



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:11 am GMT

PDB ID : 5EL4
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the first position
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.15 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

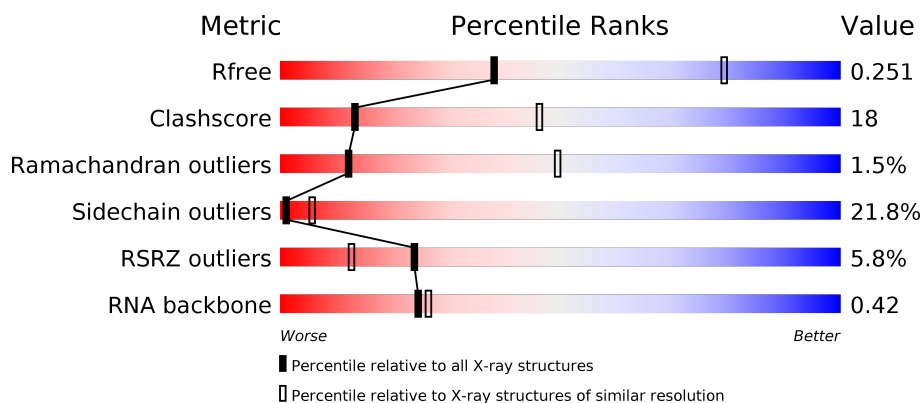
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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} | 100719 | 1259 (3.20-3.12) |
| Clashscore | 112137 | 1397 (3.20-3.12) |
| Ramachandran outliers | 110173 | 1368 (3.20-3.12) |
| Sidechain outliers | 110143 | 1367 (3.20-3.12) |
| RSRZ outliers | 101464 | 1264 (3.20-3.12) |
| RNA backbone | 2435 | 1000 (3.52-2.80) |

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. 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 | |
| 25 | 4K | 27 | |
| 25 | 4L | 27 | |
| 26 | 14 | 2917 | |
| 26 | 1H | 2917 | |
| 27 | 16 | 122 | |
| 27 | 1J | 122 | |
| 28 | 7I | 229 | |
| 29 | 11 | 276 | |

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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | M8 | 71 | |
| 53 | J5 | 60 | |
| 53 | N8 | 60 | |
| 54 | L5 | 49 | |
| 54 | P8 | 49 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55 | M5 | 65 | |
| 55 | Q8 | 65 | |
| 56 | 1L | 76 | |
| 57 | 3L | 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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 13 | 1604 | - | - | - | X |
| 58 | MG | 13 | 1608 | - | - | - | X |
| 58 | MG | 13 | 1613 | - | - | - | X |
| 58 | MG | 13 | 1621 | - | - | - | X |
| 58 | MG | 13 | 1622 | - | - | - | X |
| 58 | MG | 13 | 1638 | - | - | - | X |
| 58 | MG | 13 | 1639 | - | - | - | X |
| 58 | MG | 13 | 1645 | - | - | - | X |
| 58 | MG | 13 | 1646 | - | - | - | X |
| 58 | MG | 13 | 1654 | - | - | - | X |
| 58 | MG | 13 | 1655 | - | - | - | X |
| 58 | MG | 13 | 1664 | - | - | - | X |
| 58 | MG | 13 | 1672 | - | - | - | X |
| 58 | MG | 13 | 1677 | - | - | - | X |
| 58 | MG | 13 | 1686 | - | - | - | X |
| 58 | MG | 13 | 1694 | - | - | - | X |
| 58 | MG | 13 | 1697 | - | - | - | X |
| 58 | MG | 13 | 1699 | - | - | - | X |
| 58 | MG | 13 | 1741 | - | - | - | X |
| 58 | MG | 14 | 3003 | - | - | - | X |
| 58 | MG | 14 | 3004 | - | - | - | X |
| 58 | MG | 14 | 3006 | - | - | - | X |
| 58 | MG | 14 | 3007 | - | - | - | X |
| 58 | MG | 14 | 3009 | - | - | - | X |
| 58 | MG | 14 | 3015 | - | - | - | X |
| 58 | MG | 14 | 3016 | - | - | - | X |
| 58 | MG | 14 | 3024 | - | - | - | X |
| 58 | MG | 14 | 3029 | - | - | - | X |
| 58 | MG | 14 | 3030 | - | - | - | X |
| 58 | MG | 14 | 3035 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 14 | 3037 | - | - | - | X |
| 58 | MG | 14 | 3038 | - | - | - | X |
| 58 | MG | 14 | 3049 | - | - | - | X |
| 58 | MG | 14 | 3050 | - | - | - | X |
| 58 | MG | 14 | 3054 | - | - | - | X |
| 58 | MG | 14 | 3056 | - | - | - | X |
| 58 | MG | 14 | 3057 | - | - | - | X |
| 58 | MG | 14 | 3063 | - | - | - | X |
| 58 | MG | 14 | 3067 | - | - | - | X |
| 58 | MG | 14 | 3073 | - | - | - | X |
| 58 | MG | 14 | 3074 | - | - | - | X |
| 58 | MG | 14 | 3075 | - | - | - | X |
| 58 | MG | 14 | 3078 | - | - | - | X |
| 58 | MG | 14 | 3079 | - | - | - | X |
| 58 | MG | 14 | 3083 | - | - | - | X |
| 58 | MG | 14 | 3085 | - | - | - | X |
| 58 | MG | 14 | 3095 | - | - | - | X |
| 58 | MG | 14 | 3097 | - | - | - | X |
| 58 | MG | 14 | 3099 | - | - | - | X |
| 58 | MG | 14 | 3117 | - | - | - | X |
| 58 | MG | 14 | 3123 | - | - | - | X |
| 58 | MG | 14 | 3143 | - | - | - | X |
| 58 | MG | 14 | 3149 | - | - | - | X |
| 58 | MG | 14 | 3157 | - | - | - | X |
| 58 | MG | 14 | 3158 | - | - | - | X |
| 58 | MG | 14 | 3160 | - | - | - | X |
| 58 | MG | 14 | 3164 | - | - | - | X |
| 58 | MG | 14 | 3165 | - | - | - | X |
| 58 | MG | 14 | 3176 | - | - | - | X |
| 58 | MG | 14 | 3177 | - | - | - | X |
| 58 | MG | 14 | 3178 | - | - | - | X |
| 58 | MG | 14 | 3179 | - | - | - | X |
| 58 | MG | 14 | 3185 | - | - | - | X |
| 58 | MG | 14 | 3186 | - | - | - | X |
| 58 | MG | 14 | 3190 | - | - | - | X |
| 58 | MG | 14 | 3192 | - | - | - | X |
| 58 | MG | 14 | 3193 | - | - | - | X |
| 58 | MG | 14 | 3194 | - | - | - | X |
| 58 | MG | 14 | 3198 | - | - | - | X |
| 58 | MG | 14 | 3205 | - | - | - | X |
| 58 | MG | 14 | 3206 | - | - | - | X |
| 58 | MG | 14 | 3212 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 14 | 3213 | - | - | - | X |
| 58 | MG | 14 | 3215 | - | - | - | X |
| 58 | MG | 14 | 3216 | - | - | - | X |
| 58 | MG | 14 | 3224 | - | - | - | X |
| 58 | MG | 14 | 3233 | - | - | - | X |
| 58 | MG | 14 | 3242 | - | - | - | X |
| 58 | MG | 14 | 3249 | - | - | - | X |
| 58 | MG | 14 | 3252 | - | - | - | X |
| 58 | MG | 14 | 3253 | - | - | - | X |
| 58 | MG | 14 | 3255 | - | - | - | X |
| 58 | MG | 14 | 3258 | - | - | - | X |
| 58 | MG | 14 | 3260 | - | - | - | X |
| 58 | MG | 14 | 3277 | - | - | - | X |
| 58 | MG | 14 | 3287 | - | - | - | X |
| 58 | MG | 16 | 204 | - | - | - | X |
| 58 | MG | 16 | 205 | - | - | - | X |
| 58 | MG | 1G | 1601 | - | - | - | X |
| 58 | MG | 1G | 1602 | - | - | - | X |
| 58 | MG | 1G | 1608 | - | - | - | X |
| 58 | MG | 1G | 1614 | - | - | - | X |
| 58 | MG | 1G | 1624 | - | - | - | X |
| 58 | MG | 1G | 1626 | - | - | - | X |
| 58 | MG | 1G | 1632 | - | - | - | X |
| 58 | MG | 1G | 1644 | - | - | - | X |
| 58 | MG | 1G | 1649 | - | - | - | X |
| 58 | MG | 1G | 1653 | - | - | - | X |
| 58 | MG | 1G | 1678 | - | - | - | X |
| 58 | MG | 1H | 3001 | - | - | - | X |
| 58 | MG | 1H | 3010 | - | - | - | X |
| 58 | MG | 1H | 3012 | - | - | - | X |
| 58 | MG | 1H | 3014 | - | - | - | X |
| 58 | MG | 1H | 3016 | - | - | - | X |
| 58 | MG | 1H | 3017 | - | - | - | X |
| 58 | MG | 1H | 3019 | - | - | - | X |
| 58 | MG | 1H | 3028 | - | - | - | X |
| 58 | MG | 1H | 3029 | - | - | - | X |
| 58 | MG | 1H | 3036 | - | - | - | X |
| 58 | MG | 1H | 3042 | - | - | - | X |
| 58 | MG | 1H | 3046 | - | - | - | X |
| 58 | MG | 1H | 3051 | - | - | - | X |
| 58 | MG | 1H | 3053 | - | - | - | X |
| 58 | MG | 1H | 3054 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 1H | 3061 | - | - | - | X |
| 58 | MG | 1H | 3062 | - | - | - | X |
| 58 | MG | 1H | 3065 | - | - | - | X |
| 58 | MG | 1H | 3070 | - | - | - | X |
| 58 | MG | 1H | 3071 | - | - | - | X |
| 58 | MG | 1H | 3074 | - | - | - | X |
| 58 | MG | 1H | 3079 | - | - | - | X |
| 58 | MG | 1H | 3080 | - | - | - | X |
| 58 | MG | 1H | 3082 | - | - | - | X |
| 58 | MG | 1H | 3084 | - | - | - | X |
| 58 | MG | 1H | 3085 | - | - | - | X |
| 58 | MG | 1H | 3086 | - | - | - | X |
| 58 | MG | 1H | 3088 | - | - | - | X |
| 58 | MG | 1H | 3089 | - | - | - | X |
| 58 | MG | 1H | 3094 | - | - | - | X |
| 58 | MG | 1H | 3097 | - | - | - | X |
| 58 | MG | 1H | 3099 | - | - | - | X |
| 58 | MG | 1H | 3100 | - | - | - | X |
| 58 | MG | 1H | 3115 | - | - | - | X |
| 58 | MG | 1H | 3116 | - | - | - | X |
| 58 | MG | 1H | 3124 | - | - | - | X |
| 58 | MG | 1H | 3131 | - | - | - | X |
| 58 | MG | 1H | 3134 | - | - | - | X |
| 58 | MG | 1H | 3137 | - | - | - | X |
| 58 | MG | 1H | 3142 | - | - | - | X |
| 58 | MG | 1H | 3154 | - | - | - | X |
| 58 | MG | 1H | 3155 | - | - | - | X |
| 58 | MG | 1H | 3167 | - | - | - | X |
| 58 | MG | 1H | 3168 | - | - | - | X |
| 58 | MG | 1H | 3174 | - | - | - | X |
| 58 | MG | 1H | 3179 | - | - | - | X |
| 58 | MG | 1H | 3180 | - | - | - | X |
| 58 | MG | 1H | 3186 | - | - | - | X |
| 58 | MG | 1H | 3191 | - | - | - | X |
| 58 | MG | 1H | 3195 | - | - | - | X |
| 58 | MG | 1H | 3225 | - | - | - | X |
| 58 | MG | 1H | 3226 | - | - | - | X |
| 58 | MG | 1H | 3236 | - | - | - | X |
| 58 | MG | 1H | 3237 | - | - | - | X |
| 58 | MG | 1H | 3240 | - | - | - | X |
| 58 | MG | 1H | 3243 | - | - | - | X |
| 58 | MG | 1H | 3245 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 1H | 3246 | - | - | - | X |
| 58 | MG | 1H | 3253 | - | - | - | X |
| 58 | MG | 1H | 3258 | - | - | - | X |
| 58 | MG | 1H | 3260 | - | - | - | X |
| 58 | MG | 1H | 3270 | - | - | - | X |
| 58 | MG | 1H | 3273 | - | - | - | X |
| 58 | MG | 1H | 3285 | - | - | - | X |
| 58 | MG | 1H | 3291 | - | - | - | X |
| 58 | MG | 1H | 3303 | - | - | - | X |
| 58 | MG | 1H | 3309 | - | - | - | X |
| 58 | MG | 1H | 3333 | - | - | - | X |
| 58 | MG | 1H | 3343 | - | - | - | X |
| 58 | MG | 1H | 3344 | - | - | - | X |
| 58 | MG | 1H | 3347 | - | - | - | X |
| 58 | MG | 1H | 3348 | - | - | - | X |
| 58 | MG | 1H | 3443 | - | - | - | X |
| 58 | MG | 1H | 3479 | - | - | - | X |
| 58 | MG | 1K | 101 | - | - | - | X |
| 58 | MG | 29 | 302 | - | - | - | X |
| 58 | MG | 2K | 101 | - | - | - | X |
| 58 | MG | 2L | 101 | - | - | - | X |
| 58 | MG | 39 | 301 | - | - | - | X |
| 58 | MG | 5I | 101 | - | - | - | X |
| 58 | MG | N8 | 101 | - | - | - | X |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 294304 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 | 1507 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32391 | 14418 | 6004 | 10463 | 1506 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-------------|
| 13 | 1542 | G | - | insertion | GB 55771382 |
| 13 | 1543 | C | - | insertion | GB 55771382 |
| 13 | 1544 | U | - | insertion | GB 55771382 |
| 1G | 1542 | G | - | insertion | GB 55771382 |
| 1G | 1543 | C | - | insertion | GB 55771382 |
| 1G | 1544 | U | - | insertion | GB 55771382 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | 1E | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1874 | 1199 | 334 | 336 | 5 | | | |
| 2 | 12 | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1711 | 1094 | 307 | 306 | 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 | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1529 | 967 | 296 | 265 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | 4E | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1142 | 722 | 216 | 200 | 4 | | | |
| 5 | 42 | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1123 | 709 | 214 | 196 | 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 | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1214 | 754 | 244 | 210 | 6 | | | |
| 7 | 62 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 689 | 221 | 194 | 6 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9 | 8E | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1005 | 637 | 197 | 171 | | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | 82 | 124 | Total | C | N | O | 0 | 0 | 0 |
| | | | 983 | 624 | 190 | 169 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | 1I | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 144 | 130 | 1 | | | |
| 10 | 1A | 78 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 626 | 388 | 126 | 112 | | | | |

- 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 | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 947 | 597 | 191 | 158 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | 4I | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 928 | 574 | 191 | 161 | 2 | | | |
| 13 | 4A | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 888 | 549 | 182 | 155 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | 5I | 61 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 496 | 315 | 105 | 72 | 4 | | | |
| 14 | 5A | 57 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 466 | 297 | 97 | 68 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | 6I | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 733 | 459 | 147 | 125 | 2 | | | |
| 15 | 6A | 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 | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 671 | 427 | 132 | 111 | 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 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 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 | 67 | Total | C | N | O | 0 | 0 | 0 |
| | | | 544 | 349 | 104 | 91 | | | |
| 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 | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 643 | 411 | 118 | 112 | 2 | | | |
| 19 | AA | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 471 | 300 | 83 | 86 | 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 | | | |
| 20 | BA | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 757 | 467 | 161 | 127 | 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 | 24 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 208 | 128 | 50 | 30 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 22 | 1K | 69 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1477 | 662 | 257 | 488 | 69 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23 | 2K | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1646 | 735 | 297 | 536 | 77 | 1 | | | |
| 23 | 2L | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1626 | 726 | 295 | 528 | 76 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 24 | 3K | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1611 | 721 | 281 | 534 | 75 | | | |

- Molecule 25 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 25 | 4K | 20 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 439 | 197 | 91 | 131 | 20 | | | |
| 25 | 4L | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 373 | 167 | 76 | 113 | 17 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------|------------|------------|------------|-----------|---------|---------|-------|
| 26 | 1H | 2833 | Total 61028 | C 27159 | N 11418 | O 19618 | P 2833 | 0 | 0 | 0 |
| 26 | 14 | 2861 | Total 61630 | C 27429 | N 11535 | O 19806 | P 2860 | 0 | 0 | 0 |

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 2617 | C 1166 | N 486 | O 844 | P 121 | 0 | 0 | 0 |
| 27 | 1J | 122 | Total 2617 | C 1166 | N 486 | O 844 | P 121 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| 28 | 71 | 133 | Total 1033 | C 651 | N 194 | O 187 | S 1 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 71 | 19 | ILE | VAL | conflict | UNP Q5SLP7 |
| 71 | 27 | HIS | ARG | conflict | UNP Q5SLP7 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | 21 | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1563 | 988 | 299 | 270 | 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 | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1606 | 1024 | 300 | 280 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | 41 | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1464 | 936 | 266 | 258 | 4 | | | |
| 32 | 49 | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1464 | 936 | 266 | 258 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | 51 | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1327 | 842 | 249 | 235 | 1 | | | |
| 33 | 59 | 69 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 539 | 339 | 109 | 91 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | 61 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 723 | 200 | 207 | 1 | | | |
| 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 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 35 | 15 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1096 | 707 | 205 | 181 | 3 | | | |

- 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 | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1130 | 704 | 230 | 193 | 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 |
| | | | 1113 | 709 | 210 | 187 | 7 | | | |
| 38 | 45 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1099 | 702 | 208 | 183 | 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 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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 | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1118 | 696 | 229 | 192 | 1 | | | |
| 41 | 75 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 704 | 232 | 195 | 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 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 493 | 137 | 132 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | E8 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 175 | 153 | 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 | 96 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 751 | 489 | 135 | 127 | | | | |
| 45 | B5 | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 479 | 133 | 125 | 1 | | | |

- 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 |
| | | | 783 | 504 | 148 | 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 | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1222 | 781 | 221 | 217 | 3 | | | |
| 47 | D5 | 126 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1034 | 667 | 187 | 178 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | I8 | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 616 | 381 | 130 | 104 | 1 | | | |
| 48 | E5 | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 616 | 381 | 130 | 104 | 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 |
| | | | 571 | 355 | 115 | 100 | 1 | | | |
| 50 | G5 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 573 | 355 | 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 | S | 0 | 0 | 0 |
| | | | 459 | 293 | 89 | 77 | | | | |
| 51 | H5 | 58 | Total | C | N | O | S | 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 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 366 | 234 | 61 | 66 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | N8 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 381 | 238 | 76 | 62 | 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 tRNA-Lys.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 56 | 1L | 74 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1570 | 702 | 271 | 523 | 74 | | | |

- Molecule 57 is a RNA chain called tRNA-Lys.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 57 | 3L | 74 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1571 | 703 | 277 | 518 | 73 | | | |

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

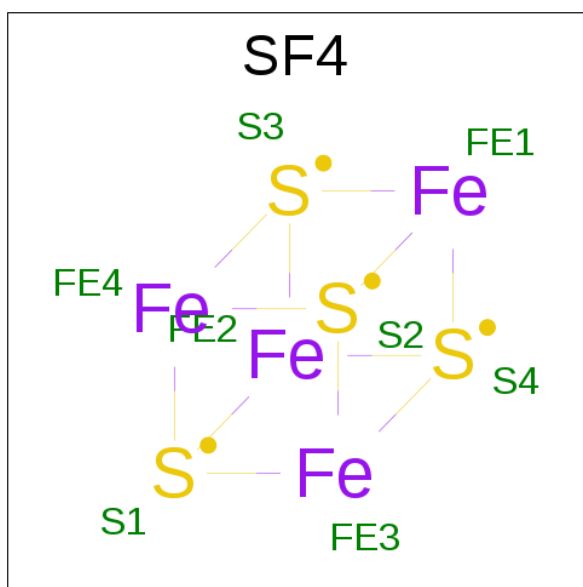
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 58 | 45 | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 58 | P8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 2I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 13 | 142 | Total | Mg | 0 | 0 |
| | | | 142 | 142 | | |
| 58 | 1J | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 58 | 5I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 16 | 11 | Total | Mg | 0 | 0 |
| | | | 11 | 11 | | |
| 58 | 25 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 21 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 58 | 2K | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 58 | Q8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 4I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 3I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | I8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 1I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 58 | 29 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 78 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | J8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 39 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 1G | 95 | Total 95 | Mg 95 | 0 | 0 |
| 58 | 11 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1H | 495 | Total 495 | Mg 495 | 0 | 0 |
| 58 | 7I | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | E5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 88 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | N8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 14 | 421 | Total 421 | Mg 421 | 0 | 0 |
| 58 | 19 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 3L | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 4K | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1K | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 41 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2L | 2 | Total 2 | Mg 2 | 0 | 0 |

- 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 | 207 | Total | O | 0 | 0 |
| | | | 207 | 207 | | |
| 61 | 3E | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 61 | 4E | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 61 | 8E | 1 | Total O 1 1 | 0 | 0 |
| 61 | 1I | 1 | Total O 1 1 | 0 | 0 |
| 61 | 3I | 2 | Total O 2 2 | 0 | 0 |
| 61 | 5I | 2 | Total O 2 2 | 0 | 0 |
| 61 | 6I | 1 | Total O 1 1 | 0 | 0 |
| 61 | 4K | 4 | Total O 4 4 | 0 | 0 |
| 61 | 1H | 819 | Total O 819 819 | 0 | 0 |
| 61 | 16 | 22 | Total O 22 22 | 0 | 0 |
| 61 | 11 | 9 | Total O 9 9 | 0 | 0 |
| 61 | 21 | 6 | Total O 6 6 | 0 | 0 |
| 61 | 31 | 4 | Total O 4 4 | 0 | 0 |
| 61 | 78 | 1 | Total O 1 1 | 0 | 0 |
| 61 | B8 | 1 | Total O 1 1 | 0 | 0 |
| 61 | C8 | 3 | Total O 3 3 | 0 | 0 |
| 61 | F8 | 1 | Total O 1 1 | 0 | 0 |
| 61 | I8 | 5 | Total O 5 5 | 0 | 0 |
| 61 | J8 | 2 | Total O 2 2 | 0 | 0 |
| 61 | L8 | 3 | Total O 3 3 | 0 | 0 |
| 61 | 1G | 117 | Total O 117 117 | 0 | 0 |
| 61 | 32 | 2 | Total O 2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O 1 1 | 0 | 0 |

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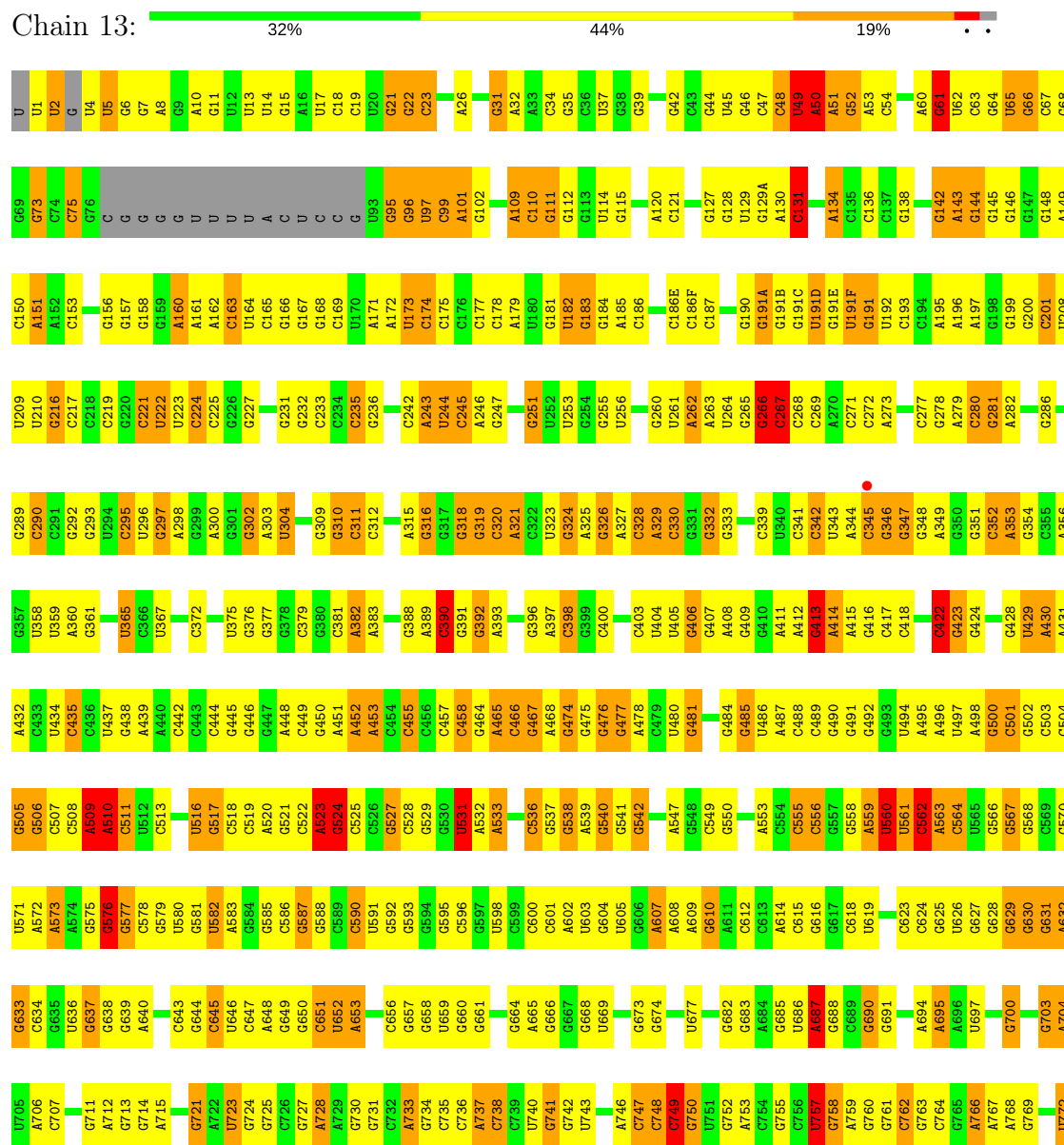
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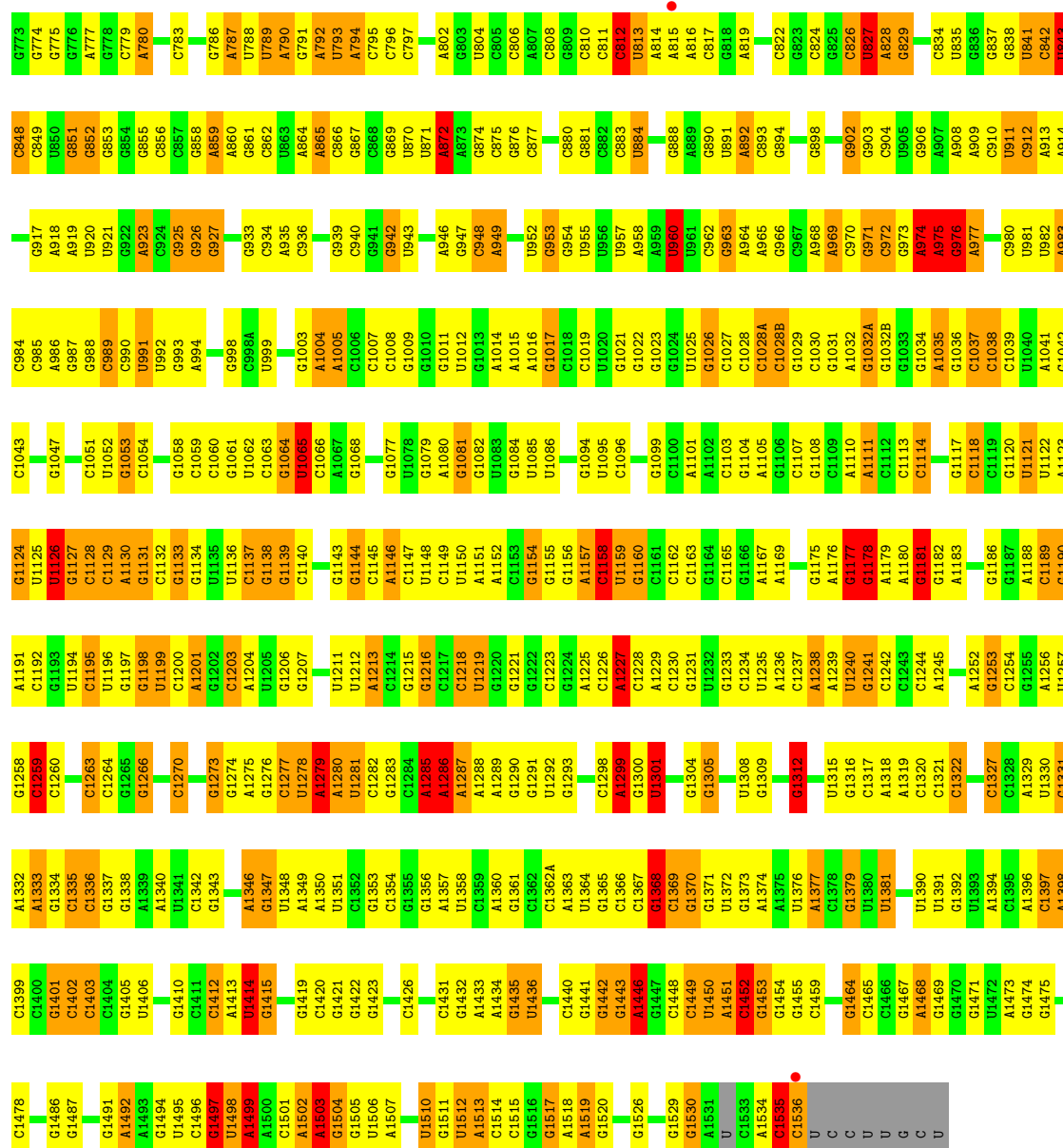
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | 6A | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 7A | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BA | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 14 | 717 | Total 717 | O 717 | 0 | 0 |
| 61 | 1J | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 19 | 10 | Total 10 | O 10 | 0 | 0 |
| 61 | 29 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 39 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 15 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 35 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 75 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 85 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | M5 | 3 | Total 3 | O 3 | 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.

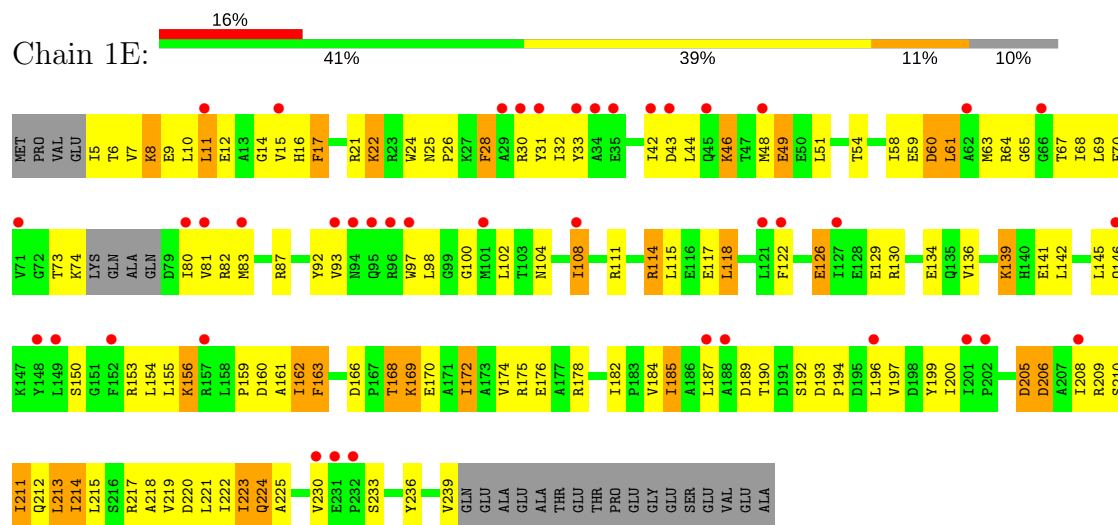
• Molecule 1: 16S ribosomal RNA



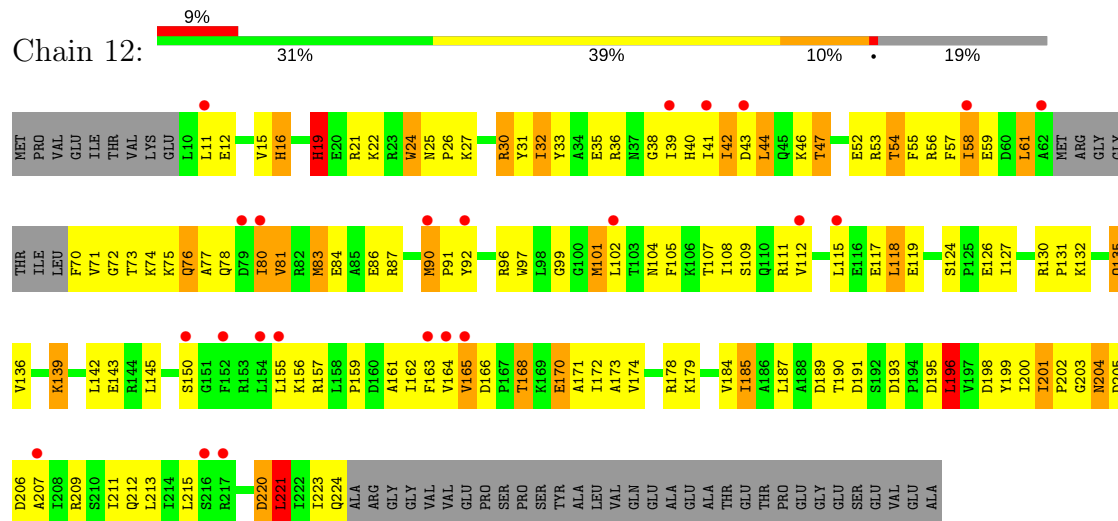




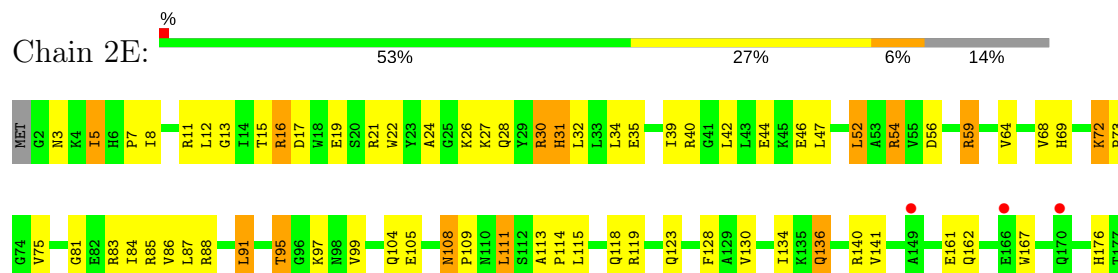
- Molecule 2: 30S ribosomal protein S2

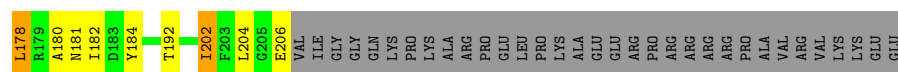


- Molecule 2: 30S ribosomal protein S2

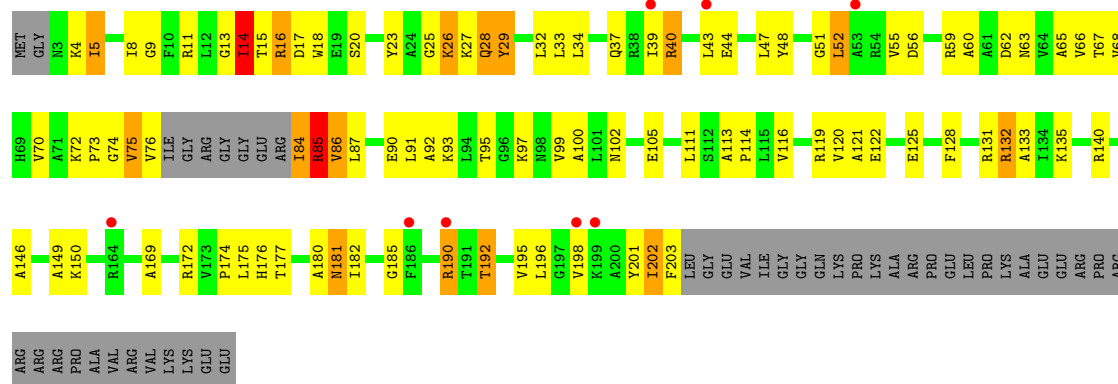
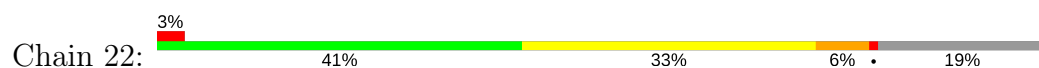


- Molecule 3: 30S ribosomal protein S3

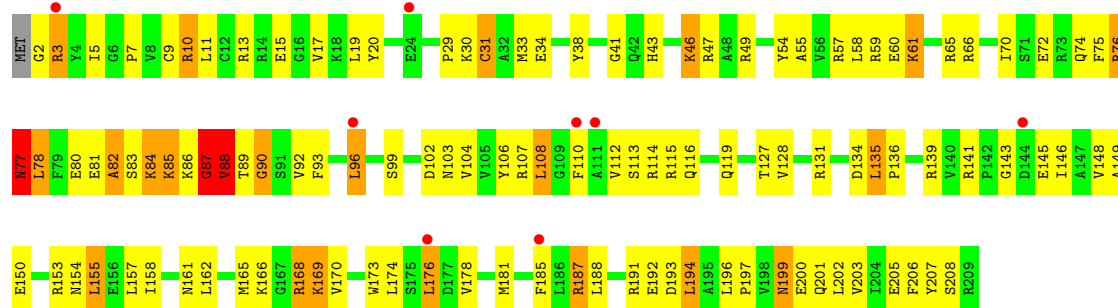
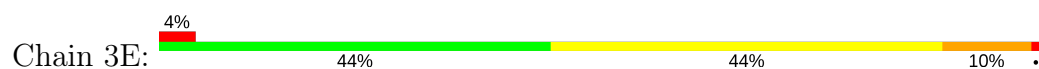




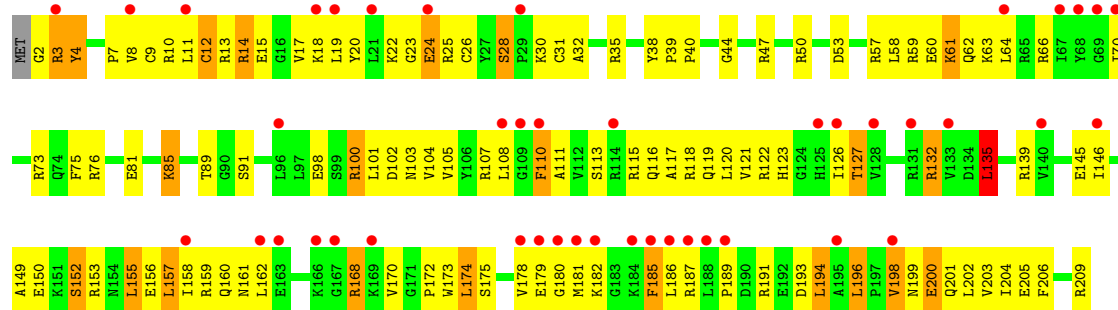
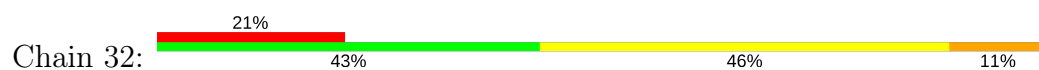
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

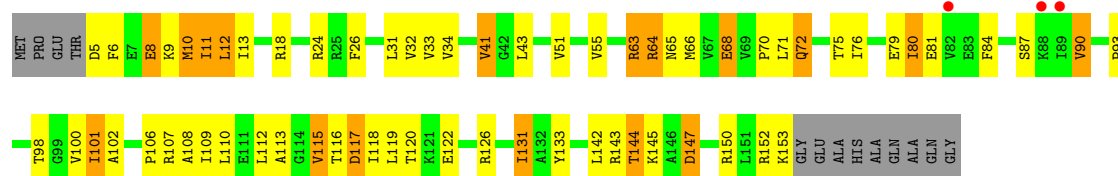


• Molecule 4: 30S ribosomal protein S4

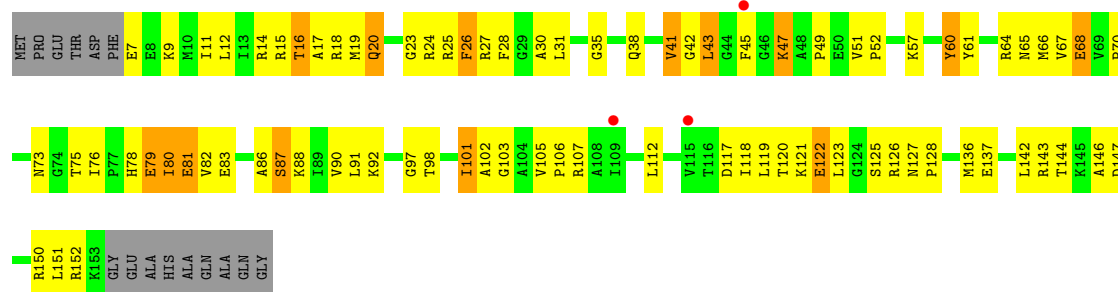
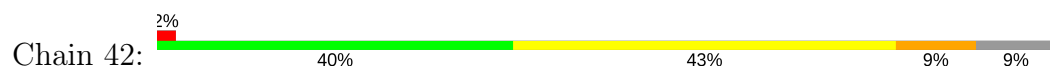


• Molecule 5: 30S ribosomal protein S5

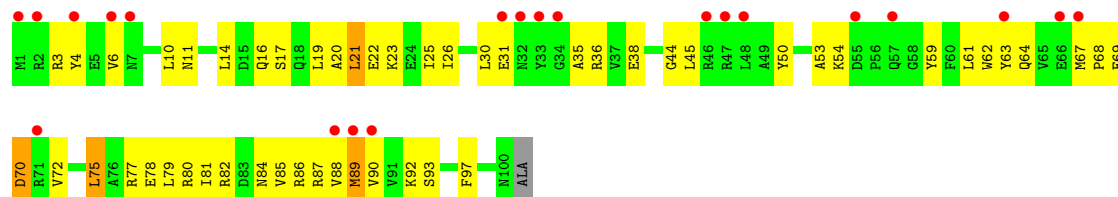




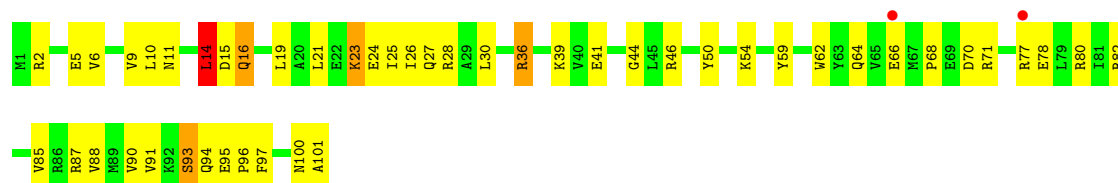
• Molecule 5: 30S ribosomal protein S5



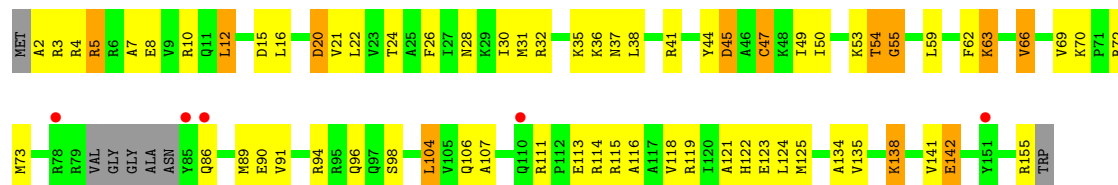
• Molecule 6: 30S ribosomal protein S6



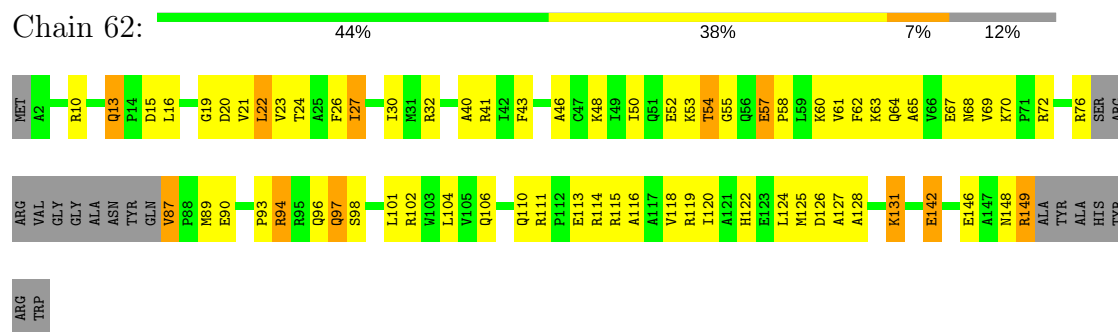
• Molecule 6: 30S ribosomal protein S6



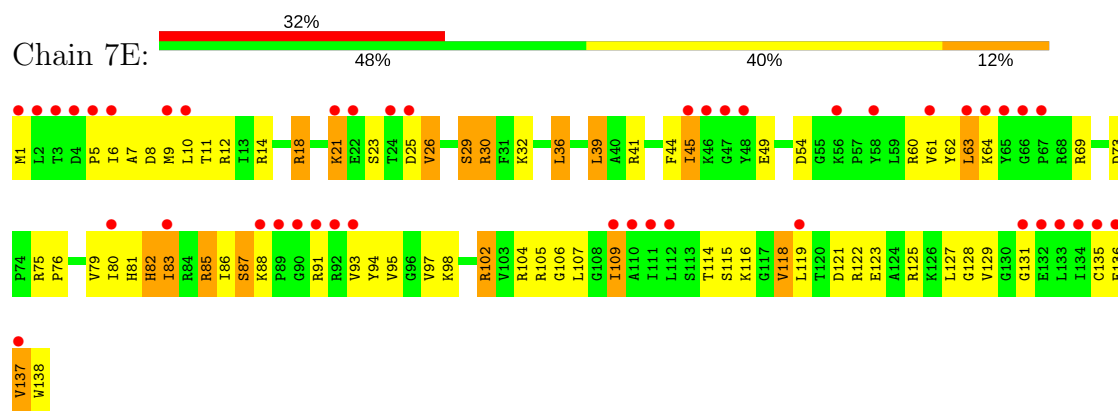
• Molecule 7: 30S ribosomal protein S7



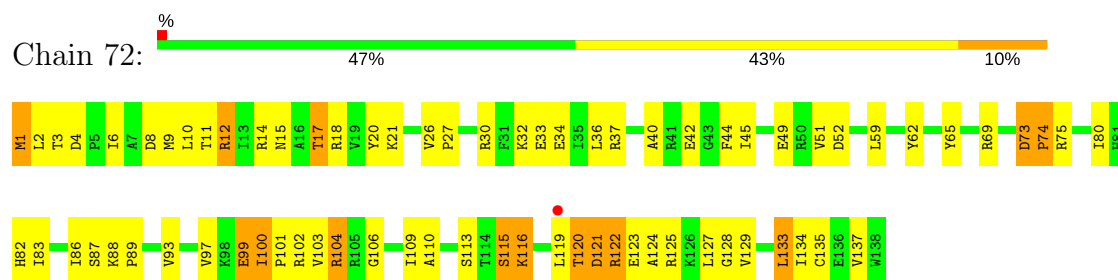
- Molecule 7: 30S ribosomal protein S7



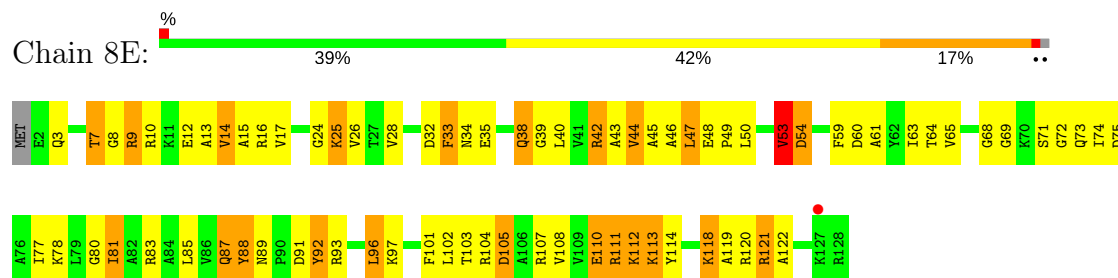
- Molecule 8: 30S ribosomal protein S8



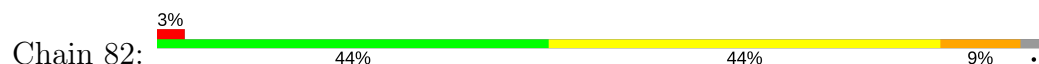
- Molecule 8: 30S ribosomal protein S8

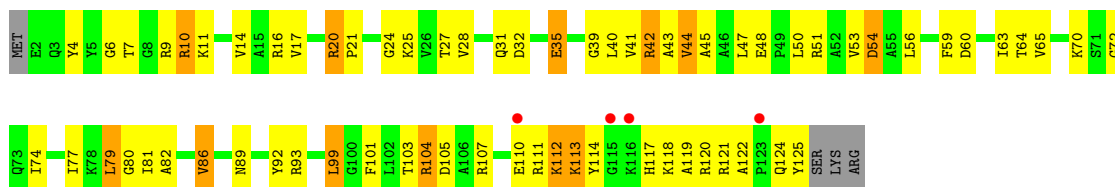


- Molecule 9: 30S ribosomal protein S9

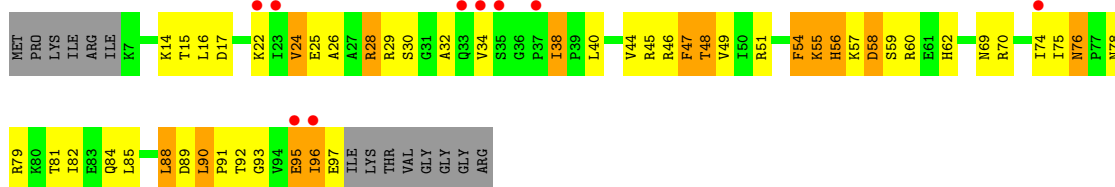


- Molecule 9: 30S ribosomal protein S9

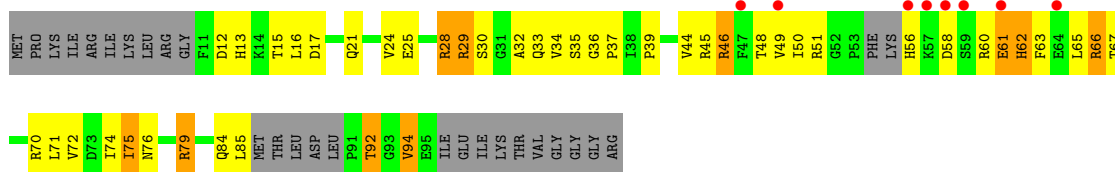




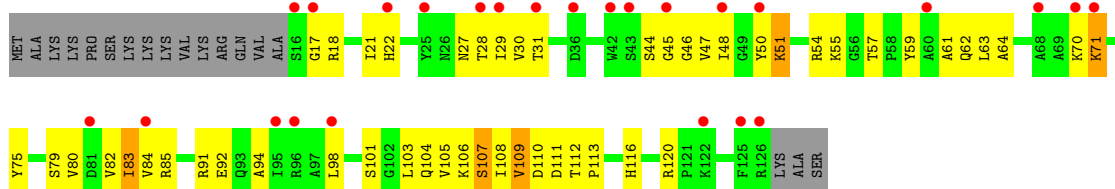
• Molecule 10: 30S ribosomal protein S10



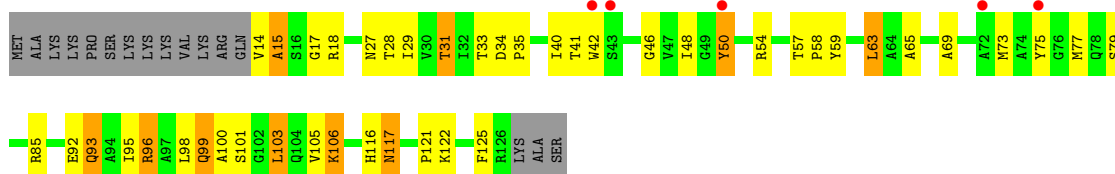
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

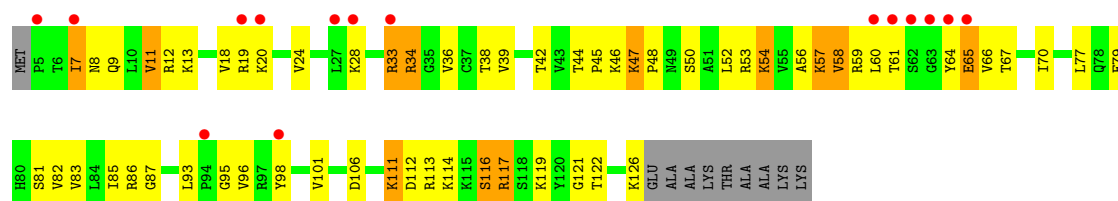


• Molecule 11: 30S ribosomal protein S11

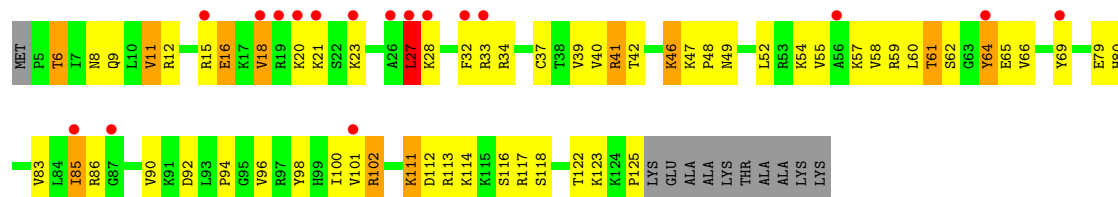


• Molecule 12: 30S ribosomal protein S12

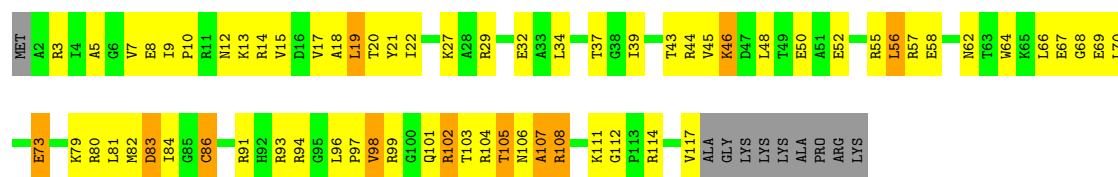




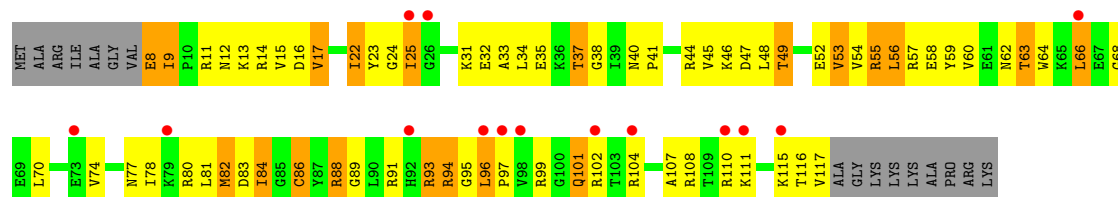
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



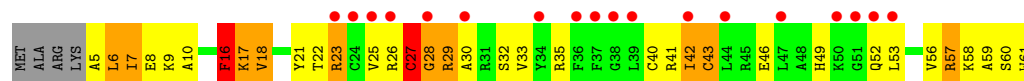
• Molecule 13: 30S ribosomal protein S13



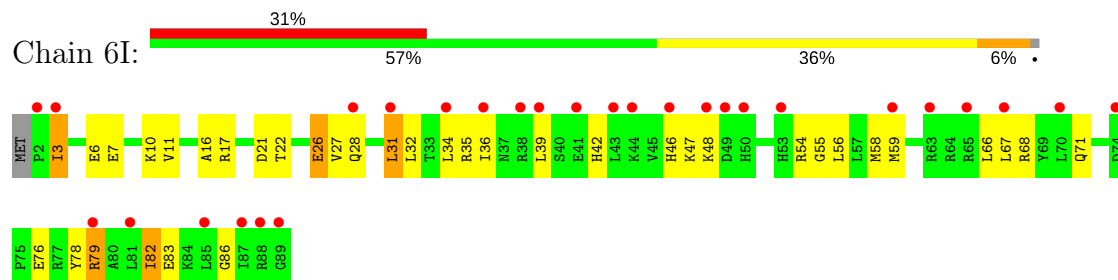
• Molecule 14: 30S ribosomal protein S14 type Z



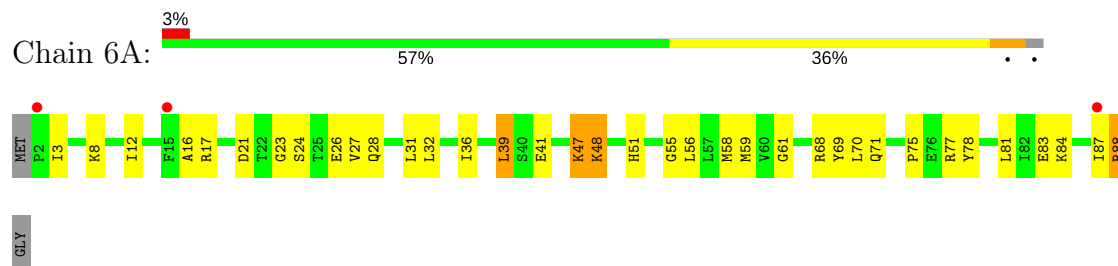
• Molecule 14: 30S ribosomal protein S14 type Z



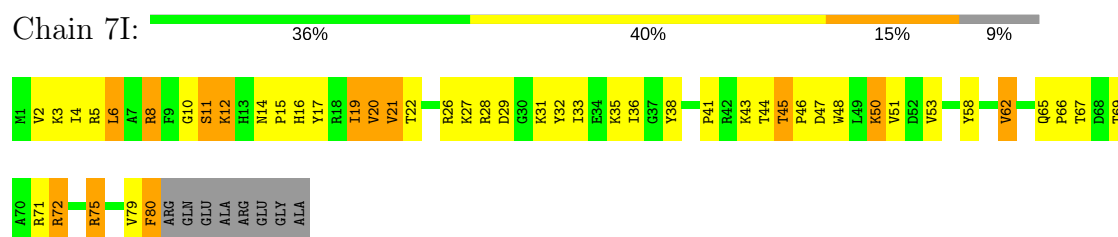
- Molecule 15: 30S ribosomal protein S15



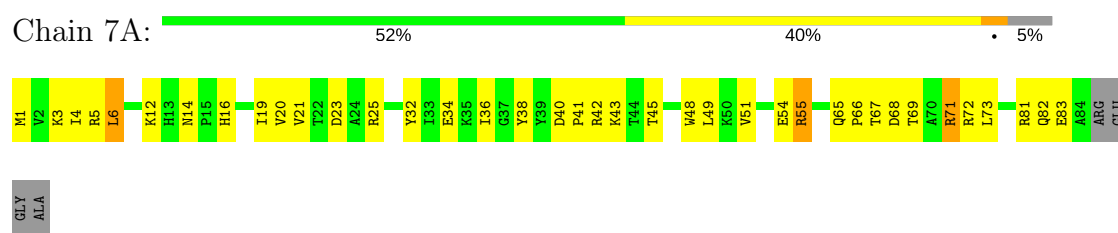
- Molecule 15: 30S ribosomal protein S15



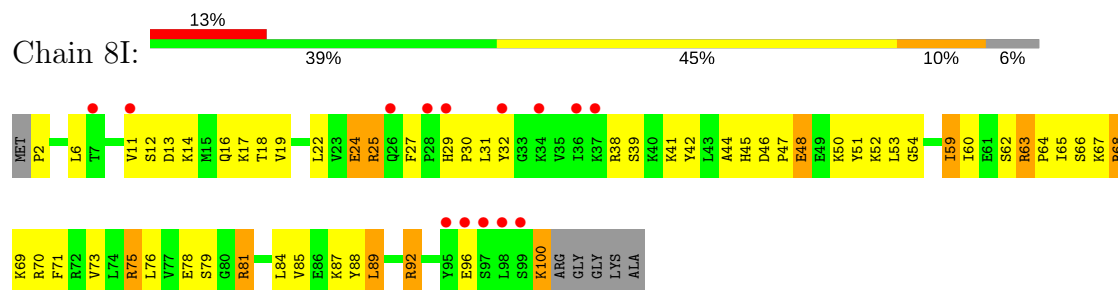
- Molecule 16: 30S ribosomal protein S16



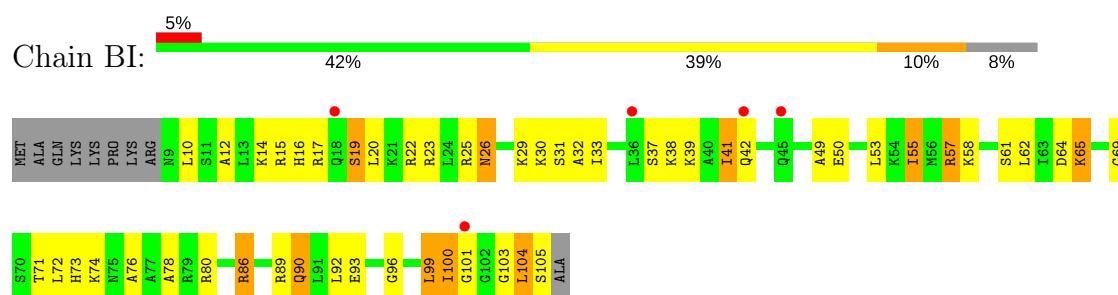
- Molecule 16: 30S ribosomal protein S16



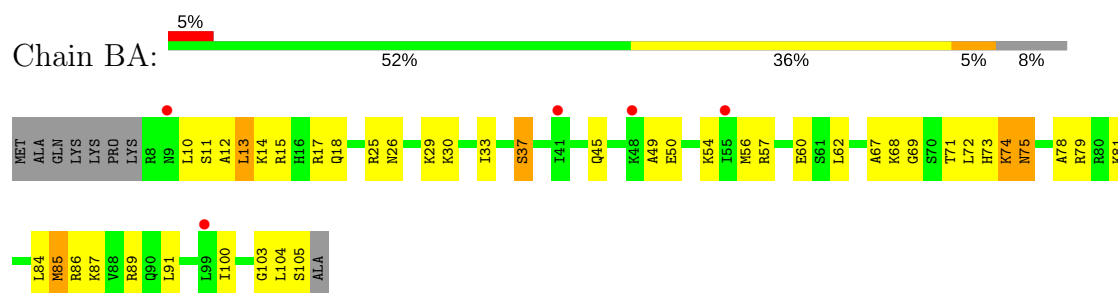
- Molecule 17: 30S ribosomal protein S17



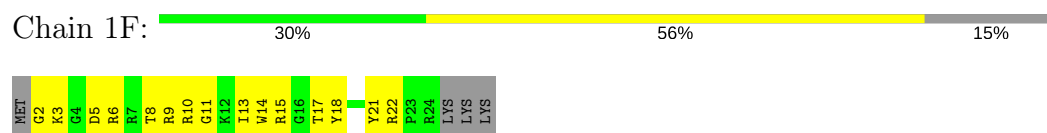
- Molecule 17: 30S ribosomal protein S17



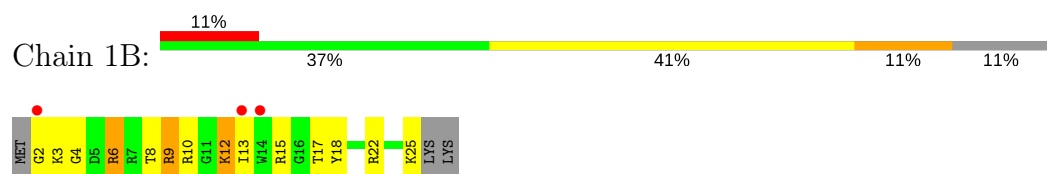
- Molecule 20: 30S ribosomal protein S20



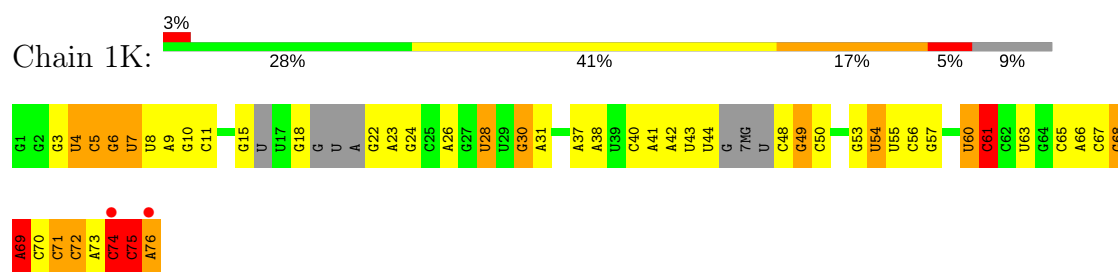
- Molecule 21: 30S ribosomal protein Thx



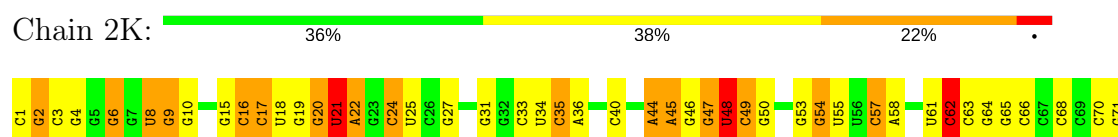
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA-Lys



- Molecule 23: tRNA-fMet





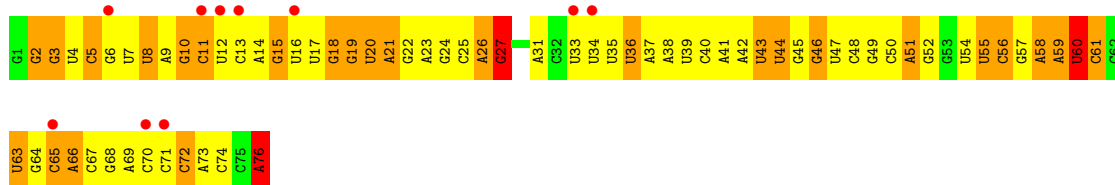
• Molecule 23: tRNA-fMet

Chain 2L: 42% 38% 16% . .



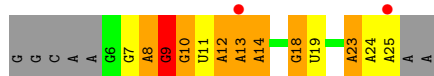
• Molecule 24: tRNA-Lys

Chain 3K: 13% 11% 51% 34% .



• Molecule 25: mRNA

Chain 4K: 7% 26% 19% 26% . 26%



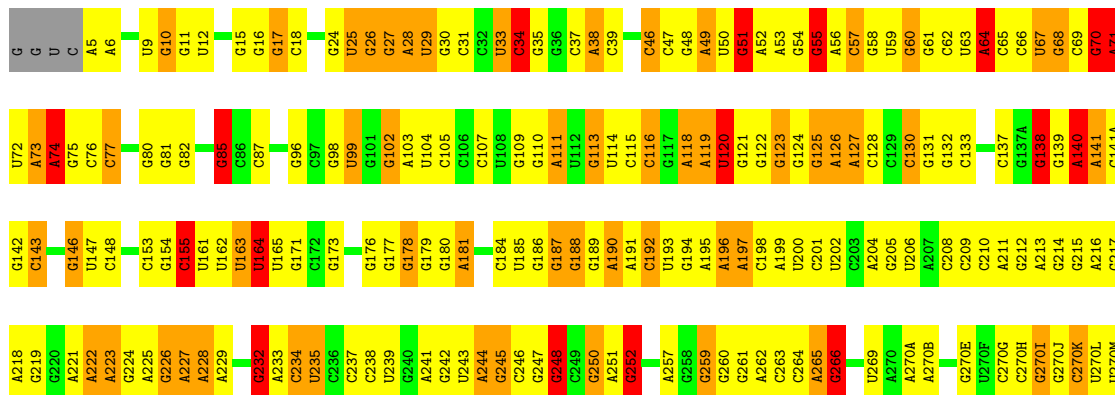
• Molecule 25: mRNA

Chain 4L: 19% 22% 22% 37%



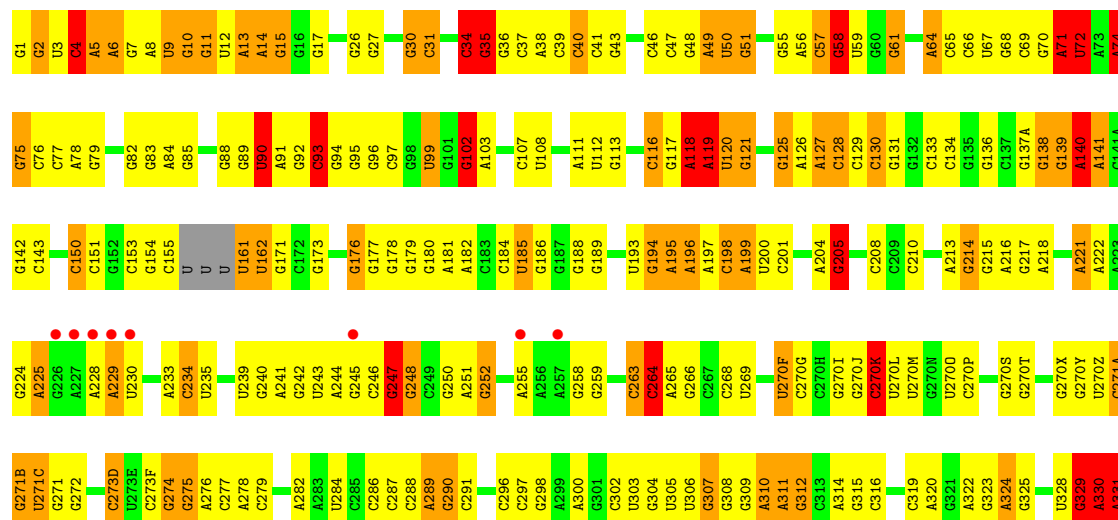
• Molecule 26: 23S ribosomal RNA

Chain 1H: 25% 41% 25% 6% .



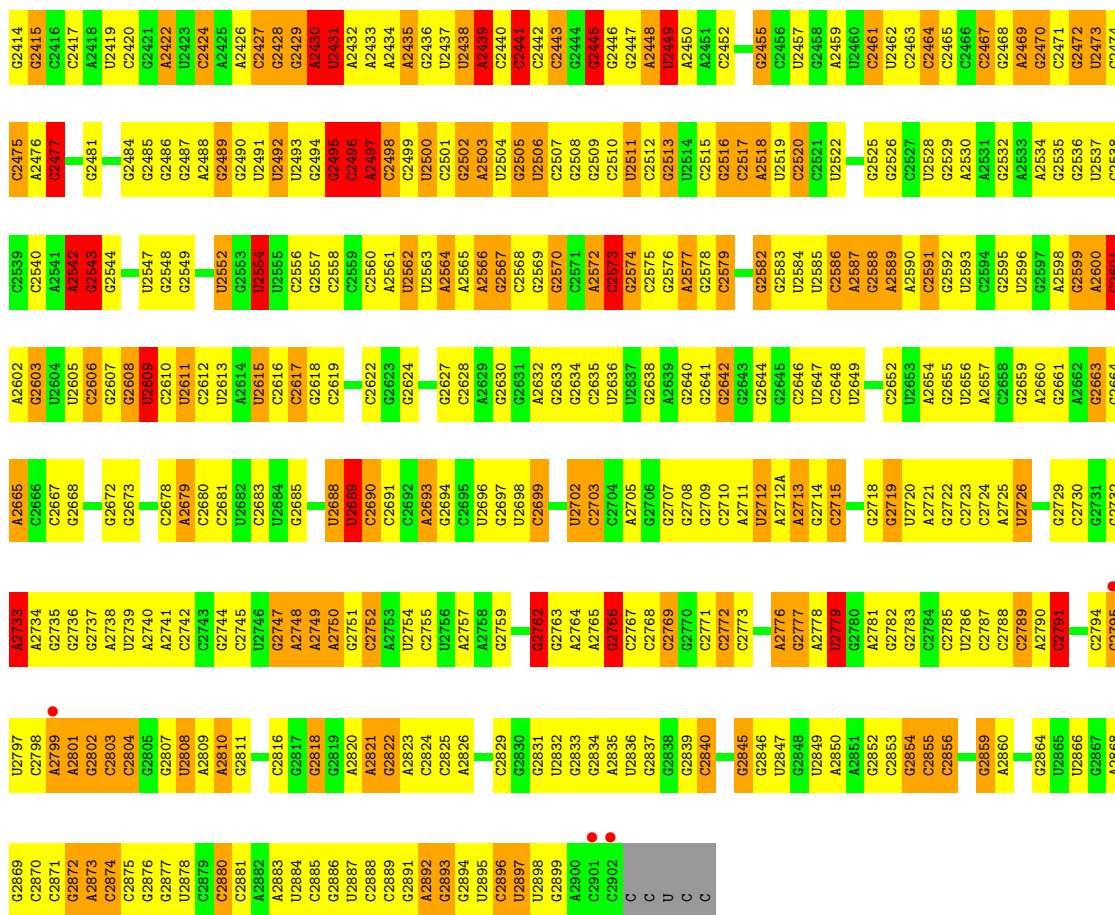


| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|--------|-------|-------|
| U2233 | G2093 | G1959 | G1896 | A1819 | G1758 | G1666 | C1604 | U1540 | G1475 | A1412 | G1348 | A1284 |
| G2234 | G2094 | A1960 | G1897 | U1820 | A1759 | G1667 | C1605 | U1541 | G1478 | A1413 | A1349 | G1285 |
| G2237 | G2095 | C1961 | U1898 | A1821 | A1760 | A1668 | G1606 | A1542 | G1479 | G1414 | A1350 | A1286 |
| G2238 | U2096 | C1962 | G1899 | G1822 | C1761 | A1669 | C1607 | A1543 | G1479 | G1415 | C1351 | A1287 |
| G2239 | G2101 | U1963 | A1900 | G1823 | A1762 | U1673 | A1609 | A1544 | G1483 | U1416 | U1352 | U1288 |
| G2240 | U1102 | G1964 | A1901 | G1824 | G1763 | G1674 | A1610 | A1545A | G1484 | G1417 | A1353 | C1289 |
| A2241 | G2105 | C1965 | C1902 | A1825 | G1764 | C1675 | A1611 | G1546 | G1485 | G1418 | A1354 | C1290 |
| G2165 | G2106 | A1966 | G1903 | G1826 | C1765 | A1676 | C1612 | C1547 | A1486 | A1419 | G1355 | C1291 |
| G2167 | G2107 | G1967 | G1904 | G1827 | U1766 | A1677 | G1613 | C1548 | G1487 | G1421 | G1356 | U1292 |
| U2243 | C2107 | G1968 | C1905 | G1828 | C1767 | G1678 | A1614 | C1549 | U1488 | G1422 | G1358 | U1292 |
| U2244 | G2108 | A1969 | G1906 | A1829 | U1768 | G1679 | C1615 | C1550 | U1489 | G1423 | A1359 | C1297 |
| G2245 | U1109 | A1970 | G1907 | G1830 | G1769 | U1680 | C1616 | C1551 | A1490 | G1424 | A1360 | C1298 |
| G2246 | U1110 | C1971 | C1908 | G1831 | G1770 | G1681 | C1617 | G1552 | G1491 | G1425 | G1362 | C1299 |
| A2171 | G2111 | A1972 | C1909 | C1832 | C1771 | G1682 | A1618 | A1553 | C1492 | G1426 | G1363 | U1300 |
| G2248 | G2112 | G1973 | U1910 | U1833 | G1772 | C1683 | G1619 | A1554 | C1493 | G1427 | U1301 | A1301 |
| U2249 | C2112 | C1974 | G1911 | U1834 | A1773 | C1684 | G1620 | G1557 | A1496 | A1428 | A1364 | A1302 |
| G2250 | U2113 | G1975 | A1912 | G1835 | C1774 | C1685 | U1621 | A1558 | U1497 | C1429 | A1365 | A1303 |
| G2251 | A2114 | U1976 | A1913 | G1836 | U1775 | C1686 | U1622 | G1559 | C1498 | C1430 | A1366 | C1304 |
| G2252 | G2115 | A1977 | G1914 | G1837 | G1776 | G1687 | G1622 | G1560 | C1499 | U1431 | G1367 | C1305 |
| G2253 | G2116 | A1978 | U1915 | C1838 | U1777 | G1688 | C1625 | G1561 | C1500 | U1432 | G1368 | C1306 |
| C2177 | A2117 | C1979 | A1916 | G1839 | U1778 | U1689 | U1626 | G1564 | C1501 | U1433 | G1370 | A1307 |
| C2178 | G2118 | G1980 | G2049 | U1840 | A1779 | A1690 | G1627 | C1565 | C1502 | U1434 | G1371 | A1308 |
| U2180 | U2119 | A1981 | A1917 | G1841 | U1780 | U1691 | G1628 | C1566 | U1503 | C1437 | G1372 | G1309 |
| G2181 | G2120 | G1982 | A1918 | G1842 | C1781 | U1692 | U1629 | C1567 | C1504 | U1438 | A1373 | G1310 |
| G2182 | G2121 | C1983 | A1919 | C1843 | G1782 | U1693 | G1630 | A1568 | C1505 | U1439 | G1374 | G1311 |
| C2183 | U1222 | G1984 | C1920 | C1844 | A1783 | C1694 | G1633 | A1569 | C1506 | U1440 | G1375 | U1312 |
| G2184 | G2123 | A1985 | U1923 | A1847 | A1784 | G1695 | G1634 | A1570 | A1507 | G1441 | G1376 | U1313 |
| G2185 | G2124 | G1986 | C1924 | A1848 | A1785 | C1696 | U1635 | A1571 | C1508 | G1442 | G1377 | C1314 |
| G2186 | G2125 | G1987 | U1925 | G1849 | A1786 | G1697 | A1634 | C1572 | C1509 | G1443 | A1378 | C1315 |
| G2187 | G2126 | G1988 | U1926 | U1850 | U1787 | G1698 | G1635 | C1573 | A1510 | G1444 | A1379 | U1316 |
| G2188 | G2127 | G1989 | A1927 | C1852 | C1788 | G1699 | C1636 | C1574 | G1512 | A1444A | G1380 | A1317 |
| U2189 | C2128 | C1990 | U1928 | A1853 | A1789 | G1699 | A1637 | C1577 | C1513 | C1446 | G1381 | C1318 |
| U2190 | C2129 | U1991 | G1929 | G1856 | C1790 | A1700 | C1638 | G1574 | U1514 | G1447 | A1383 | A1321 |
| A2267 | U1232 | G1992 | G1930 | G1857 | G1791 | G1705 | U1639 | G1577 | C1515 | G1448 | G1384 | G1324 |
| A2268 | G2133 | U1993 | A1932 | G1858 | C1793 | U1706 | C1640 | A1578 | U1516 | A1449 | G1385 | G1325 |
| A2198 | A2134 | G1987 | G1933 | A1859 | U1794 | U1709 | G1642 | A1579 | G1517 | G1448 | G1386 | U1326 |
| A2199 | A2135 | G1988 | C1934 | G1860 | C1795 | C1710 | G1643 | A1580 | C1518 | A1449 | G1387 | G1327 |
| C2205 | C2136 | C1999 | G1935 | U1864 | U1796 | G1717 | G1645 | C1581 | C1519 | G1450 | G1388 | G1328 |
| C2206 | C2137 | G2000 | A1936 | U1869 | C1797 | G1718 | C1646 | C1582 | U1520 | A1453 | G1389 | G1329 |
| C2207 | C2138 | A2001 | A1937 | G1870 | U1798 | G1719 | C1647 | C1585 | G1521 | U1454 | U1390 | U1330 |
| U2208 | C2139 | G2002 | A1938 | C1871 | G1800 | G1725 | C1648 | A1586 | G1522 | G1455 | U1391 | C1331 |
| C2209 | C2140 | G2003 | U1939 | A1871 | G1801 | G1728 | C1649 | A1587 | U1523 | G1456 | A1392 | G1332 |
| G2210 | G2141 | G2004 | U1940 | A1872 | A1802 | G1729 | G1651 | C1588 | U1524 | G1459 | A1393 | C1333 |
| G2211 | C2142 | C1941 | C1942 | G1878 | A1803 | U1729 | A1652 | C1589 | G1525 | A1460 | U1394 | G1334 |
| A2212 | C2143 | G2009 | C1943 | C1879 | C1804 | U1730 | G1653 | C1590 | G1526 | G1461 | A1395 | G1334 |
| C2213 | U2144 | G2010 | U1943 | G1882 | U1805 | G1731 | A1654 | G1591 | G1527 | C1462 | U1396 | G1337 |
| G2215 | C2145 | U2011 | U1946 | G1883 | C1806 | A1732 | A1655 | C1592 | A1528 | C1463 | U1397 | G1338 |
| G2216 | C2146 | G2012 | U1947 | C1884 | G1807 | G1742 | C1656 | G1593 | G1530 | C1464 | G1398 | G1339 |
| G2217 | G2147 | A2013 | G1948 | C1886 | G1810 | C1748 | C1657 | G1594 | G1533 | C1467 | G1403 | U1340 |
| G2218 | G2148 | A2014 | G1949 | C1887 | A1811 | G1749 | C1658 | A1596 | G1534 | C1468 | C1404 | A1342 |
| G2219 | G2149 | A2015 | G1950 | G1888 | G1812 | A1749 | U1659 | A1597 | U1535 | G1469 | U1405 | G1343 |
| G2220 | U2150 | G2016 | C1951 | A1889 | A1812 | G1753 | C1660 | G1595 | G1536 | G1470 | U1406 | G1344 |
| A2225 | G2151 | U2017 | U1951 | A1890 | G1813 | C1754 | G1661 | G1596 | C1537 | A1471 | C1407 | G1345 |
| G2226 | G2152 | G2018 | A1952 | A1891 | G1814 | C1755 | C1662 | G1597 | U1537 | A1472 | C1408 | G1346 |
| G2227 | G2153 | G2019 | A1953 | C1892 | A1815 | A1756 | C1663 | G1600 | G1538 | G1473 | U1409 | G1347 |
| G2228 | G2154 | U1955 | U1956 | C1893 | A1816 | C1757 | C1664 | G1601 | C1539 | G1474 | C1409 | G1347 |
| U2291 | G2155 | C2020 | C1957 | C1894 | G1817 | A1758 | C1665 | G1602 | G1539 | G1475 | C1409 | G1347 |
| C2292 | G2156 | U2022 | U1958 | C1895 | U1818 | U1757 | A1665 | A1603 | G1539 | G1476 | C1409 | G1347 |
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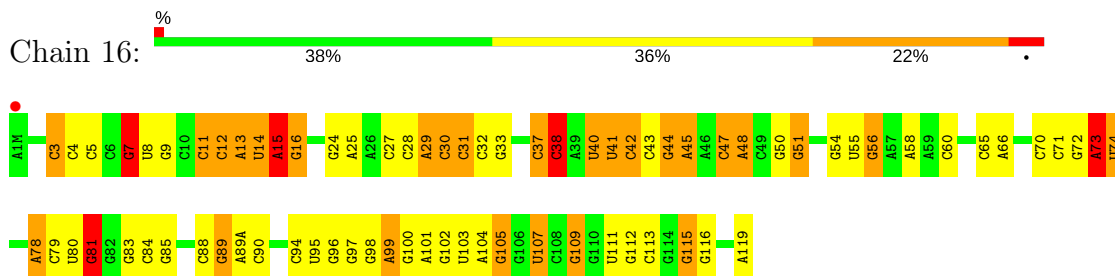


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| G1324 | C1258 | G1192 | A | A1000 | C936 | G873 | U811 | C749 | C679 | U639 | U568 | A492 | U421 | G333 |
| G1325 | G1259 | U1130 | G | A1001 | U937 | C876 | C812 | A750 | G680 | C540 | U569 | G493 | A422 | C336 |
| U1326 | G1260 | G1131 | A1069 | G1002 | U938 | C877 | U813 | A751 | G681 | C541 | G570 | G494 | A423 | C343 |
| G1327 | C1261 | A1132 | C1070 | C1006 | G940 | U877 | C814 | A752 | G682 | G642 | A571 | G495 | G424 | C343 |
| G1328 | U1133 | U1133 | G1071 | C1007 | A941 | U878 | C815 | C753 | G683 | C545 | G573 | A347 | G425 | C343 |
| U1139 | G1135 | G1135 | C1072 | C1008 | G942 | G879 | C816 | C754 | G684 | A646 | C574 | A498 | C426 | A347 |
| C1200 | G1136 | G1136 | A1073 | G1009 | U943 | G | C817 | C755 | G686 | G647 | C575 | U499 | G427 | G352 |
| G1201 | G1137 | G1138 | G1074 | A1010 | G944 | G | A819 | C756 | G687 | G648 | U576 | A501 | A428 | G352 |
| G1202 | G1138 | G1139 | C1075 | G1011 | A945 | G | A820 | U757 | U688 | G649 | G577 | A502 | A432 | U358 |
| G1203 | G1139 | G1140 | C1076 | G1012 | G946 | C | A821 | G760 | A689 | C650 | A578 | A503 | A433 | U358 |
| A1204 | U | C1140 | U | U1013 | G947 | C | U822 | A761 | G690 | G651 | G579 | U504 | U434 | G361 |
| U1205 | C | U141 | C | U1014 | G948 | C | C823 | G764 | C692 | A653 | C580 | U505 | U435 | U362 |
| G1206 | A1085 | U142 | A | G1015 | C949 | A | A824 | A765 | G693 | G654 | C581 | A508 | C436 | U363 |
| C1207 | A1086 | A1142A | U | G1016 | G950 | C | U827 | G766 | C694 | A654A | G585 | U441 | G442 | U363E |
| G1271 | U | A1143 | U | G1017 | C951 | C | U828 | U767 | G695 | C654B | G586 | G443 | G443 | A363F |
| A1272 | U | G1144 | U | G1018 | G952 | A | A829 | G768 | A689 | G654C | C587 | C444 | C444 | A363F |
| U1273 | U | C1145 | U | U1019 | A953 | C | C830 | G769 | G700 | C | C588 | G445 | C445 | G370 |
| A1274 | A | G1146 | A | G1020 | G954 | C | C831 | G770 | G701 | C | A513 | A449 | G450 | A371 |
| U1275 | A1085 | G1147 | A | A1021 | C955 | C | U832 | G771 | G702 | C | A514 | A451 | G451 | U373 |
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| A1277 | A1087 | G1149 | U | U1023 | C957 | A | C834 | G773 | U704 | C | A516 | C376 | C376 | C375 |
| A1278 | A1088 | C1150 | U | G1024 | U958 | C | C835 | A774 | G705 | A | C517 | C453 | C453 | C377 |
| G1279 | A1089 | G1151 | U | G1025 | A959 | A | A836 | G775 | A705 | C | U524 | A454 | A454 | U380 |
| U1280 | G1091 | C1152 | U | U1026 | A960 | C | C837 | G776 | G707 | G | U525 | A455 | A455 | G382 |
| C1281 | C1092 | G1153 | U | A1027 | C961 | C | U838 | A777 | G708 | C | U526 | A456 | A456 | G383 |
| U1282 | G1093 | A1154 | U | A1028 | G968 | C | U839 | G778 | C708 | C | C501 | A457 | A457 | G384 |
| G1283 | C1094 | G1155 | U | G1029 | U969 | C | C840 | U779 | G713 | G | G602 | A458 | A458 | G385 |
| A1284 | A1095 | A1156 | U | G1030 | C970 | C | C843 | G780 | G717 | C | A603 | A459 | A459 | U390 |
| C1285 | U | A1157 | U | G1031 | C971 | C | C844 | A781 | G717 | C | G604 | A460 | A460 | G388 |
| A1286 | A | A1158 | U | A1032 | G972 | C | C845 | A782 | G717 | C | C505 | A461 | A461 | G389 |
| C1287 | U | C1159 | U | U1033 | G973 | C | C846 | A783 | A722 | C | G531 | C462 | C462 | G391 |
| U1288 | A1098 | G1160 | U | G1036 | C974 | C | U847 | G785 | G723 | C | A532 | G463 | G463 | U397 |
| C1289 | C1100 | C1162 | U | G1037 | A975 | C | C848 | G786 | U724 | C | G533 | U464 | U464 | G398 |
| U1290 | U1101 | G1165 | U | C1041 | C976 | C | A849 | U787 | G725 | C | U534 | A465 | A465 | G399 |
| C1291 | G1102 | C1166 | U | G1042 | G977 | C | C850 | A788 | G726 | C | C535 | A466 | A466 | U400 |
| C1292 | A1103 | U1167 | U | C1043 | C978 | C | U851 | A789 | A727 | C | A536 | G467 | G467 | A401 |
| G1293 | C1104 | G1168 | U | G1044 | G979 | C | C852 | C790 | G728 | C | C537 | U475 | U475 | A402 |
| C1298 | U1105 | G1169 | U | A1045 | C980 | C | C853 | C791 | G729 | C | G539 | G468 | G468 | U403 |
| G1299 | G1106 | G1170 | U | A | A980 | C | C854 | G792 | C730 | C | G540 | A469 | A469 | U404 |
| A1300 | G1107 | G1171 | U | A | A981 | C | C855 | A793 | G731 | C | C543 | A470 | A470 | U405 |
| C1301 | U1108 | C1172 | U | G1047 | C982 | C | C856 | G794 | G732 | C | G620 | A471 | A471 | C397 |
| G1302 | C1109 | G1173 | U | A1048 | A983 | C | C857 | C795 | G733 | C | A621 | A472 | A472 | G400 |
| C1303 | G1110 | U1174 | U | C1049 | A984 | C | U858 | C796 | A734 | C | C546 | G473 | G473 | A401 |
| G1304 | C1111 | G1175 | U | A1050 | C985 | C | U859 | C797 | A735 | C | G623 | U474 | U474 | A402 |
| A1308 | G1112 | C1176 | U | A1054 | C986 | C | U860 | G798 | G736 | C | G624 | G476 | G476 | U403 |
| G1309 | U1113 | C1177 | U | G1055 | A987 | C | A861 | C799 | C737 | C | A627 | A479 | A479 | U404 |
| C1310 | G1114 | C1178 | U | G1056 | A988 | C | C862 | A800 | G738 | C | G556 | A480 | A480 | U405 |
| U1311 | C1115 | C1179 | U | G1057 | A989 | C | A863 | G801 | G739 | C | U557 | A481 | A481 | C407 |
| G1312 | C1116 | C1180 | U | A1058 | C991 | C | C864 | A802 | U740 | C | G630 | G482 | G482 | G408 |
| U1313 | C1117 | C1181 | U | U1059 | C992 | C | C865 | U803 | G741 | C | A631 | A483 | A483 | C409 |
| C1314 | C1118 | G1182 | U | G1060 | G993 | C | A866 | A804 | G742 | C | A632 | A484 | A484 | G410 |
| A1247 | G1119 | C1183 | U | U1061 | C994 | C | C867 | G805 | G743 | C | U562 | C485 | C485 | G411 |
| G1248 | C1120 | C1184 | U | G1062 | C995 | C | U868 | C806 | G744 | C | G563 | C486 | C486 | G412 |
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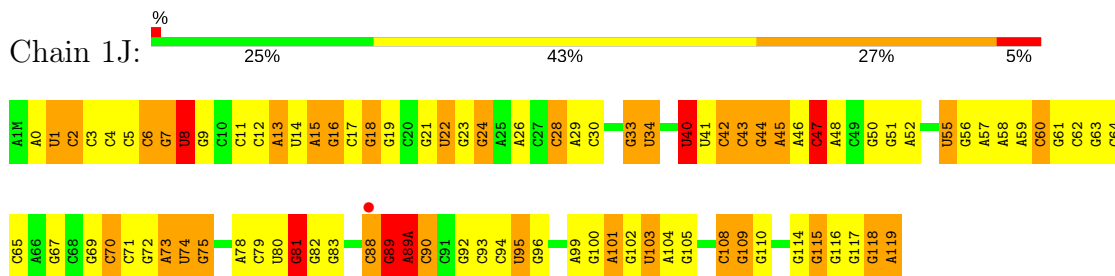




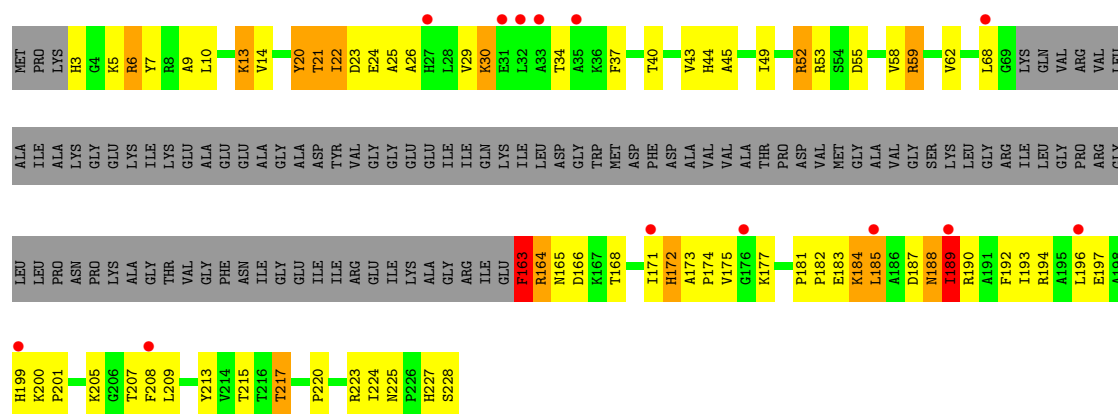
• Molecule 27: 5S ribosomal RNA



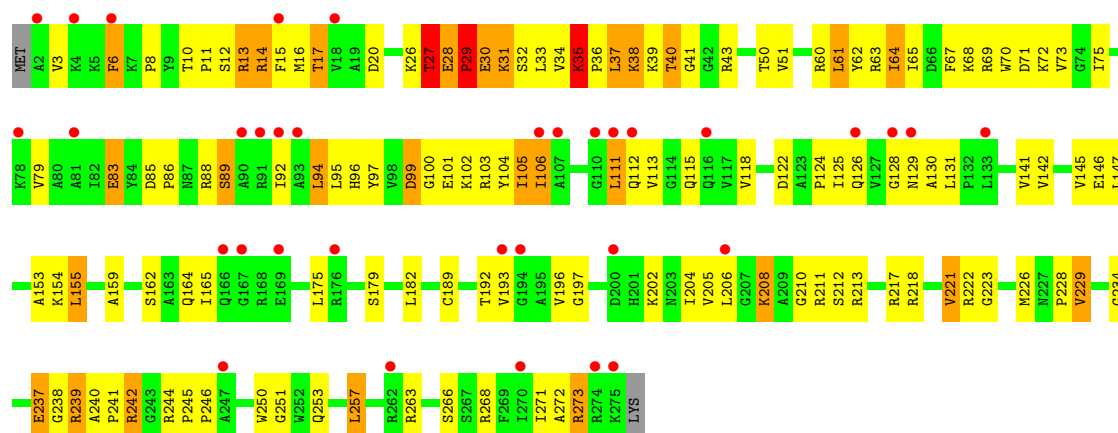
• Molecule 27: 5S ribosomal RNA



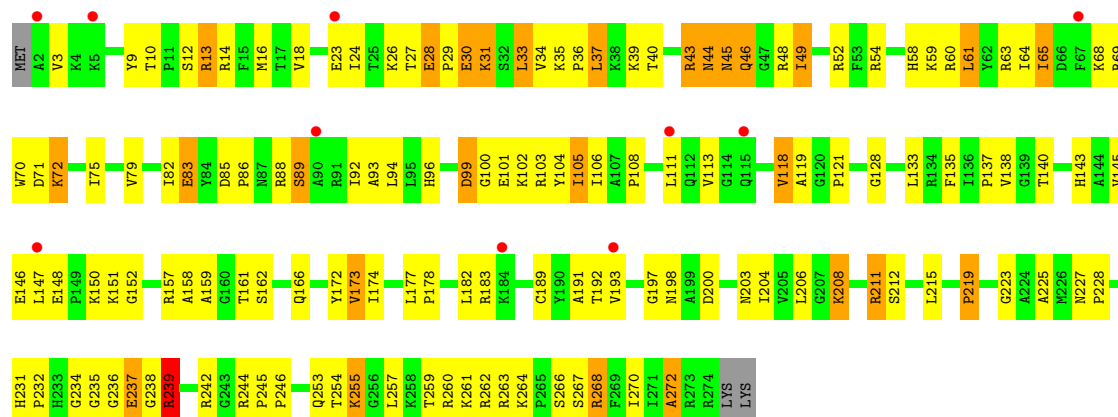
• Molecule 28: 50S ribosomal protein L1



• Molecule 29: 50S ribosomal protein L2

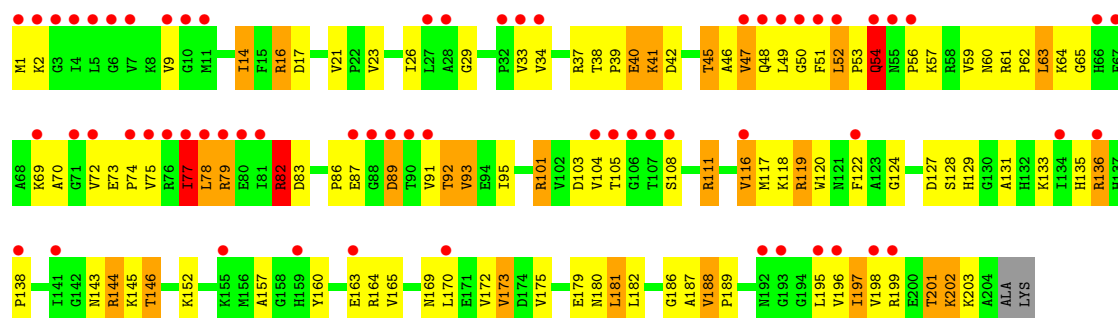


• Molecule 29: 50S ribosomal protein L2

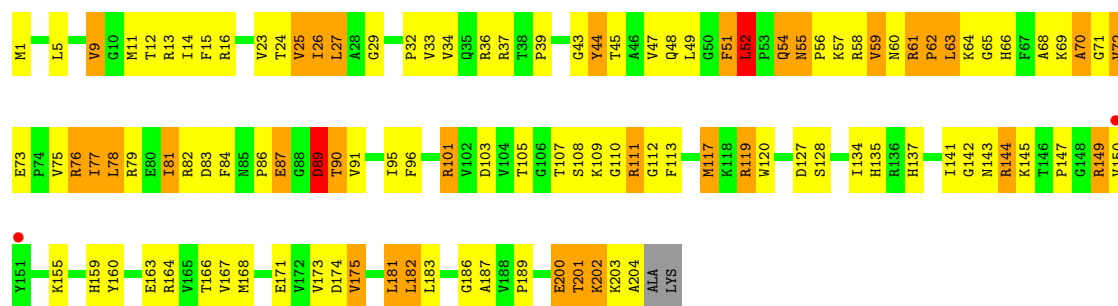
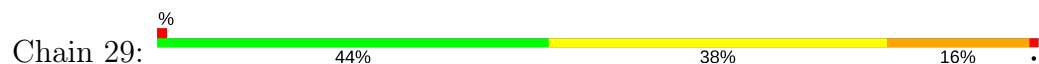


• Molecule 30: 50S ribosomal protein L3

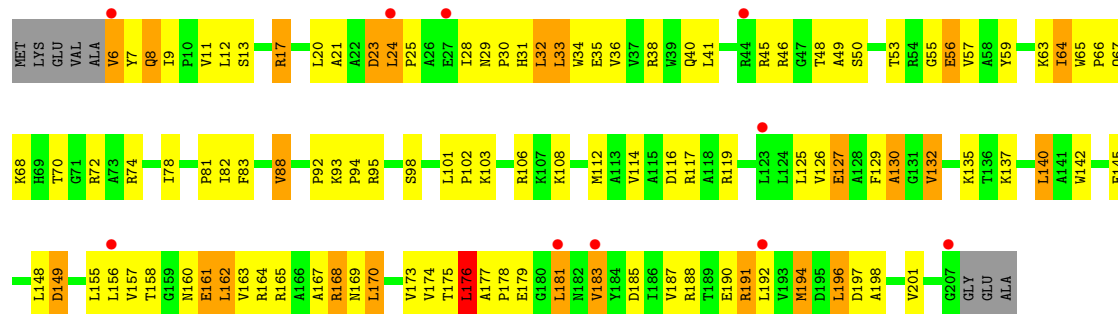
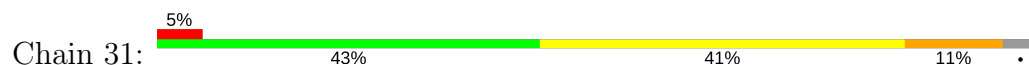




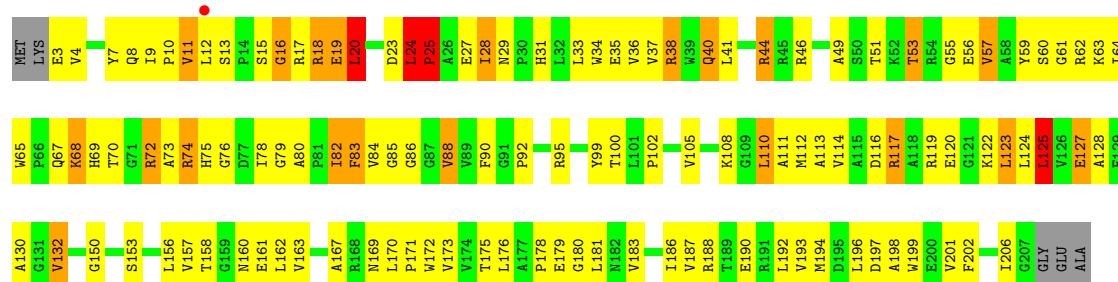
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4



• Molecule 31: 50S ribosomal protein L4



Chain 41:

2% 43% 46% 9%

Met P2 L3 D4 V5 A6 L7 K8 R9 K10 Y11 Y12 E13 E14 V15 R16 P17 E18 L19 L20 L21 R22 R23 Q24 V25 V26 Q27 V28 V31 P32 R33 L34 A35 E36 K37 V38 L43 G44 A45 A46 K47 E48 R51 L52 L53 A56 A57 L60 A61 L63 T64 G65 G66 Q67

P68 A69 V70 S76 L77 S78 R79 F80 K81 L82 R83 R84 G85 M86 M87 P88 E89 L90 R91 V92 Y93 T94 R94 A95 R96 D97 R98 R99 M100 I101 F102 L103 E104 K105 L106 L107 L108 V109 A110 L111 P112 R113 L114 R115 D116 F117 R118 N121 P122 M123 S124 R128 Y131 L135 R136 T137

Chain 49:

| Amino Acid | Segment |
|------------|---------|
| Met | Red |
| P2 | Red |
| L3 | Red |
| D4 | Red |
| V5 | Red |
| A6 | Red |
| L7 | Red |
| R9 | Red |
| K10 | Red |
| Y11 | Red |
| Y12 | Red |
| E13 | Red |
| E14 | Red |
| V15 | Red |
| R16 | Red |
| P17 | Red |
| E18 | Red |
| L19 | Red |
| I20 | Red |
| R21 | Red |
| R22 | Red |
| F23 | Red |
| G24 | Red |
| Y25 | Red |
| Q26 | Red |
| N27 | Red |
| V28 | Red |
| W29 | Red |
| P32 | Red |
| R33 | Red |
| L34 | Red |
| E35 | Red |
| K36 | Red |
| V37 | Red |
| V38 | Red |
| I39 | Red |
| N40 | Red |
| Q41 | Red |
| G42 | Red |
| L43 | Red |
| G44 | Red |
| E45 | Red |
| A46 | Red |
| K47 | Red |
| E48 | Red |
| D49 | Red |
| A50 | Red |
| R51 | Red |
| I52 | Red |
| L53 | Red |
| E54 | Red |
| K55 | Red |
| A56 | Red |
| A57 | Red |
| Q58 | Red |
| E59 | Red |
| L60 | Red |
| A61 | Red |
| L62 | Red |
| I63 | Red |
| T64 | Red |
| K67 | Red |
| P68 | Red |
| A69 | Red |
| V70 | Red |
| T71 | Red |
| R72 | Red |
| K75 | Red |
| S76 | Red |
| I77 | Red |
| F80 | Red |
| K81 | Red |
| L82 | Red |
| K83 | Red |
| A84 | Red |
| G85 | Red |
| M86 | Red |
| P87 | Red |
| I88 | Red |
| G89 | Red |
| L90 | Red |
| R91 | Red |
| V92 | Red |
| T93 | Red |
| L94 | Red |
| R95 | Red |
| R96 | Red |
| D97 | Red |
| R98 | Red |
| M99 | Red |
| W100 | Red |
| I101 | Red |
| F102 | Red |
| L103 | Red |
| E104 | Red |
| K105 | Red |
| L106 | Red |
| L107 | Red |
| L111 | Red |
| I114 | Red |
| R115 | Red |
| D116 | Red |
| F117 | Red |
| R118 | Red |
| G119 | Red |
| L120 | Red |
| N123 | Red |
| S124 | Red |
| F125 | Red |
| N130 | Red |
| Y131 | Red |
| M132 | Red |
| L133 | Red |
| G134 | Red |
| L135 | Red |
| L136 | Red |
| E137 | Red |
| L138 | Red |
| L139 | Red |
| L140 | Red |
| F141 | Red |
| P142 | Red |
| E143 | Red |
| L144 | Red |
| V145 | Red |
| V146 | Red |
| D147 | Red |
| M148 | Red |
| V149 | Red |
| D150 | Red |
| A151 | Red |
| L152 | Red |
| R153 | Red |
| G154 | Red |
| M155 | Red |
| D156 | Red |
| L157 | Red |
| A158 | Red |
| V159 | Red |
| V160 | Red |
| T161 | Red |
| F162 | Red |
| A163 | Red |
| D166 | Red |
| E167 | Red |
| R170 | Red |
| A171 | Red |
| L172 | Red |
| L173 | Red |
| E174 | Red |
| L175 | Red |
| L176 | Red |
| G177 | Red |
| F178 | Red |
| P179 | Red |
| F180 | Red |
| L181 | Red |
| Lys | Red |

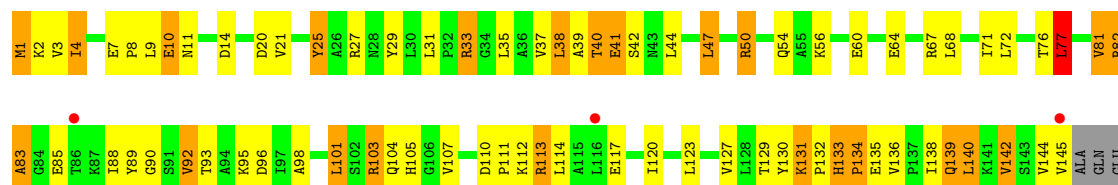
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Chain 59:

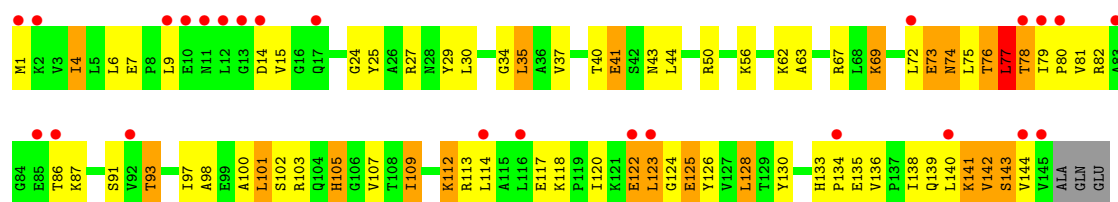
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| ARG | 1 |
| ILE | 1 |
| GLY | 1 |
| R6 | 1 |
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| V52 | 1 |
| S56 | 1 |
| D57 | 1 |
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| R59 | 1 |
| R60 | 1 |
| H61 | 1 |
| PHE | 1 |
| K62 | 1 |
| A63 | 1 |



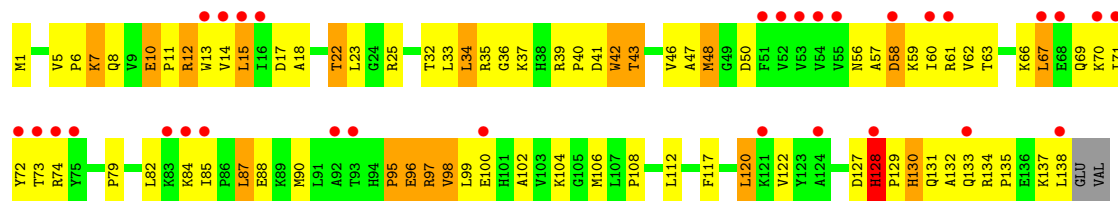
• Molecule 34: 50S ribosomal protein L9

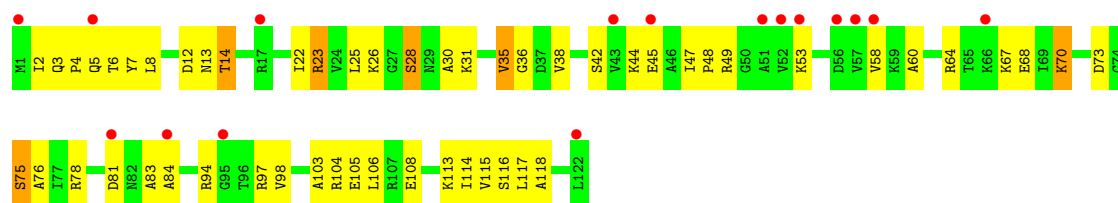


• Molecule 34: 50S ribosomal protein L9

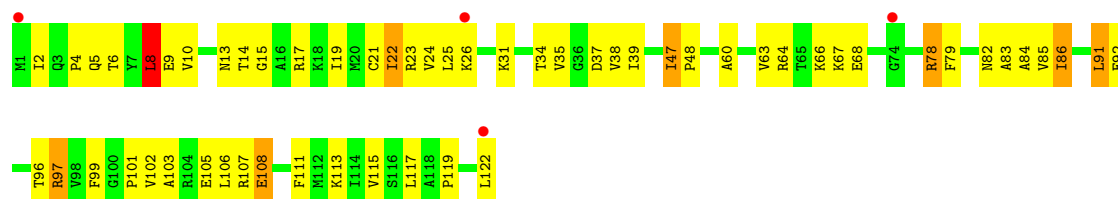


• Molecule 35: 50S ribosomal protein L13

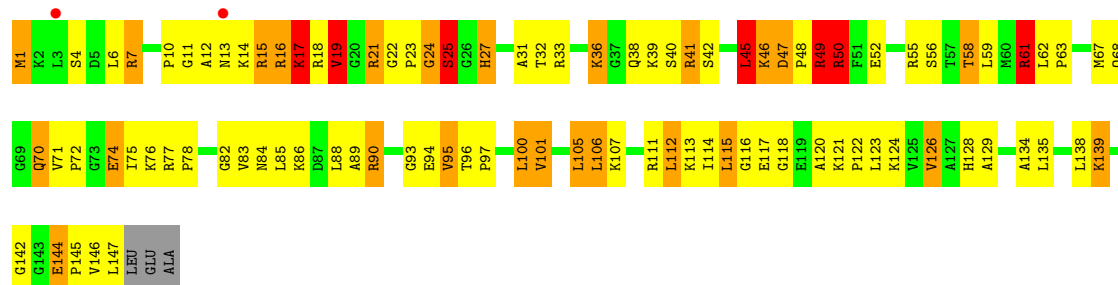




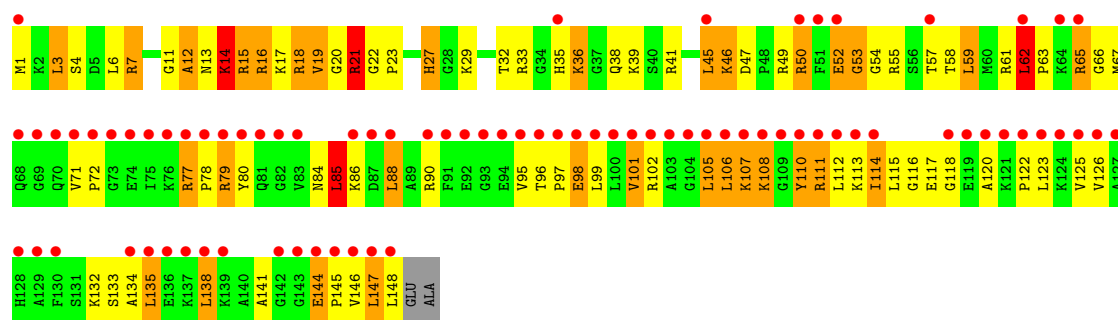
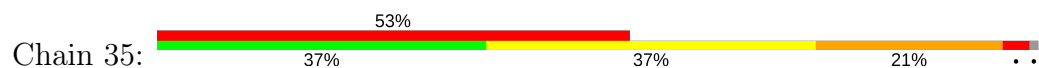
• Molecule 36: 50S ribosomal protein L14



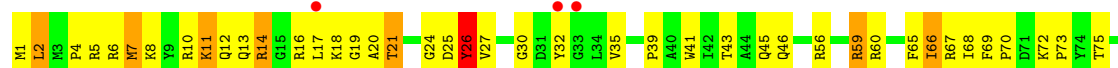
• Molecule 37: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L15

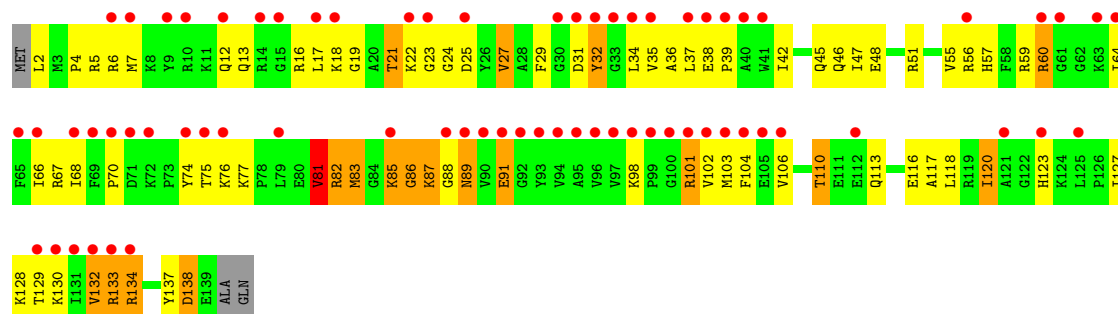
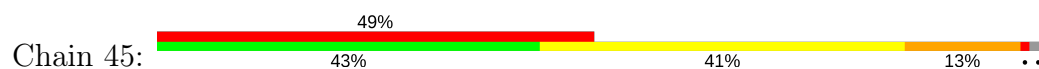


• Molecule 38: 50S ribosomal protein L16

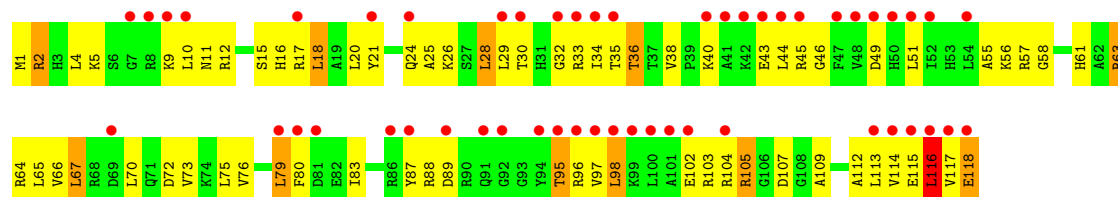




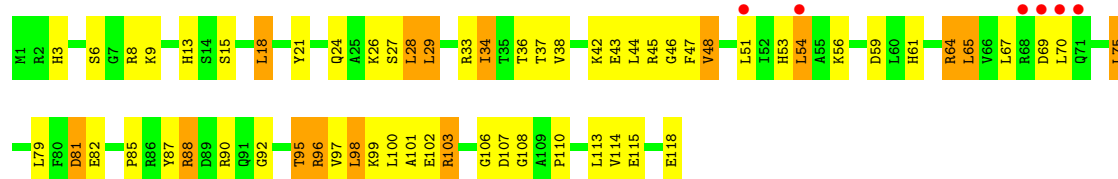
• Molecule 38: 50S ribosomal protein L16



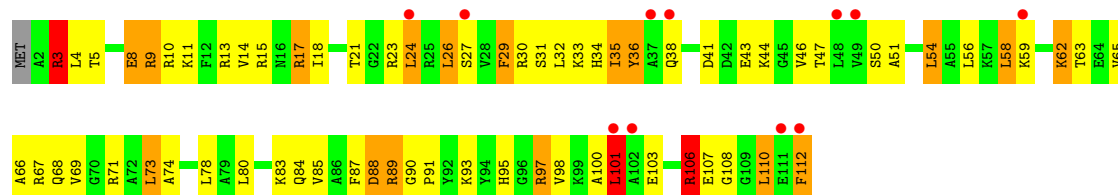
• Molecule 39: 50S ribosomal protein L17



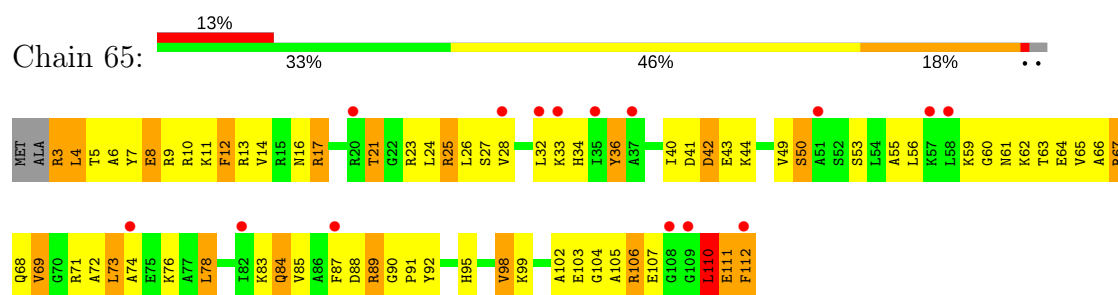
• Molecule 39: 50S ribosomal protein L17



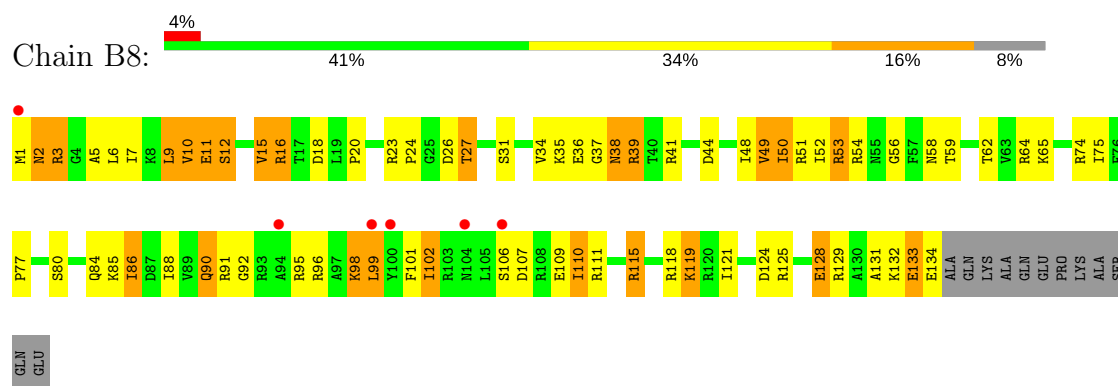
• Molecule 40: 50S ribosomal protein L18



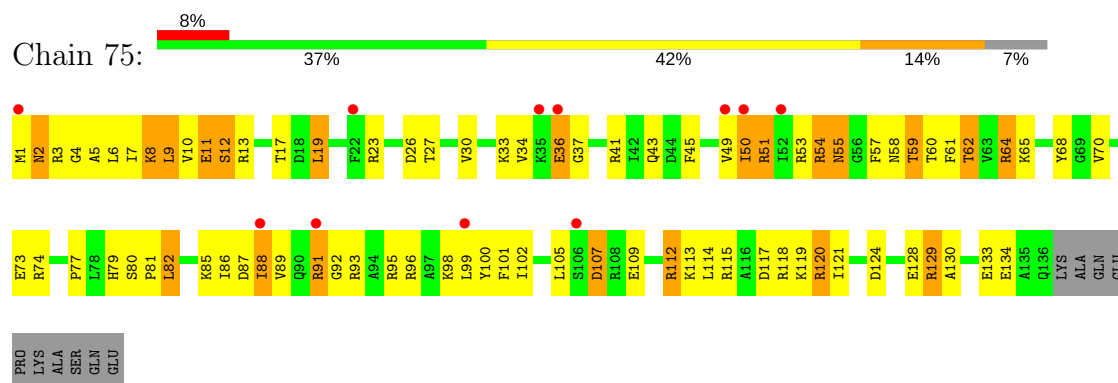
• Molecule 40: 50S ribosomal protein L18



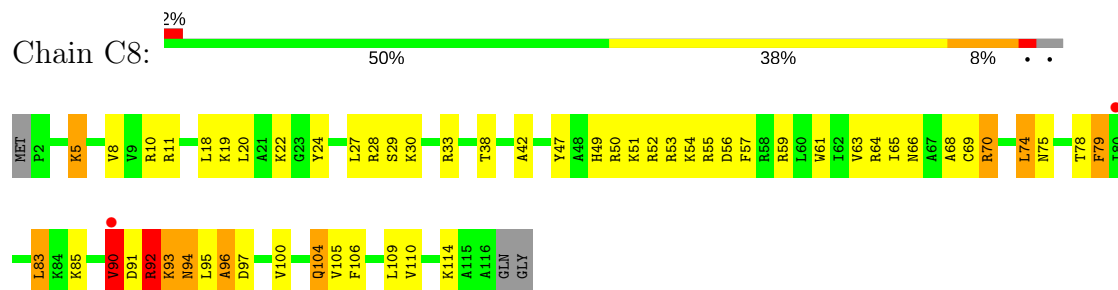
• Molecule 41: 50S ribosomal protein L19



• Molecule 41: 50S ribosomal protein L19

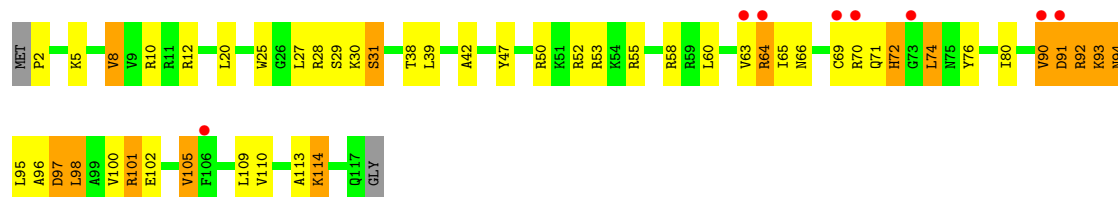


• Molecule 42: 50S ribosomal protein L20

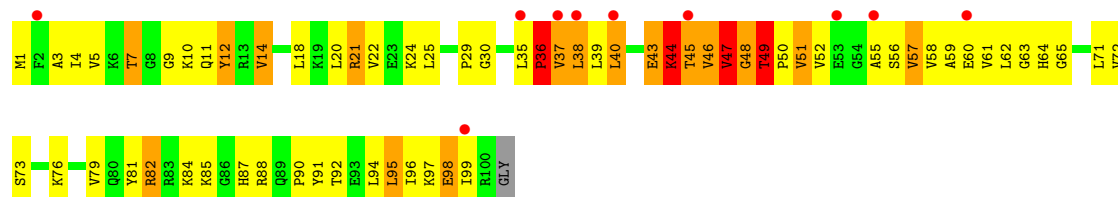


• Molecule 42: 50S ribosomal protein L20

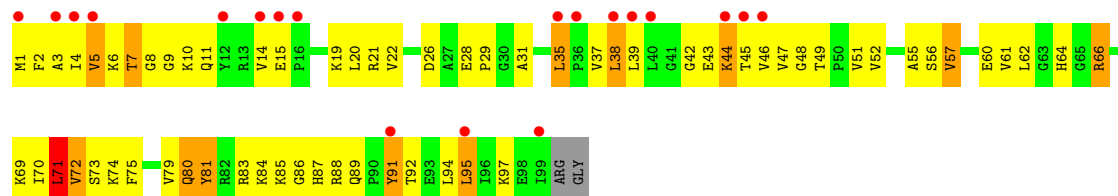




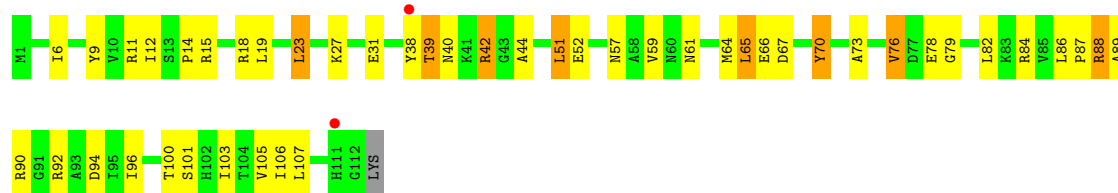
• Molecule 43: 50S ribosomal protein L21



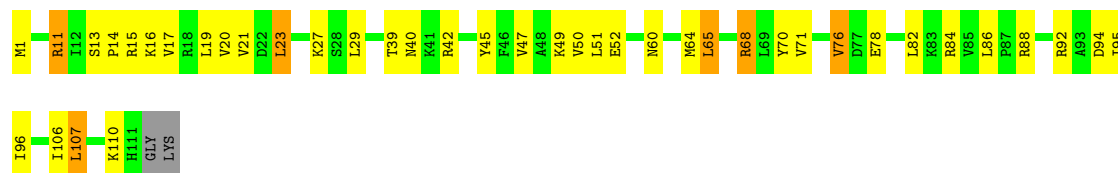
• Molecule 43: 50S ribosomal protein L21



• Molecule 44: 50S ribosomal protein L22



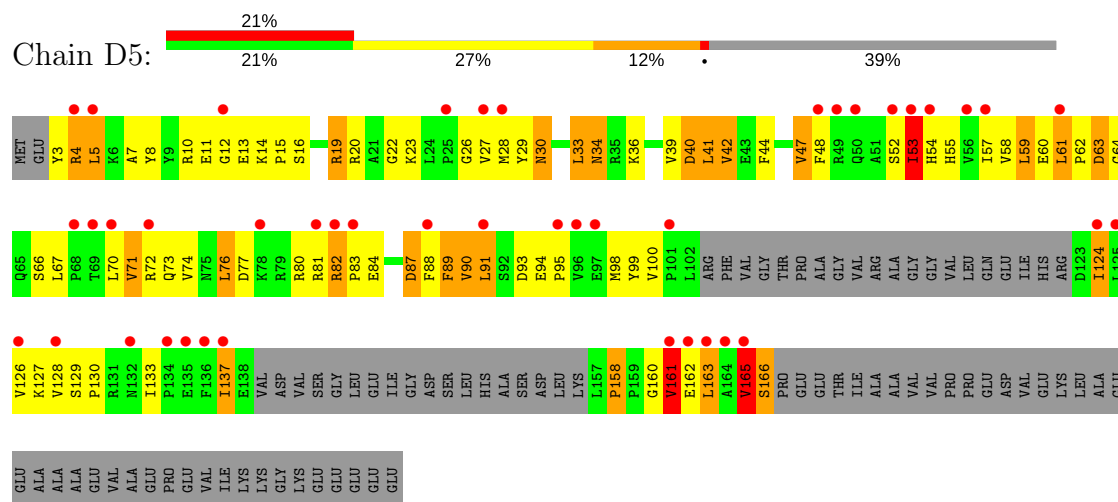
• Molecule 44: 50S ribosomal protein L22



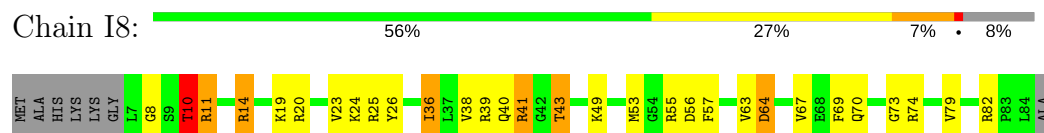
• Molecule 45: 50S ribosomal protein L23

GLU
GLU
GLU

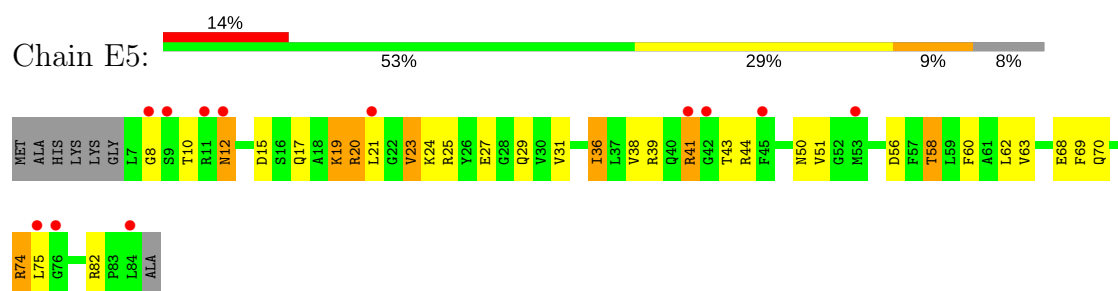
• Molecule 47: 50S ribosomal protein L25



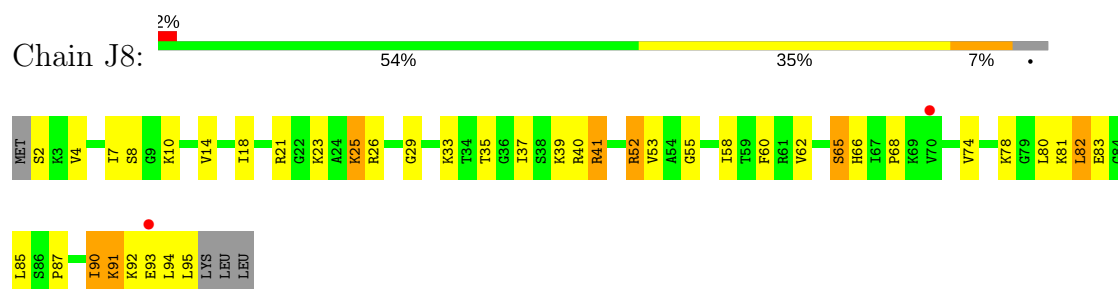
• Molecule 48: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L27

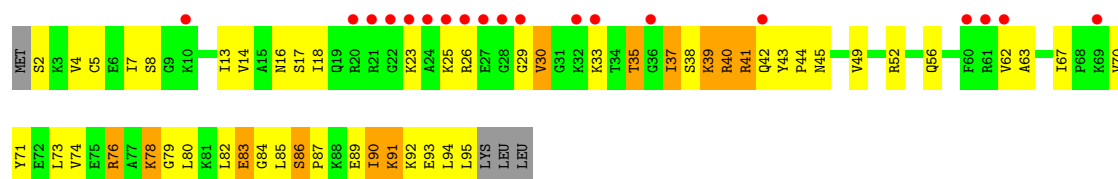


• Molecule 49: 50S ribosomal protein L28

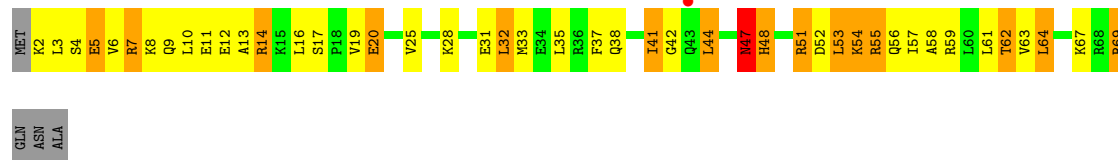


• Molecule 49: 50S ribosomal protein L28

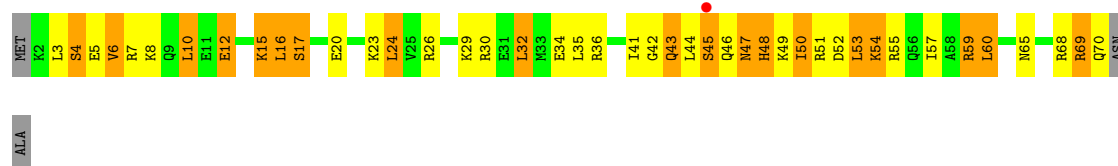




- Molecule 50: 50S ribosomal protein L29



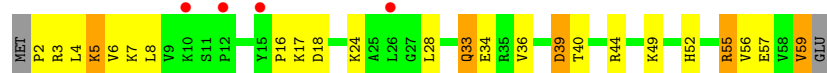
- Molecule 50: 50S ribosomal protein L29



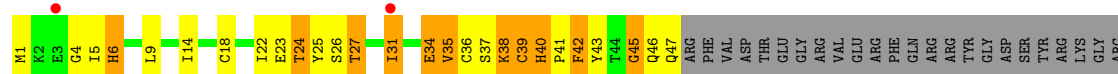
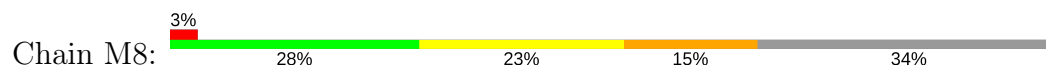
- Molecule 51: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L30

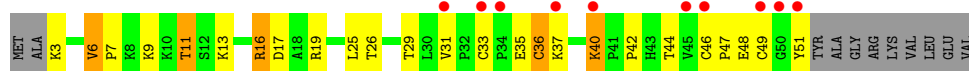


- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32





- Molecule 53: 50S ribosomal protein L32



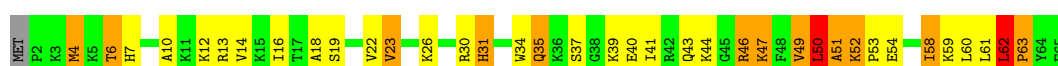
- Molecule 54: 50S ribosomal protein L34



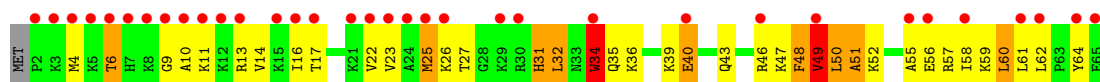
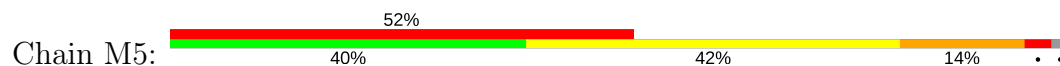
- Molecule 54: 50S ribosomal protein L34



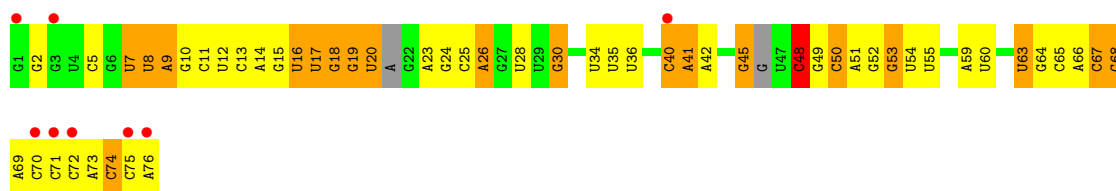
- Molecule 55: 50S ribosomal protein L35



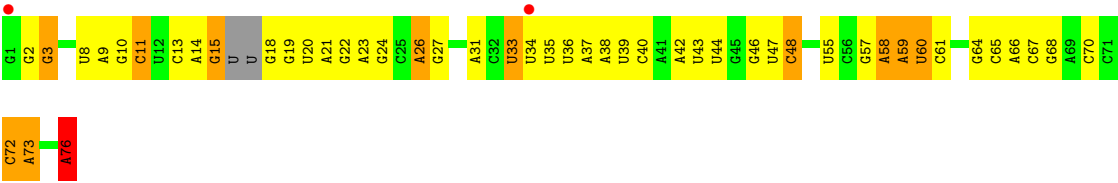
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA-Lys



- Molecule 57: tRNA-Lys



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.90Å 447.80Å 617.50Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 151.53 – 3.15 161.39 – 3.15 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (151.53-3.15) 93.3 (161.39-3.15) | Depositor EDS |
| R_{merge} | 0.31 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.57 (at 3.13Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.193 , 0.251 0.193 , 0.251 | Depositor DCC |
| R_{free} test set | 1974 reflections (0.20%) | DCC |
| Wilson B-factor (Å ²) | 84.4 | Xtriage |
| Anisotropy | 0.281 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 70.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 294304 | wwPDB-VP |
| Average B, all atoms (Å ²) | 106.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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, U8U, 7MG, SF4, MG, 4SU, T6A, 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 | 0.78 | 5/35994 (0.0%) | 1.45 | 459/56171 (0.8%) |
| 1 | 1G | 0.66 | 0/36258 | 1.30 | 243/56589 (0.4%) |
| 2 | 12 | 0.49 | 0/1742 | 0.74 | 1/2346 (0.0%) |
| 2 | 1E | 0.46 | 0/1908 | 0.69 | 0/2573 |
| 3 | 22 | 0.43 | 0/1552 | 0.70 | 2/2093 (0.1%) |
| 3 | 2E | 0.53 | 0/1629 | 0.72 | 0/2195 |
| 4 | 32 | 0.47 | 0/1732 | 0.72 | 2/2318 (0.1%) |
| 4 | 3E | 0.61 | 0/1732 | 0.79 | 2/2318 (0.1%) |
| 5 | 42 | 0.52 | 0/1138 | 0.73 | 1/1532 (0.1%) |
| 5 | 4E | 0.57 | 0/1158 | 0.75 | 0/1559 |
| 6 | 52 | 0.52 | 0/855 | 0.69 | 1/1154 (0.1%) |
| 6 | 5E | 0.53 | 0/850 | 0.70 | 0/1147 |
| 7 | 62 | 0.45 | 0/1122 | 0.68 | 0/1500 |
| 7 | 6E | 0.47 | 0/1230 | 0.65 | 0/1645 |
| 8 | 72 | 0.42 | 0/1135 | 0.61 | 0/1527 |
| 8 | 7E | 0.51 | 0/1135 | 0.74 | 0/1527 |
| 9 | 82 | 0.44 | 0/1002 | 0.65 | 0/1346 |
| 9 | 8E | 0.48 | 0/1024 | 0.70 | 1/1374 (0.1%) |
| 10 | 1A | 0.43 | 0/636 | 0.65 | 0/855 |
| 10 | 1I | 0.47 | 0/747 | 0.71 | 2/1006 (0.2%) |
| 11 | 2A | 0.47 | 0/850 | 0.67 | 0/1150 |
| 11 | 2I | 0.54 | 0/838 | 0.73 | 0/1133 |
| 12 | 3A | 0.54 | 0/963 | 0.76 | 1/1290 (0.1%) |
| 12 | 3I | 0.74 | 0/972 | 0.92 | 0/1301 |
| 13 | 4A | 0.47 | 0/898 | 0.69 | 1/1204 (0.1%) |
| 13 | 4I | 0.54 | 0/938 | 0.76 | 1/1258 (0.1%) |
| 14 | 5A | 0.46 | 0/475 | 0.76 | 1/632 (0.2%) |
| 14 | 5I | 0.58 | 0/505 | 0.76 | 0/671 |
| 15 | 6A | 0.46 | 0/740 | 0.65 | 1/987 (0.1%) |
| 15 | 6I | 0.51 | 0/744 | 0.69 | 0/992 |
| 16 | 7A | 0.49 | 0/721 | 0.69 | 0/970 |
| 16 | 7I | 0.48 | 0/687 | 0.74 | 0/925 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | 8A | 0.49 | 0/836 | 0.63 | 0/1117 |
| 17 | 8I | 0.64 | 2/836 (0.2%) | 0.77 | 0/1117 |
| 18 | 9A | 0.51 | 0/549 | 0.72 | 1/732 (0.1%) |
| 18 | 9I | 0.54 | 0/549 | 0.74 | 0/732 |
| 19 | AA | 0.45 | 0/480 | 0.76 | 0/648 |
| 19 | AI | 0.58 | 0/657 | 0.86 | 0/885 |
| 20 | BA | 0.46 | 0/759 | 0.69 | 0/1000 |
| 20 | BI | 0.44 | 0/748 | 0.63 | 0/986 |
| 21 | 1B | 0.43 | 0/212 | 0.60 | 0/277 |
| 21 | 1F | 0.44 | 0/203 | 0.67 | 0/266 |
| 22 | 1K | 0.64 | 0/1516 | 1.28 | 12/2350 (0.5%) |
| 23 | 2K | 0.83 | 0/1721 | 1.52 | 28/2682 (1.0%) |
| 23 | 2L | 0.68 | 0/1698 | 1.29 | 10/2644 (0.4%) |
| 24 | 3K | 0.62 | 0/1799 | 1.27 | 16/2801 (0.6%) |
| 25 | 4K | 0.90 | 0/495 | 1.40 | 4/771 (0.5%) |
| 25 | 4L | 0.70 | 0/420 | 1.09 | 0/654 |
| 26 | 14 | 0.94 | 73/69023 (0.1%) | 1.67 | 1714/107740 (1.6%) |
| 26 | 1H | 1.08 | 148/68351 (0.2%) | 1.86 | 2473/106700 (2.3%) |
| 27 | 16 | 0.83 | 0/2928 | 1.65 | 60/4568 (1.3%) |
| 27 | 1J | 0.74 | 1/2928 (0.0%) | 1.45 | 28/4568 (0.6%) |
| 28 | 71 | 0.56 | 1/1055 (0.1%) | 0.80 | 3/1425 (0.2%) |
| 29 | 11 | 0.83 | 2/2175 (0.1%) | 1.03 | 7/2933 (0.2%) |
| 29 | 19 | 0.83 | 1/2170 (0.0%) | 0.97 | 4/2926 (0.1%) |
| 30 | 21 | 0.70 | 0/1596 | 0.93 | 3/2153 (0.1%) |
| 30 | 29 | 0.66 | 0/1596 | 0.93 | 1/2153 (0.0%) |
| 31 | 31 | 0.76 | 0/1620 | 0.93 | 3/2194 (0.1%) |
| 31 | 39 | 0.65 | 0/1641 | 0.90 | 1/2223 (0.0%) |
| 32 | 41 | 0.55 | 0/1489 | 0.74 | 0/2005 |
| 32 | 49 | 0.43 | 0/1489 | 0.71 | 0/2005 |
| 33 | 51 | 0.60 | 0/1353 | 0.89 | 3/1830 (0.2%) |
| 33 | 59 | 0.51 | 0/548 | 0.78 | 0/738 |
| 34 | 61 | 0.51 | 0/1146 | 0.74 | 1/1551 (0.1%) |
| 34 | 69 | 0.50 | 0/1146 | 0.78 | 2/1551 (0.1%) |
| 35 | 15 | 0.47 | 0/1123 | 0.72 | 0/1515 |
| 35 | 58 | 0.62 | 0/1131 | 0.84 | 1/1525 (0.1%) |
| 36 | 25 | 0.61 | 0/942 | 0.79 | 1/1269 (0.1%) |
| 36 | 68 | 0.67 | 0/942 | 0.82 | 1/1269 (0.1%) |
| 37 | 35 | 0.69 | 0/1147 | 1.06 | 4/1525 (0.3%) |
| 37 | 78 | 0.76 | 0/1139 | 1.14 | 8/1514 (0.5%) |
| 38 | 45 | 0.66 | 0/1120 | 0.90 | 2/1498 (0.1%) |
| 38 | 88 | 0.79 | 0/1134 | 0.95 | 2/1519 (0.1%) |
| 39 | 55 | 0.65 | 0/981 | 0.83 | 0/1312 |
| 39 | 98 | 0.61 | 0/981 | 0.85 | 2/1312 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 40 | 65 | 0.55 | 0/886 | 0.83 | 2/1180 (0.2%) |
| 40 | A8 | 0.67 | 0/891 | 0.94 | 3/1187 (0.3%) |
| 41 | 75 | 0.64 | 0/1146 | 0.88 | 0/1531 |
| 41 | B8 | 0.70 | 0/1132 | 0.88 | 0/1512 |
| 42 | 85 | 0.59 | 0/977 | 0.75 | 0/1301 |
| 42 | C8 | 0.71 | 0/968 | 0.84 | 1/1289 (0.1%) |
| 43 | 95 | 0.74 | 0/774 | 0.91 | 2/1038 (0.2%) |
| 43 | D8 | 0.69 | 0/785 | 0.88 | 3/1052 (0.3%) |
| 44 | A5 | 0.63 | 0/897 | 0.82 | 0/1204 |
| 44 | E8 | 0.75 | 0/901 | 0.91 | 0/1209 |
| 45 | B5 | 0.76 | 0/752 | 0.87 | 1/1010 (0.1%) |
| 45 | F8 | 0.83 | 0/765 | 0.91 | 2/1029 (0.2%) |
| 46 | C5 | 0.65 | 0/807 | 0.88 | 1/1076 (0.1%) |
| 46 | G8 | 0.82 | 0/796 | 1.08 | 2/1062 (0.2%) |
| 47 | D5 | 0.49 | 0/1057 | 0.76 | 0/1430 |
| 47 | H8 | 0.51 | 0/1248 | 0.78 | 1/1687 (0.1%) |
| 48 | E5 | 0.61 | 0/624 | 0.83 | 0/832 |
| 48 | I8 | 0.78 | 0/624 | 0.94 | 1/832 (0.1%) |
| 49 | F5 | 0.67 | 0/744 | 0.83 | 0/989 |
| 49 | J8 | 0.73 | 0/744 | 0.97 | 1/989 (0.1%) |
| 50 | G5 | 0.61 | 0/575 | 0.81 | 0/762 |
| 50 | K8 | 0.87 | 2/573 (0.3%) | 0.84 | 0/759 |
| 51 | H5 | 0.51 | 0/464 | 0.69 | 0/623 |
| 51 | L8 | 0.59 | 0/464 | 0.80 | 0/623 |
| 52 | M8 | 0.52 | 0/375 | 0.86 | 1/507 (0.2%) |
| 53 | J5 | 0.65 | 1/448 (0.2%) | 0.83 | 0/606 |
| 53 | N8 | 0.74 | 0/394 | 0.92 | 0/534 |
| 54 | L5 | 0.71 | 0/409 | 0.93 | 1/540 (0.2%) |
| 54 | P8 | 0.88 | 0/409 | 1.05 | 0/540 |
| 55 | M5 | 0.85 | 1/524 (0.2%) | 0.92 | 1/691 (0.1%) |
| 55 | Q8 | 0.80 | 0/524 | 1.05 | 3/691 (0.4%) |
| 56 | 1L | 0.62 | 0/1705 | 1.20 | 6/2649 (0.2%) |
| 57 | 3L | 0.60 | 0/1732 | 1.14 | 8/2695 (0.3%) |
| All | All | 0.84 | 237/316396 (0.1%) | 1.46 | 5154/474130 (1.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | 12 | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | 1E | 0 | 1 |
| 4 | 32 | 0 | 2 |
| 4 | 3E | 0 | 4 |
| 7 | 62 | 0 | 1 |
| 7 | 6E | 0 | 1 |
| 10 | 1A | 0 | 1 |
| 12 | 3A | 0 | 2 |
| 12 | 3I | 0 | 2 |
| 13 | 4I | 0 | 2 |
| 14 | 5A | 0 | 1 |
| 19 | AA | 0 | 1 |
| 19 | AI | 0 | 3 |
| 28 | 71 | 0 | 1 |
| 29 | 11 | 0 | 4 |
| 29 | 19 | 0 | 2 |
| 30 | 21 | 0 | 2 |
| 30 | 29 | 0 | 6 |
| 31 | 31 | 0 | 2 |
| 31 | 39 | 0 | 6 |
| 32 | 41 | 0 | 1 |
| 32 | 49 | 0 | 2 |
| 33 | 51 | 0 | 3 |
| 33 | 59 | 0 | 1 |
| 34 | 61 | 0 | 3 |
| 34 | 69 | 0 | 1 |
| 35 | 58 | 0 | 1 |
| 37 | 35 | 0 | 10 |
| 37 | 78 | 0 | 7 |
| 38 | 45 | 0 | 4 |
| 38 | 88 | 0 | 1 |
| 40 | 65 | 0 | 1 |
| 40 | A8 | 0 | 1 |
| 41 | 75 | 0 | 3 |
| 41 | B8 | 0 | 4 |
| 42 | 85 | 0 | 2 |
| 42 | C8 | 0 | 3 |
| 43 | D8 | 0 | 3 |
| 45 | B5 | 0 | 3 |
| 45 | F8 | 0 | 1 |
| 46 | C5 | 0 | 4 |
| 46 | G8 | 0 | 2 |
| 47 | D5 | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 47 | H8 | 0 | 2 |
| 50 | G5 | 0 | 3 |
| 52 | M8 | 0 | 2 |
| 55 | M5 | 0 | 2 |
| 55 | Q8 | 0 | 2 |
| All | All | 0 | 119 |

The worst 5 of 237 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 26 | 1H | 774 | A | N9-C4 | -13.80 | 1.29 | 1.37 |
| 26 | 1H | 676 | A | N9-C4 | -13.67 | 1.29 | 1.37 |
| 26 | 14 | 783 | A | N9-C4 | -10.88 | 1.31 | 1.37 |
| 26 | 1H | 472 | A | N3-C4 | -10.55 | 1.28 | 1.34 |
| 26 | 1H | 783 | A | N3-C4 | -10.35 | 1.28 | 1.34 |

The worst 5 of 5154 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 26 | 1H | 1899 | G | N3-C4-N9 | -22.91 | 112.25 | 126.00 |
| 26 | 1H | 676 | A | C2-N3-C4 | -20.00 | 100.60 | 110.60 |
| 26 | 1H | 945 | A | N1-C6-N6 | 19.59 | 130.36 | 118.60 |
| 26 | 1H | 945 | A | C6-C5-N7 | -18.66 | 119.24 | 132.30 |
| 26 | 1H | 1332 | G | C2-N3-C4 | -18.37 | 102.72 | 111.90 |

There are no chirality outliers.

5 of 119 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | 1E | 169 | LYS | Peptide |
| 4 | 3E | 77 | ASN | Peptide |
| 4 | 3E | 82 | ALA | Peptide |
| 4 | 3E | 87 | GLY | Peptide |
| 4 | 3E | 88 | VAL | 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 | 16233 | 797 | 0 |
| 1 | 1G | 32391 | 0 | 16352 | 818 | 1 |
| 2 | 12 | 1711 | 0 | 1751 | 90 | 0 |
| 2 | 1E | 1874 | 0 | 1926 | 86 | 0 |
| 3 | 22 | 1529 | 0 | 1592 | 72 | 0 |
| 3 | 2E | 1605 | 0 | 1668 | 50 | 0 |
| 4 | 32 | 1702 | 0 | 1766 | 96 | 0 |
| 4 | 3E | 1702 | 0 | 1762 | 103 | 0 |
| 5 | 42 | 1123 | 0 | 1191 | 56 | 0 |
| 5 | 4E | 1142 | 0 | 1204 | 44 | 0 |
| 6 | 52 | 842 | 0 | 857 | 31 | 0 |
| 6 | 5E | 837 | 0 | 852 | 47 | 0 |
| 7 | 62 | 1110 | 0 | 1163 | 53 | 0 |
| 7 | 6E | 1214 | 0 | 1259 | 41 | 0 |
| 8 | 72 | 1115 | 0 | 1177 | 46 | 0 |
| 8 | 7E | 1115 | 0 | 1177 | 53 | 0 |
| 9 | 82 | 983 | 0 | 1006 | 57 | 0 |
| 9 | 8E | 1005 | 0 | 1033 | 76 | 0 |
| 10 | 1A | 626 | 0 | 639 | 34 | 0 |
| 10 | 1I | 734 | 0 | 761 | 51 | 0 |
| 11 | 2A | 835 | 0 | 847 | 38 | 0 |
| 11 | 2I | 823 | 0 | 833 | 33 | 0 |
| 12 | 3A | 947 | 0 | 1033 | 50 | 0 |
| 12 | 3I | 956 | 0 | 1046 | 43 | 0 |
| 13 | 4A | 888 | 0 | 941 | 64 | 0 |
| 13 | 4I | 928 | 0 | 987 | 50 | 0 |
| 14 | 5A | 466 | 0 | 499 | 38 | 0 |
| 14 | 5I | 496 | 0 | 535 | 25 | 0 |
| 15 | 6A | 729 | 0 | 768 | 29 | 0 |
| 15 | 6I | 733 | 0 | 771 | 23 | 0 |
| 16 | 7A | 705 | 0 | 725 | 31 | 0 |
| 16 | 7I | 671 | 0 | 693 | 40 | 0 |
| 17 | 8A | 823 | 0 | 891 | 34 | 0 |
| 17 | 8I | 823 | 0 | 891 | 48 | 0 |
| 18 | 9A | 544 | 0 | 605 | 30 | 0 |
| 18 | 9I | 544 | 0 | 605 | 28 | 0 |
| 19 | AA | 471 | 0 | 464 | 35 | 0 |
| 19 | AI | 643 | 0 | 662 | 36 | 0 |
| 20 | BA | 757 | 0 | 856 | 34 | 0 |
| 20 | BI | 746 | 0 | 843 | 42 | 0 |
| 21 | 1B | 208 | 0 | 221 | 26 | 0 |
| 21 | 1F | 199 | 0 | 208 | 7 | 0 |
| 22 | 1K | 1477 | 0 | 758 | 32 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23 | 2K | 1646 | 0 | 844 | 30 | 0 |
| 23 | 2L | 1626 | 0 | 835 | 30 | 0 |
| 24 | 3K | 1611 | 0 | 817 | 57 | 0 |
| 25 | 4K | 439 | 0 | 218 | 14 | 0 |
| 25 | 4L | 373 | 0 | 185 | 9 | 0 |
| 26 | 14 | 61630 | 0 | 31070 | 1393 | 1 |
| 26 | 1H | 61028 | 0 | 30763 | 1409 | 0 |
| 27 | 16 | 2617 | 0 | 1328 | 71 | 0 |
| 27 | 1J | 2617 | 0 | 1328 | 87 | 0 |
| 28 | 71 | 1033 | 0 | 1048 | 54 | 0 |
| 29 | 11 | 2125 | 0 | 2199 | 118 | 0 |
| 29 | 19 | 2120 | 0 | 2197 | 118 | 0 |
| 30 | 21 | 1563 | 0 | 1629 | 92 | 0 |
| 30 | 29 | 1563 | 0 | 1629 | 110 | 0 |
| 31 | 31 | 1585 | 0 | 1632 | 101 | 0 |
| 31 | 39 | 1606 | 0 | 1652 | 93 | 0 |
| 32 | 41 | 1464 | 0 | 1522 | 74 | 0 |
| 32 | 49 | 1464 | 0 | 1522 | 73 | 0 |
| 33 | 51 | 1327 | 0 | 1405 | 62 | 0 |
| 33 | 59 | 539 | 0 | 563 | 34 | 0 |
| 34 | 61 | 1131 | 0 | 1218 | 51 | 0 |
| 34 | 69 | 1131 | 0 | 1218 | 55 | 0 |
| 35 | 15 | 1096 | 0 | 1168 | 61 | 0 |
| 35 | 58 | 1104 | 0 | 1180 | 69 | 0 |
| 36 | 25 | 932 | 0 | 996 | 42 | 0 |
| 36 | 68 | 932 | 0 | 996 | 41 | 0 |
| 37 | 35 | 1130 | 0 | 1217 | 98 | 0 |
| 37 | 78 | 1122 | 0 | 1206 | 91 | 0 |
| 38 | 45 | 1099 | 0 | 1154 | 67 | 0 |
| 38 | 88 | 1113 | 0 | 1157 | 54 | 0 |
| 39 | 55 | 967 | 0 | 1033 | 46 | 0 |
| 39 | 98 | 967 | 0 | 1033 | 48 | 0 |
| 40 | 65 | 876 | 0 | 938 | 81 | 0 |
| 40 | A8 | 881 | 0 | 943 | 61 | 0 |
| 41 | 75 | 1132 | 0 | 1189 | 75 | 0 |
| 41 | B8 | 1118 | 0 | 1176 | 62 | 0 |
| 42 | 85 | 959 | 0 | 1019 | 64 | 0 |
| 42 | C8 | 950 | 0 | 1011 | 54 | 0 |
| 43 | 95 | 763 | 0 | 836 | 71 | 0 |
| 43 | D8 | 774 | 0 | 849 | 52 | 0 |
| 44 | A5 | 886 | 0 | 948 | 23 | 0 |
| 44 | E8 | 890 | 0 | 951 | 29 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 45 | B5 | 738 | 0 | 792 | 36 | 0 |
| 45 | F8 | 751 | 0 | 807 | 40 | 0 |
| 46 | C5 | 794 | 0 | 886 | 53 | 0 |
| 46 | G8 | 783 | 0 | 873 | 67 | 0 |
| 47 | D5 | 1034 | 0 | 1061 | 68 | 0 |
| 47 | H8 | 1222 | 0 | 1247 | 80 | 0 |
| 48 | E5 | 616 | 0 | 633 | 38 | 0 |
| 48 | I8 | 616 | 0 | 633 | 24 | 0 |
| 49 | F5 | 737 | 0 | 813 | 44 | 0 |
| 49 | J8 | 737 | 0 | 813 | 39 | 0 |
| 50 | G5 | 573 | 0 | 616 | 33 | 0 |
| 50 | K8 | 571 | 0 | 623 | 37 | 0 |
| 51 | H5 | 459 | 0 | 512 | 17 | 0 |
| 51 | L8 | 459 | 0 | 512 | 18 | 0 |
| 52 | M8 | 366 | 0 | 370 | 31 | 0 |
| 53 | J5 | 434 | 0 | 454 | 18 | 0 |
| 53 | N8 | 381 | 0 | 397 | 27 | 0 |
| 54 | L5 | 401 | 0 | 436 | 18 | 0 |
| 54 | P8 | 401 | 0 | 436 | 21 | 0 |
| 55 | M5 | 516 | 0 | 582 | 36 | 0 |
| 55 | Q8 | 516 | 0 | 582 | 34 | 0 |
| 56 | 1L | 1570 | 0 | 798 | 34 | 0 |
| 57 | 3L | 1571 | 0 | 798 | 34 | 0 |
| 58 | 11 | 1 | 0 | 0 | 0 | 0 |
| 58 | 13 | 142 | 0 | 0 | 0 | 0 |
| 58 | 14 | 421 | 0 | 0 | 0 | 0 |
| 58 | 16 | 11 | 0 | 0 | 0 | 0 |
| 58 | 19 | 1 | 0 | 0 | 0 | 0 |
| 58 | 1G | 95 | 0 | 0 | 0 | 0 |
| 58 | 1H | 495 | 0 | 0 | 0 | 0 |
| 58 | 1I | 1 | 0 | 0 | 0 | 0 |
| 58 | 1J | 6 | 0 | 0 | 0 | 0 |
| 58 | 1K | 1 | 0 | 0 | 0 | 0 |
| 58 | 21 | 2 | 0 | 0 | 0 | 0 |
| 58 | 25 | 1 | 0 | 0 | 0 | 0 |
| 58 | 29 | 3 | 0 | 0 | 0 | 0 |
| 58 | 2I | 1 | 0 | 0 | 0 | 0 |
| 58 | 2K | 2 | 0 | 0 | 0 | 0 |
| 58 | 2L | 2 | 0 | 0 | 0 | 0 |
| 58 | 39 | 2 | 0 | 0 | 0 | 0 |
| 58 | 3I | 1 | 0 | 0 | 0 | 0 |
| 58 | 3L | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58 | 4I | 1 | 0 | 0 | 0 | 0 |
| 58 | 45 | 3 | 0 | 0 | 0 | 0 |
| 58 | 4I | 1 | 0 | 0 | 0 | 0 |
| 58 | 4K | 1 | 0 | 0 | 0 | 0 |
| 58 | 5I | 1 | 0 | 0 | 0 | 0 |
| 58 | 78 | 1 | 0 | 0 | 0 | 0 |
| 58 | 7I | 1 | 0 | 0 | 0 | 0 |
| 58 | 88 | 3 | 0 | 0 | 0 | 0 |
| 58 | E5 | 1 | 0 | 0 | 0 | 0 |
| 58 | I8 | 1 | 0 | 0 | 0 | 0 |
| 58 | J8 | 1 | 0 | 0 | 0 | 0 |
| 58 | N8 | 1 | 0 | 0 | 0 | 0 |
| 58 | P8 | 1 | 0 | 0 | 0 | 0 |
| 58 | Q8 | 1 | 0 | 0 | 0 | 0 |
| 59 | 32 | 8 | 0 | 0 | 0 | 0 |
| 59 | 3E | 8 | 0 | 0 | 0 | 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 | 9 | 0 | 0 | 2 | 0 |
| 61 | 13 | 207 | 0 | 0 | 37 | 0 |
| 61 | 14 | 717 | 0 | 0 | 118 | 0 |
| 61 | 15 | 1 | 0 | 0 | 0 | 0 |
| 61 | 16 | 22 | 0 | 0 | 3 | 0 |
| 61 | 19 | 10 | 0 | 0 | 4 | 0 |
| 61 | 1G | 117 | 0 | 0 | 23 | 0 |
| 61 | 1H | 819 | 0 | 0 | 163 | 0 |
| 61 | 1I | 1 | 0 | 0 | 0 | 0 |
| 61 | 1J | 6 | 0 | 0 | 0 | 0 |
| 61 | 21 | 6 | 0 | 0 | 3 | 0 |
| 61 | 29 | 3 | 0 | 0 | 0 | 0 |
| 61 | 2A | 1 | 0 | 0 | 0 | 0 |
| 61 | 31 | 4 | 0 | 0 | 1 | 0 |
| 61 | 32 | 2 | 0 | 0 | 0 | 0 |
| 61 | 35 | 3 | 0 | 0 | 0 | 0 |
| 61 | 39 | 3 | 0 | 0 | 0 | 0 |
| 61 | 3E | 2 | 0 | 0 | 0 | 0 |
| 61 | 3I | 2 | 0 | 0 | 0 | 0 |
| 61 | 4E | 2 | 0 | 0 | 0 | 0 |
| 61 | 4K | 4 | 0 | 0 | 0 | 0 |
| 61 | 5I | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | 6A | 2 | 0 | 0 | 1 | 0 |
| 61 | 6I | 1 | 0 | 0 | 0 | 0 |
| 61 | 75 | 2 | 0 | 0 | 0 | 0 |
| 61 | 78 | 1 | 0 | 0 | 0 | 0 |
| 61 | 7A | 1 | 0 | 0 | 0 | 0 |
| 61 | 85 | 3 | 0 | 0 | 1 | 0 |
| 61 | 8E | 1 | 0 | 0 | 0 | 0 |
| 61 | B8 | 1 | 0 | 0 | 0 | 0 |
| 61 | BA | 1 | 0 | 0 | 0 | 0 |
| 61 | C8 | 3 | 0 | 0 | 1 | 0 |
| 61 | F8 | 1 | 0 | 0 | 0 | 0 |
| 61 | I8 | 5 | 0 | 0 | 0 | 0 |
| 61 | J8 | 2 | 0 | 0 | 0 | 0 |
| 61 | L8 | 3 | 0 | 0 | 0 | 0 |
| 61 | M5 | 3 | 0 | 0 | 0 | 0 |
| All | All | 294304 | 0 | 195547 | 8554 | 1 |

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

The worst 5 of 8554 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) |
|-------------------|------------------|--------------------------|-------------------|
| 30:21:135:HIS:NE2 | 61:21:401:HOH:O | 1.87 | 1.06 |
| 1:13:788:U:H2' | 1:13:789:U:H5' | 1.29 | 1.06 |
| 26:1H:511:U:OP2 | 61:1H:3501:HOH:O | 1.72 | 1.05 |
| 47:H8:5:LEU:HD11 | 47:H8:44:PHE:HA | 1.40 | 1.02 |
| 26:14:1899:G:H21 | 26:14:1902:C:N4 | 1.56 | 1.02 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|--------------------------|--------------------------|-------------------|
| 1:1G:82:U:O2' | 26:14:271(C):U:O4[3_545] | 2.15 | 0.05 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | 12 | 204/256 (80%) | 170 (83%) | 32 (16%) | 2 (1%) | 18 | 60 |
| 2 | 1E | 227/256 (89%) | 191 (84%) | 34 (15%) | 2 (1%) | 20 | 62 |
| 3 | 22 | 190/239 (80%) | 173 (91%) | 15 (8%) | 2 (1%) | 17 | 57 |
| 3 | 2E | 203/239 (85%) | 187 (92%) | 16 (8%) | 0 | 100 | 100 |
| 4 | 32 | 206/209 (99%) | 183 (89%) | 22 (11%) | 1 (0%) | 32 | 73 |
| 4 | 3E | 206/209 (99%) | 188 (91%) | 13 (6%) | 5 (2%) | 7 | 37 |
| 5 | 42 | 145/162 (90%) | 136 (94%) | 8 (6%) | 1 (1%) | 25 | 67 |
| 5 | 4E | 147/162 (91%) | 139 (95%) | 7 (5%) | 1 (1%) | 25 | 67 |
| 6 | 52 | 99/101 (98%) | 93 (94%) | 6 (6%) | 0 | 100 | 100 |
| 6 | 5E | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | 62 | 134/156 (86%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |
| 7 | 6E | 145/156 (93%) | 136 (94%) | 9 (6%) | 0 | 100 | 100 |
| 8 | 72 | 136/138 (99%) | 126 (93%) | 8 (6%) | 2 (2%) | 12 | 49 |
| 8 | 7E | 136/138 (99%) | 129 (95%) | 7 (5%) | 0 | 100 | 100 |
| 9 | 82 | 122/128 (95%) | 111 (91%) | 11 (9%) | 0 | 100 | 100 |
| 9 | 8E | 125/128 (98%) | 111 (89%) | 13 (10%) | 1 (1%) | 22 | 64 |
| 10 | 1A | 72/105 (69%) | 64 (89%) | 8 (11%) | 0 | 100 | 100 |
| 10 | 1I | 89/105 (85%) | 81 (91%) | 7 (8%) | 1 (1%) | 17 | 57 |
| 11 | 2A | 111/129 (86%) | 99 (89%) | 11 (10%) | 1 (1%) | 20 | 62 |
| 11 | 2I | 109/129 (84%) | 99 (91%) | 8 (7%) | 2 (2%) | 10 | 45 |
| 12 | 3A | 119/132 (90%) | 99 (83%) | 19 (16%) | 1 (1%) | 22 | 64 |
| 12 | 3I | 120/132 (91%) | 104 (87%) | 15 (12%) | 1 (1%) | 22 | 64 |
| 13 | 4A | 108/126 (86%) | 87 (81%) | 20 (18%) | 1 (1%) | 20 | 62 |
| 13 | 4I | 114/126 (90%) | 93 (82%) | 19 (17%) | 2 (2%) | 10 | 45 |
| 14 | 5A | 55/61 (90%) | 46 (84%) | 8 (14%) | 1 (2%) | 10 | 45 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14 | 5I | 59/61 (97%) | 51 (86%) | 8 (14%) | 0 | 100 | 100 |
| 15 | 6A | 85/89 (96%) | 79 (93%) | 6 (7%) | 0 | 100 | 100 |
| 15 | 6I | 86/89 (97%) | 75 (87%) | 10 (12%) | 1 (1%) | 15 | 55 |
| 16 | 7A | 82/88 (93%) | 77 (94%) | 5 (6%) | 0 | 100 | 100 |
| 16 | 7I | 78/88 (89%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 17 | 8A | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 17 | 8I | 97/105 (92%) | 92 (95%) | 5 (5%) | 0 | 100 | 100 |
| 18 | 9A | 65/88 (74%) | 61 (94%) | 4 (6%) | 0 | 100 | 100 |
| 18 | 9I | 65/88 (74%) | 63 (97%) | 1 (2%) | 1 (2%) | 12 | 49 |
| 19 | AA | 54/93 (58%) | 45 (83%) | 5 (9%) | 4 (7%) | 1 | 7 |
| 19 | AI | 78/93 (84%) | 68 (87%) | 6 (8%) | 4 (5%) | 2 | 17 |
| 20 | BA | 96/106 (91%) | 88 (92%) | 8 (8%) | 0 | 100 | 100 |
| 20 | BI | 95/106 (90%) | 82 (86%) | 13 (14%) | 0 | 100 | 100 |
| 21 | 1B | 22/27 (82%) | 21 (96%) | 1 (4%) | 0 | 100 | 100 |
| 21 | 1F | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 28 | 7I | 129/229 (56%) | 120 (93%) | 9 (7%) | 0 | 100 | 100 |
| 29 | 11 | 272/276 (99%) | 247 (91%) | 16 (6%) | 9 (3%) | 4 | 27 |
| 29 | 19 | 271/276 (98%) | 249 (92%) | 17 (6%) | 5 (2%) | 10 | 45 |
| 30 | 21 | 202/206 (98%) | 173 (86%) | 25 (12%) | 4 (2%) | 9 | 42 |
| 30 | 29 | 202/206 (98%) | 153 (76%) | 36 (18%) | 13 (6%) | 1 | 11 |
| 31 | 31 | 200/210 (95%) | 179 (90%) | 19 (10%) | 2 (1%) | 18 | 60 |
| 31 | 39 | 203/210 (97%) | 174 (86%) | 24 (12%) | 5 (2%) | 6 | 35 |
| 32 | 41 | 178/182 (98%) | 152 (85%) | 23 (13%) | 3 (2%) | 11 | 46 |
| 32 | 49 | 178/182 (98%) | 158 (89%) | 18 (10%) | 2 (1%) | 17 | 57 |
| 33 | 51 | 171/180 (95%) | 132 (77%) | 35 (20%) | 4 (2%) | 7 | 38 |
| 33 | 59 | 63/180 (35%) | 45 (71%) | 17 (27%) | 1 (2%) | 11 | 48 |
| 34 | 61 | 143/148 (97%) | 116 (81%) | 25 (18%) | 2 (1%) | 13 | 51 |
| 34 | 69 | 143/148 (97%) | 116 (81%) | 27 (19%) | 0 | 100 | 100 |
| 35 | 15 | 135/140 (96%) | 123 (91%) | 11 (8%) | 1 (1%) | 25 | 67 |
| 35 | 58 | 136/140 (97%) | 116 (85%) | 17 (12%) | 3 (2%) | 8 | 39 |
| 36 | 25 | 120/122 (98%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 36 | 68 | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 37 | 35 | 146/150 (97%) | 112 (77%) | 27 (18%) | 7 (5%) | 2 | 18 |
| 37 | 78 | 145/150 (97%) | 118 (81%) | 20 (14%) | 7 (5%) | 2 | 18 |
| 38 | 45 | 136/141 (96%) | 111 (82%) | 22 (16%) | 3 (2%) | 8 | 39 |
| 38 | 88 | 139/141 (99%) | 114 (82%) | 19 (14%) | 6 (4%) | 3 | 21 |
| 39 | 55 | 116/118 (98%) | 110 (95%) | 6 (5%) | 0 | 100 | 100 |
| 39 | 98 | 116/118 (98%) | 102 (88%) | 14 (12%) | 0 | 100 | 100 |
| 40 | 65 | 108/112 (96%) | 92 (85%) | 14 (13%) | 2 (2%) | 9 | 43 |
| 40 | A8 | 109/112 (97%) | 94 (86%) | 13 (12%) | 2 (2%) | 10 | 45 |
| 41 | 75 | 134/146 (92%) | 115 (86%) | 18 (13%) | 1 (1%) | 25 | 67 |
| 41 | B8 | 132/146 (90%) | 118 (89%) | 14 (11%) | 0 | 100 | 100 |
| 42 | 85 | 114/118 (97%) | 103 (90%) | 10 (9%) | 1 (1%) | 20 | 62 |
| 42 | C8 | 113/118 (96%) | 105 (93%) | 6 (5%) | 2 (2%) | 10 | 45 |
| 43 | 95 | 97/101 (96%) | 78 (80%) | 15 (16%) | 4 (4%) | 3 | 22 |
| 43 | D8 | 98/101 (97%) | 87 (89%) | 8 (8%) | 3 (3%) | 5 | 29 |
| 44 | A5 | 109/113 (96%) | 99 (91%) | 10 (9%) | 0 | 100 | 100 |
| 44 | E8 | 110/113 (97%) | 103 (94%) | 7 (6%) | 0 | 100 | 100 |
| 45 | B5 | 92/96 (96%) | 85 (92%) | 6 (6%) | 1 (1%) | 17 | 57 |
| 45 | F8 | 94/96 (98%) | 83 (88%) | 8 (8%) | 3 (3%) | 5 | 28 |
| 46 | C5 | 102/110 (93%) | 69 (68%) | 26 (26%) | 7 (7%) | 1 | 9 |
| 46 | G8 | 101/110 (92%) | 90 (89%) | 9 (9%) | 2 (2%) | 9 | 42 |
| 47 | D5 | 120/206 (58%) | 92 (77%) | 24 (20%) | 4 (3%) | 4 | 27 |
| 47 | H8 | 142/206 (69%) | 120 (84%) | 15 (11%) | 7 (5%) | 2 | 18 |
| 48 | E5 | 76/85 (89%) | 73 (96%) | 3 (4%) | 0 | 100 | 100 |
| 48 | I8 | 76/85 (89%) | 67 (88%) | 8 (10%) | 1 (1%) | 14 | 53 |
| 49 | F5 | 92/98 (94%) | 83 (90%) | 7 (8%) | 2 (2%) | 8 | 39 |
| 49 | J8 | 92/98 (94%) | 88 (96%) | 3 (3%) | 1 (1%) | 17 | 57 |
| 50 | G5 | 67/72 (93%) | 60 (90%) | 5 (8%) | 2 (3%) | 5 | 30 |
| 50 | K8 | 66/72 (92%) | 62 (94%) | 3 (4%) | 1 (2%) | 12 | 49 |
| 51 | H5 | 56/60 (93%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 51 | L8 | 56/60 (93%) | 54 (96%) | 2 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 52 | M8 | 45/71 (63%) | 26 (58%) | 18 (40%) | 1 (2%) | 8 | 39 |
| 53 | J5 | 54/60 (90%) | 47 (87%) | 7 (13%) | 0 | 100 | 100 |
| 53 | N8 | 47/60 (78%) | 43 (92%) | 4 (8%) | 0 | 100 | 100 |
| 54 | L5 | 45/49 (92%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | P8 | 45/49 (92%) | 42 (93%) | 3 (7%) | 0 | 100 | 100 |
| 55 | M5 | 62/65 (95%) | 50 (81%) | 9 (14%) | 3 (5%) | 2 | 18 |
| 55 | Q8 | 62/65 (95%) | 54 (87%) | 4 (6%) | 4 (6%) | 1 | 11 |
| All | All | 10880/12104 (90%) | 9578 (88%) | 1134 (10%) | 168 (2%) | 12 | 49 |

5 of 168 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 3E | 88 | VAL |
| 18 | 9I | 22 | VAL |
| 29 | 11 | 40 | THR |
| 29 | 11 | 237 | GLU |
| 37 | 78 | 16 | ARG |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | 12 | 182/220 (83%) | 138 (76%) | 44 (24%) | 1 | 3 |
| 2 | 1E | 200/220 (91%) | 152 (76%) | 48 (24%) | 1 | 3 |
| 3 | 22 | 153/188 (81%) | 126 (82%) | 27 (18%) | 2 | 10 |
| 3 | 2E | 159/188 (85%) | 129 (81%) | 30 (19%) | 2 | 9 |
| 4 | 32 | 180/181 (99%) | 145 (81%) | 35 (19%) | 1 | 8 |
| 4 | 3E | 180/181 (99%) | 149 (83%) | 31 (17%) | 2 | 11 |
| 5 | 42 | 113/123 (92%) | 85 (75%) | 28 (25%) | 1 | 3 |
| 5 | 4E | 115/123 (94%) | 91 (79%) | 24 (21%) | 1 | 6 |
| 6 | 52 | 90/90 (100%) | 80 (89%) | 10 (11%) | 7 | 29 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6 | 5E | 90/90 (100%) | 80 (89%) | 10 (11%) | 7 | 29 |
| 7 | 62 | 114/127 (90%) | 94 (82%) | 20 (18%) | 2 | 10 |
| 7 | 6E | 123/127 (97%) | 91 (74%) | 32 (26%) | 0 | 2 |
| 8 | 72 | 119/119 (100%) | 98 (82%) | 21 (18%) | 2 | 10 |
| 8 | 7E | 119/119 (100%) | 95 (80%) | 24 (20%) | 1 | 7 |
| 9 | 82 | 95/99 (96%) | 75 (79%) | 20 (21%) | 1 | 6 |
| 9 | 8E | 97/99 (98%) | 70 (72%) | 27 (28%) | 0 | 1 |
| 10 | 1A | 69/92 (75%) | 53 (77%) | 16 (23%) | 1 | 4 |
| 10 | 1I | 81/92 (88%) | 62 (76%) | 19 (24%) | 1 | 4 |
| 11 | 2A | 85/99 (86%) | 73 (86%) | 12 (14%) | 4 | 18 |
| 11 | 2I | 84/99 (85%) | 68 (81%) | 16 (19%) | 2 | 9 |
| 12 | 3A | 102/109 (94%) | 82 (80%) | 20 (20%) | 1 | 8 |
| 12 | 3I | 103/109 (94%) | 81 (79%) | 22 (21%) | 1 | 6 |
| 13 | 4A | 91/101 (90%) | 65 (71%) | 26 (29%) | 0 | 1 |
| 13 | 4I | 94/101 (93%) | 74 (79%) | 20 (21%) | 1 | 6 |
| 14 | 5A | 47/50 (94%) | 31 (66%) | 16 (34%) | 0 | 0 |
| 14 | 5I | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 10 |
| 15 | 6A | 79/80 (99%) | 71 (90%) | 8 (10%) | 9 | 32 |
| 15 | 6I | 79/80 (99%) | 68 (86%) | 11 (14%) | 4 | 18 |
| 16 | 7A | 72/74 (97%) | 62 (86%) | 10 (14%) | 4 | 18 |
| 16 | 7I | 69/74 (93%) | 50 (72%) | 19 (28%) | 0 | 1 |
| 17 | 8A | 94/97 (97%) | 82 (87%) | 12 (13%) | 5 | 22 |
| 17 | 8I | 94/97 (97%) | 73 (78%) | 21 (22%) | 1 | 5 |
| 18 | 9A | 58/77 (75%) | 45 (78%) | 13 (22%) | 1 | 5 |
| 18 | 9I | 58/77 (75%) | 48 (83%) | 10 (17%) | 2 | 11 |
| 19 | AA | 52/80 (65%) | 34 (65%) | 18 (35%) | 0 | 0 |
| 19 | AI | 70/80 (88%) | 57 (81%) | 13 (19%) | 2 | 9 |
| 20 | BA | 76/82 (93%) | 65 (86%) | 11 (14%) | 4 | 17 |
| 20 | BI | 75/82 (92%) | 62 (83%) | 13 (17%) | 2 | 11 |
| 21 | 1B | 19/22 (86%) | 16 (84%) | 3 (16%) | 3 | 13 |
| 21 | 1F | 18/22 (82%) | 14 (78%) | 4 (22%) | 1 | 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 28 | 71 | 109/181 (60%) | 76 (70%) | 33 (30%) | 0 | 1 |
| 29 | 11 | 214/218 (98%) | 169 (79%) | 45 (21%) | 1 | 6 |
| 29 | 19 | 214/218 (98%) | 164 (77%) | 50 (23%) | 1 | 4 |
| 30 | 21 | 165/166 (99%) | 128 (78%) | 37 (22%) | 1 | 5 |
| 30 | 29 | 165/166 (99%) | 134 (81%) | 31 (19%) | 2 | 9 |
| 31 | 31 | 161/166 (97%) | 126 (78%) | 35 (22%) | 1 | 6 |
| 31 | 39 | 163/166 (98%) | 128 (78%) | 35 (22%) | 1 | 6 |
| 32 | 41 | 154/156 (99%) | 118 (77%) | 36 (23%) | 1 | 4 |
| 32 | 49 | 154/156 (99%) | 123 (80%) | 31 (20%) | 1 | 7 |
| 33 | 51 | 144/148 (97%) | 113 (78%) | 31 (22%) | 1 | 6 |
| 33 | 59 | 56/148 (38%) | 41 (73%) | 15 (27%) | 0 | 2 |
| 34 | 61 | 122/124 (98%) | 93 (76%) | 29 (24%) | 1 | 3 |
| 34 | 69 | 122/124 (98%) | 90 (74%) | 32 (26%) | 0 | 2 |
| 35 | 15 | 116/119 (98%) | 92 (79%) | 24 (21%) | 1 | 6 |
| 35 | 58 | 117/119 (98%) | 91 (78%) | 26 (22%) | 1 | 5 |
| 36 | 25 | 100/100 (100%) | 85 (85%) | 15 (15%) | 3 | 16 |
| 36 | 68 | 100/100 (100%) | 82 (82%) | 18 (18%) | 2 | 10 |
| 37 | 35 | 115/116 (99%) | 82 (71%) | 33 (29%) | 0 | 1 |
| 37 | 78 | 114/116 (98%) | 79 (69%) | 35 (31%) | 0 | 1 |
| 38 | 45 | 109/111 (98%) | 85 (78%) | 24 (22%) | 1 | 5 |
| 38 | 88 | 109/111 (98%) | 89 (82%) | 20 (18%) | 2 | 10 |
| 39 | 55 | 101/101 (100%) | 81 (80%) | 20 (20%) | 1 | 8 |
| 39 | 98 | 101/101 (100%) | 76 (75%) | 25 (25%) | 1 | 3 |
| 40 | 65 | 87/88 (99%) | 66 (76%) | 21 (24%) | 1 | 3 |
| 40 | A8 | 87/88 (99%) | 60 (69%) | 27 (31%) | 0 | 1 |
| 41 | 75 | 119/127 (94%) | 88 (74%) | 31 (26%) | 0 | 2 |
| 41 | B8 | 118/127 (93%) | 87 (74%) | 31 (26%) | 0 | 2 |
| 42 | 85 | 93/94 (99%) | 77 (83%) | 16 (17%) | 2 | 11 |
| 42 | C8 | 92/94 (98%) | 77 (84%) | 15 (16%) | 3 | 12 |
| 43 | 95 | 81/82 (99%) | 61 (75%) | 20 (25%) | 1 | 3 |
| 43 | D8 | 82/82 (100%) | 57 (70%) | 25 (30%) | 0 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 44 | A5 | 91/92 (99%) | 74 (81%) | 17 (19%) | 2 | 9 |
| 44 | E8 | 91/92 (99%) | 71 (78%) | 20 (22%) | 1 | 5 |
| 45 | B5 | 75/78 (96%) | 60 (80%) | 15 (20%) | 1 | 7 |
| 45 | F8 | 76/78 (97%) | 63 (83%) | 13 (17%) | 2 | 11 |
| 46 | C5 | 85/91 (93%) | 62 (73%) | 23 (27%) | 0 | 1 |
| 46 | G8 | 84/91 (92%) | 59 (70%) | 25 (30%) | 0 | 1 |
| 47 | D5 | 115/179 (64%) | 82 (71%) | 33 (29%) | 0 | 1 |
| 47 | H8 | 137/179 (76%) | 103 (75%) | 34 (25%) | 1 | 3 |
| 48 | E5 | 62/67 (92%) | 51 (82%) | 11 (18%) | 2 | 10 |
| 48 | I8 | 62/67 (92%) | 50 (81%) | 12 (19%) | 1 | 8 |
| 49 | F5 | 79/83 (95%) | 56 (71%) | 23 (29%) | 0 | 1 |
| 49 | J8 | 79/83 (95%) | 65 (82%) | 14 (18%) | 2 | 10 |
| 50 | G5 | 62/67 (92%) | 39 (63%) | 23 (37%) | 0 | 0 |
| 50 | K8 | 63/67 (94%) | 43 (68%) | 20 (32%) | 0 | 1 |
| 51 | H5 | 50/52 (96%) | 42 (84%) | 8 (16%) | 3 | 13 |
| 51 | L8 | 50/52 (96%) | 42 (84%) | 8 (16%) | 3 | 13 |
| 52 | M8 | 42/63 (67%) | 34 (81%) | 8 (19%) | 2 | 9 |
| 53 | J5 | 48/52 (92%) | 39 (81%) | 9 (19%) | 2 | 9 |
| 53 | N8 | 44/52 (85%) | 32 (73%) | 12 (27%) | 0 | 1 |
| 54 | L5 | 38/42 (90%) | 32 (84%) | 6 (16%) | 3 | 13 |
| 54 | P8 | 38/42 (90%) | 31 (82%) | 7 (18%) | 2 | 10 |
| 55 | M5 | 54/55 (98%) | 37 (68%) | 17 (32%) | 0 | 1 |
| 55 | Q8 | 54/55 (98%) | 40 (74%) | 14 (26%) | 0 | 2 |
| All | All | 9210/10012 (92%) | 7199 (78%) | 2011 (22%) | 1 | 6 |

5 of 2011 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | G8 | 33 | LYS |
| 3 | 22 | 181 | ASN |
| 46 | C5 | 11 | ASP |
| 47 | H8 | 19 | ARG |
| 52 | M8 | 34 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 12 | 135 | GLN |
| 3 | 22 | 181 | ASN |
| 32 | 49 | 79 | ASN |
| 2 | 12 | 19 | HIS |
| 40 | 65 | 95 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 13 | 1492/1522 (98%) | 374 (25%) | 0 |
| 1 | 1G | 1505/1522 (98%) | 376 (24%) | 0 |
| 22 | 1K | 64/76 (84%) | 31 (48%) | 0 |
| 23 | 2K | 76/77 (98%) | 22 (28%) | 0 |
| 23 | 2L | 74/77 (96%) | 19 (25%) | 0 |
| 24 | 3K | 75/76 (98%) | 43 (57%) | 0 |
| 25 | 4K | 19/27 (70%) | 9 (47%) | 0 |
| 25 | 4L | 16/27 (59%) | 7 (43%) | 0 |
| 26 | 14 | 2852/2917 (97%) | 732 (25%) | 0 |
| 26 | 1H | 2828/2917 (96%) | 709 (25%) | 0 |
| 27 | 16 | 121/122 (99%) | 25 (20%) | 0 |
| 27 | 1J | 121/122 (99%) | 41 (33%) | 0 |
| 56 | 1L | 71/76 (93%) | 31 (43%) | 0 |
| 57 | 3L | 72/76 (94%) | 21 (29%) | 0 |
| All | All | 9386/9634 (97%) | 2440 (25%) | 0 |

5 of 2440 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 13 | 2 | U |
| 1 | 13 | 5 | U |
| 1 | 13 | 6 | G |
| 1 | 13 | 11 | G |
| 1 | 13 | 31 | G |

There are no RNA pucker outliers to report.

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

18 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$ |
| 22 | U8U | 1K | 34 | 25,22 | 15,24,25 | 2.55 | 4 (26%) | 18,34,37 | 1.82 | 2 (11%) |
| 22 | T6A | 1K | 37 | 22 | 24,34,35 | 2.55 | 5 (20%) | 23,49,52 | 3.59 | 7 (30%) |
| 22 | PSU | 1K | 39 | 22 | 16,21,22 | 1.01 | 1 (6%) | 20,30,33 | 3.64 | 7 (35%) |
| 22 | 5MU | 1K | 54 | 22 | 14,22,23 | 1.69 | 2 (14%) | 16,32,35 | 1.84 | 2 (12%) |
| 22 | PSU | 1K | 55 | 22 | 16,21,22 | 1.17 | 1 (6%) | 20,30,33 | 3.94 | 6 (30%) |
| 56 | 5MU | 1L | 54 | 56 | 14,22,23 | 1.75 | 2 (14%) | 16,32,35 | 1.76 | 2 (12%) |
| 56 | PSU | 1L | 55 | 56 | 16,21,22 | 1.02 | 1 (6%) | 20,30,33 | 3.73 | 5 (25%) |
| 23 | OMC | 2K | 33 | 23 | 15,22,23 | 2.11 | 4 (26%) | 19,31,34 | 1.13 | 2 (10%) |
| 23 | 7MG | 2K | 47 | 23 | 20,26,27 | 3.49 | 6 (30%) | 22,39,42 | 2.15 | 7 (31%) |
| 23 | 5MU | 2K | 55 | 23 | 14,22,23 | 1.74 | 2 (14%) | 16,32,35 | 1.82 | 2 (12%) |
| 23 | PSU | 2K | 56 | 23 | 16,21,22 | 1.19 | 1 (6%) | 20,30,33 | 3.76 | 4 (20%) |
| 23 | 4SU | 2K | 8 | 23 | 14,21,22 | 3.13 | 2 (14%) | 15,30,33 | 1.17 | 2 (13%) |
| 23 | OMC | 2L | 33 | 23 | 15,22,23 | 2.28 | 4 (26%) | 19,31,34 | 1.45 | 2 (10%) |
| 23 | 7MG | 2L | 47 | 23 | 20,26,27 | 3.42 | 6 (30%) | 22,39,42 | 2.09 | 8 (36%) |
| 23 | 5MU | 2L | 55 | 23 | 14,22,23 | 1.74 | 2 (14%) | 16,32,35 | 1.81 | 2 (12%) |
| 23 | PSU | 2L | 56 | 23 | 16,21,22 | 1.23 | 2 (12%) | 20,30,33 | 3.70 | 5 (25%) |
| 23 | 4SU | 2L | 8 | 23 | 14,21,22 | 3.15 | 2 (14%) | 15,30,33 | 1.26 | 2 (13%) |
| 57 | PSU | 3L | 39 | 57 | 16,21,22 | 1.10 | 1 (6%) | 20,30,33 | 3.76 | 6 (30%) |

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 |
|-----|------|-------|-----|-------|---------|------------|---------|
| 22 | U8U | 1K | 34 | 25,22 | - | 0/5/28/29 | 0/2/2/2 |
| 22 | T6A | 1K | 37 | 22 | - | 0/15/41/42 | 0/3/3/3 |
| 22 | PSU | 1K | 39 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | 1K | 54 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | PSU | 1K | 55 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 5MU | 1L | 54 | 56 | - | 0/3/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 56 | PSU | 1L | 55 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | OMC | 2K | 33 | 23 | - | 0/5/27/28 | 0/2/2/2 |
| 23 | 7MG | 2K | 47 | 23 | - | 0/7/37/38 | 0/3/3/3 |
| 23 | 5MU | 2K | 55 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 23 | PSU | 2K | 56 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 4SU | 2K | 8 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 23 | OMC | 2L | 33 | 23 | - | 0/5/27/28 | 0/2/2/2 |
| 23 | 7MG | 2L | 47 | 23 | - | 0/7/37/38 | 0/3/3/3 |
| 23 | 5MU | 2L | 55 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 23 | PSU | 2L | 56 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 4SU | 2L | 8 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | PSU | 3L | 39 | 57 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 48 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23 | 2L | 47 | 7MG | C5-C4 | -5.63 | 1.24 | 1.39 |
| 23 | 2K | 47 | 7MG | C5-C4 | -5.37 | 1.24 | 1.39 |
| 22 | 1K | 37 | T6A | C5-C4 | -3.39 | 1.32 | 1.40 |
| 23 | 2L | 55 | 5MU | C4-N3 | -2.98 | 1.27 | 1.33 |
| 56 | 1L | 54 | 5MU | C4-N3 | -2.94 | 1.27 | 1.33 |

The worst 5 of 73 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 57 | 3L | 39 | PSU | N1-C2-N3 | -12.90 | 119.12 | 128.40 |
| 22 | 1K | 39 | PSU | N1-C2-N3 | -12.76 | 119.22 | 128.40 |
| 22 | 1K | 37 | T6A | N3-C2-N1 | -12.63 | 117.86 | 128.86 |
| 23 | 2L | 56 | PSU | N1-C2-N3 | -12.33 | 119.53 | 128.40 |
| 22 | 1K | 55 | PSU | N1-C2-N3 | -12.24 | 119.59 | 128.40 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | 1K | 37 | T6A | 1 | 0 |
| 22 | 1K | 54 | 5MU | 3 | 0 |
| 22 | 1K | 55 | PSU | 1 | 0 |
| 23 | 2K | 33 | OMC | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | 2K | 47 | 7MG | 1 | 0 |
| 23 | 2K | 55 | 5MU | 3 | 0 |
| 23 | 2K | 8 | 4SU | 1 | 0 |
| 23 | 2L | 33 | OMC | 1 | 0 |
| 23 | 2L | 47 | 7MG | 1 | 0 |
| 23 | 2L | 55 | 5MU | 1 | 0 |
| 23 | 2L | 8 | 4SU | 2 | 0 |
| 57 | 3L | 39 | PSU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1213 ligands modelled in this entry, 1211 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 59 | SF4 | 32 | 301 | - | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 59 | SF4 | 3E | 301 | 4 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |

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 | 32 | 301 | - | - | 0/0/48/48 | 0/6/5/5 |
| 59 | SF4 | 3E | 301 | 4 | - | 0/0/48/48 | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%) | -0.52 | 3 (0%) 94 93 | 61, 106, 170, 196 | 0 |
| 1 | 1G | 1507/1522 (99%) | -0.58 | 2 (0%) 95 94 | 74, 126, 175, 200 | 0 |
| 2 | 12 | 208/256 (81%) | 0.59 | 23 (11%) 6 3 | 134, 156, 168, 176 | 0 |
| 2 | 1E | 231/256 (90%) | 1.07 | 42 (18%) 1 1 | 116, 144, 162, 166 | 0 |
| 3 | 22 | 194/239 (81%) | 0.03 | 8 (4%) 38 23 | 129, 148, 164, 167 | 0 |
| 3 | 2E | 205/239 (85%) | -0.25 | 3 (1%) 74 60 | 89, 111, 139, 148 | 0 |
| 4 | 32 | 208/209 (99%) | 1.11 | 44 (21%) 1 1 | 105, 125, 146, 151 | 0 |
| 4 | 3E | 208/209 (99%) | 0.18 | 8 (3%) 41 25 | 85, 106, 126, 135 | 0 |
| 5 | 42 | 147/162 (90%) | 0.04 | 3 (2%) 65 49 | 112, 126, 138, 145 | 0 |
| 5 | 4E | 149/162 (91%) | 0.22 | 3 (2%) 65 49 | 81, 103, 122, 131 | 0 |
| 6 | 52 | 101/101 (100%) | 0.14 | 2 (1%) 65 49 | 92, 111, 128, 134 | 0 |
| 6 | 5E | 100/101 (99%) | 1.07 | 21 (21%) 1 1 | 90, 109, 127, 132 | 0 |
| 7 | 62 | 138/156 (88%) | -0.15 | 0 100 100 | 122, 133, 142, 148 | 0 |
| 7 | 6E | 149/156 (95%) | 0.04 | 5 (3%) 46 29 | 107, 124, 143, 149 | 0 |
| 8 | 72 | 138/138 (100%) | -0.22 | 1 (0%) 87 80 | 112, 131, 141, 149 | 0 |
| 8 | 7E | 138/138 (100%) | 1.36 | 44 (31%) 0 0 | 92, 115, 130, 139 | 0 |
| 9 | 82 | 124/128 (96%) | -0.06 | 4 (3%) 48 31 | 121, 153, 162, 166 | 0 |
| 9 | 8E | 127/128 (99%) | -0.38 | 1 (0%) 86 77 | 91, 137, 154, 159 | 0 |
| 10 | 1A | 78/105 (74%) | -0.26 | 8 (10%) 7 4 | 119, 148, 159, 161 | 0 |
| 10 | 1I | 91/105 (86%) | 0.39 | 9 (9%) 8 4 | 87, 128, 157, 163 | 0 |
| 11 | 2A | 113/129 (87%) | 0.46 | 5 (4%) 35 20 | 89, 115, 135, 141 | 0 |
| 11 | 2I | 111/129 (86%) | 1.18 | 25 (22%) 1 1 | 82, 110, 127, 140 | 0 |
| 12 | 3A | 121/132 (91%) | 0.62 | 17 (14%) 3 2 | 93, 113, 129, 148 | 0 |
| 12 | 3I | 122/132 (92%) | 0.91 | 15 (12%) 5 2 | 72, 80, 103, 132 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | 4A | 110/126 (87%) | 0.35 | 14 (12%) 4 2 | 135, 149, 160, 164 | 0 |
| 13 | 4I | 116/126 (92%) | -0.27 | 0 100 100 | 94, 127, 141, 150 | 0 |
| 14 | 5A | 57/61 (93%) | 1.33 | 18 (31%) 0 0 | 134, 146, 155, 158 | 0 |
| 14 | 5I | 61/61 (100%) | -0.57 | 0 100 100 | 86, 100, 118, 123 | 0 |
| 15 | 6A | 87/89 (97%) | 0.27 | 3 (3%) 46 29 | 93, 119, 139, 144 | 0 |
| 15 | 6I | 88/89 (98%) | 1.54 | 28 (31%) 0 0 | 81, 104, 125, 134 | 0 |
| 16 | 7A | 84/88 (95%) | 0.03 | 0 100 100 | 95, 114, 137, 148 | 0 |
| 16 | 7I | 80/88 (90%) | -0.18 | 0 100 100 | 101, 115, 133, 142 | 0 |
| 17 | 8A | 99/105 (94%) | 0.39 | 3 (3%) 51 33 | 102, 119, 130, 135 | 0 |
| 17 | 8I | 99/105 (94%) | 0.86 | 14 (14%) 3 2 | 93, 109, 125, 130 | 0 |
| 18 | 9A | 67/88 (76%) | -0.19 | 0 100 100 | 101, 118, 136, 139 | 0 |
| 18 | 9I | 67/88 (76%) | 0.18 | 1 (1%) 74 60 | 94, 112, 132, 136 | 0 |
| 19 | AA | 60/93 (64%) | 0.57 | 7 (11%) 5 3 | 133, 161, 167, 171 | 0 |
| 19 | AI | 80/93 (86%) | -0.85 | 0 100 100 | 105, 121, 143, 150 | 0 |
| 20 | BA | 98/106 (92%) | 0.51 | 5 (5%) 29 15 | 87, 115, 141, 154 | 0 |
| 20 | BI | 97/106 (91%) | 0.33 | 5 (5%) 28 14 | 114, 126, 152, 156 | 0 |
| 21 | 1B | 24/27 (88%) | 0.66 | 3 (12%) 4 2 | 128, 144, 156, 160 | 0 |
| 21 | 1F | 23/27 (85%) | -0.07 | 0 100 100 | 106, 114, 122, 128 | 0 |
| 22 | 1K | 64/76 (84%) | 0.02 | 2 (3%) 49 32 | 96, 170, 182, 184 | 0 |
| 23 | 2K | 72/77 (93%) | -0.29 | 0 100 100 | 74, 103, 134, 154 | 0 |
| 23 | 2L | 71/77 (92%) | -0.16 | 0 100 100 | 84, 121, 153, 157 | 0 |
| 24 | 3K | 76/76 (100%) | 0.35 | 10 (13%) 4 2 | 79, 183, 195, 202 | 0 |
| 25 | 4K | 20/27 (74%) | 0.37 | 2 (10%) 8 4 | 78, 145, 186, 186 | 0 |
| 25 | 4L | 17/27 (62%) | 0.47 | 0 100 100 | 104, 160, 189, 189 | 0 |
| 26 | 14 | 2861/2917 (98%) | -0.29 | 15 (0%) 90 85 | 54, 88, 183, 207 | 0 |
| 26 | 1H | 2833/2917 (97%) | -0.37 | 7 (0%) 94 93 | 45, 77, 169, 200 | 0 |
| 27 | 16 | 122/122 (100%) | -0.63 | 1 (0%) 86 77 | 70, 97, 122, 187 | 0 |
| 27 | 1J | 122/122 (100%) | -0.55 | 1 (0%) 86 77 | 94, 131, 151, 186 | 0 |
| 28 | 7I | 133/229 (58%) | 0.49 | 13 (9%) 8 5 | 126, 158, 171, 177 | 0 |
| 29 | 11 | 274/276 (99%) | 1.01 | 34 (12%) 4 2 | 47, 69, 89, 99 | 0 |
| 29 | 19 | 273/276 (98%) | 0.53 | 10 (3%) 42 26 | 51, 76, 92, 113 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 30 | 21 | 204/206 (99%) | 1.43 | 63 (30%) 0 0 | 52, 92, 133, 150 | 0 |
| 30 | 29 | 204/206 (99%) | 0.09 | 2 (0%) 82 71 | 59, 96, 131, 135 | 0 |
| 31 | 31 | 202/210 (96%) | 0.48 | 10 (4%) 30 15 | 51, 81, 113, 135 | 0 |
| 31 | 39 | 205/210 (97%) | 0.10 | 1 (0%) 90 85 | 61, 104, 144, 171 | 0 |
| 32 | 41 | 180/182 (98%) | 0.11 | 4 (2%) 62 46 | 90, 110, 144, 155 | 0 |
| 32 | 49 | 180/182 (98%) | 1.40 | 47 (26%) 1 0 | 124, 143, 162, 169 | 0 |
| 33 | 51 | 173/180 (96%) | 0.31 | 11 (6%) 20 11 | 87, 109, 124, 137 | 0 |
| 33 | 59 | 69/180 (38%) | 0.40 | 15 (21%) 1 1 | 136, 158, 168, 170 | 0 |
| 34 | 61 | 145/148 (97%) | -0.18 | 3 (2%) 64 48 | 84, 133, 147, 158 | 0 |
| 34 | 69 | 145/148 (97%) | 0.69 | 25 (17%) 2 1 | 87, 127, 146, 152 | 0 |
| 35 | 15 | 137/140 (97%) | 0.45 | 4 (2%) 52 35 | 78, 109, 138, 155 | 0 |
| 35 | 58 | 138/140 (98%) | 1.14 | 31 (22%) 1 1 | 69, 92, 132, 145 | 0 |
| 36 | 25 | 122/122 (100%) | 0.53 | 4 (3%) 47 30 | 70, 92, 109, 116 | 0 |
| 36 | 68 | 122/122 (100%) | 0.86 | 16 (13%) 4 2 | 60, 81, 99, 113 | 0 |
| 37 | 35 | 148/150 (98%) | 2.27 | 80 (54%) 0 0 | 59, 105, 140, 156 | 0 |
| 37 | 78 | 147/150 (98%) | -0.09 | 2 (1%) 75 62 | 52, 84, 108, 119 | 0 |
| 38 | 45 | 138/141 (97%) | 2.25 | 69 (50%) 0 0 | 75, 110, 134, 149 | 0 |
| 38 | 88 | 141/141 (100%) | 0.12 | 4 (2%) 53 37 | 58, 85, 105, 122 | 0 |
| 39 | 55 | 118/118 (100%) | 0.49 | 6 (5%) 29 15 | 64, 84, 102, 119 | 0 |
| 39 | 98 | 118/118 (100%) | 1.89 | 51 (43%) 0 0 | 66, 87, 108, 130 | 0 |
| 40 | 65 | 110/112 (98%) | 0.80 | 15 (13%) 3 2 | 92, 120, 137, 143 | 0 |
| 40 | A8 | 111/112 (99%) | 0.64 | 11 (9%) 8 4 | 75, 93, 115, 135 | 0 |
| 41 | 75 | 136/146 (93%) | 0.70 | 11 (8%) 13 7 | 80, 100, 138, 155 | 0 |
| 41 | B8 | 134/146 (91%) | 0.17 | 6 (4%) 34 20 | 74, 95, 137, 155 | 0 |
| 42 | 85 | 116/118 (98%) | 0.47 | 8 (6%) 18 9 | 68, 97, 129, 138 | 0 |
| 42 | C8 | 115/118 (97%) | -0.12 | 2 (1%) 70 56 | 57, 83, 110, 117 | 0 |
| 43 | 95 | 99/101 (98%) | 1.11 | 19 (19%) 1 1 | 65, 123, 136, 145 | 0 |
| 43 | D8 | 100/101 (99%) | 0.69 | 10 (10%) 8 4 | 59, 102, 124, 139 | 0 |
| 44 | A5 | 111/113 (98%) | 0.09 | 0 100 100 | 65, 77, 107, 135 | 0 |
| 44 | E8 | 112/113 (99%) | 0.15 | 2 (1%) 69 53 | 61, 75, 105, 140 | 0 |
| 45 | B5 | 94/96 (97%) | 0.29 | 2 (2%) 64 48 | 69, 90, 111, 123 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 45 | F8 | 96/96 (100%) | 0.25 | 0 100 100 | 53, 74, 112, 125 | 0 |
| 46 | C5 | 104/110 (94%) | 0.62 | 13 (12%) 4 2 | 91, 119, 148, 157 | 0 |
| 46 | G8 | 103/110 (93%) | 0.36 | 3 (2%) 52 35 | 74, 93, 127, 130 | 0 |
| 47 | D5 | 126/206 (61%) | 1.43 | 43 (34%) 0 0 | 117, 137, 159, 164 | 0 |
| 47 | H8 | 148/206 (71%) | 0.08 | 1 (0%) 87 80 | 86, 121, 154, 160 | 0 |
| 48 | E5 | 78/85 (91%) | 0.89 | 12 (15%) 2 1 | 73, 93, 110, 138 | 0 |
| 48 | I8 | 78/85 (91%) | -0.07 | 0 100 100 | 62, 77, 98, 110 | 0 |
| 49 | F5 | 94/98 (95%) | 1.07 | 19 (20%) 1 1 | 65, 86, 123, 133 | 0 |
| 49 | J8 | 94/98 (95%) | 0.18 | 2 (2%) 64 48 | 57, 79, 115, 126 | 0 |
| 50 | G5 | 69/72 (95%) | -0.20 | 1 (1%) 75 62 | 89, 109, 131, 150 | 0 |
| 50 | K8 | 68/72 (94%) | 0.11 | 1 (1%) 74 60 | 64, 81, 98, 126 | 0 |
| 51 | H5 | 58/60 (96%) | 0.74 | 4 (6%) 18 9 | 77, 103, 128, 137 | 0 |
| 51 | L8 | 58/60 (96%) | 0.49 | 4 (6%) 18 9 | 66, 81, 110, 129 | 0 |
| 52 | M8 | 47/71 (66%) | 0.51 | 2 (4%) 36 21 | 114, 147, 163, 171 | 0 |
| 53 | J5 | 56/60 (93%) | -0.01 | 0 100 100 | 61, 87, 134, 143 | 0 |
| 53 | N8 | 49/60 (81%) | 0.96 | 10 (20%) 1 1 | 55, 82, 140, 150 | 0 |
| 54 | L5 | 47/49 (95%) | -0.05 | 0 100 100 | 57, 62, 79, 91 | 0 |
| 54 | P8 | 47/49 (95%) | -0.17 | 0 100 100 | 49, 55, 78, 89 | 0 |
| 55 | M5 | 64/65 (98%) | 2.11 | 34 (53%) 0 0 | 72, 82, 97, 124 | 0 |
| 55 | Q8 | 64/65 (98%) | 0.28 | 0 100 100 | 56, 73, 86, 101 | 0 |
| 56 | 1L | 72/76 (94%) | 0.39 | 8 (11%) 6 3 | 127, 184, 195, 204 | 0 |
| 57 | 3L | 73/76 (96%) | -0.16 | 2 (2%) 55 39 | 84, 172, 185, 193 | 0 |
| All | All | 20506/21738 (94%) | 0.10 | 1185 (5%) 24 13 | 45, 104, 163, 207 | 0 |

The worst 5 of 1185 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 37 | 35 | 110 | TYR | 11.7 |
| 43 | 95 | 1 | MET | 9.5 |
| 43 | 95 | 45 | THR | 9.3 |
| 37 | 35 | 148 | LEU | 8.7 |
| 38 | 45 | 91 | GLU | 8.0 |

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 56 | PSU | 1L | 55 | 20/21 | 0.88 | 0.12 | - | 137,155,161,162 | 0 |
| 22 | 5MU | 1K | 54 | 21/22 | 0.91 | 0.14 | - | 118,129,141,147 | 0 |
| 22 | PSU | 1K | 39 | 20/21 | 0.93 | 0.14 | - | 104,124,130,132 | 0 |
| 23 | PSU | 2L | 56 | 20/21 | 0.91 | 0.15 | - | 133,136,141,142 | 0 |
| 56 | 5MU | 1L | 54 | 21/22 | 0.92 | 0.11 | - | 143,156,161,162 | 0 |
| 22 | T6A | 1K | 37 | 32/33 | 0.91 | 0.18 | - | 89,102,123,128 | 0 |
| 57 | PSU | 3L | 39 | 20/21 | 0.91 | 0.13 | - | 147,156,160,160 | 0 |
| 22 | U8U | 1K | 34 | 23/24 | 0.96 | 0.14 | - | 88,99,103,104 | 0 |
| 23 | 5MU | 2K | 55 | 21/22 | 0.94 | 0.15 | - | 117,123,131,135 | 0 |
| 23 | 7MG | 2L | 47 | 24/25 | 0.96 | 0.13 | - | 133,141,147,149 | 0 |
| 23 | 7MG | 2K | 47 | 24/25 | 0.94 | 0.16 | - | 103,111,119,127 | 0 |
| 23 | 5MU | 2L | 55 | 21/22 | 0.94 | 0.12 | - | 131,139,146,151 | 0 |
| 23 | 4SU | 2K | 8 | 20/21 | 0.93 | 0.18 | - | 90,100,108,111 | 0 |
| 23 | PSU | 2K | 56 | 20/21 | 0.91 | 0.12 | - | 103,115,124,125 | 0 |
| 23 | OMC | 2K | 33 | 21/22 | 0.96 | 0.20 | - | 80,86,90,95 | 0 |
| 23 | 4SU | 2L | 8 | 20/21 | 0.90 | 0.16 | - | 110,128,130,136 | 0 |
| 23 | OMC | 2L | 33 | 21/22 | 0.93 | 0.17 | - | 106,117,118,119 | 0 |
| 22 | PSU | 1K | 55 | 20/21 | 0.86 | 0.12 | - | 121,129,137,142 | 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 58 | MG | 14 | 3242 | 1/1 | 0.87 | 1.24 | 60.82 | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 1G | 1644 | 1/1 | 0.92 | 0.47 | 48.60 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3277 | 1/1 | 0.72 | 0.65 | 37.83 | 98,98,98,98 | 0 |
| 58 | MG | 1H | 3070 | 1/1 | 0.88 | 0.36 | 31.24 | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3252 | 1/1 | 0.89 | 0.90 | 30.41 | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3137 | 1/1 | 0.95 | 0.46 | 29.96 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3028 | 1/1 | 0.92 | 0.45 | 29.46 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3014 | 1/1 | 0.94 | 0.35 | 28.76 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3333 | 1/1 | 0.83 | 0.63 | 28.47 | 88,88,88,88 | 0 |
| 58 | MG | 13 | 1699 | 1/1 | 0.92 | 0.31 | 27.13 | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3216 | 1/1 | 0.73 | 0.55 | 26.68 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3258 | 1/1 | 0.90 | 0.57 | 26.24 | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3164 | 1/1 | 0.83 | 0.52 | 26.12 | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3075 | 1/1 | 0.98 | 0.40 | 25.81 | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3344 | 1/1 | 0.90 | 0.47 | 24.31 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3255 | 1/1 | 0.90 | 0.52 | 23.73 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3089 | 1/1 | 0.96 | 0.36 | 23.21 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3131 | 1/1 | 0.92 | 0.52 | 21.05 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3224 | 1/1 | 0.92 | 0.55 | 20.74 | 59,59,59,59 | 0 |
| 58 | MG | 13 | 1686 | 1/1 | 0.41 | 0.36 | 20.42 | 94,94,94,94 | 0 |
| 58 | MG | 14 | 3178 | 1/1 | 0.97 | 0.41 | 19.56 | 65,65,65,65 | 0 |
| 58 | MG | 13 | 1638 | 1/1 | 0.96 | 0.33 | 19.28 | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3179 | 1/1 | 0.93 | 0.31 | 18.96 | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3042 | 1/1 | 0.88 | 0.47 | 18.93 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3053 | 1/1 | 0.99 | 0.31 | 18.36 | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3347 | 1/1 | 0.76 | 0.36 | 17.62 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3012 | 1/1 | 0.91 | 0.28 | 17.53 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3249 | 1/1 | 0.67 | 0.35 | 17.06 | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3237 | 1/1 | 0.98 | 0.32 | 16.80 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3001 | 1/1 | 0.98 | 0.39 | 16.28 | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1645 | 1/1 | 0.88 | 0.38 | 16.12 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3186 | 1/1 | 0.74 | 0.47 | 15.79 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3099 | 1/1 | 0.72 | 0.40 | 15.70 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3143 | 1/1 | 0.95 | 0.33 | 15.49 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3057 | 1/1 | 0.95 | 0.42 | 15.23 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3036 | 1/1 | 0.97 | 0.35 | 14.74 | 126,126,126,126 | 0 |
| 58 | MG | 1H | 3154 | 1/1 | 0.94 | 0.34 | 14.25 | 42,42,42,42 | 0 |
| 58 | MG | 14 | 3054 | 1/1 | 0.91 | 0.39 | 14.06 | 54,54,54,54 | 0 |
| 58 | MG | 14 | 3097 | 1/1 | 0.98 | 0.35 | 14.02 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3253 | 1/1 | 0.95 | 0.28 | 14.00 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3195 | 1/1 | 0.93 | 0.40 | 13.75 | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3309 | 1/1 | 0.63 | 0.33 | 13.38 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 1H | 3186 | 1/1 | 0.90 | 0.24 | 13.05 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3191 | 1/1 | 0.83 | 0.40 | 12.80 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3009 | 1/1 | 0.90 | 0.57 | 12.65 | 73,73,73,73 | 0 |
| 58 | MG | 1H | 3088 | 1/1 | 0.98 | 0.28 | 12.64 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3054 | 1/1 | 0.97 | 0.38 | 12.63 | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3179 | 1/1 | 0.97 | 0.32 | 12.60 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3206 | 1/1 | 0.93 | 0.46 | 12.59 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3074 | 1/1 | 0.92 | 0.41 | 12.35 | 44,44,44,44 | 0 |
| 58 | MG | 1G | 1602 | 1/1 | 0.91 | 0.43 | 12.14 | 79,79,79,79 | 0 |
| 58 | MG | 1K | 101 | 1/1 | 0.56 | 0.45 | 11.90 | 147,147,147,147 | 0 |
| 58 | MG | 1H | 3168 | 1/1 | 0.77 | 0.33 | 11.85 | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3094 | 1/1 | 0.88 | 0.30 | 11.81 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3124 | 1/1 | 0.75 | 0.31 | 11.78 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3479 | 1/1 | 0.74 | 0.20 | 11.75 | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3205 | 1/1 | 0.86 | 0.40 | 11.60 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3258 | 1/1 | 0.94 | 0.25 | 11.45 | 100,100,100,100 | 0 |
| 58 | MG | 14 | 3038 | 1/1 | 0.98 | 0.41 | 11.43 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3004 | 1/1 | 0.98 | 0.42 | 11.12 | 57,57,57,57 | 0 |
| 58 | MG | 13 | 1677 | 1/1 | 0.98 | 0.28 | 10.86 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3285 | 1/1 | 0.82 | 0.33 | 10.77 | 61,61,61,61 | 0 |
| 58 | MG | 14 | 3160 | 1/1 | 0.91 | 0.29 | 10.57 | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3029 | 1/1 | 0.95 | 0.53 | 10.56 | 67,67,67,67 | 0 |
| 58 | MG | 2K | 101 | 1/1 | 0.97 | 0.37 | 10.55 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3067 | 1/1 | 0.98 | 0.35 | 10.54 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3253 | 1/1 | 0.71 | 0.33 | 10.51 | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3016 | 1/1 | 0.98 | 0.28 | 10.43 | 52,52,52,52 | 0 |
| 58 | MG | 2L | 101 | 1/1 | 0.94 | 0.46 | 10.17 | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3073 | 1/1 | 0.96 | 0.46 | 10.15 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3212 | 1/1 | 0.84 | 0.32 | 9.93 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3194 | 1/1 | 0.55 | 0.30 | 9.93 | 74,74,74,74 | 0 |
| 58 | MG | 13 | 1697 | 1/1 | 0.93 | 0.34 | 9.76 | 95,95,95,95 | 0 |
| 58 | MG | 13 | 1694 | 1/1 | 0.64 | 0.48 | 9.72 | 88,88,88,88 | 0 |
| 58 | MG | 13 | 1608 | 1/1 | 0.82 | 0.27 | 9.69 | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3343 | 1/1 | 0.94 | 0.28 | 9.58 | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3015 | 1/1 | 0.97 | 0.40 | 9.28 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3225 | 1/1 | 0.89 | 0.32 | 9.22 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3240 | 1/1 | 0.95 | 0.25 | 9.21 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3079 | 1/1 | 0.86 | 0.34 | 9.21 | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3061 | 1/1 | 0.94 | 0.28 | 9.05 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3198 | 1/1 | 0.93 | 0.37 | 9.02 | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3100 | 1/1 | 0.98 | 0.35 | 8.94 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3074 | 1/1 | 0.96 | 0.49 | 8.67 | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3071 | 1/1 | 0.89 | 0.29 | 8.64 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3291 | 1/1 | 0.97 | 0.34 | 8.63 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3019 | 1/1 | 0.87 | 0.35 | 8.47 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3029 | 1/1 | 0.96 | 0.38 | 8.46 | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3190 | 1/1 | 0.75 | 0.27 | 8.33 | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3157 | 1/1 | 0.95 | 0.43 | 8.30 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3007 | 1/1 | 0.98 | 0.29 | 8.26 | 52,52,52,52 | 0 |
| 58 | MG | 1H | 3142 | 1/1 | 0.95 | 0.28 | 8.17 | 62,62,62,62 | 0 |
| 58 | MG | 13 | 1613 | 1/1 | 0.97 | 0.23 | 8.14 | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3082 | 1/1 | 0.96 | 0.30 | 8.12 | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3006 | 1/1 | 0.97 | 0.38 | 8.10 | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3176 | 1/1 | 0.90 | 0.42 | 8.10 | 92,92,92,92 | 0 |
| 58 | MG | 1G | 1614 | 1/1 | 0.91 | 0.24 | 8.05 | 120,120,120,120 | 0 |
| 58 | MG | 1H | 3246 | 1/1 | 0.64 | 0.21 | 7.86 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3185 | 1/1 | 0.93 | 0.24 | 7.83 | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3287 | 1/1 | 0.83 | 0.42 | 7.69 | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3149 | 1/1 | 0.76 | 0.20 | 7.62 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3085 | 1/1 | 0.83 | 0.29 | 7.33 | 59,59,59,59 | 0 |
| 58 | MG | 1H | 3115 | 1/1 | 0.97 | 0.37 | 6.97 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3155 | 1/1 | 0.84 | 0.25 | 6.89 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3273 | 1/1 | 0.94 | 0.31 | 6.87 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3226 | 1/1 | 0.86 | 0.26 | 6.79 | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3213 | 1/1 | 0.82 | 0.25 | 6.74 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3050 | 1/1 | 0.96 | 0.43 | 6.65 | 71,71,71,71 | 0 |
| 58 | MG | 13 | 1622 | 1/1 | 0.85 | 0.17 | 6.56 | 109,109,109,109 | 0 |
| 58 | MG | 1G | 1653 | 1/1 | 0.98 | 0.33 | 6.48 | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3085 | 1/1 | 0.90 | 0.27 | 6.40 | 54,54,54,54 | 0 |
| 58 | MG | 13 | 1654 | 1/1 | 0.91 | 0.26 | 6.39 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3158 | 1/1 | 0.68 | 0.30 | 6.29 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3003 | 1/1 | 0.95 | 0.31 | 6.21 | 74,74,74,74 | 0 |
| 58 | MG | N8 | 101 | 1/1 | 0.96 | 0.32 | 5.85 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3236 | 1/1 | 0.71 | 0.24 | 5.81 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3233 | 1/1 | 0.96 | 0.30 | 5.81 | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3192 | 1/1 | 0.92 | 0.32 | 5.80 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3083 | 1/1 | 0.98 | 0.30 | 5.72 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3095 | 1/1 | 0.96 | 0.30 | 5.65 | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3024 | 1/1 | 0.97 | 0.26 | 5.56 | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3079 | 1/1 | 0.98 | 0.30 | 5.45 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3174 | 1/1 | 0.87 | 0.31 | 5.34 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3117 | 1/1 | 0.98 | 0.29 | 5.33 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3215 | 1/1 | 0.94 | 0.26 | 5.23 | 73,73,73,73 | 0 |
| 58 | MG | 1H | 3010 | 1/1 | 0.94 | 0.29 | 5.23 | 57,57,57,57 | 0 |
| 58 | MG | 1H | 3080 | 1/1 | 0.89 | 0.20 | 5.15 | 65,65,65,65 | 0 |
| 58 | MG | 14 | 3037 | 1/1 | 0.94 | 0.23 | 5.12 | 55,55,55,55 | 0 |
| 58 | MG | 14 | 3030 | 1/1 | 0.98 | 0.26 | 5.06 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3097 | 1/1 | 0.99 | 0.27 | 4.94 | 56,56,56,56 | 0 |
| 58 | MG | 1G | 1678 | 1/1 | 0.57 | 0.20 | 4.76 | 120,120,120,120 | 0 |
| 58 | MG | 14 | 3260 | 1/1 | 0.89 | 0.23 | 4.66 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3046 | 1/1 | 0.98 | 0.29 | 4.60 | 55,55,55,55 | 0 |
| 58 | MG | 13 | 1639 | 1/1 | 0.98 | 0.33 | 4.57 | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3193 | 1/1 | 0.92 | 0.24 | 4.53 | 69,69,69,69 | 0 |
| 58 | MG | 13 | 1664 | 1/1 | 0.94 | 0.25 | 4.51 | 82,82,82,82 | 0 |
| 58 | MG | 1G | 1632 | 1/1 | 0.86 | 0.34 | 4.47 | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3099 | 1/1 | 0.96 | 0.27 | 4.44 | 69,69,69,69 | 0 |
| 58 | MG | 1G | 1649 | 1/1 | 0.95 | 0.25 | 4.40 | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3123 | 1/1 | 0.52 | 0.34 | 4.39 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3051 | 1/1 | 0.98 | 0.32 | 4.37 | 45,45,45,45 | 0 |
| 58 | MG | 13 | 1646 | 1/1 | 0.85 | 0.19 | 4.33 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3177 | 1/1 | 0.87 | 0.28 | 4.27 | 75,75,75,75 | 0 |
| 58 | MG | 16 | 204 | 1/1 | 0.79 | 0.29 | 4.16 | 80,80,80,80 | 0 |
| 58 | MG | 29 | 302 | 1/1 | 0.70 | 0.49 | 4.13 | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3063 | 1/1 | 0.96 | 0.23 | 4.12 | 73,73,73,73 | 0 |
| 58 | MG | 13 | 1672 | 1/1 | 0.92 | 0.20 | 3.91 | 112,112,112,112 | 0 |
| 58 | MG | 14 | 3078 | 1/1 | 0.94 | 0.39 | 3.88 | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3134 | 1/1 | 0.76 | 0.24 | 3.88 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3180 | 1/1 | 0.89 | 0.22 | 3.83 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3270 | 1/1 | 0.96 | 0.24 | 3.81 | 43,43,43,43 | 0 |
| 58 | MG | 1H | 3167 | 1/1 | 0.90 | 0.24 | 3.79 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3017 | 1/1 | 0.94 | 0.28 | 3.72 | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3443 | 1/1 | 0.83 | 0.23 | 3.54 | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3165 | 1/1 | 0.85 | 0.26 | 3.53 | 47,47,47,47 | 0 |
| 58 | MG | 1G | 1626 | 1/1 | 0.99 | 0.20 | 3.42 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3035 | 1/1 | 0.96 | 0.20 | 3.39 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3348 | 1/1 | 0.82 | 0.27 | 3.26 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3116 | 1/1 | 0.96 | 0.29 | 3.05 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3065 | 1/1 | 0.89 | 0.20 | 3.04 | 64,64,64,64 | 0 |
| 58 | MG | 39 | 301 | 1/1 | 0.88 | 0.33 | 3.00 | 66,66,66,66 | 0 |
| 58 | MG | 5I | 101 | 1/1 | 0.93 | 0.18 | 2.95 | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1741 | 1/1 | 0.87 | 0.43 | 2.93 | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3303 | 1/1 | 0.81 | 0.53 | 2.93 | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3062 | 1/1 | 0.82 | 0.17 | 2.85 | 88,88,88,88 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3056 | 1/1 | 0.98 | 0.33 | 2.85 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3243 | 1/1 | 0.94 | 0.20 | 2.77 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3245 | 1/1 | 0.71 | 0.21 | 2.73 | 72,72,72,72 | 0 |
| 58 | MG | 1G | 1624 | 1/1 | 0.94 | 0.29 | 2.59 | 100,100,100,100 | 0 |
| 58 | MG | 1H | 3260 | 1/1 | 0.82 | 0.22 | 2.54 | 60,60,60,60 | 0 |
| 58 | MG | 13 | 1604 | 1/1 | 0.94 | 0.21 | 2.37 | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3086 | 1/1 | 0.70 | 0.32 | 2.34 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3016 | 1/1 | 0.77 | 0.21 | 2.28 | 61,61,61,61 | 0 |
| 58 | MG | 16 | 205 | 1/1 | 0.85 | 0.15 | 2.21 | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3084 | 1/1 | 0.82 | 0.25 | 2.20 | 49,49,49,49 | 0 |
| 58 | MG | 1G | 1601 | 1/1 | 0.97 | 0.23 | 2.16 | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1608 | 1/1 | 0.92 | 0.18 | 2.09 | 97,97,97,97 | 0 |
| 58 | MG | 13 | 1621 | 1/1 | 0.95 | 0.24 | 2.06 | 101,101,101,101 | 0 |
| 58 | MG | 13 | 1655 | 1/1 | 0.94 | 0.28 | 2.06 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3049 | 1/1 | 0.95 | 0.22 | 2.05 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3118 | 1/1 | 0.95 | 0.26 | 1.91 | 54,54,54,54 | 0 |
| 58 | MG | 1G | 1606 | 1/1 | 0.94 | 0.24 | 1.78 | 88,88,88,88 | 0 |
| 58 | MG | 1G | 1661 | 1/1 | 0.62 | 0.11 | 1.74 | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3363 | 1/1 | 0.94 | 0.20 | 1.74 | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3058 | 1/1 | 0.98 | 0.27 | 1.74 | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3173 | 1/1 | 0.94 | 0.22 | 1.74 | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3291 | 1/1 | 0.97 | 0.23 | 1.71 | 55,55,55,55 | 0 |
| 58 | MG | 13 | 1618 | 1/1 | 0.93 | 0.15 | 1.62 | 107,107,107,107 | 0 |
| 58 | MG | 1G | 1664 | 1/1 | 0.90 | 0.35 | 1.58 | 122,122,122,122 | 0 |
| 58 | MG | 1H | 3044 | 1/1 | 0.98 | 0.21 | 1.56 | 41,41,41,41 | 0 |
| 58 | MG | 1H | 3215 | 1/1 | 0.86 | 0.28 | 1.52 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3236 | 1/1 | 0.80 | 0.15 | 1.49 | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3176 | 1/1 | 0.71 | 0.14 | 1.42 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3031 | 1/1 | 0.99 | 0.22 | 1.39 | 75,75,75,75 | 0 |
| 58 | MG | 39 | 302 | 1/1 | 0.97 | 0.25 | 1.32 | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3039 | 1/1 | 0.86 | 0.33 | 1.28 | 72,72,72,72 | 0 |
| 58 | MG | 16 | 202 | 1/1 | 0.94 | 0.17 | 1.26 | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3076 | 1/1 | 0.96 | 0.22 | 1.25 | 56,56,56,56 | 0 |
| 58 | MG | Q8 | 101 | 1/1 | 0.91 | 0.32 | 1.17 | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1676 | 1/1 | 0.90 | 0.19 | 1.12 | 94,94,94,94 | 0 |
| 58 | MG | 13 | 1727 | 1/1 | 0.93 | 0.20 | 1.11 | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3091 | 1/1 | 0.96 | 0.21 | 1.11 | 66,66,66,66 | 0 |
| 58 | MG | 1G | 1613 | 1/1 | 0.96 | 0.17 | 1.11 | 89,89,89,89 | 0 |
| 58 | MG | 13 | 1648 | 1/1 | 0.98 | 0.17 | 1.09 | 76,76,76,76 | 0 |
| 58 | MG | 1G | 1634 | 1/1 | 0.95 | 0.24 | 1.08 | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1634 | 1/1 | 0.84 | 0.19 | 1.05 | 81,81,81,81 | 0 |
| 58 | MG | 1G | 1656 | 1/1 | 0.93 | 0.17 | 0.97 | 126,126,126,126 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 13 | 1637 | 1/1 | 0.95 | 0.32 | 0.92 | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3129 | 1/1 | 0.95 | 0.14 | 0.88 | 68,68,68,68 | 0 |
| 58 | MG | 1G | 1647 | 1/1 | 0.90 | 0.23 | 0.85 | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3145 | 1/1 | 0.89 | 0.13 | 0.82 | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3171 | 1/1 | 0.94 | 0.30 | 0.81 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3113 | 1/1 | 0.95 | 0.20 | 0.81 | 52,52,52,52 | 0 |
| 58 | MG | 1G | 1666 | 1/1 | 0.95 | 0.24 | 0.74 | 125,125,125,125 | 0 |
| 58 | MG | 1H | 3106 | 1/1 | 0.94 | 0.21 | 0.73 | 46,46,46,46 | 0 |
| 58 | MG | 14 | 3168 | 1/1 | 0.90 | 0.25 | 0.72 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3137 | 1/1 | 0.93 | 0.21 | 0.65 | 55,55,55,55 | 0 |
| 58 | MG | 14 | 3181 | 1/1 | 0.96 | 0.19 | 0.61 | 57,57,57,57 | 0 |
| 58 | MG | 13 | 1681 | 1/1 | 0.97 | 0.18 | 0.49 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3289 | 1/1 | 0.69 | 0.17 | 0.47 | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3338 | 1/1 | 0.96 | 0.17 | 0.46 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3222 | 1/1 | 0.86 | 0.16 | 0.43 | 74,74,74,74 | 0 |
| 58 | MG | 3I | 201 | 1/1 | 0.93 | 0.18 | 0.39 | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3100 | 1/1 | 0.96 | 0.23 | 0.39 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3101 | 1/1 | 0.95 | 0.21 | 0.37 | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3419 | 1/1 | 0.96 | 0.27 | 0.34 | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3293 | 1/1 | 0.97 | 0.19 | 0.30 | 67,67,67,67 | 0 |
| 60 | ZN | 5I | 102 | 1/1 | 0.98 | 0.16 | 0.28 | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1640 | 1/1 | 0.96 | 0.20 | 0.21 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3244 | 1/1 | 0.92 | 0.20 | 0.13 | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3175 | 1/1 | 0.97 | 0.24 | 0.12 | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3128 | 1/1 | 0.89 | 0.15 | 0.02 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3217 | 1/1 | 0.92 | 0.18 | 0.01 | 67,67,67,67 | 0 |
| 58 | MG | 16 | 207 | 1/1 | 0.93 | 0.14 | -0.02 | 84,84,84,84 | 0 |
| 58 | MG | 1G | 1618 | 1/1 | 0.97 | 0.19 | -0.04 | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3289 | 1/1 | 0.74 | 0.12 | -0.04 | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1676 | 1/1 | 0.93 | 0.13 | -0.08 | 91,91,91,91 | 0 |
| 58 | MG | 13 | 1635 | 1/1 | 0.97 | 0.13 | -0.17 | 97,97,97,97 | 0 |
| 58 | MG | 4I | 201 | 1/1 | 0.92 | 0.15 | -0.18 | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3336 | 1/1 | 0.91 | 0.20 | -0.25 | 107,107,107,107 | 0 |
| 58 | MG | 13 | 1612 | 1/1 | 0.98 | 0.18 | -0.29 | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1610 | 1/1 | 0.93 | 0.18 | -0.32 | 92,92,92,92 | 0 |
| 58 | MG | 14 | 3412 | 1/1 | 0.85 | 0.13 | -0.37 | 113,113,113,113 | 0 |
| 58 | MG | 1H | 3192 | 1/1 | 0.89 | 0.14 | -0.37 | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3305 | 1/1 | 0.96 | 0.18 | -0.43 | 51,51,51,51 | 0 |
| 58 | MG | 14 | 3012 | 1/1 | 0.90 | 0.19 | -0.43 | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3110 | 1/1 | 0.91 | 0.15 | -0.48 | 66,66,66,66 | 0 |
| 58 | MG | 4I | 201 | 1/1 | 0.92 | 0.16 | -0.49 | 86,86,86,86 | 0 |
| 58 | MG | 13 | 1615 | 1/1 | 0.89 | 0.14 | -0.50 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 13 | 1658 | 1/1 | 0.98 | 0.15 | -0.51 | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3227 | 1/1 | 0.89 | 0.22 | -0.53 | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3367 | 1/1 | 0.95 | 0.17 | -0.57 | 67,67,67,67 | 0 |
| 59 | SF4 | 3E | 301 | 8/8 | 0.99 | 0.20 | -0.57 | 78,90,95,100 | 0 |
| 58 | MG | 14 | 3319 | 1/1 | 0.98 | 0.18 | -0.60 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3379 | 1/1 | 0.78 | 0.12 | -0.61 | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3023 | 1/1 | 0.85 | 0.15 | -0.63 | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1626 | 1/1 | 0.93 | 0.21 | -0.66 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3005 | 1/1 | 0.91 | 0.17 | -0.70 | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1601 | 1/1 | 0.94 | 0.20 | -0.72 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3064 | 1/1 | 0.92 | 0.20 | -0.74 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3329 | 1/1 | 0.99 | 0.16 | -0.78 | 75,75,75,75 | 0 |
| 58 | MG | 1H | 3256 | 1/1 | 0.93 | 0.18 | -0.80 | 70,70,70,70 | 0 |
| 59 | SF4 | 32 | 301 | 8/8 | 0.99 | 0.18 | -0.80 | 119,123,130,133 | 0 |
| 58 | MG | 13 | 1630 | 1/1 | 0.92 | 0.21 | -0.83 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3230 | 1/1 | 0.87 | 0.11 | -0.84 | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3320 | 1/1 | 0.98 | 0.14 | -0.86 | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1717 | 1/1 | 0.92 | 0.13 | -0.88 | 97,97,97,97 | 0 |
| 58 | MG | 13 | 1656 | 1/1 | 0.77 | 0.13 | -0.90 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3296 | 1/1 | 0.86 | 0.14 | -0.91 | 66,66,66,66 | 0 |
| 58 | MG | 1G | 1663 | 1/1 | 0.88 | 0.09 | -0.96 | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3448 | 1/1 | 0.97 | 0.13 | -0.98 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3345 | 1/1 | 0.86 | 0.12 | -1.03 | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3378 | 1/1 | 0.97 | 0.12 | -1.04 | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3007 | 1/1 | 0.97 | 0.11 | -1.06 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3373 | 1/1 | 0.97 | 0.12 | -1.06 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3415 | 1/1 | 0.92 | 0.17 | -1.09 | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3361 | 1/1 | 0.94 | 0.17 | -1.10 | 47,47,47,47 | 0 |
| 58 | MG | J8 | 101 | 1/1 | 0.95 | 0.14 | -1.10 | 77,77,77,77 | 0 |
| 58 | MG | 1G | 1685 | 1/1 | 0.97 | 0.10 | -1.11 | 109,109,109,109 | 0 |
| 58 | MG | 13 | 1631 | 1/1 | 0.93 | 0.21 | -1.12 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3140 | 1/1 | 0.99 | 0.16 | -1.13 | 61,61,61,61 | 0 |
| 60 | ZN | G8 | 201 | 1/1 | 0.97 | 0.16 | -1.13 | 147,147,147,147 | 0 |
| 58 | MG | 14 | 3251 | 1/1 | 0.95 | 0.12 | -1.13 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3221 | 1/1 | 0.83 | 0.13 | -1.14 | 63,63,63,63 | 0 |
| 60 | ZN | 5A | 101 | 1/1 | 0.97 | 0.11 | -1.15 | 128,128,128,128 | 0 |
| 58 | MG | 1H | 3157 | 1/1 | 0.89 | 0.13 | -1.20 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3238 | 1/1 | 0.95 | 0.14 | -1.21 | 63,63,63,63 | 0 |
| 58 | MG | 88 | 201 | 1/1 | 0.98 | 0.16 | -1.23 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3360 | 1/1 | 0.98 | 0.12 | -1.31 | 48,48,48,48 | 0 |
| 58 | MG | 14 | 3088 | 1/1 | 0.87 | 0.11 | -1.32 | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1742 | 1/1 | 0.88 | 0.10 | -1.32 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | ZN | C5 | 201 | 1/1 | 0.65 | 0.08 | -1.33 | 153,153,153,153 | 0 |
| 58 | MG | 13 | 1685 | 1/1 | 0.84 | 0.05 | -1.36 | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3203 | 1/1 | 0.98 | 0.11 | -1.38 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3073 | 1/1 | 0.97 | 0.17 | -1.38 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3419 | 1/1 | 0.94 | 0.10 | -1.40 | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3441 | 1/1 | 0.96 | 0.17 | -1.42 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3117 | 1/1 | 0.98 | 0.18 | -1.44 | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3390 | 1/1 | 0.96 | 0.10 | -1.45 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3111 | 1/1 | 0.90 | 0.17 | -1.48 | 39,39,39,39 | 0 |
| 58 | MG | 1H | 3213 | 1/1 | 0.97 | 0.18 | -1.50 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3135 | 1/1 | 0.94 | 0.15 | -1.52 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3424 | 1/1 | 0.98 | 0.13 | -1.52 | 66,66,66,66 | 0 |
| 58 | MG | 45 | 202 | 1/1 | 0.94 | 0.11 | -1.53 | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3334 | 1/1 | 0.78 | 0.13 | -1.57 | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3418 | 1/1 | 0.97 | 0.17 | -1.58 | 52,52,52,52 | 0 |
| 58 | MG | 1G | 1691 | 1/1 | 0.89 | 0.07 | -1.59 | 123,123,123,123 | 0 |
| 58 | MG | 14 | 3196 | 1/1 | 0.98 | 0.09 | -1.65 | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3350 | 1/1 | 0.84 | 0.15 | -1.65 | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3214 | 1/1 | 0.96 | 0.10 | -1.65 | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3139 | 1/1 | 0.91 | 0.15 | -1.66 | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3400 | 1/1 | 0.93 | 0.12 | -1.74 | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3033 | 1/1 | 0.90 | 0.16 | -1.80 | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3457 | 1/1 | 0.99 | 0.11 | -1.82 | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1619 | 1/1 | 0.92 | 0.16 | -1.84 | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3045 | 1/1 | 0.93 | 0.12 | -1.85 | 83,83,83,83 | 0 |
| 58 | MG | 1J | 204 | 1/1 | 0.88 | 0.10 | -1.86 | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1672 | 1/1 | 0.94 | 0.09 | -1.92 | 110,110,110,110 | 0 |
| 58 | MG | 88 | 202 | 1/1 | 0.98 | 0.07 | -1.94 | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3108 | 1/1 | 0.99 | 0.13 | -1.95 | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3366 | 1/1 | 0.97 | 0.12 | -1.98 | 53,53,53,53 | 0 |
| 58 | MG | 14 | 3349 | 1/1 | 0.97 | 0.13 | -2.01 | 47,47,47,47 | 0 |
| 58 | MG | 13 | 1711 | 1/1 | 0.83 | 0.09 | -2.02 | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3389 | 1/1 | 0.99 | 0.11 | -2.03 | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3046 | 1/1 | 0.97 | 0.11 | -2.08 | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3420 | 1/1 | 0.94 | 0.10 | -2.15 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3340 | 1/1 | 0.94 | 0.10 | -2.17 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3174 | 1/1 | 0.94 | 0.15 | -2.21 | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3476 | 1/1 | 0.94 | 0.12 | -2.22 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3432 | 1/1 | 0.97 | 0.12 | -2.24 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3494 | 1/1 | 0.97 | 0.12 | -2.25 | 44,44,44,44 | 0 |
| 58 | MG | 1G | 1658 | 1/1 | 0.72 | 0.11 | -2.28 | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3087 | 1/1 | 0.96 | 0.13 | -2.28 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 14 | 3308 | 1/1 | 0.97 | 0.15 | -2.30 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3169 | 1/1 | 0.90 | 0.10 | -2.32 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3152 | 1/1 | 0.97 | 0.12 | -2.32 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3402 | 1/1 | 0.98 | 0.07 | -2.32 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3125 | 1/1 | 0.94 | 0.12 | -2.34 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3403 | 1/1 | 0.86 | 0.07 | -2.35 | 119,119,119,119 | 0 |
| 58 | MG | 1H | 3121 | 1/1 | 0.94 | 0.12 | -2.42 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3180 | 1/1 | 0.91 | 0.10 | -2.42 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3380 | 1/1 | 0.98 | 0.09 | -2.43 | 56,56,56,56 | 0 |
| 58 | MG | 13 | 1667 | 1/1 | 0.85 | 0.14 | -2.43 | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1722 | 1/1 | 0.98 | 0.15 | -2.45 | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3254 | 1/1 | 0.88 | 0.11 | -2.46 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3278 | 1/1 | 0.83 | 0.15 | -2.58 | 61,61,61,61 | 0 |
| 58 | MG | 13 | 1705 | 1/1 | 0.88 | 0.07 | -2.58 | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3294 | 1/1 | 0.95 | 0.11 | -2.60 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3242 | 1/1 | 0.95 | 0.11 | -2.65 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3374 | 1/1 | 0.97 | 0.12 | -2.75 | 63,63,63,63 | 0 |
| 58 | MG | 13 | 1706 | 1/1 | 0.97 | 0.07 | -2.75 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3395 | 1/1 | 0.97 | 0.10 | -2.76 | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1712 | 1/1 | 0.98 | 0.07 | -2.78 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3369 | 1/1 | 0.97 | 0.13 | -2.83 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3444 | 1/1 | 0.94 | 0.13 | -2.87 | 50,50,50,50 | 0 |
| 58 | MG | 13 | 1703 | 1/1 | 0.97 | 0.12 | -2.88 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3220 | 1/1 | 0.85 | 0.12 | -2.88 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3310 | 1/1 | 0.95 | 0.13 | -2.95 | 59,59,59,59 | 0 |
| 58 | MG | 1H | 3358 | 1/1 | 0.95 | 0.14 | -2.95 | 54,54,54,54 | 0 |
| 58 | MG | 1G | 1675 | 1/1 | 0.95 | 0.12 | -2.97 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3063 | 1/1 | 0.91 | 0.12 | -2.98 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3353 | 1/1 | 0.97 | 0.12 | -3.10 | 54,54,54,54 | 0 |
| 58 | MG | 14 | 3311 | 1/1 | 0.97 | 0.14 | -3.17 | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3421 | 1/1 | 0.96 | 0.05 | -3.20 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3387 | 1/1 | 0.95 | 0.10 | -3.26 | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3422 | 1/1 | 0.82 | 0.09 | -3.31 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3412 | 1/1 | 0.96 | 0.10 | -3.35 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3355 | 1/1 | 0.97 | 0.13 | -3.37 | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3434 | 1/1 | 0.99 | 0.11 | -3.40 | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3362 | 1/1 | 0.99 | 0.08 | -3.41 | 42,42,42,42 | 0 |
| 58 | MG | 14 | 3298 | 1/1 | 0.98 | 0.14 | -3.52 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3348 | 1/1 | 0.98 | 0.09 | -3.53 | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3048 | 1/1 | 0.96 | 0.08 | -3.53 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3368 | 1/1 | 0.94 | 0.07 | -3.54 | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3145 | 1/1 | 0.87 | 0.11 | -3.57 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 1H | 3049 | 1/1 | 0.98 | 0.14 | -3.58 | 57,57,57,57 | 0 |
| 58 | MG | 1H | 3403 | 1/1 | 0.99 | 0.14 | -3.59 | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3445 | 1/1 | 0.96 | 0.12 | -3.64 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3411 | 1/1 | 0.98 | 0.08 | -3.77 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3392 | 1/1 | 0.99 | 0.10 | -3.78 | 50,50,50,50 | 0 |
| 58 | MG | 13 | 1661 | 1/1 | 0.98 | 0.07 | -3.92 | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3292 | 1/1 | 0.95 | 0.06 | -4.05 | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3364 | 1/1 | 0.95 | 0.12 | -4.18 | 48,48,48,48 | 0 |
| 58 | MG | 14 | 3304 | 1/1 | 0.91 | 0.12 | -4.25 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3442 | 1/1 | 0.94 | 0.06 | -4.29 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3356 | 1/1 | 0.94 | 0.10 | -4.31 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3354 | 1/1 | 0.96 | 0.12 | -4.32 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3398 | 1/1 | 0.94 | 0.11 | -4.46 | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3472 | 1/1 | 0.95 | 0.09 | -4.48 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3314 | 1/1 | 0.90 | 0.13 | -4.53 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3369 | 1/1 | 0.99 | 0.13 | -4.70 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3391 | 1/1 | 0.98 | 0.10 | -4.79 | 61,61,61,61 | 0 |
| 58 | MG | 14 | 3207 | 1/1 | 0.72 | 0.12 | -4.81 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3120 | 1/1 | 0.94 | 0.09 | -4.82 | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3217 | 1/1 | 0.94 | 0.14 | -4.85 | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3415 | 1/1 | 0.91 | 0.07 | -5.27 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3318 | 1/1 | 0.93 | 0.08 | -5.34 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3375 | 1/1 | 0.97 | 0.09 | -5.48 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3446 | 1/1 | 0.92 | 0.07 | -5.64 | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3323 | 1/1 | 0.95 | 0.10 | -5.69 | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3066 | 1/1 | 0.92 | 0.11 | -5.74 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3363 | 1/1 | 0.94 | 0.08 | -6.08 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3488 | 1/1 | 0.84 | 0.05 | -6.08 | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3351 | 1/1 | 0.97 | 0.05 | -6.26 | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3322 | 1/1 | 0.99 | 0.06 | -6.29 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3366 | 1/1 | 0.90 | 0.10 | -6.35 | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3296 | 1/1 | 0.95 | 0.08 | -6.48 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3414 | 1/1 | 0.90 | 0.12 | -6.52 | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3218 | 1/1 | 0.97 | 0.11 | -6.63 | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3384 | 1/1 | 0.97 | 0.11 | -6.69 | 45,45,45,45 | 0 |
| 58 | MG | 1G | 1681 | 1/1 | 0.88 | 0.10 | -7.10 | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3418 | 1/1 | 0.90 | 0.06 | -7.20 | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3327 | 1/1 | 0.86 | 0.06 | -7.60 | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3316 | 1/1 | 0.99 | 0.06 | -7.63 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3380 | 1/1 | 0.97 | 0.08 | -8.06 | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3365 | 1/1 | 0.94 | 0.07 | -8.19 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3438 | 1/1 | 0.93 | 0.06 | -8.33 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 58 | MG | 1H | 3473 | 1/1 | 0.91 | 0.05 | -8.99 | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3356 | 1/1 | 0.97 | 0.09 | -9.11 | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3414 | 1/1 | 0.95 | 0.08 | -9.83 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3300 | 1/1 | 0.97 | 0.11 | -10.46 | 57,57,57,57 | 0 |
| 58 | MG | 1H | 3393 | 1/1 | 0.99 | 0.06 | -10.51 | 51,51,51,51 | 0 |
| 58 | MG | 14 | 3295 | 1/1 | 0.93 | 0.07 | -11.56 | 61,61,61,61 | 0 |
| 58 | MG | 14 | 3303 | 1/1 | 0.84 | 0.06 | -11.95 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3183 | 1/1 | 0.95 | 0.29 | - | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3280 | 1/1 | 0.90 | 0.45 | - | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3247 | 1/1 | 0.89 | 0.36 | - | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1694 | 1/1 | 0.93 | 0.09 | - | 129,129,129,129 | 0 |
| 58 | MG | 1H | 3043 | 1/1 | 0.92 | 0.45 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3177 | 1/1 | 0.94 | 0.17 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3262 | 1/1 | 0.69 | 0.27 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3482 | 1/1 | 0.89 | 0.08 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3081 | 1/1 | 0.95 | 0.28 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3057 | 1/1 | 0.99 | 0.32 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3209 | 1/1 | 0.84 | 0.45 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3017 | 1/1 | 0.58 | 0.28 | - | 87,87,87,87 | 0 |
| 58 | MG | 1G | 1623 | 1/1 | 0.94 | 0.42 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3386 | 1/1 | 0.96 | 0.10 | - | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3170 | 1/1 | 0.98 | 0.46 | - | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3162 | 1/1 | 0.90 | 0.22 | - | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1654 | 1/1 | 0.81 | 0.28 | - | 132,132,132,132 | 0 |
| 58 | MG | 14 | 3210 | 1/1 | 0.86 | 0.23 | - | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3109 | 1/1 | 0.94 | 0.20 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3272 | 1/1 | 0.99 | 0.10 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3349 | 1/1 | 0.86 | 0.24 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1622 | 1/1 | 0.96 | 0.46 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3087 | 1/1 | 0.94 | 0.24 | - | 46,46,46,46 | 0 |
| 58 | MG | 14 | 3061 | 1/1 | 0.99 | 0.28 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3231 | 1/1 | 0.98 | 0.41 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3325 | 1/1 | 0.97 | 0.06 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3208 | 1/1 | 0.85 | 0.78 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3264 | 1/1 | 0.68 | 0.48 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3371 | 1/1 | 0.97 | 0.09 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1657 | 1/1 | 0.73 | 0.59 | - | 84,84,84,84 | 0 |
| 58 | MG | 13 | 1663 | 1/1 | 0.98 | 0.46 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3275 | 1/1 | 0.91 | 0.50 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3342 | 1/1 | 0.91 | 0.04 | - | 129,129,129,129 | 0 |
| 58 | MG | 13 | 1683 | 1/1 | 0.50 | 0.21 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3018 | 1/1 | 0.94 | 0.55 | - | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3271 | 1/1 | 0.77 | 0.35 | - | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1698 | 1/1 | 0.90 | 0.28 | - | 104,104,104,104 | 0 |
| 58 | MG | 21 | 302 | 1/1 | 0.82 | 0.22 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3011 | 1/1 | 0.90 | 0.50 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3324 | 1/1 | 0.69 | 0.11 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3034 | 1/1 | 0.97 | 0.38 | - | 53,53,53,53 | 0 |
| 58 | MG | 13 | 1607 | 1/1 | 0.66 | 0.65 | - | 84,84,84,84 | 0 |
| 58 | MG | 1G | 1668 | 1/1 | 0.95 | 0.44 | - | 141,141,141,141 | 0 |
| 58 | MG | 1H | 3495 | 1/1 | 0.93 | 0.06 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3307 | 1/1 | 0.95 | 0.09 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3406 | 1/1 | 0.94 | 0.06 | - | 100,100,100,100 | 0 |
| 58 | MG | 1G | 1628 | 1/1 | 0.63 | 0.49 | - | 102,102,102,102 | 0 |
| 58 | MG | 13 | 1623 | 1/1 | 0.94 | 0.18 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3355 | 1/1 | 0.99 | 0.08 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3416 | 1/1 | 0.93 | 0.18 | - | 108,108,108,108 | 0 |
| 58 | MG | 13 | 1614 | 1/1 | 0.95 | 0.06 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3466 | 1/1 | 0.93 | 0.08 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3267 | 1/1 | 0.79 | 0.15 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3254 | 1/1 | 0.74 | 0.52 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3006 | 1/1 | 0.96 | 0.19 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3311 | 1/1 | 0.89 | 0.19 | - | 127,127,127,127 | 0 |
| 58 | MG | 14 | 3072 | 1/1 | 0.99 | 0.37 | - | 43,43,43,43 | 0 |
| 58 | MG | 1G | 1684 | 1/1 | 0.98 | 0.08 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3204 | 1/1 | 0.83 | 0.66 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3320 | 1/1 | 0.90 | 0.29 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3390 | 1/1 | 0.90 | 0.13 | - | 118,118,118,118 | 0 |
| 58 | MG | 14 | 3066 | 1/1 | 0.96 | 0.44 | - | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3153 | 1/1 | 0.78 | 0.65 | - | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1619 | 1/1 | 0.95 | 0.22 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3463 | 1/1 | 0.89 | 0.31 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3391 | 1/1 | 0.94 | 0.15 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3341 | 1/1 | 0.87 | 0.24 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3014 | 1/1 | 0.53 | 0.65 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3055 | 1/1 | 0.98 | 0.26 | - | 50,50,50,50 | 0 |
| 58 | MG | 13 | 1724 | 1/1 | 0.88 | 0.16 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3301 | 1/1 | 0.97 | 0.10 | - | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3469 | 1/1 | 0.86 | 0.12 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3426 | 1/1 | 0.83 | 0.11 | - | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3301 | 1/1 | 0.69 | 0.44 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3382 | 1/1 | 0.95 | 0.07 | - | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3154 | 1/1 | 0.95 | 0.33 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3135 | 1/1 | 0.97 | 0.83 | - | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3288 | 1/1 | 0.90 | 0.34 | - | 56,56,56,56 | 0 |
| 58 | MG | 13 | 1738 | 1/1 | 0.94 | 0.13 | - | 105,105,105,105 | 0 |
| 58 | MG | 1H | 3455 | 1/1 | 0.98 | 0.06 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3200 | 1/1 | 0.94 | 0.40 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3010 | 1/1 | 0.97 | 0.29 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3126 | 1/1 | 0.77 | 0.56 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3069 | 1/1 | 0.94 | 0.23 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3144 | 1/1 | 0.91 | 0.14 | - | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3026 | 1/1 | 0.90 | 0.24 | - | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3477 | 1/1 | 0.89 | 0.07 | - | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3286 | 1/1 | 0.55 | 0.26 | - | 100,100,100,100 | 0 |
| 58 | MG | 13 | 1715 | 1/1 | 0.93 | 0.06 | - | 106,106,106,106 | 0 |
| 58 | MG | 1H | 3091 | 1/1 | 0.99 | 0.23 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3171 | 1/1 | 0.95 | 0.14 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3146 | 1/1 | 0.81 | 0.39 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3308 | 1/1 | 0.88 | 0.35 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3201 | 1/1 | 0.44 | 0.27 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3184 | 1/1 | 0.93 | 0.40 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3030 | 1/1 | 0.88 | 0.26 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3406 | 1/1 | 0.92 | 0.09 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3274 | 1/1 | 0.59 | 0.27 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3377 | 1/1 | 0.98 | 0.14 | - | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3127 | 1/1 | 0.92 | 0.30 | - | 64,64,64,64 | 0 |
| 58 | MG | 1G | 1639 | 1/1 | 0.90 | 0.36 | - | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3200 | 1/1 | 0.90 | 0.22 | - | 84,84,84,84 | 0 |
| 58 | MG | 1G | 1646 | 1/1 | 0.89 | 0.50 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3256 | 1/1 | 0.97 | 0.52 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3141 | 1/1 | 0.83 | 0.41 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3111 | 1/1 | 0.98 | 0.28 | - | 48,48,48,48 | 0 |
| 58 | MG | 1G | 1633 | 1/1 | 0.90 | 0.15 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3409 | 1/1 | 0.93 | 0.09 | - | 58,58,58,58 | 0 |
| 58 | MG | 1G | 1611 | 1/1 | 0.94 | 0.39 | - | 105,105,105,105 | 0 |
| 58 | MG | 1G | 1631 | 1/1 | 0.84 | 0.53 | - | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3288 | 1/1 | 0.72 | 0.28 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3350 | 1/1 | 0.78 | 0.10 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1659 | 1/1 | 0.81 | 0.11 | - | 107,107,107,107 | 0 |
| 58 | MG | 14 | 3002 | 1/1 | 0.98 | 0.38 | - | 53,53,53,53 | 0 |
| 58 | MG | 14 | 3405 | 1/1 | 0.84 | 0.09 | - | 107,107,107,107 | 0 |
| 58 | MG | 1G | 1662 | 1/1 | 0.73 | 0.15 | - | 84,84,84,84 | 0 |
| 58 | MG | 13 | 1734 | 1/1 | 0.77 | 0.07 | - | 130,130,130,130 | 0 |
| 58 | MG | 1G | 1683 | 1/1 | 0.96 | 0.05 | - | 106,106,106,106 | 0 |
| 58 | MG | 1H | 3468 | 1/1 | 0.79 | 0.19 | - | 108,108,108,108 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3081 | 1/1 | 0.95 | 0.25 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1735 | 1/1 | 0.64 | 0.08 | - | 124,124,124,124 | 0 |
| 58 | MG | 1H | 3193 | 1/1 | 0.79 | 0.39 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1604 | 1/1 | 0.97 | 0.31 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3266 | 1/1 | 0.77 | 0.22 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3188 | 1/1 | 0.75 | 0.57 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3040 | 1/1 | 0.96 | 0.12 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3388 | 1/1 | 0.96 | 0.15 | - | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1690 | 1/1 | 0.91 | 0.27 | - | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3221 | 1/1 | 0.74 | 0.56 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3133 | 1/1 | 0.98 | 0.21 | - | 60,60,60,60 | 0 |
| 58 | MG | 13 | 1659 | 1/1 | 0.87 | 0.25 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3126 | 1/1 | 0.90 | 0.60 | - | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1669 | 1/1 | 0.69 | 0.52 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3464 | 1/1 | 0.88 | 0.07 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3156 | 1/1 | 0.96 | 0.39 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3325 | 1/1 | 0.95 | 0.12 | - | 82,82,82,82 | 0 |
| 58 | MG | 1G | 1674 | 1/1 | 0.71 | 0.33 | - | 110,110,110,110 | 0 |
| 58 | MG | 1H | 3033 | 1/1 | 0.91 | 0.38 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3160 | 1/1 | 0.86 | 0.31 | - | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3261 | 1/1 | 0.98 | 0.07 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1641 | 1/1 | 0.57 | 0.19 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3430 | 1/1 | 0.83 | 0.28 | - | 112,112,112,112 | 0 |
| 58 | MG | 1H | 3052 | 1/1 | 0.98 | 0.18 | - | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3112 | 1/1 | 0.87 | 0.39 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3294 | 1/1 | 0.88 | 0.42 | - | 141,141,141,141 | 0 |
| 58 | MG | 1H | 3252 | 1/1 | 0.78 | 0.30 | - | 77,77,77,77 | 0 |
| 58 | MG | 1G | 1687 | 1/1 | 0.91 | 0.13 | - | 116,116,116,116 | 0 |
| 58 | MG | 14 | 3107 | 1/1 | 0.87 | 0.08 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3239 | 1/1 | 0.85 | 0.26 | - | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3095 | 1/1 | 0.95 | 0.50 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3297 | 1/1 | 0.81 | 0.32 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3219 | 1/1 | 0.94 | 0.23 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1700 | 1/1 | 0.95 | 0.24 | - | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3214 | 1/1 | 0.97 | 0.14 | - | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3279 | 1/1 | 0.83 | 0.24 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3481 | 1/1 | 0.94 | 0.05 | - | 100,100,100,100 | 0 |
| 58 | MG | 1G | 1607 | 1/1 | 0.97 | 0.21 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3279 | 1/1 | 0.74 | 0.40 | - | 71,71,71,71 | 0 |
| 58 | MG | 13 | 1625 | 1/1 | 0.87 | 0.35 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3164 | 1/1 | 0.83 | 0.39 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3386 | 1/1 | 0.98 | 0.05 | - | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3361 | 1/1 | 0.91 | 0.14 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3212 | 1/1 | 0.96 | 0.27 | - | 42,42,42,42 | 0 |
| 58 | MG | 14 | 3166 | 1/1 | 0.99 | 0.21 | - | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3071 | 1/1 | 0.97 | 0.28 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3121 | 1/1 | 0.89 | 0.47 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3271 | 1/1 | 0.91 | 0.44 | - | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1736 | 1/1 | 0.88 | 0.10 | - | 116,116,116,116 | 0 |
| 58 | MG | 1H | 3268 | 1/1 | 0.70 | 0.29 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3068 | 1/1 | 0.94 | 0.44 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3471 | 1/1 | 0.98 | 0.21 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1718 | 1/1 | 0.88 | 0.10 | - | 100,100,100,100 | 0 |
| 58 | MG | 1H | 3326 | 1/1 | 0.98 | 0.45 | - | 119,119,119,119 | 0 |
| 58 | MG | 14 | 3333 | 1/1 | 0.97 | 0.11 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3358 | 1/1 | 0.98 | 0.05 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3257 | 1/1 | 0.42 | 0.71 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3202 | 1/1 | 0.88 | 0.28 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3427 | 1/1 | 0.87 | 0.15 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3281 | 1/1 | 0.89 | 0.51 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3385 | 1/1 | 0.92 | 0.12 | - | 60,60,60,60 | 0 |
| 58 | MG | 13 | 1651 | 1/1 | 0.80 | 0.38 | - | 105,105,105,105 | 0 |
| 58 | MG | 13 | 1723 | 1/1 | 0.97 | 0.05 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3381 | 1/1 | 0.91 | 0.24 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3267 | 1/1 | 0.88 | 0.31 | - | 94,94,94,94 | 0 |
| 58 | MG | 1H | 3420 | 1/1 | 0.93 | 0.13 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3387 | 1/1 | 0.91 | 0.24 | - | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3389 | 1/1 | 0.92 | 0.08 | - | 94,94,94,94 | 0 |
| 58 | MG | 1G | 1635 | 1/1 | 0.77 | 0.51 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3277 | 1/1 | 0.90 | 0.45 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1684 | 1/1 | 0.83 | 0.16 | - | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3409 | 1/1 | 0.82 | 0.08 | - | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3144 | 1/1 | 0.96 | 0.20 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3316 | 1/1 | 0.87 | 0.65 | - | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3115 | 1/1 | 0.89 | 0.17 | - | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3312 | 1/1 | 0.90 | 0.21 | - | 80,80,80,80 | 0 |
| 58 | MG | 13 | 1678 | 1/1 | 0.82 | 0.36 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3431 | 1/1 | 0.99 | 0.03 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3323 | 1/1 | 0.96 | 0.06 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3092 | 1/1 | 0.95 | 0.15 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3159 | 1/1 | 0.72 | 0.26 | - | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1611 | 1/1 | 0.92 | 0.22 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3450 | 1/1 | 0.98 | 0.13 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3334 | 1/1 | 0.77 | 0.38 | - | 96,96,96,96 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3060 | 1/1 | 0.94 | 0.26 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3264 | 1/1 | 0.94 | 0.15 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3312 | 1/1 | 0.98 | 0.17 | - | 56,56,56,56 | 0 |
| 58 | MG | 14 | 3393 | 1/1 | 0.96 | 0.12 | - | 140,140,140,140 | 0 |
| 58 | MG | 13 | 1602 | 1/1 | 0.98 | 0.32 | - | 74,74,74,74 | 0 |
| 58 | MG | 1G | 1689 | 1/1 | 0.97 | 0.07 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3362 | 1/1 | 0.97 | 0.11 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3230 | 1/1 | 0.78 | 0.29 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3211 | 1/1 | 0.62 | 0.37 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3401 | 1/1 | 0.97 | 0.06 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3028 | 1/1 | 0.99 | 0.22 | - | 53,53,53,53 | 0 |
| 58 | MG | 4K | 101 | 1/1 | 0.89 | 0.23 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3239 | 1/1 | 0.90 | 0.53 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3223 | 1/1 | 0.66 | 0.23 | - | 92,92,92,92 | 0 |
| 58 | MG | 14 | 3359 | 1/1 | 0.99 | 0.08 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3268 | 1/1 | 0.80 | 0.32 | - | 79,79,79,79 | 0 |
| 58 | MG | 29 | 301 | 1/1 | 0.97 | 0.25 | - | 58,58,58,58 | 0 |
| 58 | MG | 13 | 1714 | 1/1 | 0.92 | 0.06 | - | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3118 | 1/1 | 0.86 | 0.21 | - | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3050 | 1/1 | 0.98 | 0.31 | - | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3175 | 1/1 | 0.67 | 0.43 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3487 | 1/1 | 0.88 | 0.21 | - | 117,117,117,117 | 0 |
| 58 | MG | 1H | 3150 | 1/1 | 0.81 | 0.38 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3283 | 1/1 | 0.93 | 0.56 | - | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1688 | 1/1 | 0.95 | 0.35 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1621 | 1/1 | 0.83 | 0.74 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3206 | 1/1 | 0.97 | 0.47 | - | 69,69,69,69 | 0 |
| 58 | MG | 1G | 1680 | 1/1 | 0.82 | 0.07 | - | 127,127,127,127 | 0 |
| 58 | MG | 1H | 3305 | 1/1 | 0.90 | 0.35 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3022 | 1/1 | 0.98 | 0.33 | - | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3404 | 1/1 | 0.92 | 0.06 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3090 | 1/1 | 0.96 | 0.26 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3023 | 1/1 | 0.99 | 0.26 | - | 42,42,42,42 | 0 |
| 58 | MG | 13 | 1728 | 1/1 | 0.96 | 0.07 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3269 | 1/1 | 0.80 | 0.12 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3191 | 1/1 | 0.85 | 0.54 | - | 81,81,81,81 | 0 |
| 58 | MG | 13 | 1710 | 1/1 | 0.96 | 0.07 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3152 | 1/1 | 0.79 | 0.41 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3344 | 1/1 | 0.82 | 0.10 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3104 | 1/1 | 0.93 | 0.43 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3437 | 1/1 | 0.93 | 0.16 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3223 | 1/1 | 0.96 | 0.15 | - | 81,81,81,81 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3194 | 1/1 | 0.85 | 0.42 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3047 | 1/1 | 0.96 | 0.33 | - | 43,43,43,43 | 0 |
| 58 | MG | 13 | 1702 | 1/1 | 0.93 | 0.21 | - | 157,157,157,157 | 0 |
| 58 | MG | 2L | 102 | 1/1 | 0.62 | 0.45 | - | 94,94,94,94 | 0 |
| 58 | MG | 1H | 3037 | 1/1 | 0.95 | 0.29 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3234 | 1/1 | 0.91 | 0.24 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3103 | 1/1 | 0.91 | 0.53 | - | 75,75,75,75 | 0 |
| 58 | MG | 1H | 3317 | 1/1 | 0.94 | 0.77 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3106 | 1/1 | 0.96 | 0.23 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3034 | 1/1 | 0.67 | 0.22 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3139 | 1/1 | 0.80 | 0.49 | - | 55,55,55,55 | 0 |
| 58 | MG | 16 | 208 | 1/1 | 0.92 | 0.49 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3229 | 1/1 | 0.85 | 0.43 | - | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3020 | 1/1 | 0.92 | 0.46 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3183 | 1/1 | 0.96 | 0.49 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3021 | 1/1 | 0.67 | 0.35 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3070 | 1/1 | 0.93 | 0.40 | - | 72,72,72,72 | 0 |
| 58 | MG | 1G | 1636 | 1/1 | 0.91 | 0.46 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3287 | 1/1 | 0.93 | 0.21 | - | 77,77,77,77 | 0 |
| 58 | MG | 16 | 211 | 1/1 | 0.89 | 0.08 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3002 | 1/1 | 0.99 | 0.26 | - | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3275 | 1/1 | 0.92 | 0.35 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3098 | 1/1 | 0.93 | 0.81 | - | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3372 | 1/1 | 0.95 | 0.05 | - | 119,119,119,119 | 0 |
| 58 | MG | 14 | 3408 | 1/1 | 0.91 | 0.17 | - | 108,108,108,108 | 0 |
| 58 | MG | 1G | 1693 | 1/1 | 0.92 | 0.10 | - | 123,123,123,123 | 0 |
| 58 | MG | 1G | 1616 | 1/1 | 0.90 | 0.35 | - | 116,116,116,116 | 0 |
| 58 | MG | 14 | 3008 | 1/1 | 0.83 | 0.39 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3129 | 1/1 | 0.97 | 0.47 | - | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3337 | 1/1 | 0.92 | 0.23 | - | 53,53,53,53 | 0 |
| 58 | MG | 1G | 1629 | 1/1 | 0.98 | 0.36 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3297 | 1/1 | 0.93 | 0.09 | - | 55,55,55,55 | 0 |
| 58 | MG | 14 | 3231 | 1/1 | 0.90 | 0.20 | - | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1721 | 1/1 | 0.97 | 0.19 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3447 | 1/1 | 0.63 | 0.28 | - | 87,87,87,87 | 0 |
| 58 | MG | P8 | 101 | 1/1 | 0.83 | 0.26 | - | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3343 | 1/1 | 0.93 | 0.18 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3284 | 1/1 | 0.85 | 0.38 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1695 | 1/1 | 0.92 | 0.24 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3331 | 1/1 | 0.90 | 0.23 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3151 | 1/1 | 0.97 | 0.53 | - | 65,65,65,65 | 0 |
| 58 | MG | 1G | 1603 | 1/1 | 0.55 | 0.63 | - | 100,100,100,100 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3299 | 1/1 | 0.88 | 0.16 | - | 98,98,98,98 | 0 |
| 58 | MG | 1H | 3208 | 1/1 | 0.92 | 0.56 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3093 | 1/1 | 0.92 | 0.46 | - | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3321 | 1/1 | 0.94 | 0.18 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3378 | 1/1 | 0.96 | 0.09 | - | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1610 | 1/1 | 0.98 | 0.11 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3243 | 1/1 | 0.73 | 0.40 | - | 118,118,118,118 | 0 |
| 58 | MG | 1H | 3440 | 1/1 | 0.80 | 0.13 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3060 | 1/1 | 0.95 | 0.19 | - | 47,47,47,47 | 0 |
| 58 | MG | 1H | 3396 | 1/1 | 0.97 | 0.07 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3105 | 1/1 | 0.90 | 0.43 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3161 | 1/1 | 0.85 | 0.36 | - | 71,71,71,71 | 0 |
| 58 | MG | 13 | 1665 | 1/1 | 0.93 | 0.14 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3347 | 1/1 | 0.97 | 0.11 | - | 83,83,83,83 | 0 |
| 58 | MG | 1G | 1638 | 1/1 | 0.90 | 0.38 | - | 131,131,131,131 | 0 |
| 58 | MG | 14 | 3069 | 1/1 | 0.97 | 0.43 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3084 | 1/1 | 0.95 | 0.42 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3065 | 1/1 | 0.85 | 0.43 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3013 | 1/1 | 0.98 | 0.39 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3078 | 1/1 | 0.96 | 0.39 | - | 56,56,56,56 | 0 |
| 58 | MG | 14 | 3261 | 1/1 | 0.95 | 0.23 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3375 | 1/1 | 0.96 | 0.16 | - | 49,49,49,49 | 0 |
| 58 | MG | 1G | 1686 | 1/1 | 0.88 | 0.09 | - | 126,126,126,126 | 0 |
| 58 | MG | 1H | 3008 | 1/1 | 0.96 | 0.17 | - | 90,90,90,90 | 0 |
| 58 | MG | 14 | 3273 | 1/1 | 0.69 | 1.01 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3371 | 1/1 | 0.93 | 0.15 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3449 | 1/1 | 0.87 | 0.07 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3338 | 1/1 | 0.91 | 0.44 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3400 | 1/1 | 0.88 | 0.12 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3025 | 1/1 | 0.97 | 0.27 | - | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1679 | 1/1 | 0.87 | 0.21 | - | 117,117,117,117 | 0 |
| 58 | MG | 1H | 3247 | 1/1 | 0.97 | 0.44 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3489 | 1/1 | 0.91 | 0.20 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1680 | 1/1 | 0.68 | 0.18 | - | 149,149,149,149 | 0 |
| 58 | MG | 14 | 3064 | 1/1 | 0.92 | 0.42 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3395 | 1/1 | 0.93 | 0.07 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3156 | 1/1 | 0.77 | 0.27 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3335 | 1/1 | 0.90 | 0.12 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3257 | 1/1 | 0.91 | 0.24 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3062 | 1/1 | 0.93 | 0.29 | - | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1652 | 1/1 | 0.92 | 0.28 | - | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3189 | 1/1 | 0.84 | 0.56 | - | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 13 | 1627 | 1/1 | 0.96 | 0.21 | - | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3302 | 1/1 | 0.15 | 0.30 | - | 94,94,94,94 | 0 |
| 58 | MG | 1H | 3421 | 1/1 | 0.85 | 0.15 | - | 118,118,118,118 | 0 |
| 58 | MG | 14 | 3047 | 1/1 | 0.95 | 0.23 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3439 | 1/1 | 0.93 | 0.13 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3309 | 1/1 | 0.98 | 0.18 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3365 | 1/1 | 0.98 | 0.07 | - | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3123 | 1/1 | 0.90 | 0.22 | - | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3382 | 1/1 | 0.78 | 0.07 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3019 | 1/1 | 0.92 | 0.30 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1649 | 1/1 | 0.71 | 0.37 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1636 | 1/1 | 0.97 | 0.29 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3461 | 1/1 | 0.96 | 0.06 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3416 | 1/1 | 0.97 | 0.31 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1620 | 1/1 | 0.92 | 0.11 | - | 87,87,87,87 | 0 |
| 58 | MG | 1G | 1625 | 1/1 | 0.94 | 0.36 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3128 | 1/1 | 0.79 | 0.37 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3077 | 1/1 | 0.92 | 0.56 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3307 | 1/1 | 0.75 | 0.32 | - | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3339 | 1/1 | 0.76 | 0.19 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3196 | 1/1 | 0.81 | 0.30 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3011 | 1/1 | 0.99 | 0.43 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3459 | 1/1 | 0.95 | 0.11 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1642 | 1/1 | 0.92 | 0.40 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3101 | 1/1 | 0.97 | 0.32 | - | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3357 | 1/1 | 0.98 | 0.09 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3399 | 1/1 | 0.97 | 0.09 | - | 40,40,40,40 | 0 |
| 58 | MG | 1H | 3342 | 1/1 | 0.90 | 0.28 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3405 | 1/1 | 0.97 | 0.09 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3140 | 1/1 | 0.73 | 0.30 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3107 | 1/1 | 0.88 | 0.30 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3417 | 1/1 | 0.89 | 0.07 | - | 113,113,113,113 | 0 |
| 58 | MG | 13 | 1737 | 1/1 | 0.82 | 0.13 | - | 111,111,111,111 | 0 |
| 58 | MG | 14 | 3240 | 1/1 | 0.74 | 0.58 | - | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3385 | 1/1 | 0.92 | 0.20 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3379 | 1/1 | 0.95 | 0.37 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3132 | 1/1 | 0.90 | 0.38 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3198 | 1/1 | 0.88 | 0.33 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3090 | 1/1 | 0.97 | 0.29 | - | 48,48,48,48 | 0 |
| 58 | MG | 14 | 3326 | 1/1 | 0.98 | 0.12 | - | 77,77,77,77 | 0 |
| 58 | MG | 16 | 201 | 1/1 | 0.89 | 0.06 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3114 | 1/1 | 0.99 | 0.26 | - | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3155 | 1/1 | 0.93 | 0.47 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3184 | 1/1 | 0.69 | 0.40 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3141 | 1/1 | 0.95 | 0.16 | - | 47,47,47,47 | 0 |
| 58 | MG | 1H | 3234 | 1/1 | 0.72 | 0.42 | - | 78,78,78,78 | 0 |
| 58 | MG | 1J | 203 | 1/1 | 0.75 | 0.29 | - | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3354 | 1/1 | 0.89 | 0.07 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3429 | 1/1 | 0.93 | 0.09 | - | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3232 | 1/1 | 0.85 | 0.25 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3292 | 1/1 | 0.89 | 0.12 | - | 68,68,68,68 | 0 |
| 58 | MG | 13 | 1713 | 1/1 | 0.93 | 0.09 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3096 | 1/1 | 0.99 | 0.36 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3138 | 1/1 | 0.87 | 0.32 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3146 | 1/1 | 0.92 | 0.49 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3417 | 1/1 | 0.96 | 0.08 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3454 | 1/1 | 0.96 | 0.17 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3027 | 1/1 | 1.00 | 0.27 | - | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3110 | 1/1 | 0.96 | 0.29 | - | 60,60,60,60 | 0 |
| 58 | MG | 11 | 301 | 1/1 | 0.94 | 0.18 | - | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3336 | 1/1 | 0.95 | 0.20 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3345 | 1/1 | 0.85 | 0.23 | - | 68,68,68,68 | 0 |
| 58 | MG | 1G | 1630 | 1/1 | 0.70 | 0.40 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3163 | 1/1 | 0.93 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 13 | 1674 | 1/1 | 0.91 | 0.14 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3328 | 1/1 | 0.94 | 0.13 | - | 105,105,105,105 | 0 |
| 58 | MG | 1G | 1650 | 1/1 | 0.69 | 0.38 | - | 102,102,102,102 | 0 |
| 58 | MG | 13 | 1641 | 1/1 | 0.88 | 0.33 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3045 | 1/1 | 0.91 | 0.25 | - | 52,52,52,52 | 0 |
| 58 | MG | 1H | 3490 | 1/1 | 0.95 | 0.05 | - | 95,95,95,95 | 0 |
| 58 | MG | 1H | 3143 | 1/1 | 0.95 | 0.19 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3229 | 1/1 | 0.65 | 0.42 | - | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1729 | 1/1 | 0.97 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3055 | 1/1 | 0.90 | 0.48 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3280 | 1/1 | 0.90 | 0.16 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3038 | 1/1 | 0.94 | 0.30 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3453 | 1/1 | 0.95 | 0.06 | - | 98,98,98,98 | 0 |
| 58 | MG | 16 | 203 | 1/1 | 0.87 | 0.39 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3172 | 1/1 | 0.90 | 0.16 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3372 | 1/1 | 0.97 | 0.09 | - | 73,73,73,73 | 0 |
| 58 | MG | 13 | 1671 | 1/1 | 0.92 | 0.17 | - | 121,121,121,121 | 0 |
| 58 | MG | 1H | 3460 | 1/1 | 0.91 | 0.17 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3182 | 1/1 | 0.98 | 0.50 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3251 | 1/1 | 0.97 | 0.82 | - | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3082 | 1/1 | 0.97 | 0.34 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3041 | 1/1 | 0.99 | 0.20 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3332 | 1/1 | 0.75 | 0.17 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3470 | 1/1 | 0.97 | 0.04 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1739 | 1/1 | 0.77 | 0.06 | - | 110,110,110,110 | 0 |
| 58 | MG | 14 | 3068 | 1/1 | 0.67 | 0.83 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3021 | 1/1 | 0.96 | 0.28 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3295 | 1/1 | 0.88 | 0.53 | - | 88,88,88,88 | 0 |
| 58 | MG | 13 | 1732 | 1/1 | 0.93 | 0.13 | - | 120,120,120,120 | 0 |
| 58 | MG | 14 | 3398 | 1/1 | 0.99 | 0.07 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3187 | 1/1 | 0.88 | 0.24 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3109 | 1/1 | 0.98 | 0.32 | - | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3346 | 1/1 | 0.48 | 0.09 | - | 144,144,144,144 | 0 |
| 58 | MG | 1H | 3072 | 1/1 | 0.84 | 0.27 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3300 | 1/1 | 0.92 | 0.38 | - | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1605 | 1/1 | 0.93 | 0.23 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3436 | 1/1 | 0.96 | 0.07 | - | 73,73,73,73 | 0 |
| 58 | MG | 13 | 1730 | 1/1 | 0.93 | 0.07 | - | 95,95,95,95 | 0 |
| 58 | MG | 13 | 1682 | 1/1 | 0.81 | 0.30 | - | 151,151,151,151 | 0 |
| 58 | MG | 1H | 3367 | 1/1 | 0.95 | 0.06 | - | 59,59,59,59 | 0 |
| 58 | MG | 1H | 3319 | 1/1 | 0.85 | 0.26 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3276 | 1/1 | 0.83 | 0.60 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3285 | 1/1 | 0.79 | 0.22 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3331 | 1/1 | 0.90 | 0.10 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3003 | 1/1 | 0.99 | 0.29 | - | 38,38,38,38 | 0 |
| 58 | MG | 13 | 1716 | 1/1 | 0.97 | 0.14 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3235 | 1/1 | 0.84 | 0.25 | - | 76,76,76,76 | 0 |
| 58 | MG | 1G | 1673 | 1/1 | 0.78 | 0.22 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3394 | 1/1 | 0.95 | 0.09 | - | 101,101,101,101 | 0 |
| 58 | MG | 1H | 3485 | 1/1 | 0.73 | 0.10 | - | 116,116,116,116 | 0 |
| 58 | MG | 1H | 3224 | 1/1 | 0.97 | 0.41 | - | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3248 | 1/1 | 0.88 | 0.72 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3474 | 1/1 | 0.91 | 0.11 | - | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3185 | 1/1 | 0.96 | 0.33 | - | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3133 | 1/1 | 0.93 | 0.41 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3324 | 1/1 | 0.51 | 0.38 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3048 | 1/1 | 0.96 | 0.33 | - | 43,43,43,43 | 0 |
| 58 | MG | 13 | 1633 | 1/1 | 0.87 | 0.37 | - | 91,91,91,91 | 0 |
| 58 | MG | 1G | 1640 | 1/1 | 0.89 | 0.57 | - | 75,75,75,75 | 0 |
| 58 | MG | 1H | 3114 | 1/1 | 0.95 | 0.59 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3310 | 1/1 | 0.66 | 0.16 | - | 126,126,126,126 | 0 |
| 58 | MG | 1H | 3032 | 1/1 | 0.93 | 0.54 | - | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1G | 1609 | 1/1 | 0.95 | 0.20 | - | 98,98,98,98 | 0 |
| 58 | MG | 13 | 1720 | 1/1 | 0.87 | 0.06 | - | 111,111,111,111 | 0 |
| 58 | MG | 14 | 3131 | 1/1 | 0.93 | 0.49 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3232 | 1/1 | 0.93 | 0.50 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3284 | 1/1 | 0.85 | 0.41 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3352 | 1/1 | 0.93 | 0.11 | - | 70,70,70,70 | 0 |
| 58 | MG | 3L | 101 | 1/1 | 0.17 | 0.24 | - | 160,160,160,160 | 0 |
| 58 | MG | 13 | 1709 | 1/1 | 0.94 | 0.07 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1740 | 1/1 | 0.95 | 0.28 | - | 93,93,93,93 | 0 |
| 58 | MG | 1G | 1695 | 1/1 | 0.87 | 0.06 | - | 136,136,136,136 | 0 |
| 58 | MG | 1I | 201 | 1/1 | 0.65 | 0.26 | - | 79,79,79,79 | 0 |
| 58 | MG | 1G | 1648 | 1/1 | 0.84 | 0.35 | - | 90,90,90,90 | 0 |
| 58 | MG | 14 | 3052 | 1/1 | 0.85 | 0.36 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1653 | 1/1 | 0.90 | 0.12 | - | 86,86,86,86 | 0 |
| 58 | MG | 13 | 1691 | 1/1 | 0.92 | 0.23 | - | 89,89,89,89 | 0 |
| 58 | MG | 13 | 1704 | 1/1 | 0.82 | 0.19 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3024 | 1/1 | 0.90 | 0.21 | - | 74,74,74,74 | 0 |
| 58 | MG | 13 | 1719 | 1/1 | 0.96 | 0.07 | - | 95,95,95,95 | 0 |
| 58 | MG | 1H | 3056 | 1/1 | 0.92 | 0.36 | - | 50,50,50,50 | 0 |
| 58 | MG | 1G | 1665 | 1/1 | 0.77 | 0.21 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3172 | 1/1 | 0.94 | 0.33 | - | 75,75,75,75 | 0 |
| 58 | MG | 25 | 201 | 1/1 | 0.82 | 0.22 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3475 | 1/1 | 0.96 | 0.09 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3182 | 1/1 | 0.76 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3158 | 1/1 | 0.83 | 0.42 | - | 78,78,78,78 | 0 |
| 58 | MG | 1G | 1677 | 1/1 | 0.84 | 0.11 | - | 130,130,130,130 | 0 |
| 58 | MG | 14 | 3352 | 1/1 | 0.95 | 0.06 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3199 | 1/1 | 0.92 | 0.41 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3492 | 1/1 | 0.95 | 0.11 | - | 95,95,95,95 | 0 |
| 58 | MG | 1H | 3329 | 1/1 | 0.69 | 0.27 | - | 91,91,91,91 | 0 |
| 58 | MG | 1G | 1692 | 1/1 | 0.91 | 0.13 | - | 130,130,130,130 | 0 |
| 58 | MG | 14 | 3163 | 1/1 | 0.85 | 0.68 | - | 65,65,65,65 | 0 |
| 58 | MG | 1J | 206 | 1/1 | 0.68 | 0.08 | - | 115,115,115,115 | 0 |
| 58 | MG | 1H | 3125 | 1/1 | 0.96 | 0.16 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3265 | 1/1 | 0.46 | 0.26 | - | 115,115,115,115 | 0 |
| 58 | MG | 13 | 1693 | 1/1 | 0.87 | 0.62 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3216 | 1/1 | 0.94 | 0.11 | - | 57,57,57,57 | 0 |
| 58 | MG | 1H | 3132 | 1/1 | 0.83 | 0.31 | - | 74,74,74,74 | 0 |
| 58 | MG | 1G | 1651 | 1/1 | 0.82 | 0.37 | - | 100,100,100,100 | 0 |
| 58 | MG | 13 | 1662 | 1/1 | 0.76 | 0.13 | - | 81,81,81,81 | 0 |
| 58 | MG | I8 | 101 | 1/1 | 0.86 | 0.15 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3105 | 1/1 | 0.81 | 0.36 | - | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3313 | 1/1 | 0.68 | 0.38 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3374 | 1/1 | 0.97 | 0.14 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3080 | 1/1 | 0.99 | 0.26 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3228 | 1/1 | 0.94 | 0.55 | - | 68,68,68,68 | 0 |
| 58 | MG | 45 | 203 | 1/1 | 0.75 | 0.46 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3151 | 1/1 | 0.74 | 0.36 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3411 | 1/1 | 0.94 | 0.04 | - | 113,113,113,113 | 0 |
| 58 | MG | 1H | 3119 | 1/1 | 0.82 | 0.28 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3248 | 1/1 | 0.95 | 0.30 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3027 | 1/1 | 0.72 | 0.56 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1707 | 1/1 | 0.89 | 0.13 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3098 | 1/1 | 0.83 | 0.29 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3314 | 1/1 | 0.90 | 0.30 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3401 | 1/1 | 0.94 | 0.10 | - | 71,71,71,71 | 0 |
| 58 | MG | E5 | 101 | 1/1 | 0.93 | 0.24 | - | 53,53,53,53 | 0 |
| 58 | MG | 14 | 3226 | 1/1 | 0.91 | 0.50 | - | 99,99,99,99 | 0 |
| 58 | MG | 13 | 1603 | 1/1 | 0.80 | 0.39 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3032 | 1/1 | 0.98 | 0.33 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3306 | 1/1 | 0.97 | 0.24 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3283 | 1/1 | 0.90 | 0.44 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3150 | 1/1 | 0.87 | 0.27 | - | 78,78,78,78 | 0 |
| 58 | MG | 78 | 201 | 1/1 | 0.90 | 0.35 | - | 76,76,76,76 | 0 |
| 58 | MG | 29 | 303 | 1/1 | 0.93 | 0.28 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3330 | 1/1 | 0.98 | 0.06 | - | 73,73,73,73 | 0 |
| 58 | MG | 14 | 3353 | 1/1 | 0.96 | 0.11 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3167 | 1/1 | 0.90 | 0.24 | - | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3127 | 1/1 | 0.89 | 0.37 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3467 | 1/1 | 0.93 | 0.16 | - | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3058 | 1/1 | 0.97 | 0.23 | - | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3067 | 1/1 | 0.96 | 0.34 | - | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3197 | 1/1 | 0.71 | 0.30 | - | 146,146,146,146 | 0 |
| 58 | MG | 13 | 1731 | 1/1 | 0.95 | 0.08 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3218 | 1/1 | 0.71 | 0.12 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3018 | 1/1 | 0.99 | 0.43 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3263 | 1/1 | 0.88 | 0.51 | - | 106,106,106,106 | 0 |
| 58 | MG | 1H | 3408 | 1/1 | 0.96 | 0.10 | - | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3346 | 1/1 | 0.87 | 0.24 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3483 | 1/1 | 0.95 | 0.05 | - | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1652 | 1/1 | 0.89 | 0.11 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3159 | 1/1 | 0.77 | 0.25 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1708 | 1/1 | 0.89 | 0.12 | - | 76,76,76,76 | 0 |
| 58 | MG | 13 | 1660 | 1/1 | 0.93 | 0.38 | - | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3484 | 1/1 | 0.83 | 0.08 | - | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3480 | 1/1 | 0.93 | 0.09 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3306 | 1/1 | 0.87 | 0.18 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3370 | 1/1 | 0.94 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3188 | 1/1 | 0.94 | 0.15 | - | 73,73,73,73 | 0 |
| 58 | MG | 14 | 3040 | 1/1 | 0.95 | 0.26 | - | 49,49,49,49 | 0 |
| 58 | MG | 1G | 1671 | 1/1 | 0.82 | 0.28 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3020 | 1/1 | 0.98 | 0.48 | - | 52,52,52,52 | 0 |
| 58 | MG | 14 | 3315 | 1/1 | 0.95 | 0.07 | - | 81,81,81,81 | 0 |
| 58 | MG | 1G | 1620 | 1/1 | 0.95 | 0.35 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3263 | 1/1 | 0.32 | 0.45 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3290 | 1/1 | 0.80 | 0.30 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3096 | 1/1 | 0.98 | 0.25 | - | 51,51,51,51 | 0 |
| 58 | MG | 13 | 1632 | 1/1 | 0.98 | 0.14 | - | 57,57,57,57 | 0 |
| 58 | MG | 21 | 301 | 1/1 | 0.99 | 0.23 | - | 48,48,48,48 | 0 |
| 58 | MG | 13 | 1675 | 1/1 | 0.61 | 0.35 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3250 | 1/1 | 0.84 | 0.53 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3259 | 1/1 | 0.96 | 0.48 | - | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3265 | 1/1 | 0.82 | 0.55 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1696 | 1/1 | 0.23 | 0.41 | - | 105,105,105,105 | 0 |
| 58 | MG | 13 | 1701 | 1/1 | 0.71 | 0.30 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1692 | 1/1 | 0.77 | 0.36 | - | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3402 | 1/1 | 0.94 | 0.07 | - | 110,110,110,110 | 0 |
| 58 | MG | 14 | 3299 | 1/1 | 0.77 | 0.06 | - | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3190 | 1/1 | 0.86 | 0.39 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3244 | 1/1 | 0.87 | 0.21 | - | 100,100,100,100 | 0 |
| 58 | MG | 14 | 3302 | 1/1 | 0.91 | 0.11 | - | 67,67,67,67 | 0 |
| 58 | MG | 1G | 1682 | 1/1 | 0.85 | 0.05 | - | 113,113,113,113 | 0 |
| 58 | MG | 1H | 3201 | 1/1 | 0.91 | 0.12 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3351 | 1/1 | 0.92 | 0.17 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3059 | 1/1 | 0.96 | 0.26 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3130 | 1/1 | 0.89 | 0.60 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3102 | 1/1 | 0.94 | 0.31 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3187 | 1/1 | 0.94 | 0.16 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3089 | 1/1 | 0.92 | 0.10 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3394 | 1/1 | 0.90 | 0.25 | - | 104,104,104,104 | 0 |
| 58 | MG | 1G | 1617 | 1/1 | 0.83 | 0.09 | - | 101,101,101,101 | 0 |
| 58 | MG | 1H | 3340 | 1/1 | 0.94 | 0.28 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3093 | 1/1 | 0.94 | 0.41 | - | 52,52,52,52 | 0 |
| 58 | MG | 1H | 3493 | 1/1 | 0.95 | 0.07 | - | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3407 | 1/1 | 0.92 | 0.16 | - | 59,59,59,59 | 0 |
| 58 | MG | 1G | 1655 | 1/1 | 0.90 | 0.71 | - | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3228 | 1/1 | 0.92 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3428 | 1/1 | 0.99 | 0.08 | - | 64,64,64,64 | 0 |
| 58 | MG | 1G | 1643 | 1/1 | 0.53 | 0.29 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1643 | 1/1 | 0.92 | 0.16 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3370 | 1/1 | 0.98 | 0.12 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3199 | 1/1 | 0.89 | 0.30 | - | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3339 | 1/1 | 0.77 | 0.12 | - | 109,109,109,109 | 0 |
| 58 | MG | 14 | 3410 | 1/1 | 0.96 | 0.09 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3051 | 1/1 | 0.87 | 0.35 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3376 | 1/1 | 0.95 | 0.11 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3392 | 1/1 | 0.95 | 0.05 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3315 | 1/1 | 0.90 | 0.39 | - | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3330 | 1/1 | 0.72 | 0.25 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3041 | 1/1 | 0.80 | 0.43 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3304 | 1/1 | 0.81 | 0.40 | - | 94,94,94,94 | 0 |
| 58 | MG | 14 | 3136 | 1/1 | 0.88 | 0.31 | - | 79,79,79,79 | 0 |
| 58 | MG | 7I | 101 | 1/1 | 0.59 | 0.19 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3281 | 1/1 | 0.85 | 0.20 | - | 93,93,93,93 | 0 |
| 58 | MG | 1J | 205 | 1/1 | 0.87 | 0.18 | - | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3399 | 1/1 | 0.92 | 0.09 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3359 | 1/1 | 0.98 | 0.07 | - | 43,43,43,43 | 0 |
| 58 | MG | 1H | 3255 | 1/1 | 0.54 | 0.45 | - | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3092 | 1/1 | 0.90 | 0.18 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3397 | 1/1 | 0.95 | 0.06 | - | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3270 | 1/1 | 0.85 | 0.20 | - | 90,90,90,90 | 0 |
| 58 | MG | 14 | 3237 | 1/1 | 0.89 | 0.51 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3452 | 1/1 | 0.90 | 0.10 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3076 | 1/1 | 0.93 | 0.23 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3491 | 1/1 | 0.98 | 0.03 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3298 | 1/1 | 0.92 | 0.42 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3004 | 1/1 | 0.90 | 0.25 | - | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3465 | 1/1 | 0.84 | 0.07 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3134 | 1/1 | 0.86 | 0.48 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3249 | 1/1 | 0.67 | 0.25 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3327 | 1/1 | 0.93 | 0.34 | - | 134,134,134,134 | 0 |
| 58 | MG | 1H | 3241 | 1/1 | 0.94 | 0.39 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3262 | 1/1 | 0.94 | 0.74 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3337 | 1/1 | 0.86 | 0.07 | - | 78,78,78,78 | 0 |
| 58 | MG | 2K | 102 | 1/1 | 0.76 | 0.45 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3425 | 1/1 | 0.87 | 0.06 | - | 110,110,110,110 | 0 |
| 58 | MG | 1H | 3397 | 1/1 | 0.91 | 0.10 | - | 79,79,79,79 | 0 |
| 58 | MG | 13 | 1725 | 1/1 | 0.97 | 0.06 | - | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3026 | 1/1 | 0.99 | 0.33 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3322 | 1/1 | 0.84 | 0.34 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3376 | 1/1 | 0.84 | 0.11 | - | 117,117,117,117 | 0 |
| 58 | MG | 13 | 1666 | 1/1 | 0.66 | 0.28 | - | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3136 | 1/1 | 0.95 | 0.25 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3293 | 1/1 | 0.77 | 0.32 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3423 | 1/1 | 0.93 | 0.06 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3456 | 1/1 | 0.97 | 0.08 | - | 93,93,93,93 | 0 |
| 58 | MG | 13 | 1624 | 1/1 | 0.94 | 0.18 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1647 | 1/1 | 0.77 | 0.33 | - | 107,107,107,107 | 0 |
| 58 | MG | 19 | 301 | 1/1 | 0.94 | 0.39 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3377 | 1/1 | 0.89 | 0.11 | - | 105,105,105,105 | 0 |
| 58 | MG | 1H | 3274 | 1/1 | 0.78 | 0.38 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3209 | 1/1 | 0.91 | 0.24 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3022 | 1/1 | 0.99 | 0.38 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3269 | 1/1 | 0.85 | 0.51 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3148 | 1/1 | 0.88 | 0.57 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3368 | 1/1 | 0.94 | 0.06 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3075 | 1/1 | 0.97 | 0.47 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3233 | 1/1 | 0.90 | 0.29 | - | 77,77,77,77 | 0 |
| 58 | MG | 16 | 209 | 1/1 | 0.96 | 0.11 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3147 | 1/1 | 0.82 | 0.49 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3112 | 1/1 | 0.95 | 0.42 | - | 52,52,52,52 | 0 |
| 58 | MG | 14 | 3094 | 1/1 | 0.96 | 0.37 | - | 67,67,67,67 | 0 |
| 58 | MG | 1G | 1645 | 1/1 | 0.96 | 0.19 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3286 | 1/1 | 0.93 | 0.08 | - | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3009 | 1/1 | 0.97 | 0.32 | - | 69,69,69,69 | 0 |
| 58 | MG | 88 | 203 | 1/1 | 0.79 | 0.35 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3148 | 1/1 | 0.91 | 0.47 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3318 | 1/1 | 0.92 | 0.53 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3225 | 1/1 | 0.64 | 0.72 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3108 | 1/1 | 0.90 | 0.25 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3149 | 1/1 | 0.73 | 0.47 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3203 | 1/1 | 0.95 | 0.16 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3039 | 1/1 | 0.91 | 0.35 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3381 | 1/1 | 0.90 | 0.15 | - | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3189 | 1/1 | 0.98 | 0.29 | - | 90,90,90,90 | 0 |
| 58 | MG | 1J | 201 | 1/1 | 0.96 | 0.17 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3207 | 1/1 | 0.62 | 0.56 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3278 | 1/1 | 0.87 | 0.23 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3478 | 1/1 | 0.89 | 0.18 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3204 | 1/1 | 0.96 | 0.36 | - | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3104 | 1/1 | 0.97 | 0.36 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3031 | 1/1 | 0.90 | 0.34 | - | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1617 | 1/1 | 0.94 | 0.27 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3015 | 1/1 | 0.73 | 0.26 | - | 70,70,70,70 | 0 |
| 58 | MG | 1G | 1612 | 1/1 | 0.83 | 0.40 | - | 100,100,100,100 | 0 |
| 58 | MG | 1H | 3433 | 1/1 | 0.98 | 0.19 | - | 45,45,45,45 | 0 |
| 58 | MG | 14 | 3113 | 1/1 | 0.68 | 0.18 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3005 | 1/1 | 0.98 | 0.22 | - | 51,51,51,51 | 0 |
| 58 | MG | 16 | 206 | 1/1 | 0.95 | 0.32 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3235 | 1/1 | 0.88 | 0.52 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3025 | 1/1 | 0.98 | 0.29 | - | 41,41,41,41 | 0 |
| 58 | MG | 1H | 3122 | 1/1 | 0.97 | 0.29 | - | 65,65,65,65 | 0 |
| 58 | MG | 2I | 201 | 1/1 | 0.55 | 0.27 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3219 | 1/1 | 0.77 | 0.35 | - | 107,107,107,107 | 0 |
| 58 | MG | 13 | 1650 | 1/1 | 0.97 | 0.14 | - | 100,100,100,100 | 0 |
| 58 | MG | 14 | 3266 | 1/1 | 0.90 | 0.42 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3162 | 1/1 | 0.60 | 0.38 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3435 | 1/1 | 0.93 | 0.10 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3396 | 1/1 | 0.89 | 0.17 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3335 | 1/1 | 0.83 | 0.10 | - | 120,120,120,120 | 0 |
| 58 | MG | 1H | 3035 | 1/1 | 0.72 | 0.52 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3195 | 1/1 | 0.92 | 0.28 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3222 | 1/1 | 0.79 | 0.41 | - | 73,73,73,73 | 0 |
| 58 | MG | 1H | 3181 | 1/1 | 0.87 | 0.41 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3013 | 1/1 | 0.76 | 0.48 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3272 | 1/1 | 0.90 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3053 | 1/1 | 0.97 | 0.30 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3043 | 1/1 | 0.85 | 0.16 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3083 | 1/1 | 0.96 | 0.17 | - | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3197 | 1/1 | 0.73 | 0.46 | - | 91,91,91,91 | 0 |
| 58 | MG | 1G | 1688 | 1/1 | 0.92 | 0.08 | - | 122,122,122,122 | 0 |
| 58 | MG | 1H | 3169 | 1/1 | 0.89 | 0.30 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3373 | 1/1 | 0.96 | 0.16 | - | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3170 | 1/1 | 0.87 | 0.37 | - | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1657 | 1/1 | 0.81 | 0.15 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3321 | 1/1 | 0.85 | 0.14 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3388 | 1/1 | 0.96 | 0.08 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3407 | 1/1 | 0.90 | 0.10 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3241 | 1/1 | 0.83 | 0.18 | - | 115,115,115,115 | 0 |
| 58 | MG | 14 | 3384 | 1/1 | 0.97 | 0.08 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3044 | 1/1 | 0.73 | 0.33 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3220 | 1/1 | 0.98 | 0.25 | - | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3290 | 1/1 | 0.80 | 0.12 | - | 89,89,89,89 | 0 |
| 58 | MG | 13 | 1673 | 1/1 | 0.76 | 0.34 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3142 | 1/1 | 0.94 | 0.07 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3451 | 1/1 | 0.96 | 0.08 | - | 68,68,68,68 | 0 |
| 58 | MG | 1G | 1605 | 1/1 | 0.97 | 0.40 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3130 | 1/1 | 0.91 | 0.18 | - | 67,67,67,67 | 0 |
| 58 | MG | 1G | 1679 | 1/1 | 0.94 | 0.09 | - | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3103 | 1/1 | 0.85 | 0.31 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1642 | 1/1 | 0.90 | 0.24 | - | 92,92,92,92 | 0 |
| 58 | MG | 1G | 1690 | 1/1 | 0.96 | 0.08 | - | 105,105,105,105 | 0 |
| 58 | MG | 1G | 1669 | 1/1 | 0.69 | 0.19 | - | 93,93,93,93 | 0 |
| 58 | MG | 13 | 1609 | 1/1 | 0.98 | 0.28 | - | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3122 | 1/1 | 0.78 | 0.46 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3042 | 1/1 | 0.93 | 0.21 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3124 | 1/1 | 0.94 | 0.42 | - | 86,86,86,86 | 0 |
| 58 | MG | 13 | 1733 | 1/1 | 0.97 | 0.24 | - | 83,83,83,83 | 0 |
| 58 | MG | 1G | 1660 | 1/1 | 0.85 | 0.41 | - | 107,107,107,107 | 0 |
| 58 | MG | 14 | 3001 | 1/1 | 0.94 | 0.19 | - | 46,46,46,46 | 0 |
| 58 | MG | 14 | 3332 | 1/1 | 0.80 | 0.07 | - | 103,103,103,103 | 0 |
| 58 | MG | 14 | 3227 | 1/1 | 0.84 | 0.24 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3462 | 1/1 | 0.92 | 0.07 | - | 91,91,91,91 | 0 |
| 58 | MG | 13 | 1668 | 1/1 | 0.67 | 0.15 | - | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3138 | 1/1 | 0.91 | 0.39 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3259 | 1/1 | 0.84 | 0.43 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3341 | 1/1 | 0.94 | 0.05 | - | 92,92,92,92 | 0 |
| 58 | MG | 14 | 3413 | 1/1 | 0.89 | 0.10 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3282 | 1/1 | 0.81 | 0.33 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3486 | 1/1 | 0.64 | 0.22 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3119 | 1/1 | 0.84 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3238 | 1/1 | 0.88 | 0.46 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3360 | 1/1 | 0.98 | 0.11 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3282 | 1/1 | 0.81 | 0.17 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3404 | 1/1 | 0.96 | 0.04 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3250 | 1/1 | 0.84 | 0.27 | - | 69,69,69,69 | 0 |
| 58 | MG | 13 | 1606 | 1/1 | 0.91 | 0.15 | - | 124,124,124,124 | 0 |
| 58 | MG | 13 | 1644 | 1/1 | 0.94 | 0.22 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1615 | 1/1 | 0.92 | 0.13 | - | 132,132,132,132 | 0 |
| 58 | MG | 16 | 210 | 1/1 | 0.96 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3161 | 1/1 | 0.97 | 0.14 | - | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1670 | 1/1 | 0.94 | 0.44 | - | 110,110,110,110 | 0 |
| 58 | MG | 14 | 3059 | 1/1 | 0.93 | 0.39 | - | 63,63,63,63 | 0 |
| 58 | MG | 1G | 1637 | 1/1 | 0.97 | 0.42 | - | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3317 | 1/1 | 0.98 | 0.10 | - | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1616 | 1/1 | 0.76 | 0.30 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3116 | 1/1 | 0.96 | 0.50 | - | 48,48,48,48 | 0 |
| 58 | MG | 13 | 1689 | 1/1 | 0.91 | 0.77 | - | 80,80,80,80 | 0 |
| 58 | MG | 1G | 1667 | 1/1 | 0.93 | 0.28 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3246 | 1/1 | 0.71 | 0.40 | - | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1629 | 1/1 | 0.95 | 0.24 | - | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3245 | 1/1 | 0.64 | 0.29 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3413 | 1/1 | 0.93 | 0.11 | - | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1670 | 1/1 | 0.81 | 0.19 | - | 103,103,103,103 | 0 |
| 58 | MG | 1J | 202 | 1/1 | 0.87 | 0.34 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3153 | 1/1 | 0.92 | 0.49 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3086 | 1/1 | 0.91 | 0.52 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3276 | 1/1 | 0.79 | 0.41 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3166 | 1/1 | 0.93 | 0.27 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3364 | 1/1 | 0.98 | 0.09 | - | 98,98,98,98 | 0 |
| 58 | MG | 1H | 3458 | 1/1 | 0.76 | 0.10 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3173 | 1/1 | 0.95 | 0.22 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3210 | 1/1 | 0.98 | 0.49 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3165 | 1/1 | 0.96 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3328 | 1/1 | 0.82 | 0.35 | - | 65,65,65,65 | 0 |
| 58 | MG | 14 | 3313 | 1/1 | 0.95 | 0.13 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3077 | 1/1 | 0.93 | 0.64 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3211 | 1/1 | 0.94 | 0.08 | - | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1687 | 1/1 | 0.88 | 0.15 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3357 | 1/1 | 0.92 | 0.11 | - | 83,83,83,83 | 0 |
| 58 | MG | 45 | 201 | 1/1 | 0.90 | 0.12 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3036 | 1/1 | 0.81 | 0.38 | - | 115,115,115,115 | 0 |
| 58 | MG | 14 | 3202 | 1/1 | 0.91 | 0.25 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3205 | 1/1 | 0.58 | 0.43 | - | 101,101,101,101 | 0 |
| 58 | MG | 1H | 3147 | 1/1 | 0.79 | 0.28 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3178 | 1/1 | 0.86 | 0.30 | - | 76,76,76,76 | 0 |
| 58 | MG | 1G | 1627 | 1/1 | 0.80 | 0.53 | - | 103,103,103,103 | 0 |
| 58 | MG | 13 | 1628 | 1/1 | 0.69 | 0.51 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3383 | 1/1 | 0.97 | 0.13 | - | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3383 | 1/1 | 0.96 | 0.16 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3120 | 1/1 | 0.80 | 0.23 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3410 | 1/1 | 0.97 | 0.07 | - | 76,76,76,76 | 0 |
| 58 | MG | 13 | 1726 | 1/1 | 0.92 | 0.09 | - | 122,122,122,122 | 0 |
| 58 | MG | 14 | 3102 | 1/1 | 0.79 | 0.80 | - | 76,76,76,76 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.