |
| 3 | 2E | 1605 | 0 | 1668 | 76 | 0 |
| 4 | 32 | 1702 | 0 | 1764 | 95 | 0 |
| 4 | 3E | 1698 | 0 | 1760 | 125 | 0 |
| 5 | 42 | 1139 | 0 | 1202 | 85 | 0 |
| 5 | 4E | 1142 | 0 | 1204 | 68 | 0 |
| 6 | 52 | 842 | 0 | 857 | 26 | 0 |
| 6 | 5E | 837 | 0 | 852 | 39 | 0 |
| 7 | 62 | 1120 | 0 | 1167 | 82 | 0 |
| 7 | 6E | 1242 | 0 | 1286 | 80 | 0 |
| 8 | 72 | 1107 | 0 | 1165 | 65 | 0 |
| 8 | 7E | 1115 | 0 | 1177 | 92 | 0 |
| 9 | 82 | 953 | 0 | 983 | 106 | 0 |
| 9 | 8E | 1000 | 0 | 1031 | 100 | 0 |
| 10 | 1A | 646 | 0 | 662 | 81 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10 | 1I | 754 | 0 | 769 | 44 | 0 |
| 11 | 2A | 835 | 0 | 847 | 42 | 0 |
| 11 | 2I | 823 | 0 | 832 | 33 | 0 |
| 12 | 3A | 956 | 0 | 1046 | 64 | 0 |
| 12 | 3I | 956 | 0 | 1046 | 39 | 0 |
| 13 | 4A | 893 | 0 | 946 | 72 | 0 |
| 13 | 4I | 942 | 0 | 997 | 76 | 0 |
| 14 | 5A | 486 | 0 | 525 | 65 | 0 |
| 14 | 5I | 491 | 0 | 532 | 49 | 0 |
| 15 | 6A | 729 | 0 | 768 | 33 | 0 |
| 15 | 6I | 729 | 0 | 768 | 38 | 0 |
| 16 | 7A | 705 | 0 | 725 | 58 | 0 |
| 16 | 7I | 700 | 0 | 720 | 77 | 0 |
| 17 | 8A | 823 | 0 | 891 | 32 | 0 |
| 17 | 8I | 834 | 0 | 904 | 84 | 0 |
| 18 | 9A | 544 | 0 | 605 | 26 | 0 |
| 18 | 9I | 549 | 0 | 607 | 33 | 0 |
| 19 | AA | 481 | 0 | 468 | 39 | 0 |
| 19 | AI | 661 | 0 | 683 | 55 | 0 |
| 20 | BA | 762 | 0 | 861 | 44 | 0 |
| 20 | BI | 746 | 0 | 843 | 98 | 0 |
| 21 | 1B | 188 | 0 | 195 | 12 | 0 |
| 21 | 1F | 199 | 0 | 208 | 19 | 0 |
| 22 | 1K | 1540 | 0 | 787 | 25 | 0 |
| 23 | 2K | 1646 | 0 | 843 | 25 | 0 |
| 23 | 2L | 1626 | 0 | 836 | 27 | 0 |
| 24 | 3K | 1491 | 0 | 761 | 59 | 0 |
| 24 | 3L | 1513 | 0 | 770 | 34 | 0 |
| 25 | 4K | 462 | 0 | 230 | 11 | 0 |
| 25 | 4L | 417 | 0 | 207 | 12 | 0 |
| 26 | 14 | 60535 | 0 | 30516 | 1082 | 0 |
| 26 | 1H | 61195 | 0 | 30847 | 1152 | 0 |
| 27 | 16 | 2617 | 0 | 1328 | 54 | 0 |
| 27 | 1J | 2617 | 0 | 1328 | 88 | 0 |
| 28 | 7I | 1033 | 0 | 1048 | 71 | 0 |
| 28 | 79 | 456 | 0 | 460 | 21 | 0 |
| 29 | 11 | 2120 | 0 | 2197 | 112 | 0 |
| 29 | 19 | 2125 | 0 | 2199 | 96 | 0 |
| 30 | 21 | 1505 | 0 | 1526 | 85 | 0 |
| 30 | 29 | 1563 | 0 | 1629 | 139 | 0 |
| 31 | 31 | 1585 | 0 | 1632 | 61 | 0 |
| 31 | 39 | 1602 | 0 | 1649 | 118 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | 41 | 1457 | 0 | 1514 | 101 | 0 |
| 32 | 49 | 1468 | 0 | 1520 | 112 | 0 |
| 33 | 51 | 1328 | 0 | 1396 | 108 | 0 |
| 33 | 59 | 1283 | 0 | 1352 | 87 | 0 |
| 34 | 61 | 1136 | 0 | 1223 | 75 | 0 |
| 34 | 69 | 1131 | 0 | 1218 | 60 | 0 |
| 35 | 15 | 1104 | 0 | 1180 | 56 | 0 |
| 35 | 58 | 1096 | 0 | 1169 | 52 | 0 |
| 36 | 25 | 932 | 0 | 996 | 42 | 0 |
| 36 | 68 | 932 | 0 | 996 | 40 | 0 |
| 37 | 35 | 1122 | 0 | 1206 | 76 | 0 |
| 37 | 78 | 1122 | 0 | 1206 | 84 | 0 |
| 38 | 45 | 1104 | 0 | 1159 | 88 | 0 |
| 38 | 88 | 1117 | 0 | 1168 | 67 | 0 |
| 39 | 55 | 967 | 0 | 1033 | 45 | 0 |
| 39 | 98 | 967 | 0 | 1033 | 33 | 0 |
| 40 | 65 | 876 | 0 | 938 | 99 | 0 |
| 40 | A8 | 881 | 0 | 943 | 58 | 0 |
| 41 | 75 | 1109 | 0 | 1170 | 74 | 0 |
| 41 | B8 | 1124 | 0 | 1179 | 78 | 0 |
| 42 | 85 | 959 | 0 | 1019 | 59 | 0 |
| 42 | C8 | 950 | 0 | 1011 | 85 | 0 |
| 43 | 95 | 770 | 0 | 838 | 48 | 0 |
| 43 | D8 | 774 | 0 | 849 | 58 | 0 |
| 44 | A5 | 886 | 0 | 948 | 38 | 0 |
| 44 | E8 | 876 | 0 | 941 | 43 | 0 |
| 45 | B5 | 735 | 0 | 785 | 37 | 0 |
| 45 | F8 | 743 | 0 | 794 | 30 | 0 |
| 46 | C5 | 794 | 0 | 886 | 81 | 0 |
| 46 | G8 | 777 | 0 | 857 | 42 | 0 |
| 47 | D5 | 1079 | 0 | 1088 | 86 | 0 |
| 47 | H8 | 1365 | 0 | 1391 | 106 | 0 |
| 48 | E5 | 603 | 0 | 620 | 36 | 0 |
| 48 | I8 | 611 | 0 | 631 | 24 | 0 |
| 49 | F5 | 737 | 0 | 813 | 44 | 0 |
| 49 | J8 | 737 | 0 | 813 | 58 | 0 |
| 50 | G5 | 576 | 0 | 625 | 33 | 0 |
| 50 | K8 | 575 | 0 | 634 | 42 | 0 |
| 51 | H5 | 459 | 0 | 512 | 41 | 0 |
| 51 | L8 | 459 | 0 | 512 | 18 | 0 |
| 52 | I5 | 515 | 0 | 514 | 46 | 0 |
| 52 | M8 | 479 | 0 | 475 | 53 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 53 | J5 | 434 | 0 | 454 | 25 | 0 |
| 53 | N8 | 437 | 0 | 460 | 21 | 0 |
| 54 | L5 | 401 | 0 | 436 | 15 | 0 |
| 54 | P8 | 401 | 0 | 436 | 9 | 0 |
| 55 | M5 | 516 | 0 | 582 | 32 | 0 |
| 55 | Q8 | 516 | 0 | 582 | 32 | 0 |
| 56 | 1L | 1469 | 0 | 752 | 37 | 0 |
| 57 | 11 | 2 | 0 | 0 | 0 | 0 |
| 57 | 13 | 148 | 0 | 0 | 0 | 0 |
| 57 | 14 | 445 | 0 | 0 | 0 | 0 |
| 57 | 16 | 11 | 0 | 0 | 0 | 0 |
| 57 | 19 | 1 | 0 | 0 | 0 | 0 |
| 57 | 1G | 133 | 0 | 0 | 0 | 0 |
| 57 | 1H | 548 | 0 | 0 | 0 | 0 |
| 57 | 1J | 7 | 0 | 0 | 0 | 0 |
| 57 | 21 | 2 | 0 | 0 | 0 | 0 |
| 57 | 25 | 2 | 0 | 0 | 0 | 0 |
| 57 | 29 | 2 | 0 | 0 | 0 | 0 |
| 57 | 2K | 4 | 0 | 0 | 0 | 0 |
| 57 | 2L | 3 | 0 | 0 | 0 | 0 |
| 57 | 31 | 2 | 0 | 0 | 0 | 0 |
| 57 | 35 | 2 | 0 | 0 | 0 | 0 |
| 57 | 39 | 2 | 0 | 0 | 0 | 0 |
| 57 | 3A | 1 | 0 | 0 | 0 | 0 |
| 57 | 3I | 1 | 0 | 0 | 0 | 0 |
| 57 | 41 | 1 | 0 | 0 | 0 | 0 |
| 57 | 42 | 1 | 0 | 0 | 0 | 0 |
| 57 | 45 | 1 | 0 | 0 | 0 | 0 |
| 57 | 4A | 1 | 0 | 0 | 0 | 0 |
| 57 | 4E | 1 | 0 | 0 | 0 | 0 |
| 57 | 4K | 2 | 0 | 0 | 0 | 0 |
| 57 | 4L | 2 | 0 | 0 | 0 | 0 |
| 57 | 5E | 1 | 0 | 0 | 0 | 0 |
| 57 | 5I | 1 | 0 | 0 | 0 | 0 |
| 57 | 68 | 2 | 0 | 0 | 0 | 0 |
| 57 | 78 | 1 | 0 | 0 | 0 | 0 |
| 57 | 88 | 3 | 0 | 0 | 0 | 0 |
| 57 | 9A | 1 | 0 | 0 | 0 | 0 |
| 57 | B5 | 1 | 0 | 0 | 0 | 0 |
| 57 | C5 | 1 | 0 | 0 | 0 | 0 |
| 57 | E5 | 1 | 0 | 0 | 0 | 0 |
| 57 | F8 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | I8 | 1 | 0 | 0 | 0 | 0 |
| 57 | J8 | 1 | 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 |
| 57 | Q8 | 1 | 0 | 0 | 0 | 0 |
| 58 | 13 | 13 | 0 | 22 | 3 | 0 |
| 58 | 14 | 26 | 0 | 46 | 11 | 0 |
| 58 | 1G | 13 | 0 | 24 | 0 | 0 |
| 58 | 1J | 13 | 0 | 24 | 1 | 0 |
| 59 | 32 | 8 | 0 | 0 | 1 | 0 |
| 59 | 3E | 8 | 0 | 0 | 3 | 0 |
| 60 | 5A | 1 | 0 | 0 | 0 | 0 |
| 60 | 5I | 1 | 0 | 0 | 0 | 0 |
| 60 | C5 | 1 | 0 | 0 | 0 | 0 |
| 60 | G8 | 1 | 0 | 0 | 0 | 0 |
| 61 | 11 | 16 | 0 | 0 | 6 | 0 |
| 61 | 13 | 304 | 0 | 0 | 17 | 0 |
| 61 | 14 | 1135 | 0 | 0 | 56 | 0 |
| 61 | 16 | 15 | 0 | 0 | 1 | 0 |
| 61 | 19 | 8 | 0 | 0 | 0 | 0 |
| 61 | 1G | 391 | 0 | 0 | 17 | 0 |
| 61 | 1H | 1133 | 0 | 0 | 86 | 0 |
| 61 | 1I | 2 | 0 | 0 | 0 | 0 |
| 61 | 1J | 18 | 0 | 0 | 1 | 0 |
| 61 | 1K | 1 | 0 | 0 | 0 | 0 |
| 61 | 21 | 8 | 0 | 0 | 0 | 0 |
| 61 | 22 | 1 | 0 | 0 | 0 | 0 |
| 61 | 25 | 11 | 0 | 0 | 1 | 0 |
| 61 | 29 | 6 | 0 | 0 | 0 | 0 |
| 61 | 2I | 1 | 0 | 0 | 0 | 0 |
| 61 | 2K | 6 | 0 | 0 | 0 | 0 |
| 61 | 31 | 4 | 0 | 0 | 0 | 0 |
| 61 | 35 | 9 | 0 | 0 | 4 | 0 |
| 61 | 39 | 6 | 0 | 0 | 0 | 0 |
| 61 | 3A | 1 | 0 | 0 | 0 | 0 |
| 61 | 3E | 1 | 0 | 0 | 0 | 0 |
| 61 | 3I | 2 | 0 | 0 | 0 | 0 |
| 61 | 3K | 1 | 0 | 0 | 0 | 0 |
| 61 | 42 | 1 | 0 | 0 | 0 | 0 |
| 61 | 45 | 3 | 0 | 0 | 0 | 0 |
| 61 | 4E | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | 4K | 11 | 0 | 0 | 0 | 0 |
| 61 | 4L | 14 | 0 | 0 | 1 | 0 |
| 61 | 52 | 3 | 0 | 0 | 0 | 0 |
| 61 | 55 | 1 | 0 | 0 | 0 | 0 |
| 61 | 58 | 1 | 0 | 0 | 0 | 0 |
| 61 | 5I | 2 | 0 | 0 | 0 | 0 |
| 61 | 75 | 1 | 0 | 0 | 0 | 0 |
| 61 | 78 | 11 | 0 | 0 | 5 | 0 |
| 61 | 7A | 1 | 0 | 0 | 0 | 0 |
| 61 | 7I | 2 | 0 | 0 | 1 | 0 |
| 61 | 85 | 1 | 0 | 0 | 0 | 0 |
| 61 | 98 | 2 | 0 | 0 | 0 | 0 |
| 61 | 9A | 3 | 0 | 0 | 3 | 0 |
| 61 | A5 | 1 | 0 | 0 | 0 | 0 |
| 61 | A8 | 3 | 0 | 0 | 1 | 0 |
| 61 | B8 | 1 | 0 | 0 | 0 | 0 |
| 61 | BA | 2 | 0 | 0 | 0 | 0 |
| 61 | C5 | 3 | 0 | 0 | 0 | 0 |
| 61 | E5 | 5 | 0 | 0 | 0 | 0 |
| 61 | E8 | 1 | 0 | 0 | 0 | 0 |
| 61 | F5 | 3 | 0 | 0 | 0 | 0 |
| 61 | F8 | 1 | 0 | 0 | 0 | 0 |
| 61 | H5 | 1 | 0 | 0 | 0 | 0 |
| 61 | I8 | 6 | 0 | 0 | 1 | 0 |
| 61 | K8 | 1 | 0 | 0 | 0 | 0 |
| 61 | L8 | 1 | 0 | 0 | 1 | 0 |
| 61 | M5 | 7 | 0 | 0 | 1 | 0 |
| 61 | P8 | 1 | 0 | 0 | 0 | 0 |
| 61 | Q8 | 5 | 0 | 0 | 1 | 0 |
| All | All | 296743 | 0 | 197188 | 8820 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8820 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:22:173:VAL:C | 3:22:174:PRO:N | 1.71 | 1.38 |
| 4:3E:25:ARG:NH1 | 59:3E:301:SF4:S3 | 2.12 | 1.23 |
| 19:AI:3:ARG:HE | 19:AI:9:VAL:HG11 | 1.07 | 1.14 |
| 44:E8:89:ALA:O | 44:E8:92:ARG:NH1 | 1.81 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 38:45:27:VAL:HB | 38:45:28:ALA:HA | 1.12 | 1.10 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | 12 | 203/256 (79%) | 172 (85%) | 25 (12%) | 6 (3%) | 4 | 20 |
| 2 | 1E | 231/256 (90%) | 188 (81%) | 41 (18%) | 2 (1%) | 17 | 51 |
| 3 | 22 | 191/239 (80%) | 167 (87%) | 24 (13%) | 0 | 100 | 100 |
| 3 | 2E | 203/239 (85%) | 181 (89%) | 22 (11%) | 0 | 100 | 100 |
| 4 | 32 | 206/209 (99%) | 183 (89%) | 22 (11%) | 1 (0%) | 29 | 64 |
| 4 | 3E | 205/209 (98%) | 190 (93%) | 15 (7%) | 0 | 100 | 100 |
| 5 | 42 | 147/162 (91%) | 140 (95%) | 7 (5%) | 0 | 100 | 100 |
| 5 | 4E | 147/162 (91%) | 140 (95%) | 6 (4%) | 1 (1%) | 22 | 56 |
| 6 | 52 | 99/101 (98%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | 5E | 98/101 (97%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 7 | 62 | 136/156 (87%) | 123 (90%) | 13 (10%) | 0 | 100 | 100 |
| 7 | 6E | 152/156 (97%) | 140 (92%) | 12 (8%) | 0 | 100 | 100 |
| 8 | 72 | 135/138 (98%) | 125 (93%) | 7 (5%) | 3 (2%) | 6 | 28 |
| 8 | 7E | 136/138 (99%) | 124 (91%) | 11 (8%) | 1 (1%) | 22 | 56 |
| 9 | 82 | 119/128 (93%) | 101 (85%) | 17 (14%) | 1 (1%) | 19 | 53 |
| 9 | 8E | 124/128 (97%) | 101 (82%) | 19 (15%) | 4 (3%) | 4 | 19 |
| 10 | 1A | 76/105 (72%) | 70 (92%) | 6 (8%) | 0 | 100 | 100 |
| 10 | 1I | 93/105 (89%) | 82 (88%) | 10 (11%) | 1 (1%) | 14 | 46 |
| 11 | 2A | 111/129 (86%) | 102 (92%) | 7 (6%) | 2 (2%) | 8 | 33 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 11 | 2I | 109/129 (84%) | 98 (90%) | 10 (9%) | 1 (1%) | 17 | 51 |
| 12 | 3A | 120/132 (91%) | 101 (84%) | 14 (12%) | 5 (4%) | 3 | 13 |
| 12 | 3I | 120/132 (91%) | 106 (88%) | 11 (9%) | 3 (2%) | 5 | 25 |
| 13 | 4A | 109/126 (86%) | 98 (90%) | 9 (8%) | 2 (2%) | 8 | 33 |
| 13 | 4I | 117/126 (93%) | 97 (83%) | 20 (17%) | 0 | 100 | 100 |
| 14 | 5A | 57/61 (93%) | 48 (84%) | 8 (14%) | 1 (2%) | 8 | 33 |
| 14 | 5I | 58/61 (95%) | 48 (83%) | 8 (14%) | 2 (3%) | 3 | 17 |
| 15 | 6A | 85/89 (96%) | 83 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | 6I | 85/89 (96%) | 81 (95%) | 4 (5%) | 0 | 100 | 100 |
| 16 | 7A | 82/88 (93%) | 76 (93%) | 5 (6%) | 1 (1%) | 13 | 43 |
| 16 | 7I | 81/88 (92%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | 8A | 97/105 (92%) | 91 (94%) | 6 (6%) | 0 | 100 | 100 |
| 17 | 8I | 98/105 (93%) | 89 (91%) | 7 (7%) | 2 (2%) | 7 | 30 |
| 18 | 9A | 65/88 (74%) | 61 (94%) | 4 (6%) | 0 | 100 | 100 |
| 18 | 9I | 66/88 (75%) | 62 (94%) | 3 (4%) | 1 (2%) | 10 | 38 |
| 19 | AA | 56/93 (60%) | 49 (88%) | 5 (9%) | 2 (4%) | 3 | 16 |
| 19 | AI | 80/93 (86%) | 67 (84%) | 8 (10%) | 5 (6%) | 1 | 6 |
| 20 | BA | 97/106 (92%) | 85 (88%) | 10 (10%) | 2 (2%) | 7 | 29 |
| 20 | BI | 95/106 (90%) | 82 (86%) | 13 (14%) | 0 | 100 | 100 |
| 21 | 1B | 20/27 (74%) | 19 (95%) | 1 (5%) | 0 | 100 | 100 |
| 21 | 1F | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 28 | 7I | 129/229 (56%) | 116 (90%) | 12 (9%) | 1 (1%) | 19 | 53 |
| 28 | 79 | 45/229 (20%) | 40 (89%) | 4 (9%) | 1 (2%) | 6 | 28 |
| 29 | 11 | 271/276 (98%) | 241 (89%) | 21 (8%) | 9 (3%) | 4 | 18 |
| 29 | 19 | 272/276 (99%) | 243 (89%) | 25 (9%) | 4 (2%) | 10 | 38 |
| 30 | 21 | 200/206 (97%) | 154 (77%) | 37 (18%) | 9 (4%) | 2 | 12 |
| 30 | 29 | 202/206 (98%) | 155 (77%) | 35 (17%) | 12 (6%) | 1 | 7 |
| 31 | 31 | 200/210 (95%) | 179 (90%) | 18 (9%) | 3 (2%) | 10 | 38 |
| 31 | 39 | 202/210 (96%) | 159 (79%) | 35 (17%) | 8 (4%) | 3 | 14 |
| 32 | 41 | 177/182 (97%) | 156 (88%) | 18 (10%) | 3 (2%) | 9 | 34 |
| 32 | 49 | 179/182 (98%) | 159 (89%) | 19 (11%) | 1 (1%) | 25 | 60 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 33 | 51 | 172/180 (96%) | 138 (80%) | 23 (13%) | 11 (6%) | 1 | 5 |
| 33 | 59 | 165/180 (92%) | 129 (78%) | 30 (18%) | 6 (4%) | 3 | 16 |
| 34 | 61 | 144/148 (97%) | 120 (83%) | 21 (15%) | 3 (2%) | 7 | 29 |
| 34 | 69 | 143/148 (97%) | 113 (79%) | 27 (19%) | 3 (2%) | 7 | 29 |
| 35 | 15 | 136/140 (97%) | 124 (91%) | 11 (8%) | 1 (1%) | 22 | 56 |
| 35 | 58 | 135/140 (96%) | 115 (85%) | 17 (13%) | 3 (2%) | 6 | 28 |
| 36 | 25 | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 36 | 68 | 120/122 (98%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 37 | 35 | 145/150 (97%) | 117 (81%) | 27 (19%) | 1 (1%) | 22 | 56 |
| 37 | 78 | 145/150 (97%) | 116 (80%) | 21 (14%) | 8 (6%) | 2 | 8 |
| 38 | 45 | 137/141 (97%) | 115 (84%) | 19 (14%) | 3 (2%) | 6 | 28 |
| 38 | 88 | 139/141 (99%) | 121 (87%) | 12 (9%) | 6 (4%) | 2 | 12 |
| 39 | 55 | 116/118 (98%) | 109 (94%) | 6 (5%) | 1 (1%) | 17 | 51 |
| 39 | 98 | 116/118 (98%) | 107 (92%) | 7 (6%) | 2 (2%) | 9 | 34 |
| 40 | 65 | 108/112 (96%) | 91 (84%) | 16 (15%) | 1 (1%) | 17 | 51 |
| 40 | A8 | 109/112 (97%) | 92 (84%) | 15 (14%) | 2 (2%) | 8 | 33 |
| 41 | 75 | 131/146 (90%) | 120 (92%) | 8 (6%) | 3 (2%) | 6 | 27 |
| 41 | B8 | 134/146 (92%) | 120 (90%) | 12 (9%) | 2 (2%) | 10 | 38 |
| 42 | 85 | 114/118 (97%) | 102 (90%) | 12 (10%) | 0 | 100 | 100 |
| 42 | C8 | 113/118 (96%) | 105 (93%) | 3 (3%) | 5 (4%) | 2 | 12 |
| 43 | 95 | 98/101 (97%) | 81 (83%) | 14 (14%) | 3 (3%) | 4 | 19 |
| 43 | D8 | 98/101 (97%) | 88 (90%) | 8 (8%) | 2 (2%) | 7 | 30 |
| 44 | A5 | 109/113 (96%) | 103 (94%) | 5 (5%) | 1 (1%) | 17 | 51 |
| 44 | E8 | 108/113 (96%) | 100 (93%) | 8 (7%) | 0 | 100 | 100 |
| 45 | B5 | 92/96 (96%) | 81 (88%) | 9 (10%) | 2 (2%) | 6 | 28 |
| 45 | F8 | 93/96 (97%) | 87 (94%) | 5 (5%) | 1 (1%) | 14 | 46 |
| 46 | C5 | 102/110 (93%) | 71 (70%) | 24 (24%) | 7 (7%) | 1 | 4 |
| 46 | G8 | 101/110 (92%) | 82 (81%) | 15 (15%) | 4 (4%) | 3 | 14 |
| 47 | D5 | 127/206 (62%) | 102 (80%) | 21 (16%) | 4 (3%) | 4 | 19 |
| 47 | H8 | 168/206 (82%) | 132 (79%) | 32 (19%) | 4 (2%) | 6 | 26 |
| 48 | E5 | 74/85 (87%) | 66 (89%) | 7 (10%) | 1 (1%) | 11 | 39 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 48 | I8 | 75/85 (88%) | 68 (91%) | 6 (8%) | 1 (1%) | 12 | 41 |
| 49 | F5 | 92/98 (94%) | 80 (87%) | 11 (12%) | 1 (1%) | 14 | 46 |
| 49 | J8 | 92/98 (94%) | 86 (94%) | 4 (4%) | 2 (2%) | 6 | 28 |
| 50 | G5 | 67/72 (93%) | 62 (92%) | 2 (3%) | 3 (4%) | 2 | 12 |
| 50 | K8 | 66/72 (92%) | 60 (91%) | 3 (4%) | 3 (4%) | 2 | 12 |
| 51 | H5 | 56/60 (93%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 51 | L8 | 56/60 (93%) | 51 (91%) | 5 (9%) | 0 | 100 | 100 |
| 52 | I5 | 61/71 (86%) | 28 (46%) | 28 (46%) | 5 (8%) | 1 | 3 |
| 52 | M8 | 57/71 (80%) | 39 (68%) | 13 (23%) | 5 (9%) | 1 | 3 |
| 53 | J5 | 54/60 (90%) | 50 (93%) | 4 (7%) | 0 | 100 | 100 |
| 53 | N8 | 54/60 (90%) | 49 (91%) | 5 (9%) | 0 | 100 | 100 |
| 54 | L5 | 45/49 (92%) | 42 (93%) | 3 (7%) | 0 | 100 | 100 |
| 54 | P8 | 45/49 (92%) | 43 (96%) | 2 (4%) | 0 | 100 | 100 |
| 55 | M5 | 62/65 (95%) | 54 (87%) | 6 (10%) | 2 (3%) | 4 | 19 |
| 55 | Q8 | 62/65 (95%) | 52 (84%) | 7 (11%) | 3 (5%) | 2 | 11 |
| All | All | 11163/12404 (90%) | 9756 (87%) | 1192 (11%) | 215 (2%) | 8 | 32 |

5 of 215 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | 8E | 111 | ARG |
| 18 | 9I | 22 | VAL |
| 19 | AI | 41 | VAL |
| 30 | 21 | 77 | ILE |
| 37 | 78 | 25 | SER |

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 | 179/220 (81%) | 136 (76%) | 43 (24%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | 1E | 202/220 (92%) | 152 (75%) | 50 (25%) | 0 | 2 |
| 3 | 22 | 154/188 (82%) | 119 (77%) | 35 (23%) | 1 | 3 |
| 3 | 2E | 159/188 (85%) | 127 (80%) | 32 (20%) | 1 | 5 |
| 4 | 32 | 180/181 (99%) | 151 (84%) | 29 (16%) | 2 | 10 |
| 4 | 3E | 180/181 (99%) | 141 (78%) | 39 (22%) | 1 | 4 |
| 5 | 42 | 114/123 (93%) | 88 (77%) | 26 (23%) | 1 | 3 |
| 5 | 4E | 115/123 (94%) | 93 (81%) | 22 (19%) | 1 | 6 |
| 6 | 52 | 90/90 (100%) | 79 (88%) | 11 (12%) | 5 | 19 |
| 6 | 5E | 90/90 (100%) | 82 (91%) | 8 (9%) | 9 | 32 |
| 7 | 62 | 114/127 (90%) | 91 (80%) | 23 (20%) | 1 | 5 |
| 7 | 6E | 125/127 (98%) | 101 (81%) | 24 (19%) | 1 | 6 |
| 8 | 72 | 118/119 (99%) | 94 (80%) | 24 (20%) | 1 | 5 |
| 8 | 7E | 119/119 (100%) | 96 (81%) | 23 (19%) | 1 | 6 |
| 9 | 82 | 92/99 (93%) | 67 (73%) | 25 (27%) | 0 | 1 |
| 9 | 8E | 97/99 (98%) | 77 (79%) | 20 (21%) | 1 | 4 |
| 10 | 1A | 71/92 (77%) | 46 (65%) | 25 (35%) | 0 | 1 |
| 10 | 1I | 81/92 (88%) | 66 (82%) | 15 (18%) | 1 | 7 |
| 11 | 2A | 85/99 (86%) | 69 (81%) | 16 (19%) | 1 | 7 |
| 11 | 2I | 84/99 (85%) | 69 (82%) | 15 (18%) | 2 | 7 |
| 12 | 3A | 103/109 (94%) | 84 (82%) | 19 (18%) | 1 | 7 |
| 12 | 3I | 103/109 (94%) | 86 (84%) | 17 (16%) | 2 | 9 |
| 13 | 4A | 91/101 (90%) | 62 (68%) | 29 (32%) | 0 | 1 |
| 13 | 4I | 94/101 (93%) | 72 (77%) | 22 (23%) | 1 | 3 |
| 14 | 5A | 49/50 (98%) | 26 (53%) | 23 (47%) | 0 | 0 |
| 14 | 5I | 49/50 (98%) | 35 (71%) | 14 (29%) | 0 | 1 |
| 15 | 6A | 79/80 (99%) | 74 (94%) | 5 (6%) | 18 | 48 |
| 15 | 6I | 79/80 (99%) | 70 (89%) | 9 (11%) | 5 | 21 |
| 16 | 7A | 72/74 (97%) | 60 (83%) | 12 (17%) | 2 | 9 |
| 16 | 7I | 72/74 (97%) | 55 (76%) | 17 (24%) | 1 | 3 |
| 17 | 8A | 94/97 (97%) | 78 (83%) | 16 (17%) | 2 | 9 |
| 17 | 8I | 95/97 (98%) | 72 (76%) | 23 (24%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 18 | 9A | 58/77 (75%) | 45 (78%) | 13 (22%) | 1 | 3 |
| 18 | 9I | 58/77 (75%) | 43 (74%) | 15 (26%) | 0 | 2 |
| 19 | AA | 52/80 (65%) | 41 (79%) | 11 (21%) | 1 | 4 |
| 19 | AI | 72/80 (90%) | 60 (83%) | 12 (17%) | 2 | 9 |
| 20 | BA | 76/82 (93%) | 56 (74%) | 20 (26%) | 0 | 2 |
| 20 | BI | 75/82 (92%) | 57 (76%) | 18 (24%) | 0 | 2 |
| 21 | 1B | 17/22 (77%) | 13 (76%) | 4 (24%) | 1 | 3 |
| 21 | 1F | 18/22 (82%) | 15 (83%) | 3 (17%) | 2 | 9 |
| 28 | 71 | 109/181 (60%) | 84 (77%) | 25 (23%) | 1 | 3 |
| 28 | 79 | 48/181 (26%) | 37 (77%) | 11 (23%) | 1 | 3 |
| 29 | 11 | 214/218 (98%) | 189 (88%) | 25 (12%) | 5 | 20 |
| 29 | 19 | 214/218 (98%) | 179 (84%) | 35 (16%) | 2 | 9 |
| 30 | 21 | 155/166 (93%) | 121 (78%) | 34 (22%) | 1 | 4 |
| 30 | 29 | 165/166 (99%) | 145 (88%) | 20 (12%) | 5 | 19 |
| 31 | 31 | 161/166 (97%) | 139 (86%) | 22 (14%) | 3 | 15 |
| 31 | 39 | 163/166 (98%) | 129 (79%) | 34 (21%) | 1 | 4 |
| 32 | 41 | 153/156 (98%) | 131 (86%) | 22 (14%) | 3 | 13 |
| 32 | 49 | 153/156 (98%) | 112 (73%) | 41 (27%) | 0 | 2 |
| 33 | 51 | 143/148 (97%) | 104 (73%) | 39 (27%) | 0 | 1 |
| 33 | 59 | 139/148 (94%) | 113 (81%) | 26 (19%) | 1 | 7 |
| 34 | 61 | 122/124 (98%) | 97 (80%) | 25 (20%) | 1 | 5 |
| 34 | 69 | 122/124 (98%) | 93 (76%) | 29 (24%) | 0 | 2 |
| 35 | 15 | 117/119 (98%) | 100 (86%) | 17 (14%) | 3 | 13 |
| 35 | 58 | 116/119 (98%) | 100 (86%) | 16 (14%) | 3 | 14 |
| 36 | 25 | 100/100 (100%) | 83 (83%) | 17 (17%) | 2 | 9 |
| 36 | 68 | 100/100 (100%) | 88 (88%) | 12 (12%) | 5 | 19 |
| 37 | 35 | 114/116 (98%) | 89 (78%) | 25 (22%) | 1 | 4 |
| 37 | 78 | 114/116 (98%) | 91 (80%) | 23 (20%) | 1 | 5 |
| 38 | 45 | 109/111 (98%) | 82 (75%) | 27 (25%) | 0 | 2 |
| 38 | 88 | 110/111 (99%) | 92 (84%) | 18 (16%) | 2 | 9 |
| 39 | 55 | 101/101 (100%) | 86 (85%) | 15 (15%) | 3 | 12 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 39 | 98 | 101/101 (100%) | 85 (84%) | 16 (16%) | 2 | 10 |
| 40 | 65 | 87/88 (99%) | 57 (66%) | 30 (34%) | 0 | 1 |
| 40 | A8 | 87/88 (99%) | 72 (83%) | 15 (17%) | 2 | 8 |
| 41 | 75 | 117/127 (92%) | 98 (84%) | 19 (16%) | 2 | 10 |
| 41 | B8 | 117/127 (92%) | 90 (77%) | 27 (23%) | 1 | 3 |
| 42 | 85 | 93/94 (99%) | 78 (84%) | 15 (16%) | 2 | 10 |
| 42 | C8 | 92/94 (98%) | 80 (87%) | 12 (13%) | 4 | 16 |
| 43 | 95 | 81/82 (99%) | 60 (74%) | 21 (26%) | 0 | 2 |
| 43 | D8 | 82/82 (100%) | 60 (73%) | 22 (27%) | 0 | 2 |
| 44 | A5 | 91/92 (99%) | 74 (81%) | 17 (19%) | 1 | 7 |
| 44 | E8 | 90/92 (98%) | 80 (89%) | 10 (11%) | 6 | 22 |
| 45 | B5 | 74/78 (95%) | 64 (86%) | 10 (14%) | 4 | 15 |
| 45 | F8 | 75/78 (96%) | 69 (92%) | 6 (8%) | 12 | 37 |
| 46 | C5 | 85/91 (93%) | 62 (73%) | 23 (27%) | 0 | 1 |
| 46 | G8 | 83/91 (91%) | 65 (78%) | 18 (22%) | 1 | 4 |
| 47 | D5 | 118/179 (66%) | 90 (76%) | 28 (24%) | 1 | 2 |
| 47 | H8 | 151/179 (84%) | 112 (74%) | 39 (26%) | 0 | 2 |
| 48 | E5 | 61/67 (91%) | 53 (87%) | 8 (13%) | 4 | 16 |
| 48 | I8 | 62/67 (92%) | 53 (86%) | 9 (14%) | 3 | 13 |
| 49 | F5 | 79/83 (95%) | 65 (82%) | 14 (18%) | 2 | 8 |
| 49 | J8 | 79/83 (95%) | 65 (82%) | 14 (18%) | 2 | 8 |
| 50 | G5 | 63/67 (94%) | 42 (67%) | 21 (33%) | 0 | 1 |
| 50 | K8 | 64/67 (96%) | 48 (75%) | 16 (25%) | 0 | 2 |
| 51 | H5 | 50/52 (96%) | 39 (78%) | 11 (22%) | 1 | 4 |
| 51 | L8 | 50/52 (96%) | 40 (80%) | 10 (20%) | 1 | 5 |
| 52 | I5 | 57/63 (90%) | 39 (68%) | 18 (32%) | 0 | 1 |
| 52 | M8 | 52/63 (82%) | 33 (64%) | 19 (36%) | 0 | 0 |
| 53 | J5 | 48/52 (92%) | 34 (71%) | 14 (29%) | 0 | 1 |
| 53 | N8 | 49/52 (94%) | 39 (80%) | 10 (20%) | 1 | 5 |
| 54 | L5 | 38/42 (90%) | 33 (87%) | 5 (13%) | 4 | 16 |
| 54 | P8 | 38/42 (90%) | 32 (84%) | 6 (16%) | 2 | 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 55 | M5 | 54/55 (98%) | 42 (78%) | 12 (22%) | 1 | 3 |
| 55 | Q8 | 54/55 (98%) | 48 (89%) | 6 (11%) | 6 | 22 |
| All | All | 9419/10256 (92%) | 7533 (80%) | 1886 (20%) | 1 | 5 |

5 of 1886 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | K8 | 28 | LYS |
| 6 | 52 | 74 | ASP |
| 46 | C5 | 79 | CYS |
| 52 | M8 | 21 | VAL |
| 3 | 22 | 4 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 12 | 135 | GLN |
| 11 | 2A | 117 | ASN |
| 32 | 49 | 130 | ASN |
| 2 | 12 | 16 | HIS |
| 38 | 45 | 123 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 13 | 1493/1522 (98%) | 348 (23%) | 34 (2%) |
| 1 | 1G | 1505/1522 (98%) | 323 (21%) | 33 (2%) |
| 22 | 1K | 67/76 (88%) | 36 (53%) | 4 (5%) |
| 23 | 2K | 76/77 (98%) | 20 (26%) | 1 (1%) |
| 23 | 2L | 75/77 (97%) | 10 (13%) | 2 (2%) |
| 24 | 3K | 67/76 (88%) | 37 (55%) | 3 (4%) |
| 24 | 3L | 69/76 (90%) | 32 (46%) | 1 (1%) |
| 25 | 4K | 19/30 (63%) | 12 (63%) | 2 (10%) |
| 25 | 4L | 18/30 (60%) | 10 (55%) | 2 (11%) |
| 26 | 14 | 2803/2917 (96%) | 638 (22%) | 37 (1%) |
| 26 | 1H | 2836/2917 (97%) | 590 (20%) | 43 (1%) |
| 27 | 16 | 121/122 (99%) | 24 (19%) | 0 |
| 27 | 1J | 121/122 (99%) | 34 (28%) | 2 (1%) |
| 56 | 1L | 65/76 (85%) | 24 (36%) | 2 (3%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| All | All | 9335/9640 (96%) | 2138 (22%) | 166 (1%) |

5 of 2138 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 13 | 2 | U |
| 1 | 13 | 5 | U |
| 1 | 13 | 6 | G |
| 1 | 13 | 12 | U |
| 1 | 13 | 13 | U |

5 of 166 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 1900 | A |
| 1 | 1G | 250 | A |
| 26 | 14 | 2402 | C |
| 26 | 1H | 2172 | U |
| 26 | 1H | 2481 | G |

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | 7MG | 2L | 47 | 23 | 22,26,27 | 3.40 | 6 (27%) | 28,39,42 | 2.72 | 10 (35%) |
| 23 | 7MG | 2K | 47 | 23 | 22,26,27 | 3.49 | 7 (31%) | 28,39,42 | 2.49 | 11 (39%) |
| 23 | 5MU | 2L | 55 | 23 | 15,22,23 | 2.19 | 3 (20%) | 16,32,35 | 1.72 | 2 (12%) |
| 23 | OMC | 2L | 33 | 23 | 15,22,23 | 2.30 | 4 (26%) | 17,31,34 | 1.59 | 3 (17%) |
| 23 | 4SU | 2K | 8 | 23 | 14,21,22 | 3.35 | 2 (14%) | 15,30,33 | 1.01 | 1 (6%) |
| 23 | PSU | 2K | 56 | 23 | 17,21,22 | 1.14 | 2 (11%) | 20,30,33 | 2.83 | 5 (25%) |
| 22 | 5MU | 1K | 54 | 22 | 15,22,23 | 2.14 | 3 (20%) | 16,32,35 | 1.97 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | H2U | 1K | 17 | 22 | 18,21,22 | 2.13 | 4 (22%) | 21,30,33 | 2.38 | 5 (23%) |
| 22 | PSU | 1K | 55 | 22 | 17,21,22 | 1.14 | 1 (5%) | 20,30,33 | 3.46 | 4 (20%) |
| 56 | PSU | 1L | 55 | 56 | 17,21,22 | 1.21 | 1 (5%) | 20,30,33 | 3.63 | 5 (25%) |
| 22 | 6MZ | 1K | 37 | 22 | 18,25,26 | 2.22 | 4 (22%) | 16,36,39 | 2.30 | 3 (18%) |
| 23 | PSU | 2L | 56 | 23 | 17,21,22 | 1.12 | 1 (5%) | 20,30,33 | 3.35 | 5 (25%) |
| 22 | CM0 | 1K | 34 | 22 | 16,26,27 | 3.23 | 4 (25%) | 18,37,40 | 2.07 | 3 (16%) |
| 23 | OMC | 2K | 33 | 23 | 15,22,23 | 2.21 | 4 (26%) | 17,31,34 | 1.56 | 3 (17%) |
| 23 | 4SU | 2L | 8 | 23 | 14,21,22 | 3.54 | 2 (14%) | 15,30,33 | 0.92 | 1 (6%) |
| 56 | 5MU | 1L | 54 | 56 | 15,22,23 | 2.13 | 3 (20%) | 16,32,35 | 1.74 | 2 (12%) |
| 23 | 5MU | 2K | 55 | 57,23 | 15,22,23 | 2.12 | 3 (20%) | 16,32,35 | 1.67 | 2 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 23 | 7MG | 2L | 47 | 23 | - | 4/7/37/38 | 0/3/3/3 |
| 23 | 7MG | 2K | 47 | 23 | - | 0/7/37/38 | 0/3/3/3 |
| 23 | 5MU | 2L | 55 | 23 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | OMC | 2L | 33 | 23 | - | 2/7/27/28 | 0/2/2/2 |
| 23 | 4SU | 2K | 8 | 23 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | PSU | 2K | 56 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | 1K | 54 | 22 | - | 0/5/25/26 | 0/2/2/2 |
| 22 | H2U | 1K | 17 | 22 | - | 1/7/38/39 | 0/2/2/2 |
| 22 | PSU | 1K | 55 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | 1L | 55 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 6MZ | 1K | 37 | 22 | - | 2/5/27/28 | 0/3/3/3 |
| 23 | PSU | 2L | 56 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | CM0 | 1K | 34 | 22 | - | 5/8/30/31 | 0/2/2/2 |
| 23 | OMC | 2K | 33 | 23 | - | 0/7/27/28 | 0/2/2/2 |
| 23 | 4SU | 2L | 8 | 23 | - | 0/5/25/26 | 0/2/2/2 |
| 56 | 5MU | 1L | 54 | 56 | - | 0/5/25/26 | 0/2/2/2 |
| 23 | 5MU | 2K | 55 | 57,23 | - | 0/5/25/26 | 0/2/2/2 |

The worst 5 of 54 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23 | 2L | 47 | 7MG | C4-N3 | 11.59 | 1.49 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23 | 2K | 47 | 7MG | C4-N3 | 10.99 | 1.48 | 1.34 |
| 23 | 2L | 8 | 4SU | C5-C4 | 10.34 | 1.50 | 1.38 |
| 23 | 2K | 8 | 4SU | C5-C4 | 9.88 | 1.49 | 1.38 |
| 23 | 2L | 8 | 4SU | C6-N1 | 8.01 | 1.45 | 1.35 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 56 | 1L | 55 | PSU | N1-C2-N3 | -11.80 | 119.05 | 128.43 |
| 23 | 2L | 56 | PSU | N1-C2-N3 | -11.71 | 119.12 | 128.43 |
| 22 | 1K | 55 | PSU | N1-C2-N3 | -10.48 | 120.10 | 128.43 |
| 23 | 2K | 56 | PSU | N1-C2-N3 | -9.32 | 121.02 | 128.43 |
| 56 | 1L | 55 | PSU | C4-N3-C2 | 7.95 | 121.85 | 115.14 |

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | 2L | 47 | 7MG | C2'-C1'-N9-C8 |
| 23 | 2L | 33 | OMC | C2'-C1'-N1-C6 |
| 23 | 2L | 33 | OMC | O4'-C1'-N1-C6 |
| 22 | 1K | 34 | CM0 | C2'-C1'-N1-C6 |
| 22 | 1K | 34 | CM0 | O4'-C4'-C5'-O5' |

There are no ring outliers.

13 monomers are involved in 22 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | 2L | 47 | 7MG | 1 | 0 |
| 23 | 2K | 47 | 7MG | 2 | 0 |
| 23 | 2L | 55 | 5MU | 3 | 0 |
| 23 | 2L | 33 | OMC | 3 | 0 |
| 23 | 2K | 8 | 4SU | 1 | 0 |
| 22 | 1K | 54 | 5MU | 1 | 0 |
| 22 | 1K | 17 | H2U | 2 | 0 |
| 22 | 1K | 55 | PSU | 2 | 0 |
| 22 | 1K | 34 | CM0 | 1 | 0 |
| 23 | 2K | 33 | OMC | 1 | 0 |
| 23 | 2L | 8 | 4SU | 2 | 0 |
| 56 | 1L | 54 | 5MU | 1 | 0 |
| 23 | 2K | 55 | 5MU | 3 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1355 ligands modelled in this entry, 1348 are monoatomic - leaving 7 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 59 | SF4 | 3E | 301 | 4 | 0,12,12 | 0.00 | - | - | | |
| 58 | SPE | 14 | 3446 | - | 12,12,12 | 0.73 | 0 | 11,11,11 | 0.98 | 1 (9%) |
| 58 | SPE | 1G | 1733 | - | 12,12,12 | 0.40 | 0 | 11,11,11 | 0.91 | 0 |
| 59 | SF4 | 32 | 301 | 4 | 0,12,12 | 0.00 | - | - | | |
| 58 | SPE | 1J | 208 | - | 12,12,12 | 0.40 | 0 | 11,11,11 | 0.88 | 0 |
| 58 | SPE | 14 | 3445 | 26 | 12,12,12 | 0.58 | 0 | 11,11,11 | 0.89 | 0 |
| 58 | SPE | 13 | 1748 | 1 | 12,12,12 | 0.49 | 0 | 11,11,11 | 0.97 | 1 (9%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 59 | SF4 | 3E | 301 | 4 | - | - | 0/6/5/5 |
| 58 | SPE | 14 | 3446 | - | - | 5/10/10/10 | - |
| 58 | SPE | 1G | 1733 | - | - | 4/10/10/10 | - |
| 59 | SF4 | 32 | 301 | 4 | - | - | 0/6/5/5 |
| 58 | SPE | 1J | 208 | - | - | 5/10/10/10 | - |
| 58 | SPE | 14 | 3445 | 26 | - | 6/10/10/10 | - |
| 58 | SPE | 13 | 1748 | 1 | - | 7/10/10/10 | - |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|------------|-------|------------------------|---------------------|
| 58 | 13 | 1748 | SPE | C11-C10-N9 | -2.43 | 105.58 | 112.14 |
| 58 | 14 | 3446 | SPE | C11-C10-N9 | -2.39 | 105.69 | 112.14 |

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 58 | 14 | 3445 | SPE | C2-C3-C4-N5 |
| 58 | 14 | 3446 | SPE | N9-C10-C11-C12 |
| 58 | 13 | 1748 | SPE | C2-C3-C4-N5 |
| 58 | 13 | 1748 | SPE | N9-C10-C11-C12 |
| 58 | 13 | 1748 | SPE | C7-C6-N5-C4 |

There are no ring outliers.

6 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 59 | 3E | 301 | SF4 | 3 | 0 |
| 58 | 14 | 3446 | SPE | 6 | 0 |
| 59 | 32 | 301 | SF4 | 1 | 0 |
| 58 | 1J | 208 | SPE | 1 | 0 |
| 58 | 14 | 3445 | SPE | 5 | 0 |
| 58 | 13 | 1748 | SPE | 3 | 0 |

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 |
|-----|-------|------------------|
| 3 | 22 | 1 |
| 10 | 1A | 1 |
| 25 | 4K | 1 |
| 2 | 1E | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 1E | 78:GLN | C | 79:ASP | N | 4.14 |
| 1 | 4K | 25:A | O3' | 26:A | P | 3.23 |
| 1 | 22 | 173:VAL | C | 174:PRO | N | 1.71 |
| 1 | 1A | 38:ILE | C | 39:PRO | N | 1.62 |

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1 | 13 | 1496/1522 (98%) | -0.40 | 5 (0%) 94 87 | 57, 98, 164, 235 | 0 |
| 1 | 1G | 1506/1522 (98%) | -0.45 | 4 (0%) 94 87 | 68, 105, 166, 238 | 0 |
| 2 | 12 | 207/256 (80%) | 1.12 | 47 (22%) 0 0 | 121, 148, 168, 185 | 0 |
| 2 | 1E | 235/256 (91%) | 0.46 | 18 (7%) 13 7 | 108, 135, 160, 171 | 0 |
| 3 | 22 | 195/239 (81%) | 1.28 | 49 (25%) 0 0 | 113, 131, 152, 164 | 0 |
| 3 | 2E | 205/239 (85%) | 1.21 | 46 (22%) 0 0 | 85, 107, 142, 149 | 0 |
| 4 | 32 | 208/209 (99%) | 0.84 | 30 (14%) 2 1 | 84, 101, 123, 132 | 0 |
| 4 | 3E | 207/209 (99%) | 0.55 | 19 (9%) 9 5 | 77, 103, 125, 133 | 0 |
| 5 | 42 | 149/162 (91%) | 0.16 | 5 (3%) 45 29 | 91, 111, 128, 149 | 0 |
| 5 | 4E | 149/162 (91%) | 0.21 | 3 (2%) 65 48 | 79, 98, 118, 135 | 0 |
| 6 | 52 | 101/101 (100%) | 0.84 | 11 (10%) 5 3 | 81, 97, 110, 131 | 0 |
| 6 | 5E | 100/101 (99%) | 0.91 | 12 (12%) 4 2 | 83, 99, 113, 123 | 0 |
| 7 | 62 | 140/156 (89%) | 0.89 | 20 (14%) 2 1 | 103, 119, 131, 138 | 0 |
| 7 | 6E | 154/156 (98%) | 0.98 | 21 (13%) 3 1 | 98, 113, 138, 162 | 0 |
| 8 | 72 | 137/138 (99%) | -0.18 | 1 (0%) 87 76 | 90, 114, 125, 128 | 0 |
| 8 | 7E | 138/138 (100%) | 0.07 | 5 (3%) 42 28 | 87, 102, 113, 120 | 0 |
| 9 | 82 | 121/128 (94%) | 0.41 | 7 (5%) 23 14 | 101, 144, 160, 164 | 0 |
| 9 | 8E | 126/128 (98%) | 0.66 | 12 (9%) 8 5 | 84, 133, 153, 157 | 0 |
| 10 | 1A | 80/105 (76%) | 0.31 | 8 (10%) 7 4 | 111, 138, 152, 156 | 0 |
| 10 | 1I | 95/105 (90%) | 2.01 | 48 (50%) 0 0 | 80, 127, 155, 159 | 0 |
| 11 | 2A | 113/129 (87%) | 1.68 | 40 (35%) 0 0 | 78, 103, 117, 120 | 0 |
| 11 | 2I | 111/129 (86%) | 0.91 | 16 (14%) 2 1 | 70, 99, 115, 125 | 0 |
| 12 | 3A | 122/132 (92%) | 0.84 | 18 (14%) 2 1 | 74, 91, 116, 132 | 0 |
| 12 | 3I | 122/132 (92%) | 0.30 | 3 (2%) 57 40 | 65, 76, 103, 112 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | 4A | 111/126 (88%) | 0.33 | 4 (3%) 42 28 | 102, 129, 143, 152 | 0 |
| 13 | 4I | 119/126 (94%) | 0.30 | 6 (5%) 28 18 | 87, 111, 129, 139 | 0 |
| 14 | 5A | 59/61 (96%) | 1.73 | 24 (40%) 0 0 | 118, 129, 141, 142 | 0 |
| 14 | 5I | 60/61 (98%) | 0.43 | 4 (6%) 17 10 | 83, 97, 112, 119 | 0 |
| 15 | 6A | 87/89 (97%) | -0.04 | 0 100 100 | 79, 100, 115, 117 | 0 |
| 15 | 6I | 87/89 (97%) | 0.80 | 10 (11%) 4 3 | 75, 94, 109, 116 | 0 |
| 16 | 7A | 84/88 (95%) | 0.03 | 1 (1%) 79 63 | 85, 98, 119, 145 | 0 |
| 16 | 7I | 83/88 (94%) | 0.13 | 2 (2%) 59 42 | 91, 107, 132, 147 | 0 |
| 17 | 8A | 99/105 (94%) | 0.14 | 2 (2%) 65 48 | 89, 100, 117, 120 | 0 |
| 17 | 8I | 100/105 (95%) | 0.32 | 3 (3%) 50 34 | 81, 98, 108, 115 | 0 |
| 18 | 9A | 67/88 (76%) | 0.87 | 10 (14%) 2 1 | 87, 101, 125, 129 | 0 |
| 18 | 9I | 68/88 (77%) | 0.94 | 11 (16%) 1 1 | 85, 100, 125, 128 | 0 |
| 19 | AA | 62/93 (66%) | 0.27 | 5 (8%) 12 6 | 118, 142, 155, 158 | 0 |
| 19 | AI | 82/93 (88%) | 0.77 | 12 (14%) 2 1 | 95, 110, 128, 136 | 0 |
| 20 | BA | 99/106 (93%) | 0.43 | 4 (4%) 38 25 | 85, 104, 128, 140 | 0 |
| 20 | BI | 97/106 (91%) | 0.25 | 6 (6%) 20 12 | 103, 117, 139, 145 | 0 |
| 21 | 1B | 22/27 (81%) | 0.92 | 3 (13%) 3 1 | 110, 116, 124, 134 | 0 |
| 21 | 1F | 23/27 (85%) | 0.76 | 3 (13%) 3 2 | 90, 98, 106, 108 | 0 |
| 22 | 1K | 67/76 (88%) | 0.62 | 7 (10%) 6 4 | 80, 167, 196, 203 | 0 |
| 23 | 2K | 72/77 (93%) | -0.22 | 1 (1%) 75 59 | 68, 89, 116, 129 | 0 |
| 23 | 2L | 71/77 (92%) | -0.04 | 0 100 100 | 78, 100, 132, 145 | 0 |
| 24 | 3K | 70/76 (92%) | 0.66 | 11 (15%) 2 1 | 71, 198, 222, 224 | 0 |
| 24 | 3L | 71/76 (93%) | 0.66 | 9 (12%) 3 2 | 78, 191, 215, 218 | 0 |
| 25 | 4K | 21/30 (70%) | 0.83 | 2 (9%) 8 5 | 69, 129, 212, 213 | 0 |
| 25 | 4L | 19/30 (63%) | 0.27 | 1 (5%) 26 16 | 85, 144, 210, 210 | 0 |
| 26 | 14 | 2810/2917 (96%) | -0.12 | 30 (1%) 80 65 | 54, 81, 180, 237 | 0 |
| 26 | 1H | 2841/2917 (97%) | -0.12 | 27 (0%) 82 68 | 44, 70, 166, 244 | 0 |
| 27 | 16 | 122/122 (100%) | -0.66 | 1 (0%) 86 73 | 65, 87, 105, 180 | 0 |
| 27 | 1J | 122/122 (100%) | -0.71 | 0 100 100 | 79, 106, 125, 185 | 0 |
| 28 | 71 | 133/229 (58%) | 2.14 | 60 (45%) 0 0 | 137, 194, 219, 229 | 0 |
| 28 | 79 | 57/229 (24%) | 0.84 | 11 (19%) 1 0 | 136, 178, 198, 205 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 29 | 11 | 273/276 (98%) | 0.32 | 4 (1%) 73 57 | 44, 62, 78, 94 | 0 |
| 29 | 19 | 274/276 (99%) | 0.84 | 24 (8%) 10 5 | 50, 72, 87, 102 | 0 |
| 30 | 21 | 202/206 (98%) | 0.87 | 29 (14%) 2 1 | 49, 82, 115, 123 | 0 |
| 30 | 29 | 204/206 (99%) | 0.78 | 27 (13%) 3 2 | 57, 88, 125, 135 | 0 |
| 31 | 31 | 202/210 (96%) | 0.75 | 27 (13%) 3 1 | 46, 75, 108, 123 | 0 |
| 31 | 39 | 204/210 (97%) | 0.66 | 21 (10%) 6 4 | 57, 95, 139, 164 | 0 |
| 32 | 41 | 179/182 (98%) | 0.35 | 7 (3%) 39 25 | 75, 95, 124, 138 | 0 |
| 32 | 49 | 181/182 (99%) | 1.04 | 40 (22%) 0 0 | 99, 118, 142, 156 | 0 |
| 33 | 51 | 174/180 (96%) | 0.09 | 6 (3%) 45 29 | 76, 99, 116, 128 | 0 |
| 33 | 59 | 167/180 (92%) | 1.60 | 57 (34%) 0 0 | 123, 190, 216, 225 | 0 |
| 34 | 61 | 146/148 (98%) | 0.75 | 20 (13%) 3 1 | 75, 119, 134, 148 | 0 |
| 34 | 69 | 145/148 (97%) | 0.57 | 17 (11%) 4 2 | 80, 115, 138, 144 | 0 |
| 35 | 15 | 138/140 (98%) | 1.02 | 24 (17%) 1 1 | 76, 98, 124, 139 | 0 |
| 35 | 58 | 137/140 (97%) | 0.55 | 11 (8%) 12 7 | 64, 84, 113, 134 | 0 |
| 36 | 25 | 122/122 (100%) | 0.79 | 14 (11%) 4 3 | 68, 81, 97, 107 | 0 |
| 36 | 68 | 122/122 (100%) | 0.49 | 1 (0%) 86 73 | 57, 72, 87, 93 | 0 |
| 37 | 35 | 147/150 (98%) | 0.89 | 24 (16%) 1 1 | 59, 93, 121, 133 | 0 |
| 37 | 78 | 147/150 (98%) | 0.32 | 5 (3%) 45 29 | 46, 77, 98, 106 | 0 |
| 38 | 45 | 139/141 (98%) | 1.17 | 31 (22%) 0 0 | 70, 94, 112, 126 | 0 |
| 38 | 88 | 141/141 (100%) | 0.45 | 9 (6%) 19 11 | 57, 74, 97, 117 | 0 |
| 39 | 55 | 118/118 (100%) | 0.17 | 3 (2%) 57 40 | 61, 77, 92, 109 | 0 |
| 39 | 98 | 118/118 (100%) | 0.80 | 13 (11%) 5 3 | 58, 76, 94, 104 | 0 |
| 40 | 65 | 110/112 (98%) | 0.61 | 8 (7%) 15 8 | 82, 100, 119, 130 | 0 |
| 40 | A8 | 111/112 (99%) | 1.03 | 17 (15%) 2 1 | 73, 86, 104, 112 | 0 |
| 41 | 75 | 133/146 (91%) | 0.17 | 3 (2%) 60 43 | 76, 88, 117, 142 | 0 |
| 41 | B8 | 136/146 (93%) | 0.04 | 2 (1%) 73 57 | 66, 83, 121, 152 | 0 |
| 42 | 85 | 116/118 (98%) | 0.68 | 9 (7%) 13 7 | 65, 91, 116, 123 | 0 |
| 42 | C8 | 115/118 (97%) | 0.36 | 5 (4%) 35 22 | 57, 75, 96, 106 | 0 |
| 43 | 95 | 100/101 (99%) | 1.23 | 24 (24%) 0 0 | 65, 108, 126, 132 | 0 |
| 43 | D8 | 100/101 (99%) | 0.92 | 13 (13%) 3 2 | 56, 92, 111, 125 | 0 |
| 44 | A5 | 111/113 (98%) | 0.61 | 7 (6%) 20 11 | 62, 73, 95, 128 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | E8 | 110/113 (97%) | 0.47 | 6 (5%) 25 15 | 57, 69, 90, 101 | 0 |
| 45 | B5 | 94/96 (97%) | 0.41 | 7 (7%) 14 8 | 66, 80, 103, 111 | 0 |
| 45 | F8 | 95/96 (98%) | 0.13 | 2 (2%) 63 46 | 50, 66, 91, 99 | 0 |
| 46 | C5 | 104/110 (94%) | 1.58 | 26 (25%) 0 0 | 84, 110, 143, 150 | 0 |
| 46 | G8 | 103/110 (93%) | 0.21 | 2 (1%) 66 49 | 74, 91, 118, 125 | 0 |
| 47 | D5 | 133/206 (64%) | 1.70 | 48 (36%) 0 0 | 93, 123, 150, 159 | 0 |
| 47 | H8 | 170/206 (82%) | 2.15 | 78 (45%) 0 0 | 77, 112, 191, 198 | 0 |
| 48 | E5 | 76/85 (89%) | 0.06 | 1 (1%) 77 61 | 58, 82, 94, 108 | 0 |
| 48 | I8 | 77/85 (90%) | -0.17 | 2 (2%) 56 39 | 54, 70, 87, 98 | 0 |
| 49 | F5 | 94/98 (95%) | 0.67 | 5 (5%) 26 16 | 61, 76, 117, 123 | 0 |
| 49 | J8 | 94/98 (95%) | 0.53 | 5 (5%) 26 16 | 49, 70, 115, 135 | 0 |
| 50 | G5 | 69/72 (95%) | 0.64 | 5 (7%) 15 8 | 77, 96, 113, 130 | 0 |
| 50 | K8 | 68/72 (94%) | 0.07 | 1 (1%) 73 57 | 60, 76, 94, 124 | 0 |
| 51 | H5 | 58/60 (96%) | 1.35 | 15 (25%) 0 0 | 73, 90, 118, 123 | 0 |
| 51 | L8 | 58/60 (96%) | 0.09 | 0 100 100 | 59, 75, 94, 101 | 0 |
| 52 | I5 | 63/71 (88%) | 3.48 | 46 (73%) 0 0 | 133, 174, 191, 195 | 0 |
| 52 | M8 | 61/71 (85%) | 1.37 | 16 (26%) 0 0 | 96, 137, 167, 174 | 0 |
| 53 | J5 | 56/60 (93%) | 0.62 | 6 (10%) 6 3 | 57, 81, 130, 140 | 0 |
| 53 | N8 | 56/60 (93%) | 1.22 | 10 (17%) 1 1 | 50, 83, 145, 155 | 0 |
| 54 | L5 | 47/49 (95%) | 0.18 | 1 (2%) 63 46 | 51, 61, 82, 96 | 0 |
| 54 | P8 | 47/49 (95%) | 0.05 | 0 100 100 | 44, 53, 68, 89 | 0 |
| 55 | M5 | 64/65 (98%) | 0.54 | 2 (3%) 49 32 | 64, 76, 89, 114 | 0 |
| 55 | Q8 | 64/65 (98%) | 0.06 | 1 (1%) 72 55 | 52, 64, 78, 91 | 0 |
| 56 | 1L | 67/76 (88%) | 1.41 | 17 (25%) 0 0 | 98, 180, 207, 210 | 0 |
| All | All | 20742/22044 (94%) | 0.30 | 1522 (7%) 15 8 | 44, 93, 167, 244 | 0 |

The worst 5 of 1522 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | 14 | 2902 | C | 15.3 |
| 46 | C5 | 59 | GLY | 14.8 |
| 52 | I5 | 52 | THR | 11.4 |
| 26 | 14 | 2901 | C | 11.2 |
| 43 | D8 | 37 | VAL | 11.2 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 56 | PSU | 1L | 55 | 20/21 | 0.73 | 0.29 | 118,133,146,147 | 0 |
| 22 | H2U | 1K | 17 | 20/21 | 0.81 | 0.12 | 119,145,154,154 | 0 |
| 22 | PSU | 1K | 55 | 20/21 | 0.84 | 0.25 | 102,116,131,132 | 0 |
| 23 | 7MG | 2L | 47 | 24/25 | 0.84 | 0.16 | 92,112,117,118 | 0 |
| 23 | OMC | 2L | 33 | 21/22 | 0.90 | 0.18 | 83,94,97,100 | 0 |
| 56 | 5MU | 1L | 54 | 21/22 | 0.91 | 0.22 | 117,124,131,143 | 0 |
| 23 | PSU | 2K | 56 | 20/21 | 0.92 | 0.11 | 93,98,106,114 | 0 |
| 22 | 5MU | 1K | 54 | 21/22 | 0.92 | 0.19 | 100,106,117,129 | 0 |
| 23 | PSU | 2L | 56 | 20/21 | 0.93 | 0.10 | 105,114,120,120 | 0 |
| 23 | 4SU | 2L | 8 | 20/21 | 0.93 | 0.15 | 104,106,109,112 | 0 |
| 23 | 7MG | 2K | 47 | 24/25 | 0.94 | 0.12 | 90,98,109,111 | 0 |
| 23 | 4SU | 2K | 8 | 20/21 | 0.95 | 0.13 | 84,88,92,94 | 0 |
| 22 | CM0 | 1K | 34 | 25/26 | 0.95 | 0.13 | 72,89,106,107 | 0 |
| 23 | 5MU | 2K | 55 | 21/22 | 0.95 | 0.12 | 99,102,106,113 | 0 |
| 23 | OMC | 2K | 33 | 21/22 | 0.96 | 0.17 | 72,79,82,89 | 0 |
| 23 | 5MU | 2L | 55 | 21/22 | 0.96 | 0.09 | 111,115,122,127 | 0 |
| 22 | 6MZ | 1K | 37 | 23/24 | 0.97 | 0.13 | 61,79,86,90 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | 1G | 1712 | 1/1 | 0.14 | 0.13 | 142,142,142,142 | 0 |
| 57 | MG | 13 | 1736 | 1/1 | 0.20 | 0.10 | 104,104,104,104 | 0 |
| 57 | MG | 1H | 3246 | 1/1 | 0.24 | 0.48 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3386 | 1/1 | 0.28 | 0.15 | 93,93,93,93 | 0 |
| 57 | MG | 14 | 3438 | 1/1 | 0.31 | 0.12 | 101,101,101,101 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3509 | 1/1 | 0.35 | 0.18 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3327 | 1/1 | 0.41 | 0.12 | 100,100,100,100 | 0 |
| 57 | MG | 14 | 3428 | 1/1 | 0.43 | 0.16 | 109,109,109,109 | 0 |
| 57 | MG | 1J | 206 | 1/1 | 0.44 | 0.17 | 109,109,109,109 | 0 |
| 57 | MG | 14 | 3173 | 1/1 | 0.45 | 0.16 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3216 | 1/1 | 0.45 | 0.54 | 89,89,89,89 | 0 |
| 57 | MG | 4L | 101 | 1/1 | 0.46 | 0.09 | 110,110,110,110 | 0 |
| 57 | MG | 14 | 3174 | 1/1 | 0.46 | 0.45 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3436 | 1/1 | 0.46 | 0.22 | 96,96,96,96 | 0 |
| 57 | MG | 1G | 1686 | 1/1 | 0.47 | 0.10 | 107,107,107,107 | 0 |
| 57 | MG | 1G | 1714 | 1/1 | 0.47 | 0.19 | 99,99,99,99 | 0 |
| 57 | MG | 1G | 1630 | 1/1 | 0.47 | 0.49 | 106,106,106,106 | 0 |
| 57 | MG | 1H | 3118 | 1/1 | 0.47 | 0.33 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3214 | 1/1 | 0.48 | 0.76 | 93,93,93,93 | 0 |
| 57 | MG | 14 | 3349 | 1/1 | 0.49 | 0.07 | 105,105,105,105 | 0 |
| 57 | MG | 13 | 1707 | 1/1 | 0.49 | 0.17 | 92,92,92,92 | 0 |
| 57 | MG | 1G | 1717 | 1/1 | 0.49 | 0.10 | 99,99,99,99 | 0 |
| 57 | MG | 13 | 1686 | 1/1 | 0.51 | 0.33 | 104,104,104,104 | 0 |
| 57 | MG | 1H | 3198 | 1/1 | 0.51 | 0.22 | 108,108,108,108 | 0 |
| 57 | MG | 1H | 3205 | 1/1 | 0.51 | 0.32 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3210 | 1/1 | 0.51 | 0.37 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3293 | 1/1 | 0.51 | 0.15 | 72,72,72,72 | 0 |
| 57 | MG | 13 | 1726 | 1/1 | 0.51 | 0.19 | 103,103,103,103 | 0 |
| 57 | MG | 1H | 3402 | 1/1 | 0.52 | 0.10 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3515 | 1/1 | 0.53 | 0.16 | 98,98,98,98 | 0 |
| 57 | MG | 14 | 3443 | 1/1 | 0.53 | 0.14 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3423 | 1/1 | 0.54 | 0.37 | 92,92,92,92 | 0 |
| 57 | MG | 1G | 1702 | 1/1 | 0.54 | 0.13 | 95,95,95,95 | 0 |
| 57 | MG | 1G | 1691 | 1/1 | 0.54 | 0.13 | 99,99,99,99 | 0 |
| 57 | MG | 1G | 1675 | 1/1 | 0.54 | 0.12 | 107,107,107,107 | 0 |
| 57 | MG | 14 | 3216 | 1/1 | 0.54 | 0.14 | 106,106,106,106 | 0 |
| 57 | MG | 13 | 1671 | 1/1 | 0.54 | 0.79 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3274 | 1/1 | 0.55 | 0.46 | 83,83,83,83 | 0 |
| 57 | MG | 13 | 1668 | 1/1 | 0.55 | 0.13 | 121,121,121,121 | 0 |
| 57 | MG | 1H | 3266 | 1/1 | 0.56 | 0.29 | 89,89,89,89 | 0 |
| 57 | MG | 16 | 206 | 1/1 | 0.56 | 0.38 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3010 | 1/1 | 0.56 | 0.25 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3422 | 1/1 | 0.56 | 0.17 | 100,100,100,100 | 0 |
| 57 | MG | 13 | 1732 | 1/1 | 0.56 | 0.15 | 118,118,118,118 | 0 |
| 57 | MG | 1H | 3261 | 1/1 | 0.56 | 0.40 | 77,77,77,77 | 0 |
| 57 | MG | 13 | 1645 | 1/1 | 0.57 | 0.30 | 78,78,78,78 | 0 |
| 57 | MG | 1G | 1715 | 1/1 | 0.57 | 0.12 | 119,119,119,119 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1G | 1695 | 1/1 | 0.57 | 0.07 | 112,112,112,112 | 0 |
| 57 | MG | 13 | 1654 | 1/1 | 0.57 | 0.09 | 113,113,113,113 | 0 |
| 57 | MG | 1H | 3168 | 1/1 | 0.58 | 0.16 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3188 | 1/1 | 0.58 | 0.68 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3405 | 1/1 | 0.58 | 0.09 | 91,91,91,91 | 0 |
| 57 | MG | 14 | 3282 | 1/1 | 0.58 | 0.15 | 105,105,105,105 | 0 |
| 57 | MG | 1H | 3295 | 1/1 | 0.59 | 0.15 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3524 | 1/1 | 0.59 | 0.17 | 96,96,96,96 | 0 |
| 57 | MG | 1G | 1700 | 1/1 | 0.60 | 0.11 | 109,109,109,109 | 0 |
| 57 | MG | 1H | 3061 | 1/1 | 0.60 | 0.45 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3409 | 1/1 | 0.60 | 0.25 | 95,95,95,95 | 0 |
| 57 | MG | 39 | 302 | 1/1 | 0.60 | 0.30 | 67,67,67,67 | 0 |
| 57 | MG | 14 | 3031 | 1/1 | 0.60 | 0.44 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3217 | 1/1 | 0.60 | 0.42 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3238 | 1/1 | 0.61 | 0.36 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3095 | 1/1 | 0.61 | 0.33 | 69,69,69,69 | 0 |
| 57 | MG | 1G | 1643 | 1/1 | 0.62 | 0.33 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3182 | 1/1 | 0.62 | 0.26 | 90,90,90,90 | 0 |
| 57 | MG | 1G | 1684 | 1/1 | 0.62 | 0.07 | 120,120,120,120 | 0 |
| 57 | MG | 14 | 3157 | 1/1 | 0.62 | 0.69 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3520 | 1/1 | 0.62 | 0.11 | 97,97,97,97 | 0 |
| 57 | MG | 14 | 3291 | 1/1 | 0.62 | 0.14 | 90,90,90,90 | 0 |
| 57 | MG | 25 | 201 | 1/1 | 0.63 | 0.09 | 118,118,118,118 | 0 |
| 57 | MG | 14 | 3208 | 1/1 | 0.63 | 0.20 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3284 | 1/1 | 0.63 | 0.11 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3289 | 1/1 | 0.63 | 0.31 | 78,78,78,78 | 0 |
| 57 | MG | 1G | 1710 | 1/1 | 0.63 | 0.31 | 102,102,102,102 | 0 |
| 57 | MG | 1H | 3232 | 1/1 | 0.64 | 0.49 | 85,85,85,85 | 0 |
| 57 | MG | 13 | 1743 | 1/1 | 0.64 | 0.13 | 153,153,153,153 | 0 |
| 57 | MG | 13 | 1677 | 1/1 | 0.64 | 0.29 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3525 | 1/1 | 0.64 | 0.08 | 134,134,134,134 | 0 |
| 57 | MG | 1H | 3496 | 1/1 | 0.64 | 0.12 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3212 | 1/1 | 0.64 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3186 | 1/1 | 0.65 | 0.42 | 94,94,94,94 | 0 |
| 57 | MG | 14 | 3162 | 1/1 | 0.65 | 0.60 | 67,67,67,67 | 0 |
| 57 | MG | 14 | 3435 | 1/1 | 0.65 | 0.12 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3077 | 1/1 | 0.65 | 0.25 | 56,56,56,56 | 0 |
| 57 | MG | 13 | 1678 | 1/1 | 0.65 | 0.59 | 94,94,94,94 | 0 |
| 57 | MG | 1J | 205 | 1/1 | 0.65 | 0.10 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3390 | 1/1 | 0.65 | 0.18 | 108,108,108,108 | 0 |
| 57 | MG | 14 | 3086 | 1/1 | 0.65 | 0.26 | 64,64,64,64 | 0 |
| 57 | MG | 14 | 3092 | 1/1 | 0.66 | 0.49 | 81,81,81,81 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1G | 1707 | 1/1 | 0.66 | 0.22 | 108,108,108,108 | 0 |
| 57 | MG | 1H | 3415 | 1/1 | 0.66 | 0.21 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3500 | 1/1 | 0.66 | 0.09 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3104 | 1/1 | 0.66 | 0.29 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3147 | 1/1 | 0.66 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3535 | 1/1 | 0.66 | 0.24 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3508 | 1/1 | 0.66 | 0.08 | 84,84,84,84 | 0 |
| 57 | MG | 13 | 1741 | 1/1 | 0.66 | 0.12 | 110,110,110,110 | 0 |
| 57 | MG | 14 | 3218 | 1/1 | 0.67 | 0.28 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3180 | 1/1 | 0.67 | 0.38 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3397 | 1/1 | 0.67 | 0.07 | 109,109,109,109 | 0 |
| 57 | MG | 1G | 1680 | 1/1 | 0.67 | 0.29 | 91,91,91,91 | 0 |
| 57 | MG | 13 | 1733 | 1/1 | 0.67 | 0.10 | 106,106,106,106 | 0 |
| 57 | MG | 14 | 3111 | 1/1 | 0.67 | 0.48 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3008 | 1/1 | 0.67 | 0.40 | 90,90,90,90 | 0 |
| 57 | MG | 14 | 3295 | 1/1 | 0.67 | 0.29 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3263 | 1/1 | 0.68 | 0.47 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3211 | 1/1 | 0.68 | 0.49 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3218 | 1/1 | 0.68 | 0.21 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3448 | 1/1 | 0.68 | 0.19 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3133 | 1/1 | 0.68 | 0.48 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3204 | 1/1 | 0.68 | 0.41 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3479 | 1/1 | 0.68 | 0.17 | 75,75,75,75 | 0 |
| 57 | MG | 1G | 1701 | 1/1 | 0.68 | 0.08 | 101,101,101,101 | 0 |
| 57 | MG | 1H | 3439 | 1/1 | 0.68 | 0.05 | 95,95,95,95 | 0 |
| 57 | MG | 1G | 1719 | 1/1 | 0.69 | 0.06 | 119,119,119,119 | 0 |
| 57 | MG | 14 | 3136 | 1/1 | 0.69 | 0.12 | 127,127,127,127 | 0 |
| 57 | MG | 14 | 3393 | 1/1 | 0.69 | 0.08 | 118,118,118,118 | 0 |
| 57 | MG | 1H | 3120 | 1/1 | 0.69 | 0.46 | 96,96,96,96 | 0 |
| 57 | MG | 4K | 101 | 1/1 | 0.69 | 0.27 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3416 | 1/1 | 0.69 | 0.05 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3504 | 1/1 | 0.70 | 0.19 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3316 | 1/1 | 0.70 | 0.48 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3103 | 1/1 | 0.70 | 0.30 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3380 | 1/1 | 0.70 | 0.16 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3053 | 1/1 | 0.70 | 0.08 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3380 | 1/1 | 0.70 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | 2L | 102 | 1/1 | 0.70 | 0.63 | 90,90,90,90 | 0 |
| 57 | MG | 14 | 3189 | 1/1 | 0.70 | 0.66 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3154 | 1/1 | 0.70 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | 1G | 1728 | 1/1 | 0.70 | 0.05 | 114,114,114,114 | 0 |
| 57 | MG | 13 | 1650 | 1/1 | 0.70 | 0.40 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3298 | 1/1 | 0.71 | 0.24 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3282 | 1/1 | 0.71 | 0.43 | 89,89,89,89 | 0 |
| 57 | MG | 14 | 3261 | 1/1 | 0.71 | 0.20 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3078 | 1/1 | 0.71 | 0.37 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3321 | 1/1 | 0.71 | 0.37 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3373 | 1/1 | 0.71 | 0.14 | 89,89,89,89 | 0 |
| 57 | MG | 13 | 1630 | 1/1 | 0.71 | 0.25 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3199 | 1/1 | 0.71 | 0.42 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3376 | 1/1 | 0.71 | 0.12 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3083 | 1/1 | 0.71 | 0.68 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3250 | 1/1 | 0.71 | 0.38 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3483 | 1/1 | 0.71 | 0.08 | 103,103,103,103 | 0 |
| 57 | MG | 1H | 3260 | 1/1 | 0.71 | 0.43 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3517 | 1/1 | 0.71 | 0.12 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3404 | 1/1 | 0.72 | 0.15 | 100,100,100,100 | 0 |
| 57 | MG | 1H | 3464 | 1/1 | 0.72 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | 14 | 3217 | 1/1 | 0.72 | 0.20 | 77,77,77,77 | 0 |
| 57 | MG | 13 | 1683 | 1/1 | 0.72 | 0.20 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3134 | 1/1 | 0.72 | 0.42 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3222 | 1/1 | 0.72 | 0.39 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3155 | 1/1 | 0.72 | 0.21 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3227 | 1/1 | 0.72 | 0.41 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3087 | 1/1 | 0.72 | 0.54 | 58,58,58,58 | 0 |
| 57 | MG | 14 | 3402 | 1/1 | 0.73 | 0.14 | 118,118,118,118 | 0 |
| 57 | MG | 1H | 3258 | 1/1 | 0.73 | 0.39 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3086 | 1/1 | 0.73 | 0.40 | 66,66,66,66 | 0 |
| 57 | MG | 1G | 1650 | 1/1 | 0.73 | 0.15 | 114,114,114,114 | 0 |
| 57 | MG | 14 | 3148 | 1/1 | 0.73 | 0.36 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3265 | 1/1 | 0.73 | 0.15 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3009 | 1/1 | 0.73 | 0.43 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3422 | 1/1 | 0.73 | 0.14 | 101,101,101,101 | 0 |
| 57 | MG | 1H | 3036 | 1/1 | 0.73 | 0.75 | 70,70,70,70 | 0 |
| 57 | MG | 13 | 1681 | 1/1 | 0.73 | 0.25 | 68,68,68,68 | 0 |
| 57 | MG | 1G | 1651 | 1/1 | 0.73 | 0.15 | 105,105,105,105 | 0 |
| 57 | MG | 14 | 3140 | 1/1 | 0.74 | 0.34 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3443 | 1/1 | 0.74 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | 14 | 3391 | 1/1 | 0.74 | 0.24 | 103,103,103,103 | 0 |
| 57 | MG | 1G | 1696 | 1/1 | 0.74 | 0.13 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3269 | 1/1 | 0.74 | 0.36 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3434 | 1/1 | 0.74 | 0.19 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3072 | 1/1 | 0.74 | 0.66 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3207 | 1/1 | 0.74 | 0.28 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3115 | 1/1 | 0.74 | 0.91 | 84,84,84,84 | 0 |
| 57 | MG | 1G | 1731 | 1/1 | 0.74 | 0.08 | 114,114,114,114 | 0 |
| 57 | MG | 1G | 1657 | 1/1 | 0.74 | 0.21 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3097 | 1/1 | 0.74 | 0.43 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3121 | 1/1 | 0.74 | 0.94 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3396 | 1/1 | 0.74 | 0.14 | 109,109,109,109 | 0 |
| 57 | MG | 1H | 3279 | 1/1 | 0.74 | 0.46 | 76,76,76,76 | 0 |
| 57 | MG | 1G | 1652 | 1/1 | 0.74 | 0.33 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3528 | 1/1 | 0.74 | 0.11 | 96,96,96,96 | 0 |
| 57 | MG | 14 | 3244 | 1/1 | 0.74 | 0.22 | 58,58,58,58 | 0 |
| 57 | MG | 1G | 1685 | 1/1 | 0.74 | 0.12 | 91,91,91,91 | 0 |
| 57 | MG | 14 | 3426 | 1/1 | 0.74 | 0.07 | 126,126,126,126 | 0 |
| 57 | MG | 13 | 1665 | 1/1 | 0.75 | 0.30 | 88,88,88,88 | 0 |
| 57 | MG | 1H | 3187 | 1/1 | 0.75 | 1.20 | 81,81,81,81 | 0 |
| 57 | MG | 13 | 1685 | 1/1 | 0.75 | 0.38 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3189 | 1/1 | 0.75 | 0.43 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3094 | 1/1 | 0.75 | 0.94 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3278 | 1/1 | 0.75 | 0.31 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3077 | 1/1 | 0.75 | 0.20 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3322 | 1/1 | 0.75 | 0.32 | 100,100,100,100 | 0 |
| 57 | MG | 13 | 1663 | 1/1 | 0.75 | 0.25 | 90,90,90,90 | 0 |
| 57 | MG | 16 | 211 | 1/1 | 0.75 | 0.12 | 99,99,99,99 | 0 |
| 57 | MG | 14 | 3205 | 1/1 | 0.75 | 0.43 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3191 | 1/1 | 0.75 | 0.31 | 82,82,82,82 | 0 |
| 57 | MG | 13 | 1625 | 1/1 | 0.76 | 0.31 | 93,93,93,93 | 0 |
| 57 | MG | 1G | 1645 | 1/1 | 0.76 | 0.06 | 93,93,93,93 | 0 |
| 57 | MG | 14 | 3370 | 1/1 | 0.76 | 0.24 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3005 | 1/1 | 0.76 | 0.72 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3007 | 1/1 | 0.76 | 0.65 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3125 | 1/1 | 0.76 | 0.22 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3201 | 1/1 | 0.76 | 0.36 | 88,88,88,88 | 0 |
| 57 | MG | 13 | 1679 | 1/1 | 0.76 | 0.28 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3172 | 1/1 | 0.76 | 0.49 | 82,82,82,82 | 0 |
| 57 | MG | 1H | 3294 | 1/1 | 0.76 | 0.15 | 90,90,90,90 | 0 |
| 57 | MG | 13 | 1643 | 1/1 | 0.76 | 0.42 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3437 | 1/1 | 0.76 | 0.07 | 107,107,107,107 | 0 |
| 57 | MG | 1G | 1644 | 1/1 | 0.76 | 0.37 | 107,107,107,107 | 0 |
| 57 | MG | 4E | 201 | 1/1 | 0.76 | 0.46 | 85,85,85,85 | 0 |
| 57 | MG | 2K | 102 | 1/1 | 0.76 | 0.31 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3110 | 1/1 | 0.76 | 0.52 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3221 | 1/1 | 0.76 | 0.28 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3477 | 1/1 | 0.77 | 0.07 | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3179 | 1/1 | 0.77 | 0.41 | 67,67,67,67 | 0 |
| 57 | MG | 1G | 1647 | 1/1 | 0.77 | 0.26 | 102,102,102,102 | 0 |
| 57 | MG | 14 | 3230 | 1/1 | 0.77 | 0.32 | 81,81,81,81 | 0 |
| 57 | MG | 1G | 1638 | 1/1 | 0.77 | 0.11 | 93,93,93,93 | 0 |
| 57 | MG | 13 | 1702 | 1/1 | 0.77 | 0.08 | 107,107,107,107 | 0 |
| 57 | MG | 1H | 3117 | 1/1 | 0.77 | 0.37 | 54,54,54,54 | 0 |
| 57 | MG | 1G | 1653 | 1/1 | 0.77 | 0.28 | 103,103,103,103 | 0 |
| 57 | MG | 14 | 3398 | 1/1 | 0.77 | 0.07 | 99,99,99,99 | 0 |
| 57 | MG | 1G | 1621 | 1/1 | 0.77 | 0.74 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3351 | 1/1 | 0.77 | 0.18 | 104,104,104,104 | 0 |
| 57 | MG | 13 | 1687 | 1/1 | 0.77 | 1.03 | 82,82,82,82 | 0 |
| 57 | MG | 29 | 301 | 1/1 | 0.77 | 0.27 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3185 | 1/1 | 0.77 | 0.35 | 90,90,90,90 | 0 |
| 57 | MG | 14 | 3215 | 1/1 | 0.77 | 0.18 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3025 | 1/1 | 0.77 | 0.27 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3157 | 1/1 | 0.77 | 0.13 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3137 | 1/1 | 0.77 | 0.42 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3317 | 1/1 | 0.77 | 0.48 | 83,83,83,83 | 0 |
| 57 | MG | 1G | 1619 | 1/1 | 0.77 | 0.29 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3151 | 1/1 | 0.77 | 0.20 | 87,87,87,87 | 0 |
| 57 | MG | 1G | 1724 | 1/1 | 0.77 | 0.08 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3519 | 1/1 | 0.77 | 0.10 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3521 | 1/1 | 0.78 | 0.25 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3308 | 1/1 | 0.78 | 0.35 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3082 | 1/1 | 0.78 | 0.33 | 90,90,90,90 | 0 |
| 57 | MG | 13 | 1673 | 1/1 | 0.78 | 0.36 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3526 | 1/1 | 0.78 | 0.11 | 113,113,113,113 | 0 |
| 57 | MG | 1G | 1681 | 1/1 | 0.78 | 0.11 | 96,96,96,96 | 0 |
| 57 | MG | 1G | 1616 | 1/1 | 0.78 | 0.32 | 88,88,88,88 | 0 |
| 57 | MG | 1H | 3421 | 1/1 | 0.78 | 0.14 | 99,99,99,99 | 0 |
| 57 | MG | 13 | 1651 | 1/1 | 0.78 | 0.29 | 97,97,97,97 | 0 |
| 57 | MG | 1H | 3397 | 1/1 | 0.78 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | 14 | 3152 | 1/1 | 0.78 | 0.65 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3404 | 1/1 | 0.78 | 0.12 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3372 | 1/1 | 0.78 | 0.12 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3226 | 1/1 | 0.78 | 0.46 | 83,83,83,83 | 0 |
| 57 | MG | 2L | 103 | 1/1 | 0.78 | 0.43 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3058 | 1/1 | 0.78 | 0.43 | 77,77,77,77 | 0 |
| 57 | MG | 1G | 1723 | 1/1 | 0.78 | 0.16 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3313 | 1/1 | 0.78 | 0.17 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3273 | 1/1 | 0.78 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | 13 | 1746 | 1/1 | 0.78 | 0.12 | 119,119,119,119 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 13 | 1731 | 1/1 | 0.78 | 0.05 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3101 | 1/1 | 0.79 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3206 | 1/1 | 0.79 | 0.24 | 91,91,91,91 | 0 |
| 57 | MG | 1G | 1692 | 1/1 | 0.79 | 0.09 | 105,105,105,105 | 0 |
| 57 | MG | 1H | 3320 | 1/1 | 0.79 | 0.41 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3085 | 1/1 | 0.79 | 0.42 | 75,75,75,75 | 0 |
| 57 | MG | 13 | 1614 | 1/1 | 0.79 | 0.28 | 88,88,88,88 | 0 |
| 57 | MG | 13 | 1742 | 1/1 | 0.79 | 0.10 | 98,98,98,98 | 0 |
| 57 | MG | 14 | 3112 | 1/1 | 0.79 | 0.43 | 99,99,99,99 | 0 |
| 57 | MG | 13 | 1695 | 1/1 | 0.79 | 0.11 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3232 | 1/1 | 0.79 | 0.28 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3131 | 1/1 | 0.79 | 0.35 | 70,70,70,70 | 0 |
| 57 | MG | 14 | 3374 | 1/1 | 0.79 | 0.11 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3100 | 1/1 | 0.79 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3420 | 1/1 | 0.79 | 0.07 | 102,102,102,102 | 0 |
| 57 | MG | 14 | 3355 | 1/1 | 0.79 | 0.14 | 107,107,107,107 | 0 |
| 57 | MG | 1H | 3542 | 1/1 | 0.79 | 0.33 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3498 | 1/1 | 0.79 | 0.16 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3207 | 1/1 | 0.79 | 0.71 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3348 | 1/1 | 0.79 | 0.10 | 101,101,101,101 | 0 |
| 57 | MG | 68 | 201 | 1/1 | 0.79 | 0.23 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3416 | 1/1 | 0.79 | 0.06 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3171 | 1/1 | 0.79 | 0.30 | 90,90,90,90 | 0 |
| 57 | MG | 9A | 101 | 1/1 | 0.79 | 0.25 | 115,115,115,115 | 0 |
| 58 | SPE | 1J | 208 | 13/13 | 0.80 | 0.22 | 94,98,105,105 | 0 |
| 57 | MG | 1G | 1711 | 1/1 | 0.80 | 0.12 | 108,108,108,108 | 0 |
| 57 | MG | 14 | 3243 | 1/1 | 0.80 | 0.08 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3198 | 1/1 | 0.80 | 0.20 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3163 | 1/1 | 0.80 | 0.84 | 84,84,84,84 | 0 |
| 57 | MG | 16 | 203 | 1/1 | 0.80 | 0.12 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3081 | 1/1 | 0.80 | 0.35 | 81,81,81,81 | 0 |
| 57 | MG | 1G | 1632 | 1/1 | 0.80 | 0.05 | 99,99,99,99 | 0 |
| 57 | MG | 1H | 3123 | 1/1 | 0.80 | 0.60 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3161 | 1/1 | 0.80 | 0.33 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3067 | 1/1 | 0.80 | 0.17 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3374 | 1/1 | 0.80 | 0.11 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3348 | 1/1 | 0.80 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | 1G | 1683 | 1/1 | 0.80 | 0.04 | 113,113,113,113 | 0 |
| 57 | MG | 1H | 3484 | 1/1 | 0.80 | 0.15 | 84,84,84,84 | 0 |
| 57 | MG | 13 | 1690 | 1/1 | 0.80 | 0.43 | 100,100,100,100 | 0 |
| 57 | MG | 1H | 3139 | 1/1 | 0.80 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | 1H | 3003 | 1/1 | 0.80 | 0.47 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3184 | 1/1 | 0.80 | 0.24 | 93,93,93,93 | 0 |
| 57 | MG | 1G | 1676 | 1/1 | 0.80 | 0.07 | 100,100,100,100 | 0 |
| 57 | MG | 14 | 3387 | 1/1 | 0.81 | 0.12 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3330 | 1/1 | 0.81 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | 14 | 3021 | 1/1 | 0.81 | 0.15 | 76,76,76,76 | 0 |
| 57 | MG | 1G | 1674 | 1/1 | 0.81 | 0.18 | 78,78,78,78 | 0 |
| 57 | MG | 1J | 201 | 1/1 | 0.81 | 0.29 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3414 | 1/1 | 0.81 | 0.06 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3434 | 1/1 | 0.81 | 0.14 | 115,115,115,115 | 0 |
| 57 | MG | 1H | 3377 | 1/1 | 0.81 | 0.24 | 75,75,75,75 | 0 |
| 57 | MG | 14 | 3158 | 1/1 | 0.81 | 0.37 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3523 | 1/1 | 0.81 | 0.23 | 84,84,84,84 | 0 |
| 57 | MG | 14 | 3224 | 1/1 | 0.81 | 0.16 | 113,113,113,113 | 0 |
| 57 | MG | 13 | 1684 | 1/1 | 0.81 | 0.30 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3518 | 1/1 | 0.81 | 0.12 | 101,101,101,101 | 0 |
| 57 | MG | 1H | 3088 | 1/1 | 0.81 | 0.22 | 61,61,61,61 | 0 |
| 57 | MG | 1G | 1648 | 1/1 | 0.81 | 0.39 | 79,79,79,79 | 0 |
| 57 | MG | 1G | 1697 | 1/1 | 0.81 | 0.07 | 110,110,110,110 | 0 |
| 57 | MG | 14 | 3378 | 1/1 | 0.81 | 0.11 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3165 | 1/1 | 0.81 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 1G | 1620 | 1/1 | 0.81 | 0.27 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3177 | 1/1 | 0.81 | 0.31 | 82,82,82,82 | 0 |
| 57 | MG | 1G | 1664 | 1/1 | 0.81 | 0.19 | 73,73,73,73 | 0 |
| 57 | MG | 13 | 1724 | 1/1 | 0.81 | 0.17 | 73,73,73,73 | 0 |
| 57 | MG | 13 | 1657 | 1/1 | 0.81 | 0.41 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3008 | 1/1 | 0.81 | 0.47 | 75,75,75,75 | 0 |
| 57 | MG | 1G | 1694 | 1/1 | 0.81 | 0.10 | 94,94,94,94 | 0 |
| 57 | MG | L8 | 101 | 1/1 | 0.81 | 0.35 | 86,86,86,86 | 0 |
| 57 | MG | 35 | 202 | 1/1 | 0.81 | 0.35 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3315 | 1/1 | 0.81 | 0.36 | 99,99,99,99 | 0 |
| 57 | MG | 1H | 3364 | 1/1 | 0.82 | 0.12 | 72,72,72,72 | 0 |
| 57 | MG | 13 | 1723 | 1/1 | 0.82 | 0.12 | 83,83,83,83 | 0 |
| 57 | MG | 13 | 1740 | 1/1 | 0.82 | 0.05 | 132,132,132,132 | 0 |
| 57 | MG | 14 | 3411 | 1/1 | 0.82 | 0.27 | 93,93,93,93 | 0 |
| 57 | MG | 14 | 3256 | 1/1 | 0.82 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | 1H | 3235 | 1/1 | 0.82 | 0.51 | 99,99,99,99 | 0 |
| 57 | MG | 14 | 3343 | 1/1 | 0.82 | 0.08 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3527 | 1/1 | 0.82 | 0.11 | 107,107,107,107 | 0 |
| 57 | MG | 14 | 3381 | 1/1 | 0.82 | 0.28 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3220 | 1/1 | 0.82 | 0.29 | 73,73,73,73 | 0 |
| 57 | MG | 13 | 1688 | 1/1 | 0.82 | 0.52 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3223 | 1/1 | 0.82 | 0.23 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3379 | 1/1 | 0.82 | 0.09 | 99,99,99,99 | 0 |
| 57 | MG | 13 | 1728 | 1/1 | 0.82 | 0.14 | 112,112,112,112 | 0 |
| 57 | MG | 14 | 3062 | 1/1 | 0.82 | 0.86 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3324 | 1/1 | 0.82 | 0.25 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3270 | 1/1 | 0.82 | 0.35 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3084 | 1/1 | 0.82 | 0.60 | 68,68,68,68 | 0 |
| 58 | SPE | 14 | 3446 | 13/13 | 0.82 | 0.28 | 68,79,87,89 | 0 |
| 57 | MG | 14 | 3168 | 1/1 | 0.82 | 0.27 | 87,87,87,87 | 0 |
| 57 | MG | 88 | 202 | 1/1 | 0.82 | 0.32 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3462 | 1/1 | 0.82 | 0.20 | 53,53,53,53 | 0 |
| 57 | MG | 14 | 3395 | 1/1 | 0.82 | 0.10 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3340 | 1/1 | 0.82 | 0.31 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3048 | 1/1 | 0.82 | 0.25 | 43,43,43,43 | 0 |
| 57 | MG | 13 | 1691 | 1/1 | 0.82 | 0.20 | 65,65,65,65 | 0 |
| 57 | MG | 14 | 3165 | 1/1 | 0.83 | 0.44 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3149 | 1/1 | 0.83 | 0.67 | 71,71,71,71 | 0 |
| 57 | MG | 35 | 201 | 1/1 | 0.83 | 0.16 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3183 | 1/1 | 0.83 | 0.25 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3122 | 1/1 | 0.83 | 0.27 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3311 | 1/1 | 0.83 | 0.20 | 93,93,93,93 | 0 |
| 57 | MG | 13 | 1708 | 1/1 | 0.83 | 0.09 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3085 | 1/1 | 0.83 | 0.47 | 81,81,81,81 | 0 |
| 57 | MG | 13 | 1672 | 1/1 | 0.83 | 0.83 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3111 | 1/1 | 0.83 | 0.50 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3228 | 1/1 | 0.83 | 0.34 | 70,70,70,70 | 0 |
| 57 | MG | 13 | 1662 | 1/1 | 0.83 | 0.19 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3317 | 1/1 | 0.83 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3516 | 1/1 | 0.83 | 0.09 | 79,79,79,79 | 0 |
| 57 | MG | 13 | 1734 | 1/1 | 0.83 | 0.07 | 100,100,100,100 | 0 |
| 57 | MG | 14 | 3138 | 1/1 | 0.83 | 0.34 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3442 | 1/1 | 0.83 | 0.21 | 75,75,75,75 | 0 |
| 57 | MG | 1G | 1722 | 1/1 | 0.83 | 0.12 | 101,101,101,101 | 0 |
| 57 | MG | 14 | 3133 | 1/1 | 0.83 | 0.29 | 58,58,58,58 | 0 |
| 57 | MG | 1H | 3149 | 1/1 | 0.83 | 0.29 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3038 | 1/1 | 0.83 | 0.60 | 65,65,65,65 | 0 |
| 57 | MG | 14 | 3187 | 1/1 | 0.83 | 0.33 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3486 | 1/1 | 0.83 | 0.10 | 89,89,89,89 | 0 |
| 57 | MG | 1G | 1682 | 1/1 | 0.83 | 0.08 | 105,105,105,105 | 0 |
| 57 | MG | 14 | 3027 | 1/1 | 0.83 | 0.25 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3473 | 1/1 | 0.83 | 0.12 | 76,76,76,76 | 0 |
| 57 | MG | 13 | 1745 | 1/1 | 0.83 | 0.06 | 111,111,111,111 | 0 |
| 57 | MG | F8 | 101 | 1/1 | 0.83 | 0.42 | 86,86,86,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3296 | 1/1 | 0.83 | 0.30 | 81,81,81,81 | 0 |
| 57 | MG | 14 | 3274 | 1/1 | 0.83 | 0.14 | 81,81,81,81 | 0 |
| 57 | MG | 14 | 3239 | 1/1 | 0.83 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | 14 | 3104 | 1/1 | 0.83 | 0.19 | 84,84,84,84 | 0 |
| 57 | MG | 13 | 1682 | 1/1 | 0.83 | 0.28 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3327 | 1/1 | 0.83 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | 1G | 1662 | 1/1 | 0.83 | 0.90 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3087 | 1/1 | 0.83 | 0.38 | 79,79,79,79 | 0 |
| 57 | MG | 1G | 1709 | 1/1 | 0.83 | 0.14 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3530 | 1/1 | 0.83 | 0.10 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3158 | 1/1 | 0.84 | 0.48 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3325 | 1/1 | 0.84 | 0.38 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3314 | 1/1 | 0.84 | 0.13 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3307 | 1/1 | 0.84 | 0.64 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3246 | 1/1 | 0.84 | 0.18 | 72,72,72,72 | 0 |
| 57 | MG | 1G | 1720 | 1/1 | 0.84 | 0.05 | 106,106,106,106 | 0 |
| 57 | MG | 1H | 3127 | 1/1 | 0.84 | 0.37 | 84,84,84,84 | 0 |
| 57 | MG | 13 | 1653 | 1/1 | 0.84 | 0.53 | 94,94,94,94 | 0 |
| 57 | MG | 13 | 1699 | 1/1 | 0.84 | 0.09 | 102,102,102,102 | 0 |
| 57 | MG | 1H | 3098 | 1/1 | 0.84 | 0.53 | 78,78,78,78 | 0 |
| 57 | MG | 13 | 1623 | 1/1 | 0.84 | 0.40 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3522 | 1/1 | 0.84 | 0.20 | 91,91,91,91 | 0 |
| 57 | MG | 14 | 3410 | 1/1 | 0.84 | 0.07 | 116,116,116,116 | 0 |
| 57 | MG | 13 | 1697 | 1/1 | 0.84 | 0.11 | 78,78,78,78 | 0 |
| 57 | MG | 1G | 1678 | 1/1 | 0.84 | 0.15 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3418 | 1/1 | 0.84 | 0.09 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3301 | 1/1 | 0.84 | 0.07 | 117,117,117,117 | 0 |
| 57 | MG | 1H | 3248 | 1/1 | 0.84 | 0.39 | 96,96,96,96 | 0 |
| 57 | MG | 14 | 3362 | 1/1 | 0.84 | 0.09 | 97,97,97,97 | 0 |
| 57 | MG | 14 | 3427 | 1/1 | 0.84 | 0.18 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3199 | 1/1 | 0.84 | 0.56 | 68,68,68,68 | 0 |
| 57 | MG | 14 | 3116 | 1/1 | 0.84 | 0.28 | 66,66,66,66 | 0 |
| 57 | MG | 1G | 1670 | 1/1 | 0.84 | 0.21 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3421 | 1/1 | 0.84 | 0.20 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3544 | 1/1 | 0.84 | 0.08 | 84,84,84,84 | 0 |
| 57 | MG | 14 | 3213 | 1/1 | 0.84 | 0.39 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3406 | 1/1 | 0.84 | 0.10 | 90,90,90,90 | 0 |
| 57 | MG | 1G | 1704 | 1/1 | 0.84 | 0.07 | 107,107,107,107 | 0 |
| 57 | MG | 1H | 3220 | 1/1 | 0.84 | 0.15 | 89,89,89,89 | 0 |
| 57 | MG | 14 | 3190 | 1/1 | 0.84 | 0.33 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3190 | 1/1 | 0.84 | 0.41 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3281 | 1/1 | 0.84 | 0.21 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1G | 1729 | 1/1 | 0.84 | 0.10 | 104,104,104,104 | 0 |
| 57 | MG | 14 | 3161 | 1/1 | 0.84 | 0.88 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3272 | 1/1 | 0.84 | 0.07 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3211 | 1/1 | 0.84 | 0.42 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3370 | 1/1 | 0.84 | 0.17 | 59,59,59,59 | 0 |
| 58 | SPE | 13 | 1748 | 13/13 | 0.85 | 0.24 | 60,77,82,87 | 0 |
| 57 | MG | 1H | 3410 | 1/1 | 0.85 | 0.08 | 106,106,106,106 | 0 |
| 57 | MG | 14 | 3281 | 1/1 | 0.85 | 0.07 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3331 | 1/1 | 0.85 | 0.16 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3108 | 1/1 | 0.85 | 0.32 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3276 | 1/1 | 0.85 | 0.36 | 90,90,90,90 | 0 |
| 57 | MG | 13 | 1642 | 1/1 | 0.85 | 0.17 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3335 | 1/1 | 0.85 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 13 | 1669 | 1/1 | 0.85 | 0.30 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3066 | 1/1 | 0.85 | 0.36 | 59,59,59,59 | 0 |
| 57 | MG | 14 | 3271 | 1/1 | 0.85 | 0.06 | 72,72,72,72 | 0 |
| 57 | MG | 13 | 1727 | 1/1 | 0.85 | 0.17 | 90,90,90,90 | 0 |
| 57 | MG | 41 | 201 | 1/1 | 0.85 | 0.11 | 62,62,62,62 | 0 |
| 58 | SPE | 1G | 1733 | 13/13 | 0.85 | 0.10 | 98,101,104,105 | 0 |
| 57 | MG | 14 | 3041 | 1/1 | 0.85 | 0.63 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3106 | 1/1 | 0.85 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3323 | 1/1 | 0.85 | 0.23 | 75,75,75,75 | 0 |
| 57 | MG | 2K | 103 | 1/1 | 0.85 | 0.38 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3191 | 1/1 | 0.85 | 0.29 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3075 | 1/1 | 0.85 | 0.35 | 89,89,89,89 | 0 |
| 57 | MG | 14 | 3352 | 1/1 | 0.85 | 0.11 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3545 | 1/1 | 0.85 | 0.07 | 116,116,116,116 | 0 |
| 57 | MG | 14 | 3288 | 1/1 | 0.85 | 0.15 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3429 | 1/1 | 0.85 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3394 | 1/1 | 0.85 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3292 | 1/1 | 0.85 | 0.11 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3203 | 1/1 | 0.85 | 0.43 | 93,93,93,93 | 0 |
| 57 | MG | 13 | 1700 | 1/1 | 0.85 | 0.07 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3420 | 1/1 | 0.85 | 0.08 | 96,96,96,96 | 0 |
| 57 | MG | 1H | 3082 | 1/1 | 0.85 | 0.39 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3449 | 1/1 | 0.85 | 0.41 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3052 | 1/1 | 0.85 | 0.46 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3222 | 1/1 | 0.85 | 0.58 | 88,88,88,88 | 0 |
| 57 | MG | 1J | 207 | 1/1 | 0.85 | 0.10 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3286 | 1/1 | 0.85 | 0.06 | 93,93,93,93 | 0 |
| 57 | MG | 16 | 208 | 1/1 | 0.85 | 0.37 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3032 | 1/1 | 0.85 | 0.45 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3252 | 1/1 | 0.85 | 0.25 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3436 | 1/1 | 0.85 | 0.12 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3197 | 1/1 | 0.85 | 0.35 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3367 | 1/1 | 0.85 | 0.08 | 99,99,99,99 | 0 |
| 57 | MG | 31 | 302 | 1/1 | 0.85 | 0.21 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3332 | 1/1 | 0.85 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | 14 | 3368 | 1/1 | 0.85 | 0.12 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3350 | 1/1 | 0.85 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 1H | 3511 | 1/1 | 0.85 | 0.05 | 92,92,92,92 | 0 |
| 57 | MG | 42 | 201 | 1/1 | 0.85 | 0.11 | 116,116,116,116 | 0 |
| 57 | MG | 1H | 3537 | 1/1 | 0.85 | 0.21 | 61,61,61,61 | 0 |
| 57 | MG | 14 | 3181 | 1/1 | 0.85 | 0.34 | 81,81,81,81 | 0 |
| 57 | MG | M5 | 101 | 1/1 | 0.85 | 0.10 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3233 | 1/1 | 0.86 | 0.19 | 110,110,110,110 | 0 |
| 57 | MG | 1H | 3331 | 1/1 | 0.86 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | 1G | 1624 | 1/1 | 0.86 | 0.43 | 76,76,76,76 | 0 |
| 57 | MG | 3A | 201 | 1/1 | 0.86 | 0.25 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3283 | 1/1 | 0.86 | 0.09 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3164 | 1/1 | 0.86 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3099 | 1/1 | 0.86 | 0.37 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3513 | 1/1 | 0.86 | 0.11 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3259 | 1/1 | 0.86 | 0.43 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3078 | 1/1 | 0.86 | 0.35 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3458 | 1/1 | 0.86 | 0.14 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3319 | 1/1 | 0.86 | 0.10 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3004 | 1/1 | 0.86 | 0.23 | 73,73,73,73 | 0 |
| 57 | MG | 13 | 1632 | 1/1 | 0.86 | 0.39 | 90,90,90,90 | 0 |
| 57 | MG | 13 | 1615 | 1/1 | 0.86 | 0.23 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3466 | 1/1 | 0.86 | 0.03 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3378 | 1/1 | 0.86 | 0.09 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3124 | 1/1 | 0.86 | 0.52 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3424 | 1/1 | 0.86 | 0.05 | 100,100,100,100 | 0 |
| 57 | MG | 1H | 3284 | 1/1 | 0.86 | 0.34 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3444 | 1/1 | 0.86 | 0.10 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3200 | 1/1 | 0.86 | 0.34 | 73,73,73,73 | 0 |
| 57 | MG | 25 | 202 | 1/1 | 0.86 | 0.17 | 110,110,110,110 | 0 |
| 57 | MG | 14 | 3276 | 1/1 | 0.86 | 0.07 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3200 | 1/1 | 0.86 | 0.28 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3277 | 1/1 | 0.86 | 0.53 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3359 | 1/1 | 0.86 | 0.06 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3075 | 1/1 | 0.86 | 0.19 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3234 | 1/1 | 0.86 | 0.74 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3209 | 1/1 | 0.86 | 0.33 | 65,65,65,65 | 0 |
| 57 | MG | 14 | 3273 | 1/1 | 0.86 | 0.16 | 70,70,70,70 | 0 |
| 57 | MG | 1G | 1666 | 1/1 | 0.86 | 0.08 | 103,103,103,103 | 0 |
| 57 | MG | 14 | 3353 | 1/1 | 0.86 | 0.12 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3231 | 1/1 | 0.86 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3113 | 1/1 | 0.86 | 0.26 | 64,64,64,64 | 0 |
| 57 | MG | 4A | 201 | 1/1 | 0.86 | 0.21 | 96,96,96,96 | 0 |
| 57 | MG | 1H | 3352 | 1/1 | 0.86 | 0.08 | 84,84,84,84 | 0 |
| 57 | MG | 1G | 1725 | 1/1 | 0.86 | 0.11 | 113,113,113,113 | 0 |
| 57 | MG | 1H | 3388 | 1/1 | 0.86 | 0.18 | 58,58,58,58 | 0 |
| 57 | MG | 1H | 3145 | 1/1 | 0.86 | 0.61 | 62,62,62,62 | 0 |
| 57 | MG | 13 | 1674 | 1/1 | 0.86 | 0.38 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3303 | 1/1 | 0.86 | 0.47 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3429 | 1/1 | 0.86 | 0.09 | 99,99,99,99 | 0 |
| 57 | MG | 13 | 1664 | 1/1 | 0.86 | 0.19 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3488 | 1/1 | 0.87 | 0.07 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3316 | 1/1 | 0.87 | 0.09 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3056 | 1/1 | 0.87 | 0.43 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3176 | 1/1 | 0.87 | 0.35 | 69,69,69,69 | 0 |
| 57 | MG | 1G | 1623 | 1/1 | 0.87 | 0.49 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3202 | 1/1 | 0.87 | 0.98 | 82,82,82,82 | 0 |
| 57 | MG | 1H | 3177 | 1/1 | 0.87 | 0.61 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3223 | 1/1 | 0.87 | 0.31 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3225 | 1/1 | 0.87 | 0.11 | 95,95,95,95 | 0 |
| 57 | MG | 1H | 3338 | 1/1 | 0.87 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3493 | 1/1 | 0.87 | 0.05 | 102,102,102,102 | 0 |
| 57 | MG | 1H | 3450 | 1/1 | 0.87 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 1H | 3209 | 1/1 | 0.87 | 0.41 | 52,52,52,52 | 0 |
| 57 | MG | 1H | 3275 | 1/1 | 0.87 | 0.60 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3312 | 1/1 | 0.87 | 0.23 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3360 | 1/1 | 0.87 | 0.15 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3051 | 1/1 | 0.87 | 0.47 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3268 | 1/1 | 0.87 | 0.13 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3201 | 1/1 | 0.87 | 0.73 | 95,95,95,95 | 0 |
| 57 | MG | 1H | 3224 | 1/1 | 0.87 | 0.44 | 90,90,90,90 | 0 |
| 57 | MG | 14 | 3341 | 1/1 | 0.87 | 0.08 | 91,91,91,91 | 0 |
| 57 | MG | 14 | 3369 | 1/1 | 0.87 | 0.11 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3406 | 1/1 | 0.87 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | 14 | 3431 | 1/1 | 0.87 | 0.23 | 60,60,60,60 | 0 |
| 57 | MG | 14 | 3383 | 1/1 | 0.87 | 0.14 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3062 | 1/1 | 0.87 | 0.26 | 40,40,40,40 | 0 |
| 57 | MG | 14 | 3415 | 1/1 | 0.87 | 0.10 | 101,101,101,101 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3394 | 1/1 | 0.87 | 0.07 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3102 | 1/1 | 0.87 | 0.59 | 66,66,66,66 | 0 |
| 57 | MG | 14 | 3419 | 1/1 | 0.87 | 0.20 | 110,110,110,110 | 0 |
| 57 | MG | 1G | 1607 | 1/1 | 0.87 | 0.27 | 92,92,92,92 | 0 |
| 57 | MG | 13 | 1660 | 1/1 | 0.87 | 0.50 | 96,96,96,96 | 0 |
| 57 | MG | 14 | 3357 | 1/1 | 0.87 | 0.09 | 96,96,96,96 | 0 |
| 58 | SPE | 14 | 3445 | 13/13 | 0.87 | 0.36 | 70,76,79,79 | 0 |
| 57 | MG | 13 | 1737 | 1/1 | 0.87 | 0.10 | 98,98,98,98 | 0 |
| 57 | MG | 1G | 1689 | 1/1 | 0.87 | 0.16 | 89,89,89,89 | 0 |
| 57 | MG | 14 | 3093 | 1/1 | 0.87 | 0.24 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3080 | 1/1 | 0.87 | 0.52 | 103,103,103,103 | 0 |
| 57 | MG | 14 | 3334 | 1/1 | 0.87 | 0.07 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3042 | 1/1 | 0.87 | 0.41 | 67,67,67,67 | 0 |
| 57 | MG | 1G | 1727 | 1/1 | 0.87 | 0.09 | 93,93,93,93 | 0 |
| 57 | MG | 14 | 3424 | 1/1 | 0.87 | 0.13 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3292 | 1/1 | 0.87 | 0.23 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3070 | 1/1 | 0.87 | 0.40 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3129 | 1/1 | 0.87 | 0.47 | 75,75,75,75 | 0 |
| 57 | MG | 1G | 1703 | 1/1 | 0.88 | 0.08 | 113,113,113,113 | 0 |
| 57 | MG | 14 | 3264 | 1/1 | 0.88 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | 1H | 3445 | 1/1 | 0.88 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | 1H | 3245 | 1/1 | 0.88 | 0.52 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3502 | 1/1 | 0.88 | 0.10 | 90,90,90,90 | 0 |
| 57 | MG | 14 | 3210 | 1/1 | 0.88 | 0.17 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3425 | 1/1 | 0.88 | 0.17 | 74,74,74,74 | 0 |
| 57 | MG | 13 | 1620 | 1/1 | 0.88 | 0.29 | 57,57,57,57 | 0 |
| 57 | MG | 13 | 1637 | 1/1 | 0.88 | 0.11 | 79,79,79,79 | 0 |
| 57 | MG | 88 | 203 | 1/1 | 0.88 | 0.20 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3056 | 1/1 | 0.88 | 0.32 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3089 | 1/1 | 0.88 | 0.28 | 66,66,66,66 | 0 |
| 57 | MG | 1J | 202 | 1/1 | 0.88 | 0.09 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3309 | 1/1 | 0.88 | 0.72 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3242 | 1/1 | 0.88 | 0.12 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3442 | 1/1 | 0.88 | 0.21 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3280 | 1/1 | 0.88 | 0.11 | 97,97,97,97 | 0 |
| 57 | MG | 14 | 3193 | 1/1 | 0.88 | 0.38 | 95,95,95,95 | 0 |
| 57 | MG | 1G | 1693 | 1/1 | 0.88 | 0.06 | 84,84,84,84 | 0 |
| 57 | MG | 14 | 3072 | 1/1 | 0.88 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | 14 | 3375 | 1/1 | 0.88 | 0.06 | 84,84,84,84 | 0 |
| 57 | MG | 13 | 1706 | 1/1 | 0.88 | 0.09 | 103,103,103,103 | 0 |
| 57 | MG | 1H | 3367 | 1/1 | 0.88 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3155 | 1/1 | 0.88 | 0.30 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1G | 1605 | 1/1 | 0.88 | 0.31 | 82,82,82,82 | 0 |
| 57 | MG | 13 | 1739 | 1/1 | 0.88 | 0.05 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3238 | 1/1 | 0.88 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | 14 | 3358 | 1/1 | 0.88 | 0.09 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3366 | 1/1 | 0.88 | 0.12 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3395 | 1/1 | 0.88 | 0.10 | 84,84,84,84 | 0 |
| 57 | MG | 14 | 3126 | 1/1 | 0.88 | 0.22 | 75,75,75,75 | 0 |
| 57 | MG | 1G | 1633 | 1/1 | 0.88 | 0.17 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3267 | 1/1 | 0.88 | 0.53 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3134 | 1/1 | 0.88 | 0.23 | 44,44,44,44 | 0 |
| 57 | MG | 1H | 3147 | 1/1 | 0.88 | 0.43 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3474 | 1/1 | 0.88 | 0.09 | 82,82,82,82 | 0 |
| 57 | MG | 13 | 1635 | 1/1 | 0.88 | 0.22 | 99,99,99,99 | 0 |
| 57 | MG | 1H | 3297 | 1/1 | 0.88 | 0.17 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3249 | 1/1 | 0.88 | 0.30 | 68,68,68,68 | 0 |
| 57 | MG | 1G | 1661 | 1/1 | 0.88 | 0.18 | 99,99,99,99 | 0 |
| 57 | MG | 1H | 3391 | 1/1 | 0.88 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | 1H | 3301 | 1/1 | 0.88 | 0.27 | 70,70,70,70 | 0 |
| 57 | MG | 13 | 1647 | 1/1 | 0.88 | 0.27 | 91,91,91,91 | 0 |
| 57 | MG | 1G | 1669 | 1/1 | 0.88 | 0.11 | 99,99,99,99 | 0 |
| 57 | MG | 1H | 3105 | 1/1 | 0.88 | 0.43 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3204 | 1/1 | 0.88 | 0.78 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3332 | 1/1 | 0.88 | 0.10 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3094 | 1/1 | 0.88 | 0.50 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3452 | 1/1 | 0.88 | 0.09 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3203 | 1/1 | 0.88 | 0.36 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3323 | 1/1 | 0.88 | 0.12 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3286 | 1/1 | 0.88 | 0.29 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3019 | 1/1 | 0.88 | 0.30 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3533 | 1/1 | 0.88 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | 1H | 3092 | 1/1 | 0.88 | 0.18 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3227 | 1/1 | 0.88 | 0.27 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3065 | 1/1 | 0.88 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | 1G | 1721 | 1/1 | 0.88 | 0.07 | 107,107,107,107 | 0 |
| 57 | MG | 4L | 102 | 1/1 | 0.89 | 0.11 | 108,108,108,108 | 0 |
| 57 | MG | 14 | 3385 | 1/1 | 0.89 | 0.13 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3413 | 1/1 | 0.89 | 0.27 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3478 | 1/1 | 0.89 | 0.06 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3541 | 1/1 | 0.89 | 0.10 | 67,67,67,67 | 0 |
| 57 | MG | 1G | 1668 | 1/1 | 0.89 | 0.06 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3425 | 1/1 | 0.89 | 0.10 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3193 | 1/1 | 0.89 | 0.51 | 93,93,93,93 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3236 | 1/1 | 0.89 | 0.15 | 70,70,70,70 | 0 |
| 57 | MG | 1G | 1698 | 1/1 | 0.89 | 0.12 | 105,105,105,105 | 0 |
| 57 | MG | 1H | 3130 | 1/1 | 0.89 | 0.72 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3495 | 1/1 | 0.89 | 0.06 | 94,94,94,94 | 0 |
| 57 | MG | 88 | 201 | 1/1 | 0.89 | 0.16 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3401 | 1/1 | 0.89 | 0.20 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3408 | 1/1 | 0.89 | 0.07 | 111,111,111,111 | 0 |
| 57 | MG | 14 | 3154 | 1/1 | 0.89 | 0.14 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3113 | 1/1 | 0.89 | 0.31 | 57,57,57,57 | 0 |
| 57 | MG | 14 | 3287 | 1/1 | 0.89 | 0.07 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3307 | 1/1 | 0.89 | 0.15 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3172 | 1/1 | 0.89 | 0.25 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3379 | 1/1 | 0.89 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | 5I | 101 | 1/1 | 0.89 | 0.08 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3195 | 1/1 | 0.89 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | J8 | 101 | 1/1 | 0.89 | 0.61 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3400 | 1/1 | 0.89 | 0.09 | 76,76,76,76 | 0 |
| 57 | MG | 13 | 1735 | 1/1 | 0.89 | 0.08 | 111,111,111,111 | 0 |
| 57 | MG | 14 | 3178 | 1/1 | 0.89 | 0.50 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3280 | 1/1 | 0.89 | 0.54 | 68,68,68,68 | 0 |
| 57 | MG | 1G | 1618 | 1/1 | 0.89 | 0.24 | 89,89,89,89 | 0 |
| 57 | MG | P8 | 101 | 1/1 | 0.89 | 0.34 | 71,71,71,71 | 0 |
| 57 | MG | 13 | 1710 | 1/1 | 0.89 | 0.10 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3183 | 1/1 | 0.89 | 0.61 | 65,65,65,65 | 0 |
| 57 | MG | 1G | 1637 | 1/1 | 0.89 | 0.12 | 113,113,113,113 | 0 |
| 57 | MG | 1H | 3304 | 1/1 | 0.89 | 0.42 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3294 | 1/1 | 0.89 | 0.11 | 114,114,114,114 | 0 |
| 57 | MG | 14 | 3365 | 1/1 | 0.89 | 0.17 | 96,96,96,96 | 0 |
| 57 | MG | 1H | 3241 | 1/1 | 0.89 | 0.13 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3371 | 1/1 | 0.89 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3039 | 1/1 | 0.89 | 0.41 | 65,65,65,65 | 0 |
| 57 | MG | C5 | 201 | 1/1 | 0.89 | 0.08 | 103,103,103,103 | 0 |
| 57 | MG | 11 | 301 | 1/1 | 0.89 | 0.64 | 60,60,60,60 | 0 |
| 57 | MG | 13 | 1616 | 1/1 | 0.89 | 0.29 | 82,82,82,82 | 0 |
| 57 | MG | 13 | 1626 | 1/1 | 0.89 | 0.28 | 67,67,67,67 | 0 |
| 57 | MG | 14 | 3167 | 1/1 | 0.89 | 0.28 | 76,76,76,76 | 0 |
| 57 | MG | 1G | 1646 | 1/1 | 0.89 | 0.07 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3285 | 1/1 | 0.89 | 0.41 | 96,96,96,96 | 0 |
| 57 | MG | 14 | 3160 | 1/1 | 0.89 | 0.32 | 92,92,92,92 | 0 |
| 57 | MG | 1G | 1625 | 1/1 | 0.89 | 0.12 | 98,98,98,98 | 0 |
| 57 | MG | 1G | 1667 | 1/1 | 0.89 | 0.12 | 90,90,90,90 | 0 |
| 57 | MG | 14 | 3432 | 1/1 | 0.89 | 0.15 | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3433 | 1/1 | 0.89 | 0.11 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3128 | 1/1 | 0.89 | 0.14 | 79,79,79,79 | 0 |
| 57 | MG | 1G | 1611 | 1/1 | 0.89 | 0.68 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3275 | 1/1 | 0.89 | 0.07 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3099 | 1/1 | 0.89 | 0.34 | 77,77,77,77 | 0 |
| 57 | MG | 16 | 205 | 1/1 | 0.89 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3469 | 1/1 | 0.89 | 0.09 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3006 | 1/1 | 0.89 | 0.43 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3287 | 1/1 | 0.89 | 0.39 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3447 | 1/1 | 0.89 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3237 | 1/1 | 0.89 | 0.17 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3363 | 1/1 | 0.89 | 0.09 | 102,102,102,102 | 0 |
| 57 | MG | 1H | 3214 | 1/1 | 0.89 | 0.26 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3179 | 1/1 | 0.89 | 0.23 | 71,71,71,71 | 0 |
| 57 | MG | 16 | 204 | 1/1 | 0.89 | 0.26 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3392 | 1/1 | 0.89 | 0.20 | 52,52,52,52 | 0 |
| 57 | MG | 1H | 3114 | 1/1 | 0.89 | 0.66 | 67,67,67,67 | 0 |
| 57 | MG | 14 | 3024 | 1/1 | 0.90 | 0.13 | 77,77,77,77 | 0 |
| 57 | MG | 13 | 1624 | 1/1 | 0.90 | 0.12 | 93,93,93,93 | 0 |
| 57 | MG | 14 | 3418 | 1/1 | 0.90 | 0.09 | 101,101,101,101 | 0 |
| 57 | MG | 13 | 1649 | 1/1 | 0.90 | 0.23 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3389 | 1/1 | 0.90 | 0.17 | 94,94,94,94 | 0 |
| 57 | MG | 13 | 1633 | 1/1 | 0.90 | 0.21 | 87,87,87,87 | 0 |
| 57 | MG | 2K | 101 | 1/1 | 0.90 | 0.31 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3305 | 1/1 | 0.90 | 0.10 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3255 | 1/1 | 0.90 | 0.23 | 73,73,73,73 | 0 |
| 57 | MG | 1G | 1654 | 1/1 | 0.90 | 0.36 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3116 | 1/1 | 0.90 | 0.18 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3308 | 1/1 | 0.90 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | 16 | 201 | 1/1 | 0.90 | 0.16 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3140 | 1/1 | 0.90 | 0.20 | 40,40,40,40 | 0 |
| 57 | MG | 1H | 3141 | 1/1 | 0.90 | 0.31 | 66,66,66,66 | 0 |
| 57 | MG | 78 | 201 | 1/1 | 0.90 | 0.07 | 57,57,57,57 | 0 |
| 57 | MG | 1G | 1716 | 1/1 | 0.90 | 0.07 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3357 | 1/1 | 0.90 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 1G | 1636 | 1/1 | 0.90 | 0.07 | 91,91,91,91 | 0 |
| 57 | MG | 14 | 3101 | 1/1 | 0.90 | 0.26 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3044 | 1/1 | 0.90 | 0.67 | 81,81,81,81 | 0 |
| 57 | MG | 14 | 3194 | 1/1 | 0.90 | 0.69 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3267 | 1/1 | 0.90 | 0.08 | 86,86,86,86 | 0 |
| 57 | MG | 13 | 1656 | 1/1 | 0.90 | 0.25 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3171 | 1/1 | 0.90 | 0.16 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3097 | 1/1 | 0.90 | 0.49 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3126 | 1/1 | 0.90 | 0.22 | 75,75,75,75 | 0 |
| 57 | MG | 14 | 3371 | 1/1 | 0.90 | 0.10 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3390 | 1/1 | 0.90 | 0.10 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3386 | 1/1 | 0.90 | 0.16 | 48,48,48,48 | 0 |
| 57 | MG | 14 | 3392 | 1/1 | 0.90 | 0.05 | 112,112,112,112 | 0 |
| 57 | MG | 1G | 1672 | 1/1 | 0.90 | 0.10 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3423 | 1/1 | 0.90 | 0.08 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3033 | 1/1 | 0.90 | 0.22 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3040 | 1/1 | 0.90 | 0.40 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3037 | 1/1 | 0.90 | 0.35 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3119 | 1/1 | 0.90 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | 14 | 3401 | 1/1 | 0.90 | 0.29 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3167 | 1/1 | 0.90 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | 14 | 3063 | 1/1 | 0.90 | 0.36 | 52,52,52,52 | 0 |
| 57 | MG | 14 | 3005 | 1/1 | 0.90 | 0.30 | 50,50,50,50 | 0 |
| 57 | MG | 1G | 1713 | 1/1 | 0.90 | 0.13 | 113,113,113,113 | 0 |
| 57 | MG | 1H | 3531 | 1/1 | 0.90 | 0.21 | 76,76,76,76 | 0 |
| 57 | MG | 1G | 1726 | 1/1 | 0.90 | 0.06 | 113,113,113,113 | 0 |
| 57 | MG | 14 | 3377 | 1/1 | 0.90 | 0.09 | 64,64,64,64 | 0 |
| 57 | MG | 13 | 1667 | 1/1 | 0.90 | 0.85 | 96,96,96,96 | 0 |
| 57 | MG | 1H | 3162 | 1/1 | 0.90 | 0.32 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3358 | 1/1 | 0.90 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | 1H | 3356 | 1/1 | 0.90 | 0.12 | 75,75,75,75 | 0 |
| 57 | MG | 14 | 3229 | 1/1 | 0.90 | 0.17 | 90,90,90,90 | 0 |
| 57 | MG | 13 | 1619 | 1/1 | 0.90 | 0.22 | 53,53,53,53 | 0 |
| 57 | MG | 13 | 1738 | 1/1 | 0.90 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | 1G | 1610 | 1/1 | 0.90 | 0.24 | 69,69,69,69 | 0 |
| 57 | MG | 13 | 1670 | 1/1 | 0.90 | 0.23 | 100,100,100,100 | 0 |
| 57 | MG | 14 | 3440 | 1/1 | 0.90 | 0.10 | 98,98,98,98 | 0 |
| 57 | MG | 14 | 3373 | 1/1 | 0.90 | 0.13 | 97,97,97,97 | 0 |
| 57 | MG | 1H | 3194 | 1/1 | 0.90 | 0.26 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3399 | 1/1 | 0.90 | 0.14 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3296 | 1/1 | 0.90 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 14 | 3384 | 1/1 | 0.90 | 0.07 | 88,88,88,88 | 0 |
| 57 | MG | 1G | 1660 | 1/1 | 0.90 | 0.28 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3455 | 1/1 | 0.90 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | 1H | 3176 | 1/1 | 0.90 | 0.34 | 62,62,62,62 | 0 |
| 57 | MG | 14 | 3412 | 1/1 | 0.90 | 0.10 | 101,101,101,101 | 0 |
| 57 | MG | 14 | 3035 | 1/1 | 0.90 | 0.85 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3299 | 1/1 | 0.90 | 0.13 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3137 | 1/1 | 0.90 | 0.17 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3407 | 1/1 | 0.90 | 0.04 | 83,83,83,83 | 0 |
| 57 | MG | 13 | 1609 | 1/1 | 0.90 | 0.25 | 71,71,71,71 | 0 |
| 57 | MG | 13 | 1730 | 1/1 | 0.90 | 0.08 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3456 | 1/1 | 0.90 | 0.15 | 41,41,41,41 | 0 |
| 57 | MG | 13 | 1719 | 1/1 | 0.90 | 0.10 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3471 | 1/1 | 0.90 | 0.07 | 73,73,73,73 | 0 |
| 57 | MG | E5 | 101 | 1/1 | 0.90 | 0.08 | 100,100,100,100 | 0 |
| 57 | MG | 14 | 3159 | 1/1 | 0.90 | 0.39 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3109 | 1/1 | 0.91 | 0.34 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3251 | 1/1 | 0.91 | 0.22 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3336 | 1/1 | 0.91 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | 1H | 3467 | 1/1 | 0.91 | 0.08 | 85,85,85,85 | 0 |
| 57 | MG | 1G | 1622 | 1/1 | 0.91 | 0.35 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3241 | 1/1 | 0.91 | 0.09 | 100,100,100,100 | 0 |
| 57 | MG | 16 | 207 | 1/1 | 0.91 | 0.08 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3027 | 1/1 | 0.91 | 0.35 | 84,84,84,84 | 0 |
| 57 | MG | Q8 | 101 | 1/1 | 0.91 | 0.26 | 81,81,81,81 | 0 |
| 57 | MG | 14 | 3330 | 1/1 | 0.91 | 0.13 | 64,64,64,64 | 0 |
| 57 | MG | 13 | 1602 | 1/1 | 0.91 | 0.26 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3181 | 1/1 | 0.91 | 0.16 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3494 | 1/1 | 0.91 | 0.09 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3012 | 1/1 | 0.91 | 0.22 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3536 | 1/1 | 0.91 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | 14 | 3195 | 1/1 | 0.91 | 0.27 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3025 | 1/1 | 0.91 | 0.24 | 48,48,48,48 | 0 |
| 57 | MG | 14 | 3289 | 1/1 | 0.91 | 0.06 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3349 | 1/1 | 0.91 | 0.19 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3254 | 1/1 | 0.91 | 0.90 | 75,75,75,75 | 0 |
| 57 | MG | 14 | 3185 | 1/1 | 0.91 | 0.12 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3417 | 1/1 | 0.91 | 0.11 | 74,74,74,74 | 0 |
| 57 | MG | 1G | 1606 | 1/1 | 0.91 | 0.13 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3252 | 1/1 | 0.91 | 0.49 | 81,81,81,81 | 0 |
| 57 | MG | 14 | 3002 | 1/1 | 0.91 | 0.70 | 68,68,68,68 | 0 |
| 57 | MG | 14 | 3346 | 1/1 | 0.91 | 0.07 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3175 | 1/1 | 0.91 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3329 | 1/1 | 0.91 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | 14 | 3313 | 1/1 | 0.91 | 0.15 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3439 | 1/1 | 0.91 | 0.14 | 99,99,99,99 | 0 |
| 57 | MG | 1G | 1673 | 1/1 | 0.91 | 0.17 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3444 | 1/1 | 0.91 | 0.27 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3202 | 1/1 | 0.91 | 0.26 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3385 | 1/1 | 0.91 | 0.08 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3156 | 1/1 | 0.91 | 0.16 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3166 | 1/1 | 0.91 | 0.76 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3247 | 1/1 | 0.91 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3239 | 1/1 | 0.91 | 0.51 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3482 | 1/1 | 0.91 | 0.20 | 102,102,102,102 | 0 |
| 57 | MG | 1G | 1629 | 1/1 | 0.91 | 0.14 | 97,97,97,97 | 0 |
| 57 | MG | 14 | 3196 | 1/1 | 0.91 | 0.44 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3169 | 1/1 | 0.91 | 0.93 | 82,82,82,82 | 0 |
| 57 | MG | 1H | 3208 | 1/1 | 0.91 | 0.44 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3356 | 1/1 | 0.91 | 0.10 | 67,67,67,67 | 0 |
| 57 | MG | 13 | 1718 | 1/1 | 0.91 | 0.07 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3441 | 1/1 | 0.91 | 0.26 | 102,102,102,102 | 0 |
| 57 | MG | 13 | 1646 | 1/1 | 0.91 | 0.32 | 97,97,97,97 | 0 |
| 57 | MG | 1H | 3023 | 1/1 | 0.91 | 0.12 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3148 | 1/1 | 0.91 | 0.22 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3163 | 1/1 | 0.91 | 0.20 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3152 | 1/1 | 0.91 | 0.31 | 51,51,51,51 | 0 |
| 57 | MG | 1G | 1612 | 1/1 | 0.91 | 0.20 | 82,82,82,82 | 0 |
| 57 | MG | 1G | 1655 | 1/1 | 0.91 | 0.14 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3310 | 1/1 | 0.91 | 0.68 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3016 | 1/1 | 0.91 | 0.34 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3388 | 1/1 | 0.91 | 0.31 | 89,89,89,89 | 0 |
| 57 | MG | 13 | 1608 | 1/1 | 0.91 | 0.13 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3123 | 1/1 | 0.91 | 0.38 | 60,60,60,60 | 0 |
| 57 | MG | 13 | 1603 | 1/1 | 0.91 | 0.12 | 116,116,116,116 | 0 |
| 57 | MG | 1H | 3306 | 1/1 | 0.91 | 0.29 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3262 | 1/1 | 0.91 | 0.24 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3079 | 1/1 | 0.91 | 0.28 | 45,45,45,45 | 0 |
| 57 | MG | 13 | 1659 | 1/1 | 0.91 | 0.64 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3192 | 1/1 | 0.91 | 0.27 | 76,76,76,76 | 0 |
| 57 | MG | 13 | 1711 | 1/1 | 0.91 | 0.12 | 102,102,102,102 | 0 |
| 57 | MG | 14 | 3235 | 1/1 | 0.91 | 0.21 | 65,65,65,65 | 0 |
| 57 | MG | 13 | 1636 | 1/1 | 0.91 | 0.28 | 103,103,103,103 | 0 |
| 57 | MG | 14 | 3338 | 1/1 | 0.91 | 0.08 | 81,81,81,81 | 0 |
| 57 | MG | 13 | 1613 | 1/1 | 0.91 | 0.18 | 81,81,81,81 | 0 |
| 57 | MG | 13 | 1622 | 1/1 | 0.92 | 0.35 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3419 | 1/1 | 0.92 | 0.07 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3417 | 1/1 | 0.92 | 0.11 | 89,89,89,89 | 0 |
| 57 | MG | 1G | 1635 | 1/1 | 0.92 | 0.26 | 102,102,102,102 | 0 |
| 57 | MG | 14 | 3115 | 1/1 | 0.92 | 0.41 | 48,48,48,48 | 0 |
| 57 | MG | 14 | 3302 | 1/1 | 0.92 | 0.13 | 86,86,86,86 | 0 |
| 57 | MG | 1G | 1659 | 1/1 | 0.92 | 0.38 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1G | 1602 | 1/1 | 0.92 | 0.11 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3225 | 1/1 | 0.92 | 0.20 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3362 | 1/1 | 0.92 | 0.07 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3059 | 1/1 | 0.92 | 0.42 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3002 | 1/1 | 0.92 | 0.39 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3117 | 1/1 | 0.92 | 0.14 | 58,58,58,58 | 0 |
| 57 | MG | 14 | 3022 | 1/1 | 0.92 | 0.35 | 44,44,44,44 | 0 |
| 57 | MG | 1H | 3166 | 1/1 | 0.92 | 0.26 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3213 | 1/1 | 0.92 | 0.26 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3083 | 1/1 | 0.92 | 0.48 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3049 | 1/1 | 0.92 | 0.32 | 57,57,57,57 | 0 |
| 57 | MG | 14 | 3231 | 1/1 | 0.92 | 0.67 | 80,80,80,80 | 0 |
| 57 | MG | 13 | 1747 | 1/1 | 0.92 | 0.11 | 110,110,110,110 | 0 |
| 57 | MG | 1G | 1615 | 1/1 | 0.92 | 0.39 | 91,91,91,91 | 0 |
| 57 | MG | 14 | 3142 | 1/1 | 0.92 | 0.20 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3365 | 1/1 | 0.92 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3053 | 1/1 | 0.92 | 0.76 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3540 | 1/1 | 0.92 | 0.10 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3247 | 1/1 | 0.92 | 0.38 | 101,101,101,101 | 0 |
| 57 | MG | 1H | 3428 | 1/1 | 0.92 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | 14 | 3107 | 1/1 | 0.92 | 0.24 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3298 | 1/1 | 0.92 | 0.14 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3310 | 1/1 | 0.92 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3026 | 1/1 | 0.92 | 0.40 | 52,52,52,52 | 0 |
| 57 | MG | 1H | 3253 | 1/1 | 0.92 | 0.66 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3369 | 1/1 | 0.92 | 0.26 | 54,54,54,54 | 0 |
| 57 | MG | 1H | 3272 | 1/1 | 0.92 | 0.31 | 80,80,80,80 | 0 |
| 57 | MG | 13 | 1606 | 1/1 | 0.92 | 0.33 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3408 | 1/1 | 0.92 | 0.08 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3069 | 1/1 | 0.92 | 0.28 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3435 | 1/1 | 0.92 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | 1G | 1617 | 1/1 | 0.92 | 0.36 | 86,86,86,86 | 0 |
| 57 | MG | 13 | 1715 | 1/1 | 0.92 | 0.13 | 114,114,114,114 | 0 |
| 57 | MG | 14 | 3015 | 1/1 | 0.92 | 0.24 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3146 | 1/1 | 0.92 | 0.30 | 51,51,51,51 | 0 |
| 57 | MG | 1H | 3016 | 1/1 | 0.92 | 0.39 | 47,47,47,47 | 0 |
| 57 | MG | 14 | 3006 | 1/1 | 0.92 | 0.25 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3529 | 1/1 | 0.92 | 0.43 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3103 | 1/1 | 0.92 | 0.81 | 75,75,75,75 | 0 |
| 57 | MG | 13 | 1744 | 1/1 | 0.92 | 0.04 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3153 | 1/1 | 0.92 | 0.23 | 82,82,82,82 | 0 |
| 57 | MG | 1G | 1705 | 1/1 | 0.92 | 0.11 | 124,124,124,124 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3248 | 1/1 | 0.92 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 1H | 3512 | 1/1 | 0.92 | 0.17 | 97,97,97,97 | 0 |
| 57 | MG | 1H | 3066 | 1/1 | 0.92 | 0.18 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3178 | 1/1 | 0.92 | 0.24 | 57,57,57,57 | 0 |
| 57 | MG | 1H | 3090 | 1/1 | 0.92 | 0.76 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3127 | 1/1 | 0.92 | 0.35 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3271 | 1/1 | 0.92 | 0.31 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3221 | 1/1 | 0.93 | 0.12 | 91,91,91,91 | 0 |
| 57 | MG | 3I | 201 | 1/1 | 0.93 | 0.26 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3399 | 1/1 | 0.93 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | 1H | 3302 | 1/1 | 0.93 | 0.51 | 81,81,81,81 | 0 |
| 57 | MG | 14 | 3098 | 1/1 | 0.93 | 0.67 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3156 | 1/1 | 0.93 | 0.26 | 66,66,66,66 | 0 |
| 57 | MG | 14 | 3076 | 1/1 | 0.93 | 0.17 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3409 | 1/1 | 0.93 | 0.11 | 55,55,55,55 | 0 |
| 57 | MG | 14 | 3297 | 1/1 | 0.93 | 0.19 | 66,66,66,66 | 0 |
| 57 | MG | 13 | 1658 | 1/1 | 0.93 | 0.48 | 75,75,75,75 | 0 |
| 57 | MG | 14 | 3414 | 1/1 | 0.93 | 0.22 | 100,100,100,100 | 0 |
| 57 | MG | 68 | 202 | 1/1 | 0.93 | 0.22 | 83,83,83,83 | 0 |
| 57 | MG | 13 | 1652 | 1/1 | 0.93 | 0.22 | 68,68,68,68 | 0 |
| 57 | MG | 1G | 1718 | 1/1 | 0.93 | 0.11 | 91,91,91,91 | 0 |
| 57 | MG | 14 | 3130 | 1/1 | 0.93 | 0.39 | 70,70,70,70 | 0 |
| 57 | MG | 13 | 1618 | 1/1 | 0.93 | 0.58 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3170 | 1/1 | 0.93 | 0.27 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3020 | 1/1 | 0.93 | 0.26 | 47,47,47,47 | 0 |
| 57 | MG | 1H | 3268 | 1/1 | 0.93 | 0.66 | 92,92,92,92 | 0 |
| 57 | MG | 13 | 1709 | 1/1 | 0.93 | 0.04 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3260 | 1/1 | 0.93 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 14 | 3071 | 1/1 | 0.93 | 0.24 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3107 | 1/1 | 0.93 | 0.43 | 72,72,72,72 | 0 |
| 57 | MG | 1G | 1699 | 1/1 | 0.93 | 0.08 | 93,93,93,93 | 0 |
| 57 | MG | 19 | 301 | 1/1 | 0.93 | 0.39 | 57,57,57,57 | 0 |
| 57 | MG | 31 | 301 | 1/1 | 0.93 | 0.26 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3141 | 1/1 | 0.93 | 0.22 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3064 | 1/1 | 0.93 | 0.30 | 62,62,62,62 | 0 |
| 57 | MG | 1G | 1658 | 1/1 | 0.93 | 0.26 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3480 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 13 | 1720 | 1/1 | 0.93 | 0.04 | 100,100,100,100 | 0 |
| 57 | MG | 13 | 1704 | 1/1 | 0.93 | 0.10 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3001 | 1/1 | 0.93 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | 13 | 1676 | 1/1 | 0.93 | 0.34 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3054 | 1/1 | 0.93 | 0.27 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3028 | 1/1 | 0.93 | 0.42 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3461 | 1/1 | 0.93 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | 13 | 1644 | 1/1 | 0.93 | 0.06 | 82,82,82,82 | 0 |
| 57 | MG | 1H | 3543 | 1/1 | 0.93 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3407 | 1/1 | 0.93 | 0.04 | 77,77,77,77 | 0 |
| 57 | MG | 39 | 301 | 1/1 | 0.93 | 0.13 | 95,95,95,95 | 0 |
| 57 | MG | 13 | 1631 | 1/1 | 0.93 | 0.24 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3173 | 1/1 | 0.93 | 0.74 | 89,89,89,89 | 0 |
| 57 | MG | 14 | 3299 | 1/1 | 0.93 | 0.21 | 58,58,58,58 | 0 |
| 57 | MG | 1J | 203 | 1/1 | 0.93 | 0.23 | 91,91,91,91 | 0 |
| 57 | MG | 1H | 3131 | 1/1 | 0.93 | 0.34 | 75,75,75,75 | 0 |
| 57 | MG | 14 | 3344 | 1/1 | 0.93 | 0.08 | 88,88,88,88 | 0 |
| 57 | MG | 1H | 3314 | 1/1 | 0.93 | 0.19 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3043 | 1/1 | 0.93 | 0.39 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3112 | 1/1 | 0.93 | 0.32 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3034 | 1/1 | 0.93 | 0.38 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3026 | 1/1 | 0.93 | 0.12 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3250 | 1/1 | 0.93 | 0.15 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3028 | 1/1 | 0.93 | 0.31 | 61,61,61,61 | 0 |
| 57 | MG | 14 | 3186 | 1/1 | 0.93 | 0.17 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3257 | 1/1 | 0.93 | 0.36 | 51,51,51,51 | 0 |
| 57 | MG | 14 | 3018 | 1/1 | 0.93 | 0.34 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3074 | 1/1 | 0.93 | 0.41 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3046 | 1/1 | 0.93 | 0.42 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3257 | 1/1 | 0.93 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3431 | 1/1 | 0.93 | 0.09 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3229 | 1/1 | 0.93 | 0.38 | 64,64,64,64 | 0 |
| 57 | MG | 13 | 1694 | 1/1 | 0.93 | 0.05 | 94,94,94,94 | 0 |
| 57 | MG | 1G | 1730 | 1/1 | 0.93 | 0.06 | 94,94,94,94 | 0 |
| 57 | MG | 14 | 3279 | 1/1 | 0.93 | 0.26 | 83,83,83,83 | 0 |
| 57 | MG | 1G | 1609 | 1/1 | 0.93 | 0.44 | 96,96,96,96 | 0 |
| 57 | MG | 1H | 3324 | 1/1 | 0.93 | 0.40 | 66,66,66,66 | 0 |
| 57 | MG | 14 | 3182 | 1/1 | 0.93 | 0.12 | 82,82,82,82 | 0 |
| 57 | MG | 1H | 3440 | 1/1 | 0.93 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | 1G | 1641 | 1/1 | 0.93 | 0.11 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3074 | 1/1 | 0.93 | 0.27 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3073 | 1/1 | 0.93 | 0.58 | 59,59,59,59 | 0 |
| 57 | MG | 1H | 3470 | 1/1 | 0.93 | 0.07 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3024 | 1/1 | 0.93 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | 14 | 3234 | 1/1 | 0.93 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3236 | 1/1 | 0.93 | 0.36 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3354 | 1/1 | 0.94 | 0.10 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3463 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | 13 | 1634 | 1/1 | 0.94 | 0.31 | 78,78,78,78 | 0 |
| 57 | MG | 14 | 3067 | 1/1 | 0.94 | 0.35 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3230 | 1/1 | 0.94 | 0.22 | 87,87,87,87 | 0 |
| 57 | MG | 1H | 3047 | 1/1 | 0.94 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | 1H | 3032 | 1/1 | 0.94 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3033 | 1/1 | 0.94 | 0.66 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3096 | 1/1 | 0.94 | 0.31 | 53,53,53,53 | 0 |
| 57 | MG | 14 | 3382 | 1/1 | 0.94 | 0.09 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3034 | 1/1 | 0.94 | 0.24 | 48,48,48,48 | 0 |
| 57 | MG | 14 | 3184 | 1/1 | 0.94 | 0.25 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3312 | 1/1 | 0.94 | 0.07 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3093 | 1/1 | 0.94 | 0.32 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3057 | 1/1 | 0.94 | 0.45 | 84,84,84,84 | 0 |
| 57 | MG | 1G | 1688 | 1/1 | 0.94 | 0.11 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3013 | 1/1 | 0.94 | 0.32 | 37,37,37,37 | 0 |
| 57 | MG | 14 | 3091 | 1/1 | 0.94 | 0.41 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3015 | 1/1 | 0.94 | 0.40 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3150 | 1/1 | 0.94 | 0.30 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3240 | 1/1 | 0.94 | 0.37 | 67,67,67,67 | 0 |
| 57 | MG | 14 | 3106 | 1/1 | 0.94 | 0.79 | 94,94,94,94 | 0 |
| 57 | MG | 14 | 3108 | 1/1 | 0.94 | 0.84 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3342 | 1/1 | 0.94 | 0.16 | 42,42,42,42 | 0 |
| 57 | MG | 1H | 3510 | 1/1 | 0.94 | 0.07 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3244 | 1/1 | 0.94 | 0.32 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3004 | 1/1 | 0.94 | 0.71 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3073 | 1/1 | 0.94 | 0.31 | 48,48,48,48 | 0 |
| 57 | MG | 1H | 3011 | 1/1 | 0.94 | 0.23 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3029 | 1/1 | 0.94 | 0.23 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3447 | 1/1 | 0.94 | 0.53 | 69,69,69,69 | 0 |
| 60 | ZN | C5 | 202 | 1/1 | 0.94 | 0.12 | 151,151,151,151 | 0 |
| 57 | MG | 13 | 1629 | 1/1 | 0.94 | 0.33 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3153 | 1/1 | 0.94 | 0.58 | 65,65,65,65 | 0 |
| 57 | MG | 14 | 3030 | 1/1 | 0.94 | 0.44 | 89,89,89,89 | 0 |
| 57 | MG | 1G | 1640 | 1/1 | 0.94 | 0.24 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3489 | 1/1 | 0.94 | 0.09 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3080 | 1/1 | 0.94 | 0.34 | 51,51,51,51 | 0 |
| 57 | MG | 1H | 3481 | 1/1 | 0.94 | 0.07 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3118 | 1/1 | 0.94 | 0.09 | 73,73,73,73 | 0 |
| 57 | MG | 13 | 1722 | 1/1 | 0.94 | 0.12 | 77,77,77,77 | 0 |
| 57 | MG | 1G | 1708 | 1/1 | 0.94 | 0.04 | 140,140,140,140 | 0 |
| 57 | MG | 13 | 1638 | 1/1 | 0.94 | 0.08 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3277 | 1/1 | 0.94 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | 1G | 1639 | 1/1 | 0.94 | 0.12 | 103,103,103,103 | 0 |
| 57 | MG | 14 | 3212 | 1/1 | 0.94 | 0.33 | 94,94,94,94 | 0 |
| 57 | MG | 1H | 3387 | 1/1 | 0.94 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | 14 | 3013 | 1/1 | 0.94 | 0.44 | 63,63,63,63 | 0 |
| 57 | MG | 13 | 1716 | 1/1 | 0.94 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | 1G | 1677 | 1/1 | 0.94 | 0.07 | 97,97,97,97 | 0 |
| 57 | MG | 13 | 1639 | 1/1 | 0.94 | 0.17 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3285 | 1/1 | 0.94 | 0.09 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3320 | 1/1 | 0.94 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | 1G | 1628 | 1/1 | 0.94 | 0.61 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3368 | 1/1 | 0.94 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 13 | 1680 | 1/1 | 0.94 | 0.35 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3045 | 1/1 | 0.94 | 0.22 | 42,42,42,42 | 0 |
| 57 | MG | 1H | 3326 | 1/1 | 0.94 | 0.12 | 47,47,47,47 | 0 |
| 57 | MG | 14 | 3010 | 1/1 | 0.94 | 0.26 | 50,50,50,50 | 0 |
| 57 | MG | 1G | 1690 | 1/1 | 0.94 | 0.08 | 114,114,114,114 | 0 |
| 57 | MG | 1G | 1631 | 1/1 | 0.94 | 0.14 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3088 | 1/1 | 0.94 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3457 | 1/1 | 0.94 | 0.09 | 45,45,45,45 | 0 |
| 57 | MG | 14 | 3145 | 1/1 | 0.94 | 0.12 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3262 | 1/1 | 0.94 | 0.16 | 66,66,66,66 | 0 |
| 57 | MG | 14 | 3122 | 1/1 | 0.94 | 0.29 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3453 | 1/1 | 0.94 | 0.19 | 58,58,58,58 | 0 |
| 57 | MG | 1H | 3151 | 1/1 | 0.94 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | 1H | 3334 | 1/1 | 0.94 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | 14 | 3169 | 1/1 | 0.94 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3022 | 1/1 | 0.94 | 0.33 | 41,41,41,41 | 0 |
| 57 | MG | 1G | 1634 | 1/1 | 0.94 | 0.18 | 93,93,93,93 | 0 |
| 57 | MG | 13 | 1661 | 1/1 | 0.94 | 0.20 | 92,92,92,92 | 0 |
| 57 | MG | 14 | 3003 | 1/1 | 0.94 | 0.49 | 54,54,54,54 | 0 |
| 57 | MG | 13 | 1693 | 1/1 | 0.94 | 0.12 | 84,84,84,84 | 0 |
| 57 | MG | 1G | 1604 | 1/1 | 0.94 | 0.30 | 103,103,103,103 | 0 |
| 57 | MG | 1H | 3196 | 1/1 | 0.95 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3459 | 1/1 | 0.95 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | 14 | 3124 | 1/1 | 0.95 | 0.35 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3050 | 1/1 | 0.95 | 0.48 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3226 | 1/1 | 0.95 | 0.54 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3437 | 1/1 | 0.95 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | 1H | 3366 | 1/1 | 0.95 | 0.16 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3055 | 1/1 | 0.95 | 0.29 | 50,50,50,50 | 0 |
| 57 | MG | 14 | 3303 | 1/1 | 0.95 | 0.18 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3215 | 1/1 | 0.95 | 0.41 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3121 | 1/1 | 0.95 | 0.28 | 55,55,55,55 | 0 |
| 57 | MG | 1H | 3138 | 1/1 | 0.95 | 0.46 | 41,41,41,41 | 0 |
| 57 | MG | 1G | 1626 | 1/1 | 0.95 | 0.24 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3539 | 1/1 | 0.95 | 0.11 | 45,45,45,45 | 0 |
| 57 | MG | 1H | 3129 | 1/1 | 0.95 | 0.51 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3300 | 1/1 | 0.95 | 0.24 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3068 | 1/1 | 0.95 | 0.37 | 64,64,64,64 | 0 |
| 57 | MG | 14 | 3019 | 1/1 | 0.95 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3346 | 1/1 | 0.95 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3328 | 1/1 | 0.95 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | 1H | 3174 | 1/1 | 0.95 | 0.20 | 37,37,37,37 | 0 |
| 57 | MG | 14 | 3150 | 1/1 | 0.95 | 0.19 | 81,81,81,81 | 0 |
| 57 | MG | 14 | 3014 | 1/1 | 0.95 | 0.33 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3076 | 1/1 | 0.95 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | 14 | 3188 | 1/1 | 0.95 | 0.51 | 76,76,76,76 | 0 |
| 57 | MG | 14 | 3180 | 1/1 | 0.95 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3492 | 1/1 | 0.95 | 0.07 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3100 | 1/1 | 0.95 | 0.31 | 61,61,61,61 | 0 |
| 57 | MG | 13 | 1666 | 1/1 | 0.95 | 0.13 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3389 | 1/1 | 0.95 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3344 | 1/1 | 0.95 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | 13 | 1705 | 1/1 | 0.95 | 0.18 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3393 | 1/1 | 0.95 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3339 | 1/1 | 0.95 | 0.22 | 43,43,43,43 | 0 |
| 57 | MG | 1G | 1601 | 1/1 | 0.95 | 0.19 | 70,70,70,70 | 0 |
| 57 | MG | 14 | 3364 | 1/1 | 0.95 | 0.07 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3263 | 1/1 | 0.95 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3343 | 1/1 | 0.95 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | 14 | 3337 | 1/1 | 0.95 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 14 | 3430 | 1/1 | 0.95 | 0.13 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3069 | 1/1 | 0.95 | 0.13 | 93,93,93,93 | 0 |
| 57 | MG | 14 | 3058 | 1/1 | 0.95 | 0.27 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3009 | 1/1 | 0.95 | 0.26 | 68,68,68,68 | 0 |
| 57 | MG | 14 | 3139 | 1/1 | 0.95 | 0.48 | 84,84,84,84 | 0 |
| 57 | MG | 13 | 1617 | 1/1 | 0.95 | 0.69 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3007 | 1/1 | 0.95 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | 13 | 1717 | 1/1 | 0.95 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 1G | 1642 | 1/1 | 0.95 | 0.23 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3084 | 1/1 | 0.95 | 0.30 | 87,87,87,87 | 0 |
| 57 | MG | 1G | 1671 | 1/1 | 0.95 | 0.09 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3476 | 1/1 | 0.95 | 0.12 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3350 | 1/1 | 0.95 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3472 | 1/1 | 0.95 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3376 | 1/1 | 0.95 | 0.09 | 45,45,45,45 | 0 |
| 57 | MG | 1H | 3451 | 1/1 | 0.95 | 0.12 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3278 | 1/1 | 0.95 | 0.12 | 80,80,80,80 | 0 |
| 57 | MG | 1G | 1687 | 1/1 | 0.95 | 0.11 | 95,95,95,95 | 0 |
| 57 | MG | 14 | 3143 | 1/1 | 0.95 | 0.42 | 54,54,54,54 | 0 |
| 57 | MG | 14 | 3164 | 1/1 | 0.95 | 0.32 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3206 | 1/1 | 0.95 | 0.26 | 101,101,101,101 | 0 |
| 57 | MG | 1H | 3426 | 1/1 | 0.95 | 0.05 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3146 | 1/1 | 0.95 | 0.64 | 58,58,58,58 | 0 |
| 57 | MG | 1H | 3363 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | 1H | 3001 | 1/1 | 0.95 | 0.29 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3491 | 1/1 | 0.95 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | 14 | 3125 | 1/1 | 0.95 | 0.47 | 70,70,70,70 | 0 |
| 57 | MG | 14 | 3325 | 1/1 | 0.95 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | 14 | 3132 | 1/1 | 0.95 | 0.30 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3256 | 1/1 | 0.95 | 0.28 | 67,67,67,67 | 0 |
| 57 | MG | 1G | 1608 | 1/1 | 0.95 | 0.10 | 111,111,111,111 | 0 |
| 57 | MG | 16 | 210 | 1/1 | 0.95 | 0.06 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3319 | 1/1 | 0.95 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3372 | 1/1 | 0.95 | 0.13 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3403 | 1/1 | 0.95 | 0.06 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3170 | 1/1 | 0.95 | 0.34 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3336 | 1/1 | 0.95 | 0.07 | 65,65,65,65 | 0 |
| 57 | MG | 14 | 3233 | 1/1 | 0.95 | 0.26 | 54,54,54,54 | 0 |
| 57 | MG | 14 | 3219 | 1/1 | 0.95 | 0.43 | 54,54,54,54 | 0 |
| 57 | MG | 4K | 102 | 1/1 | 0.95 | 0.07 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3288 | 1/1 | 0.95 | 0.29 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3546 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | B5 | 101 | 1/1 | 0.95 | 0.12 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3337 | 1/1 | 0.95 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | 1H | 3441 | 1/1 | 0.95 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | 1H | 3031 | 1/1 | 0.95 | 0.43 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3240 | 1/1 | 0.96 | 0.12 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3432 | 1/1 | 0.96 | 0.23 | 56,56,56,56 | 0 |
| 57 | MG | 13 | 1621 | 1/1 | 0.96 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | 2L | 101 | 1/1 | 0.96 | 0.53 | 77,77,77,77 | 0 |
| 57 | MG | 1G | 1614 | 1/1 | 0.96 | 0.29 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3254 | 1/1 | 0.96 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | 14 | 3266 | 1/1 | 0.96 | 0.11 | 72,72,72,72 | 0 |
| 57 | MG | 16 | 202 | 1/1 | 0.96 | 0.31 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3057 | 1/1 | 0.96 | 0.26 | 72,72,72,72 | 0 |
| 57 | MG | 14 | 3144 | 1/1 | 0.96 | 0.30 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3446 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 57 | MG | 14 | 3038 | 1/1 | 0.96 | 0.36 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3468 | 1/1 | 0.96 | 0.11 | 68,68,68,68 | 0 |
| 57 | MG | 14 | 3011 | 1/1 | 0.96 | 0.39 | 51,51,51,51 | 0 |
| 57 | MG | 13 | 1627 | 1/1 | 0.96 | 0.24 | 85,85,85,85 | 0 |
| 57 | MG | 1H | 3040 | 1/1 | 0.96 | 0.32 | 36,36,36,36 | 0 |
| 57 | MG | 1H | 3347 | 1/1 | 0.96 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3160 | 1/1 | 0.96 | 0.43 | 68,68,68,68 | 0 |
| 57 | MG | 1G | 1679 | 1/1 | 0.96 | 0.07 | 93,93,93,93 | 0 |
| 57 | MG | 1H | 3219 | 1/1 | 0.96 | 0.54 | 82,82,82,82 | 0 |
| 57 | MG | 1H | 3485 | 1/1 | 0.96 | 0.06 | 83,83,83,83 | 0 |
| 57 | MG | 1G | 1665 | 1/1 | 0.96 | 0.20 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3534 | 1/1 | 0.96 | 0.12 | 92,92,92,92 | 0 |
| 57 | MG | 1H | 3144 | 1/1 | 0.96 | 0.41 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3475 | 1/1 | 0.96 | 0.06 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3143 | 1/1 | 0.96 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | 1G | 1663 | 1/1 | 0.96 | 0.20 | 76,76,76,76 | 0 |
| 57 | MG | 13 | 1714 | 1/1 | 0.96 | 0.08 | 100,100,100,100 | 0 |
| 57 | MG | 45 | 201 | 1/1 | 0.96 | 0.12 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3382 | 1/1 | 0.96 | 0.22 | 54,54,54,54 | 0 |
| 57 | MG | 1H | 3353 | 1/1 | 0.96 | 0.13 | 64,64,64,64 | 0 |
| 57 | MG | 14 | 3020 | 1/1 | 0.96 | 0.42 | 61,61,61,61 | 0 |
| 57 | MG | 2K | 104 | 1/1 | 0.96 | 0.06 | 89,89,89,89 | 0 |
| 57 | MG | 14 | 3360 | 1/1 | 0.96 | 0.06 | 94,94,94,94 | 0 |
| 57 | MG | I8 | 101 | 1/1 | 0.96 | 0.05 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3340 | 1/1 | 0.96 | 0.07 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3012 | 1/1 | 0.96 | 0.41 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3029 | 1/1 | 0.96 | 0.21 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3396 | 1/1 | 0.96 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3060 | 1/1 | 0.96 | 0.33 | 51,51,51,51 | 0 |
| 57 | MG | 1H | 3046 | 1/1 | 0.96 | 0.24 | 49,49,49,49 | 0 |
| 57 | MG | 1G | 1603 | 1/1 | 0.96 | 0.26 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3095 | 1/1 | 0.96 | 0.34 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3433 | 1/1 | 0.96 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3017 | 1/1 | 0.96 | 0.29 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3063 | 1/1 | 0.96 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3264 | 1/1 | 0.96 | 0.25 | 59,59,59,59 | 0 |
| 57 | MG | 13 | 1641 | 1/1 | 0.96 | 0.25 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3487 | 1/1 | 0.96 | 0.10 | 72,72,72,72 | 0 |
| 57 | MG | 13 | 1689 | 1/1 | 0.96 | 0.40 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1G | 1656 | 1/1 | 0.96 | 0.23 | 66,66,66,66 | 0 |
| 57 | MG | 14 | 3105 | 1/1 | 0.96 | 0.35 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3192 | 1/1 | 0.96 | 0.39 | 82,82,82,82 | 0 |
| 57 | MG | 13 | 1610 | 1/1 | 0.96 | 0.35 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3060 | 1/1 | 0.96 | 0.55 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3175 | 1/1 | 0.96 | 0.08 | 107,107,107,107 | 0 |
| 57 | MG | 14 | 3036 | 1/1 | 0.96 | 0.26 | 47,47,47,47 | 0 |
| 57 | MG | 13 | 1749 | 1/1 | 0.96 | 0.14 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3052 | 1/1 | 0.96 | 0.35 | 50,50,50,50 | 0 |
| 57 | MG | 13 | 1696 | 1/1 | 0.96 | 0.15 | 83,83,83,83 | 0 |
| 57 | MG | 1H | 3021 | 1/1 | 0.96 | 0.34 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3505 | 1/1 | 0.96 | 0.06 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3037 | 1/1 | 0.96 | 0.34 | 57,57,57,57 | 0 |
| 57 | MG | 13 | 1701 | 1/1 | 0.96 | 0.04 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3070 | 1/1 | 0.96 | 0.33 | 82,82,82,82 | 0 |
| 57 | MG | 13 | 1605 | 1/1 | 0.96 | 0.24 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3383 | 1/1 | 0.96 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3305 | 1/1 | 0.96 | 0.23 | 71,71,71,71 | 0 |
| 57 | MG | 21 | 301 | 1/1 | 0.96 | 0.24 | 62,62,62,62 | 0 |
| 57 | MG | 13 | 1692 | 1/1 | 0.96 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | 14 | 3315 | 1/1 | 0.96 | 0.10 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3265 | 1/1 | 0.96 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | 14 | 3102 | 1/1 | 0.96 | 0.14 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3253 | 1/1 | 0.96 | 0.22 | 53,53,53,53 | 0 |
| 57 | MG | 1H | 3381 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 57 | MG | 1H | 3497 | 1/1 | 0.96 | 0.06 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3490 | 1/1 | 0.96 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | 13 | 1648 | 1/1 | 0.96 | 0.17 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3120 | 1/1 | 0.96 | 0.28 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3427 | 1/1 | 0.96 | 0.07 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3064 | 1/1 | 0.96 | 0.36 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3228 | 1/1 | 0.96 | 1.16 | 86,86,86,86 | 0 |
| 57 | MG | 1H | 3405 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 60 | ZN | G8 | 201 | 1/1 | 0.96 | 0.10 | 131,131,131,131 | 0 |
| 57 | MG | 13 | 1655 | 1/1 | 0.96 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | 14 | 3089 | 1/1 | 0.96 | 0.43 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3110 | 1/1 | 0.96 | 0.26 | 65,65,65,65 | 0 |
| 57 | MG | 1H | 3043 | 1/1 | 0.96 | 0.41 | 66,66,66,66 | 0 |
| 57 | MG | 13 | 1725 | 1/1 | 0.96 | 0.10 | 90,90,90,90 | 0 |
| 57 | MG | 1H | 3341 | 1/1 | 0.96 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | 14 | 3347 | 1/1 | 0.96 | 0.07 | 101,101,101,101 | 0 |
| 57 | MG | 13 | 1612 | 1/1 | 0.96 | 0.21 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 13 | 1628 | 1/1 | 0.97 | 0.39 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3333 | 1/1 | 0.97 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | 13 | 1729 | 1/1 | 0.97 | 0.06 | 73,73,73,73 | 0 |
| 57 | MG | 14 | 3090 | 1/1 | 0.97 | 0.49 | 65,65,65,65 | 0 |
| 57 | MG | 16 | 209 | 1/1 | 0.97 | 0.03 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3135 | 1/1 | 0.97 | 0.20 | 42,42,42,42 | 0 |
| 57 | MG | 1H | 3465 | 1/1 | 0.97 | 0.12 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3259 | 1/1 | 0.97 | 0.06 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3361 | 1/1 | 0.97 | 0.04 | 74,74,74,74 | 0 |
| 57 | MG | 1G | 1627 | 1/1 | 0.97 | 0.20 | 77,77,77,77 | 0 |
| 57 | MG | 14 | 3329 | 1/1 | 0.97 | 0.11 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3283 | 1/1 | 0.97 | 0.35 | 146,146,146,146 | 0 |
| 57 | MG | 5E | 201 | 1/1 | 0.97 | 0.27 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3438 | 1/1 | 0.97 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | 13 | 1675 | 1/1 | 0.97 | 0.18 | 104,104,104,104 | 0 |
| 57 | MG | 14 | 3042 | 1/1 | 0.97 | 0.45 | 69,69,69,69 | 0 |
| 57 | MG | 14 | 3322 | 1/1 | 0.97 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3503 | 1/1 | 0.97 | 0.06 | 47,47,47,47 | 0 |
| 57 | MG | 14 | 3309 | 1/1 | 0.97 | 0.06 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3255 | 1/1 | 0.97 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | 14 | 3059 | 1/1 | 0.97 | 0.26 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3049 | 1/1 | 0.97 | 0.43 | 69,69,69,69 | 0 |
| 57 | MG | 13 | 1607 | 1/1 | 0.97 | 0.26 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3044 | 1/1 | 0.97 | 0.50 | 48,48,48,48 | 0 |
| 57 | MG | 29 | 302 | 1/1 | 0.97 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | 14 | 3051 | 1/1 | 0.97 | 0.31 | 72,72,72,72 | 0 |
| 57 | MG | 1H | 3454 | 1/1 | 0.97 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | 1H | 3318 | 1/1 | 0.97 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | 1G | 1613 | 1/1 | 0.97 | 0.34 | 83,83,83,83 | 0 |
| 57 | MG | 13 | 1601 | 1/1 | 0.97 | 0.32 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3548 | 1/1 | 0.97 | 0.14 | 70,70,70,70 | 0 |
| 57 | MG | 1H | 3290 | 1/1 | 0.97 | 0.13 | 87,87,87,87 | 0 |
| 57 | MG | 14 | 3023 | 1/1 | 0.97 | 0.41 | 82,82,82,82 | 0 |
| 57 | MG | 13 | 1712 | 1/1 | 0.97 | 0.09 | 101,101,101,101 | 0 |
| 57 | MG | 14 | 3361 | 1/1 | 0.97 | 0.04 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3081 | 1/1 | 0.97 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | 13 | 1640 | 1/1 | 0.97 | 0.47 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3243 | 1/1 | 0.97 | 0.22 | 79,79,79,79 | 0 |
| 57 | MG | 1H | 3293 | 1/1 | 0.97 | 0.45 | 46,46,46,46 | 0 |
| 57 | MG | 14 | 3339 | 1/1 | 0.97 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | 1G | 1734 | 1/1 | 0.97 | 0.16 | 84,84,84,84 | 0 |
| 57 | MG | 1H | 3091 | 1/1 | 0.97 | 0.39 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1H | 3055 | 1/1 | 0.97 | 0.26 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3071 | 1/1 | 0.97 | 0.41 | 57,57,57,57 | 0 |
| 57 | MG | 1H | 3291 | 1/1 | 0.97 | 0.20 | 78,78,78,78 | 0 |
| 57 | MG | 1H | 3050 | 1/1 | 0.97 | 0.30 | 54,54,54,54 | 0 |
| 57 | MG | 1H | 3514 | 1/1 | 0.97 | 0.08 | 76,76,76,76 | 0 |
| 57 | MG | 1H | 3054 | 1/1 | 0.97 | 0.29 | 37,37,37,37 | 0 |
| 57 | MG | 14 | 3342 | 1/1 | 0.97 | 0.11 | 82,82,82,82 | 0 |
| 57 | MG | 14 | 3045 | 1/1 | 0.97 | 0.32 | 61,61,61,61 | 0 |
| 57 | MG | 14 | 3354 | 1/1 | 0.97 | 0.09 | 73,73,73,73 | 0 |
| 57 | MG | 1H | 3068 | 1/1 | 0.97 | 0.57 | 71,71,71,71 | 0 |
| 57 | MG | 14 | 3318 | 1/1 | 0.97 | 0.07 | 75,75,75,75 | 0 |
| 57 | MG | 14 | 3047 | 1/1 | 0.97 | 0.26 | 81,81,81,81 | 0 |
| 57 | MG | 1H | 3018 | 1/1 | 0.97 | 0.50 | 55,55,55,55 | 0 |
| 57 | MG | 1H | 3359 | 1/1 | 0.97 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3430 | 1/1 | 0.97 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3335 | 1/1 | 0.97 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 14 | 3258 | 1/1 | 0.97 | 0.09 | 71,71,71,71 | 0 |
| 57 | MG | 1H | 3532 | 1/1 | 0.97 | 0.12 | 103,103,103,103 | 0 |
| 57 | MG | 14 | 3065 | 1/1 | 0.97 | 0.35 | 60,60,60,60 | 0 |
| 57 | MG | 14 | 3306 | 1/1 | 0.97 | 0.13 | 86,86,86,86 | 0 |
| 57 | MG | 14 | 3017 | 1/1 | 0.97 | 0.48 | 60,60,60,60 | 0 |
| 57 | MG | 1H | 3413 | 1/1 | 0.97 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | 1G | 1732 | 1/1 | 0.97 | 0.05 | 114,114,114,114 | 0 |
| 57 | MG | 14 | 3237 | 1/1 | 0.97 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | 1H | 3035 | 1/1 | 0.97 | 0.32 | 80,80,80,80 | 0 |
| 57 | MG | 1H | 3400 | 1/1 | 0.98 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | 14 | 3345 | 1/1 | 0.98 | 0.08 | 83,83,83,83 | 0 |
| 57 | MG | 14 | 3048 | 1/1 | 0.98 | 0.28 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3501 | 1/1 | 0.98 | 0.15 | 75,75,75,75 | 0 |
| 57 | MG | 1G | 1706 | 1/1 | 0.98 | 0.07 | 79,79,79,79 | 0 |
| 57 | MG | 13 | 1703 | 1/1 | 0.98 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | 1H | 3030 | 1/1 | 0.98 | 0.34 | 75,75,75,75 | 0 |
| 57 | MG | 1H | 3384 | 1/1 | 0.98 | 0.07 | 61,61,61,61 | 0 |
| 57 | MG | 1G | 1649 | 1/1 | 0.98 | 0.37 | 89,89,89,89 | 0 |
| 57 | MG | 1H | 3132 | 1/1 | 0.98 | 0.27 | 88,88,88,88 | 0 |
| 57 | MG | 14 | 3290 | 1/1 | 0.98 | 0.08 | 66,66,66,66 | 0 |
| 57 | MG | 14 | 3135 | 1/1 | 0.98 | 0.21 | 69,69,69,69 | 0 |
| 57 | MG | 1H | 3398 | 1/1 | 0.98 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | 14 | 3245 | 1/1 | 0.98 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3119 | 1/1 | 0.98 | 0.37 | 79,79,79,79 | 0 |
| 57 | MG | 14 | 3249 | 1/1 | 0.98 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | 14 | 3300 | 1/1 | 0.98 | 0.20 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3251 | 1/1 | 0.98 | 0.18 | 63,63,63,63 | 0 |
| 57 | MG | 14 | 3128 | 1/1 | 0.98 | 0.33 | 88,88,88,88 | 0 |
| 57 | MG | 1H | 3375 | 1/1 | 0.98 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | 14 | 3061 | 1/1 | 0.98 | 0.65 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3109 | 1/1 | 0.98 | 0.52 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3355 | 1/1 | 0.98 | 0.13 | 67,67,67,67 | 0 |
| 57 | MG | 1H | 3412 | 1/1 | 0.98 | 0.10 | 51,51,51,51 | 0 |
| 57 | MG | 13 | 1713 | 1/1 | 0.98 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | 21 | 302 | 1/1 | 0.98 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | 1H | 3403 | 1/1 | 0.98 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | 14 | 3326 | 1/1 | 0.98 | 0.09 | 60,60,60,60 | 0 |
| 57 | MG | 14 | 3321 | 1/1 | 0.98 | 0.07 | 64,64,64,64 | 0 |
| 57 | MG | 1H | 3507 | 1/1 | 0.98 | 0.04 | 74,74,74,74 | 0 |
| 57 | MG | 1H | 3014 | 1/1 | 0.98 | 0.38 | 43,43,43,43 | 0 |
| 57 | MG | 11 | 302 | 1/1 | 0.98 | 0.07 | 47,47,47,47 | 0 |
| 57 | MG | 13 | 1611 | 1/1 | 0.98 | 0.11 | 85,85,85,85 | 0 |
| 57 | MG | 14 | 3242 | 1/1 | 0.98 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | 1H | 3142 | 1/1 | 0.98 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | 14 | 3269 | 1/1 | 0.98 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3039 | 1/1 | 0.98 | 0.28 | 40,40,40,40 | 0 |
| 57 | MG | 13 | 1604 | 1/1 | 0.98 | 0.32 | 77,77,77,77 | 0 |
| 57 | MG | 1H | 3041 | 1/1 | 0.98 | 0.25 | 51,51,51,51 | 0 |
| 57 | MG | 1H | 3159 | 1/1 | 0.98 | 0.29 | 74,74,74,74 | 0 |
| 57 | MG | 14 | 3328 | 1/1 | 0.98 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | 14 | 3304 | 1/1 | 0.98 | 0.13 | 68,68,68,68 | 0 |
| 57 | MG | 13 | 1698 | 1/1 | 0.98 | 0.04 | 94,94,94,94 | 0 |
| 57 | MG | 14 | 3079 | 1/1 | 0.98 | 0.34 | 61,61,61,61 | 0 |
| 57 | MG | 14 | 3096 | 1/1 | 0.98 | 0.24 | 50,50,50,50 | 0 |
| 60 | ZN | 5I | 102 | 1/1 | 0.98 | 0.11 | 98,98,98,98 | 0 |
| 57 | MG | 1H | 3538 | 1/1 | 0.98 | 0.06 | 58,58,58,58 | 0 |
| 57 | MG | 1H | 3460 | 1/1 | 0.98 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | 1H | 3506 | 1/1 | 0.98 | 0.09 | 61,61,61,61 | 0 |
| 57 | MG | 1H | 3136 | 1/1 | 0.98 | 0.17 | 45,45,45,45 | 0 |
| 60 | ZN | 5A | 101 | 1/1 | 0.99 | 0.09 | 123,123,123,123 | 0 |
| 59 | SF4 | 3E | 301 | 8/8 | 0.99 | 0.17 | 86,90,100,103 | 0 |
| 57 | MG | 1H | 3345 | 1/1 | 0.99 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | 14 | 3311 | 1/1 | 0.99 | 0.10 | 68,68,68,68 | 0 |
| 57 | MG | 1H | 3351 | 1/1 | 0.99 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | 1H | 3499 | 1/1 | 0.99 | 0.09 | 52,52,52,52 | 0 |
| 57 | MG | 14 | 3114 | 1/1 | 0.99 | 0.43 | 63,63,63,63 | 0 |
| 57 | MG | 1H | 3411 | 1/1 | 0.99 | 0.09 | 80,80,80,80 | 0 |
| 57 | MG | 14 | 3333 | 1/1 | 0.99 | 0.06 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 14 | 3270 | 1/1 | 0.99 | 0.09 | 65,65,65,65 | 0 |
| 57 | MG | 1J | 204 | 1/1 | 0.99 | 0.12 | 88,88,88,88 | 0 |
| 59 | SF4 | 32 | 301 | 8/8 | 0.99 | 0.15 | 90,99,108,116 | 0 |
| 57 | MG | 13 | 1721 | 1/1 | 0.99 | 0.06 | 62,62,62,62 | 0 |
| 57 | MG | 1H | 3547 | 1/1 | 1.00 | 0.28 | 61,61,61,61 | 0 |
| 57 | MG | 14 | 3197 | 1/1 | 1.00 | 0.20 | 78,78,78,78 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.