



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:15 am BST

PDB ID : 4YPB
Title : Precleavage 70S structure of the *P. vulgaris* HigB DeltaH92 toxin bound to the AAA codon
Authors : Schureck, M.A.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2015-03-12
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

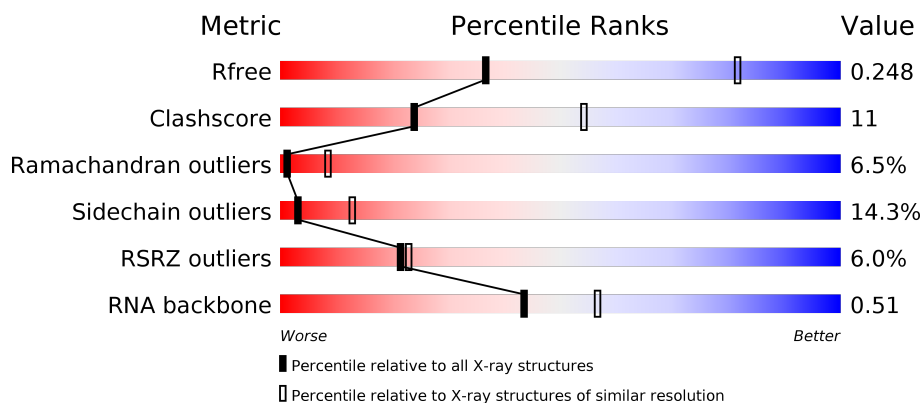
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



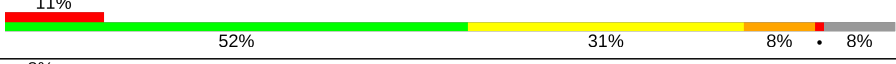

The reported resolution of this entry is 3.40 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1026 (3.48-3.32) |
| Clashscore | 141614 | 1055 (3.48-3.32) |
| Ramachandran outliers | 138981 | 1038 (3.48-3.32) |
| Sidechain outliers | 138945 | 1038 (3.48-3.32) |
| RSRZ outliers | 127900 | 2173 (3.50-3.30) |
| RNA backbone | 3102 | 1006 (3.84-2.96) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | QA | 1522 |  |
| 1 | XA | 1522 |  |
| 2 | QB | 256 |  |
| 2 | XB | 256 |  |

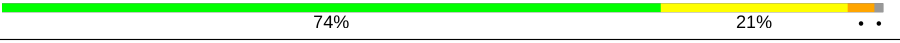





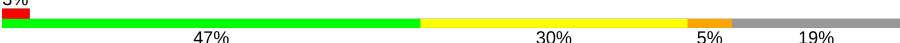
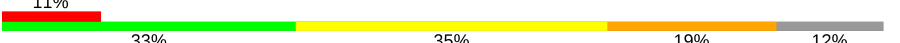
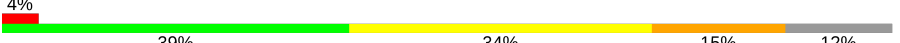


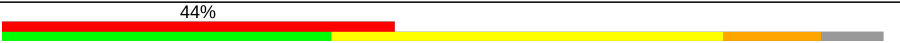
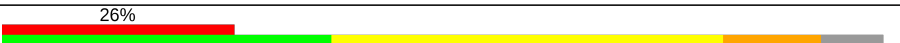





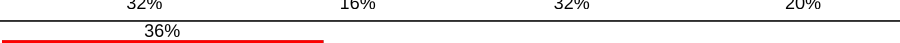

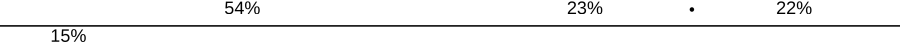
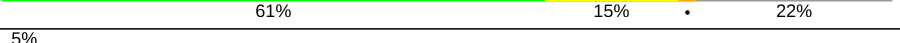



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | QC | 239 | |
| 3 | XC | 239 | |
| 4 | QD | 209 | |
| 4 | XD | 209 | |
| 5 | QE | 162 | |
| 5 | XE | 162 | |
| 6 | QF | 101 | |
| 6 | XF | 101 | |
| 7 | QG | 156 | |
| 7 | XG | 156 | |
| 8 | QH | 138 | |
| 8 | XH | 138 | |
| 9 | QI | 128 | |
| 9 | XI | 128 | |
| 10 | QJ | 105 | |
| 10 | XJ | 105 | |
| 11 | QK | 129 | |
| 11 | XK | 129 | |
| 12 | QL | 132 | |
| 12 | XL | 132 | |
| 13 | QM | 126 | |
| 13 | XM | 126 | |
| 14 | QN | 61 | |
| 14 | XN | 61 | |
| 15 | QO | 89 | |




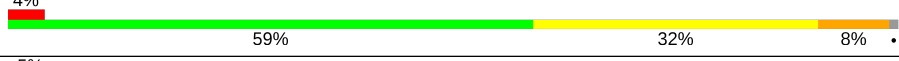
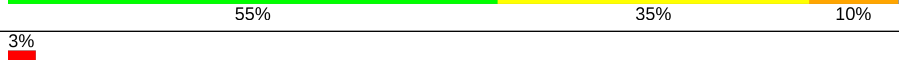
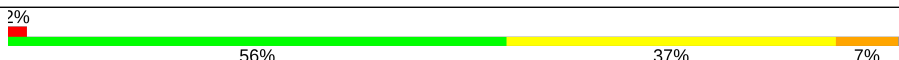
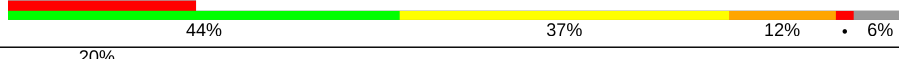
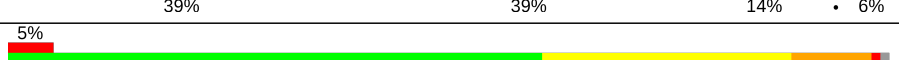





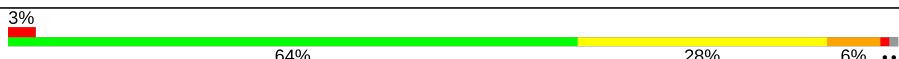


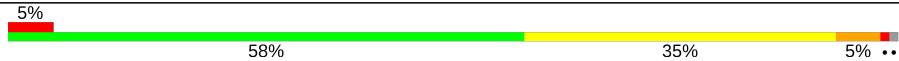

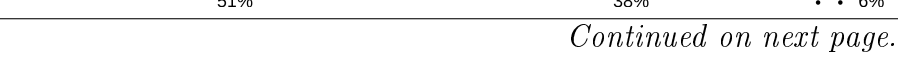






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | XO | 89 |  |
| 16 | QP | 88 |  |
| 16 | XP | 88 |  |
| 17 | QQ | 105 |  |
| 17 | XQ | 105 |  |
| 18 | QR | 88 |  |
| 18 | XR | 88 |  |
| 19 | QS | 93 |  |
| 19 | XS | 93 |  |
| 20 | QT | 106 |  |
| 20 | XT | 106 |  |
| 21 | QU | 27 |  |
| 21 | XU | 27 |  |
| 22 | QV | 77 |  |
| 22 | QW | 77 |  |
| 22 | XV | 77 |  |
| 22 | XW | 77 |  |
| 23 | QX | 25 |  |
| 23 | XX | 25 |  |
| 24 | QY | 117 |  |
| 24 | XY | 117 |  |
| 25 | RA | 2916 |  |
| 25 | YA | 2916 |  |
| 26 | RB | 124 |  |
| 26 | YB | 124 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 27 | RD | 276 |  |
| 27 | YD | 276 |  |
| 28 | RE | 206 |  |
| 28 | YE | 206 |  |
| 29 | RF | 210 |  |
| 29 | YF | 210 |  |
| 30 | RG | 182 |  |
| 30 | YG | 182 |  |
| 31 | RH | 180 |  |
| 31 | YH | 180 |  |
| 32 | RI | 148 |  |
| 32 | YI | 148 |  |
| 33 | RN | 140 |  |
| 33 | YN | 140 |  |
| 34 | RO | 122 |  |
| 34 | YO | 122 |  |
| 35 | RP | 150 |  |
| 35 | YP | 150 |  |
| 36 | RQ | 141 |  |
| 36 | YQ | 141 |  |
| 37 | RR | 118 |  |
| 37 | YR | 118 |  |
| 38 | RS | 112 |  |
| 38 | YS | 112 |  |
| 39 | RT | 146 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39 | YT | 146 | |
| 40 | RU | 118 | |
| 40 | YU | 118 | |
| 41 | RV | 101 | |
| 41 | YV | 101 | |
| 42 | RW | 113 | |
| 42 | YW | 113 | |
| 43 | RX | 96 | |
| 43 | YX | 96 | |
| 44 | RY | 110 | |
| 44 | YY | 110 | |
| 45 | RZ | 206 | |
| 45 | YZ | 206 | |
| 46 | R0 | 85 | |
| 46 | Y0 | 85 | |
| 47 | R1 | 98 | |
| 47 | Y1 | 98 | |
| 48 | R2 | 72 | |
| 48 | Y2 | 72 | |
| 49 | R3 | 60 | |
| 49 | Y3 | 60 | |
| 50 | R4 | 71 | |
| 50 | Y4 | 71 | |
| 51 | R5 | 60 | |
| 51 | Y5 | 60 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52 | R6 | 54 | |
| 52 | Y6 | 54 | |
| 53 | R7 | 49 | |
| 53 | Y7 | 49 | |
| 54 | R8 | 65 | |
| 54 | Y8 | 65 | |
| 55 | R9 | 37 | |
| 55 | Y9 | 37 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | QA | 1627 | - | - | - | X |
| 56 | MG | QA | 1636 | - | - | - | X |
| 56 | MG | QA | 1696 | - | - | - | X |
| 56 | MG | QA | 1719 | - | - | - | X |
| 56 | MG | QA | 1734 | - | - | - | X |
| 56 | MG | QA | 1746 | - | - | - | X |
| 56 | MG | RA | 3002 | - | - | - | X |
| 56 | MG | RA | 3037 | - | - | - | X |
| 56 | MG | RA | 3075 | - | - | - | X |
| 56 | MG | RA | 3108 | - | - | - | X |
| 56 | MG | RA | 3134 | - | - | - | X |
| 56 | MG | RA | 3168 | - | - | - | X |
| 56 | MG | RA | 3171 | - | - | - | X |
| 56 | MG | RA | 3220 | - | - | - | X |
| 56 | MG | RA | 3222 | - | - | - | X |
| 56 | MG | RA | 3253 | - | - | - | X |
| 56 | MG | RA | 3277 | - | - | - | X |
| 56 | MG | RA | 3295 | - | - | - | X |
| 56 | MG | RA | 3299 | - | - | - | X |
| 56 | MG | RA | 3316 | - | - | - | X |
| 56 | MG | RA | 3320 | - | - | - | X |
| 56 | MG | RA | 3326 | - | - | - | X |
| 56 | MG | RA | 3338 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | RA | 3342 | - | - | - | X |
| 56 | MG | RA | 3347 | - | - | - | X |
| 56 | MG | RA | 3360 | - | - | - | X |
| 56 | MG | RA | 3391 | - | - | - | X |
| 56 | MG | RA | 3406 | - | - | - | X |
| 56 | MG | RA | 3426 | - | - | - | X |
| 56 | MG | RQ | 202 | - | - | - | X |
| 56 | MG | RY | 201 | - | - | - | X |
| 56 | MG | XA | 1727 | - | - | - | X |
| 56 | MG | XA | 1759 | - | - | - | X |
| 56 | MG | Y5 | 102 | - | - | - | X |
| 56 | MG | Y7 | 101 | - | - | - | X |
| 56 | MG | YA | 3001 | - | - | - | X |
| 56 | MG | YA | 3068 | - | - | - | X |
| 56 | MG | YA | 3099 | - | - | - | X |
| 56 | MG | YA | 3132 | - | - | - | X |
| 56 | MG | YA | 3149 | - | - | - | X |
| 56 | MG | YA | 3163 | - | - | - | X |
| 56 | MG | YA | 3233 | - | - | - | X |
| 56 | MG | YA | 3293 | - | - | - | X |
| 56 | MG | YA | 3317 | - | - | - | X |
| 56 | MG | YA | 3322 | - | - | - | X |
| 56 | MG | YA | 3341 | - | - | - | X |
| 56 | MG | YA | 3344 | - | - | - | X |
| 56 | MG | YA | 3357 | - | - | - | X |
| 56 | MG | YA | 3361 | - | - | - | X |
| 56 | MG | YA | 3379 | - | - | - | X |
| 56 | MG | YA | 3386 | - | - | - | X |
| 56 | MG | YA | 3401 | - | - | - | X |
| 56 | MG | YA | 3406 | - | - | - | X |
| 56 | MG | YA | 3415 | - | - | - | X |
| 56 | MG | YA | 3425 | - | - | - | X |
| 56 | MG | YA | 3432 | - | - | - | X |
| 56 | MG | YA | 3436 | - | - | - | X |
| 56 | MG | YA | 3448 | - | - | - | X |
| 56 | MG | YA | 3459 | - | - | - | X |
| 56 | MG | YA | 3467 | - | - | - | X |
| 56 | MG | YA | 3472 | - | - | - | X |
| 56 | MG | YA | 3482 | - | - | - | X |
| 56 | MG | YH | 201 | - | - | - | X |

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 297549 atoms, of which 18 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 rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | QA | 1511 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32472 | 14453 | 6011 | 10497 | 1511 | | | |
| 1 | XA | 1508 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32409 | 14425 | 6001 | 10475 | 1508 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | QB | 236 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1223 | 343 | 344 | 5 | | | |
| 2 | XB | 236 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1223 | 343 | 344 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | QC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1016 | 314 | 281 | 1 | | | |
| 3 | XC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1016 | 314 | 281 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | QD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |
| 4 | XD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | QE | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1178 | 743 | 221 | 210 | 4 | | | |
| 5 | XE | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1178 | 743 | 221 | 210 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | QF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |
| 6 | XF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | QG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |
| 7 | XG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | QH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |
| 8 | XH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | QI | 128 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1018 | 644 | 198 | 175 | 1 | | | |
| 9 | XI | 128 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1018 | 644 | 198 | 175 | 1 | | | |

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | QK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 901 | 560 | 171 | 167 | 3 | | | |
| 11 | XK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 901 | 560 | 171 | 167 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | QL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |
| 12 | XL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | QM | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 937 | 579 | 193 | 163 | 2 | | | |
| 13 | XM | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 937 | 579 | 193 | 163 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | QN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 14 | XN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | QO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | XO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | QP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |
| 16 | XP | 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 | QQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | XQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | QR | 71 | Total | C | N | O | 0 | 0 | 0 |
| | | | 585 | 373 | 116 | 96 | | | |
| 18 | XR | 71 | Total | C | N | O | 0 | 0 | 0 |
| | | | 585 | 373 | 116 | 96 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | QS | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 656 | 419 | 121 | 114 | 2 | | | |
| 19 | XS | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 656 | 419 | 121 | 114 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | QT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |
| 20 | XT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | QU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | XU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called tRNA fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | QV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |
| 22 | QW | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |
| 22 | XV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |
| 22 | XW | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1640 | 732 | 297 | 535 | 76 | | | |

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|-----|----|---------|---------|-------|
| 23 | QX | 20 | Total | C | H | N | O | P | 0 | 0 | 0 |
| | | | 449 | 199 | 9 | 89 | 132 | 20 | | | |
| 23 | XX | 20 | Total | C | H | N | O | P | 0 | 0 | 0 |
| | | | 449 | 199 | 9 | 89 | 132 | 20 | | | |

- Molecule 24 is a protein called Host inhibition of growth B.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 24 | QY | 91 | Total | C | N | O | 0 | 0 | 0 |
| | | | 746 | 478 | 131 | 137 | | | |
| 24 | XY | 91 | Total | C | N | O | 0 | 0 | 0 |
| | | | 746 | 478 | 131 | 137 | | | |

There are 54 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| QY | 0 | MET | - | initiating methionine | UNP Q7A225 |
| QY | 1 | GLY | - | expression tag | UNP Q7A225 |
| QY | 92 | LYS | - | expression tag | UNP Q7A225 |
| QY | 93 | LEU | - | expression tag | UNP Q7A225 |
| QY | 94 | GLY | - | expression tag | UNP Q7A225 |
| QY | 95 | PRO | - | expression tag | UNP Q7A225 |
| QY | 96 | GLU | - | expression tag | UNP Q7A225 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| QY | 97 | GLN | - | expression tag | UNP Q7A225 |
| QY | 98 | LYS | - | expression tag | UNP Q7A225 |
| QY | 99 | LEU | - | expression tag | UNP Q7A225 |
| QY | 100 | ILE | - | expression tag | UNP Q7A225 |
| QY | 101 | SER | - | expression tag | UNP Q7A225 |
| QY | 102 | GLU | - | expression tag | UNP Q7A225 |
| QY | 103 | GLU | - | expression tag | UNP Q7A225 |
| QY | 104 | ASP | - | expression tag | UNP Q7A225 |
| QY | 105 | LEU | - | expression tag | UNP Q7A225 |
| QY | 106 | ASN | - | expression tag | UNP Q7A225 |
| QY | 107 | SER | - | expression tag | UNP Q7A225 |
| QY | 108 | ALA | - | expression tag | UNP Q7A225 |
| QY | 109 | VAL | - | expression tag | UNP Q7A225 |
| QY | 110 | ASP | - | expression tag | UNP Q7A225 |
| QY | 111 | HIS | - | expression tag | UNP Q7A225 |
| QY | 112 | HIS | - | expression tag | UNP Q7A225 |
| QY | 113 | HIS | - | expression tag | UNP Q7A225 |
| QY | 114 | HIS | - | expression tag | UNP Q7A225 |
| QY | 115 | HIS | - | expression tag | UNP Q7A225 |
| QY | 116 | HIS | - | expression tag | UNP Q7A225 |
| XY | 0 | MET | - | initiating methionine | UNP Q7A225 |
| XY | 1 | GLY | - | expression tag | UNP Q7A225 |
| XY | 92 | LYS | - | expression tag | UNP Q7A225 |
| XY | 93 | LEU | - | expression tag | UNP Q7A225 |
| XY | 94 | GLY | - | expression tag | UNP Q7A225 |
| XY | 95 | PRO | - | expression tag | UNP Q7A225 |
| XY | 96 | GLU | - | expression tag | UNP Q7A225 |
| XY | 97 | GLN | - | expression tag | UNP Q7A225 |
| XY | 98 | LYS | - | expression tag | UNP Q7A225 |
| XY | 99 | LEU | - | expression tag | UNP Q7A225 |
| XY | 100 | ILE | - | expression tag | UNP Q7A225 |
| XY | 101 | SER | - | expression tag | UNP Q7A225 |
| XY | 102 | GLU | - | expression tag | UNP Q7A225 |
| XY | 103 | GLU | - | expression tag | UNP Q7A225 |
| XY | 104 | ASP | - | expression tag | UNP Q7A225 |
| XY | 105 | LEU | - | expression tag | UNP Q7A225 |
| XY | 106 | ASN | - | expression tag | UNP Q7A225 |
| XY | 107 | SER | - | expression tag | UNP Q7A225 |
| XY | 108 | ALA | - | expression tag | UNP Q7A225 |
| XY | 109 | VAL | - | expression tag | UNP Q7A225 |
| XY | 110 | ASP | - | expression tag | UNP Q7A225 |
| XY | 111 | HIS | - | expression tag | UNP Q7A225 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| XY | 112 | HIS | - | expression tag | UNP Q7A225 |
| XY | 113 | HIS | - | expression tag | UNP Q7A225 |
| XY | 114 | HIS | - | expression tag | UNP Q7A225 |
| XY | 115 | HIS | - | expression tag | UNP Q7A225 |
| XY | 116 | HIS | - | expression tag | UNP Q7A225 |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25 | RA | 2891 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62269 | 27713 | 11649 | 20016 | 2891 | | | |
| 25 | YA | 2875 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61924 | 27560 | 11583 | 19906 | 2875 | | | |

- Molecule 26 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | RB | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |
| 26 | YB | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | RD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |
| 27 | YD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | RE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |
| 28 | YE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | RF | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1627 | 1037 | 304 | 283 | 3 | | | |
| 29 | YF | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1627 | 1037 | 304 | 283 | 3 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | RG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 30 | YG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | RH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |
| 31 | YH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | RI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |
| 32 | YI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | RN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 33 | YN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | RO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | YO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | RP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |
| 35 | YP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | RQ | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 710 | 210 | 185 | 7 | | | |
| 36 | YQ | 139 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1107 | 707 | 209 | 184 | 7 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 37 | RR | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | | |
| 37 | YR | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | | |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 38 | RS | 111 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | | |
| 38 | YS | 111 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | RT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 39 | YT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | RU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |
| 40 | YU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | RV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 41 | YV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | RW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |
| 42 | YW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43 | RX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |
| 43 | YX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | RY | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |
| 44 | YY | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | RZ | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1404 | 897 | 252 | 252 | 3 | | | |
| 45 | YZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | R0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 657 | 407 | 139 | 110 | 1 | | | |
| 46 | Y0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 657 | 407 | 139 | 110 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | R1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |
| 47 | Y1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | R2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |
| 48 | Y2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49 | R3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 49 | Y3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | R4 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 573 | 359 | 107 | 103 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | Y4 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 573 | 359 | 107 | 103 | 4 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | R5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 51 | Y5 | 57 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 442 | 278 | 88 | 71 | 5 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | R6 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 68 | 4 | | | |
| 52 | Y6 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 68 | 4 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | R7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |
| 53 | Y7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54 | R8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 54 | Y8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55 | R9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 55 | Y9 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 299 | 183 | 67 | 46 | 3 | | | |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | QA | 150 | Total 150 | Mg 150 | 0 | 0 |
| 56 | YV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RP | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | QX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YA | 487 | Total 487 | Mg 487 | 0 | 0 |
| 56 | Y5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | YH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | XS | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | Y1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QV | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | YO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XA | 163 | Total 163 | Mg 163 | 0 | 0 |
| 56 | YY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RQ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | R0 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | QL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | Y0 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | YG | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | YQ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | RY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | R1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | Y7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | R5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | RA | 441 | Total 441 | Mg 441 | 0 | 0 |
| 56 | YF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | R2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YB | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | YW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XV | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | RB | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | XD | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 56 | RF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YE | 1 | Total 1 | Mg 1 | 0 | 0 |

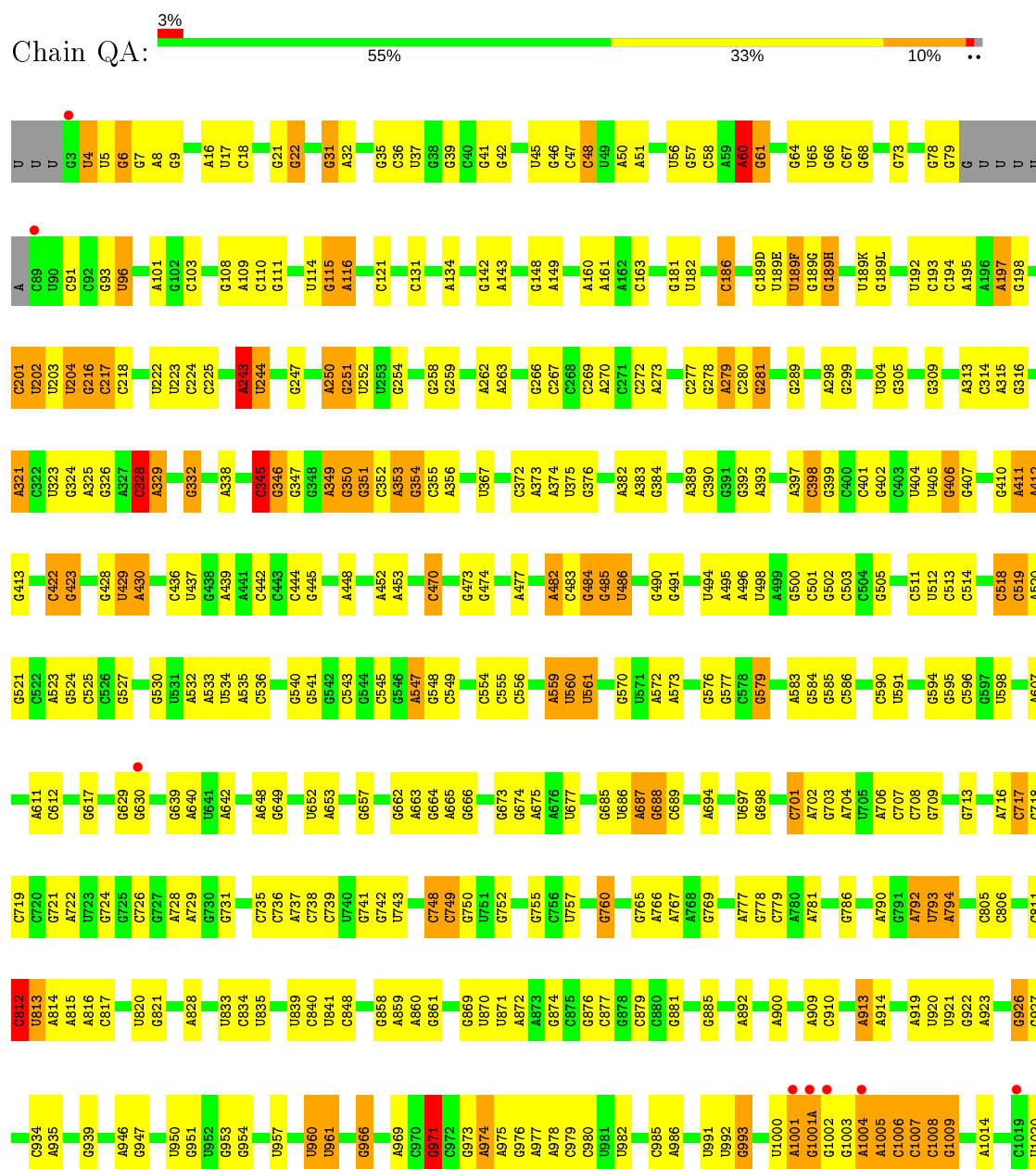
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

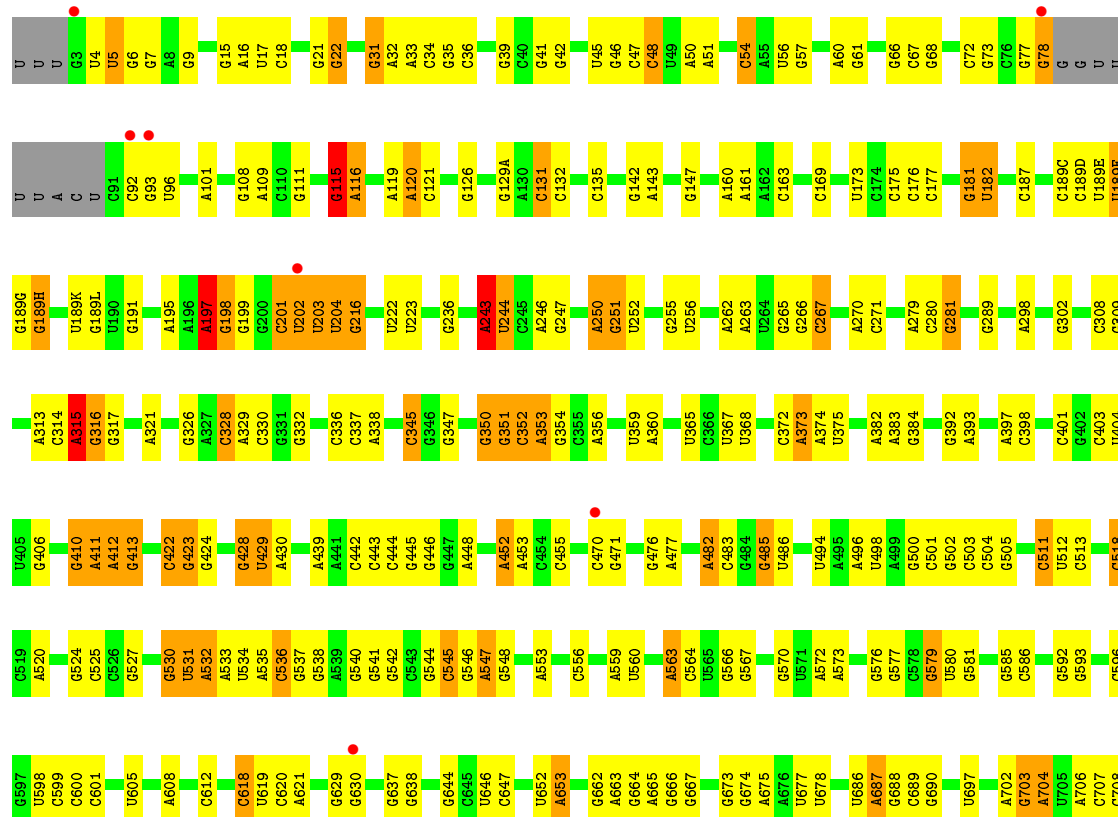
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57 | XD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | QD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | QN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | XN | 1 | Total 1 | Zn 1 | 0 | 0 |

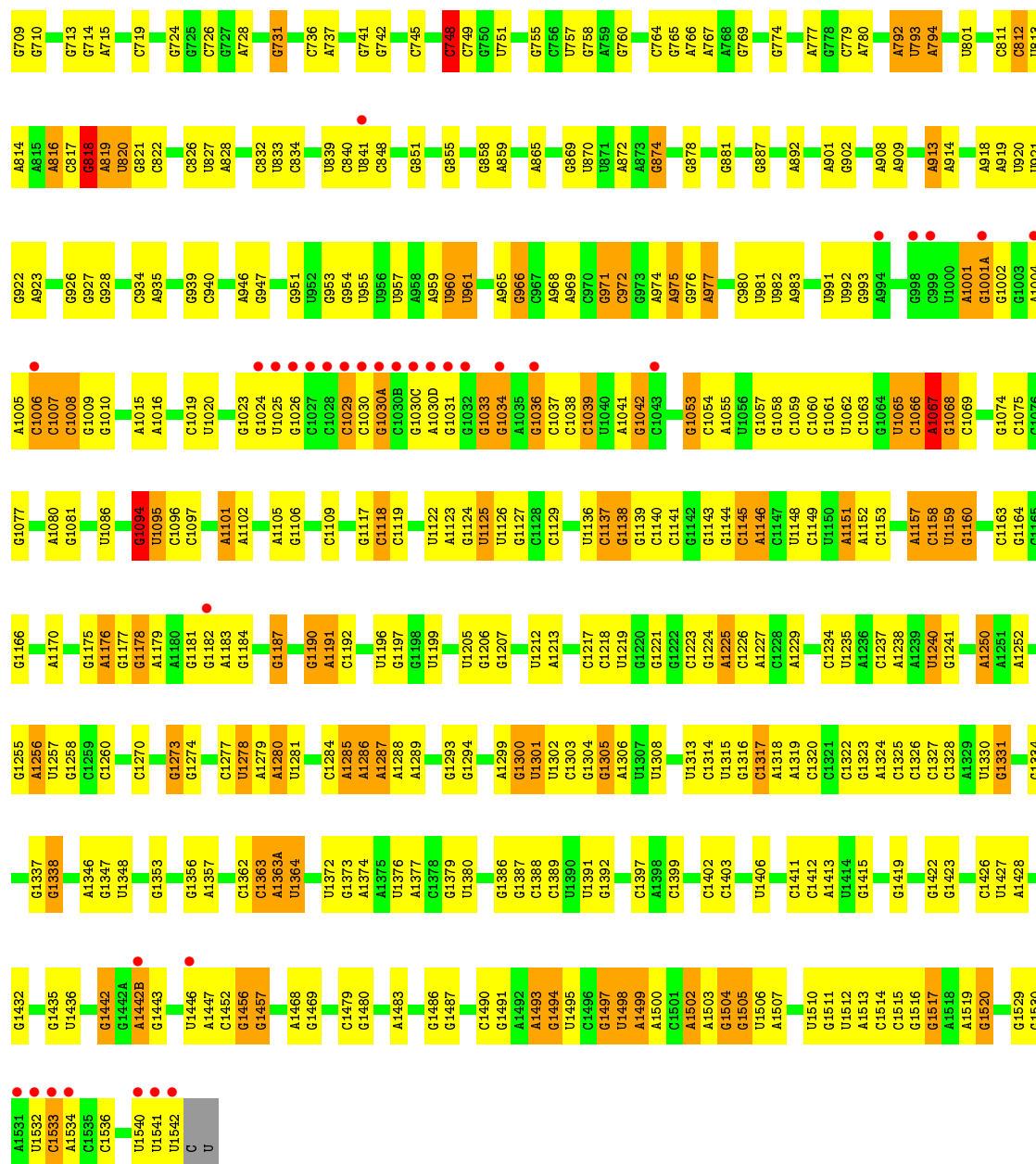
3 Residue-property plots [i](#)

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.

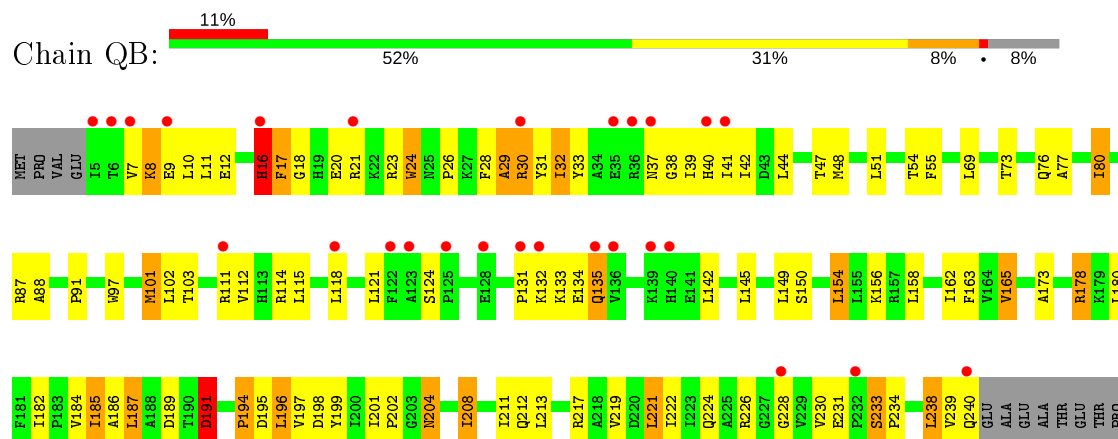
• Molecule 1: 16S rRNA

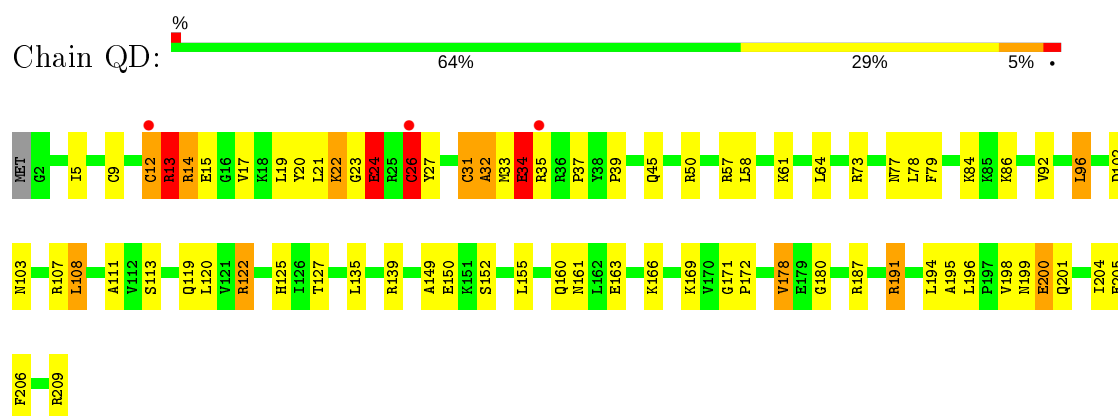




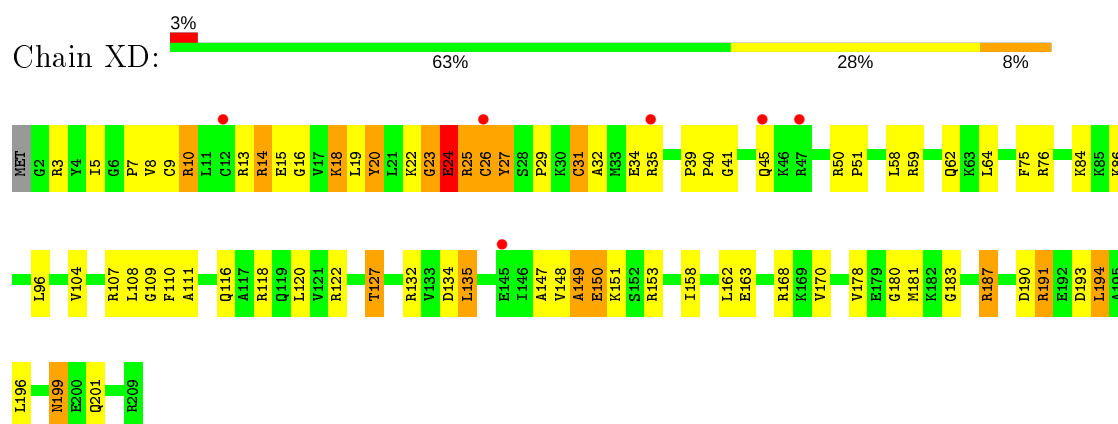


• Molecule 2: 30S ribosomal protein S2

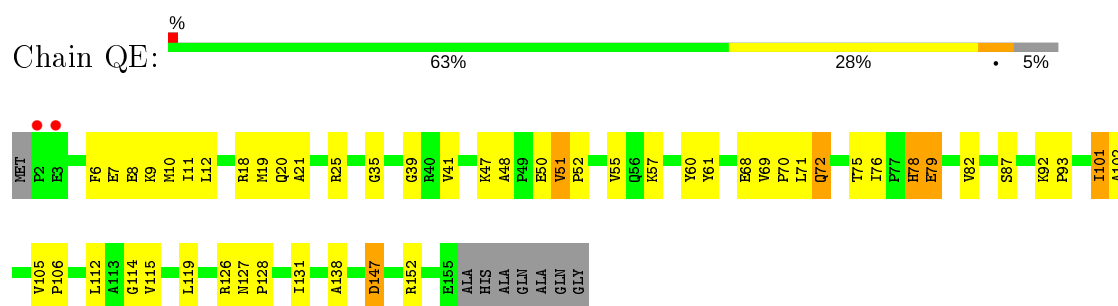


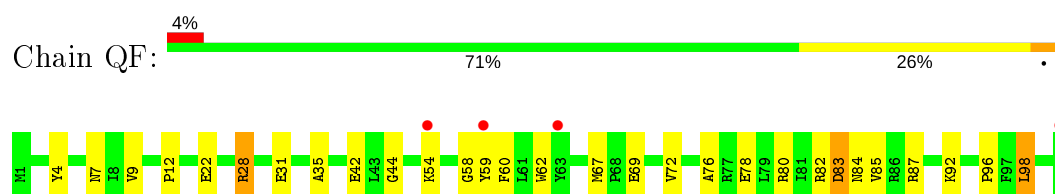


- Molecule 4: 30S ribosomal protein S4

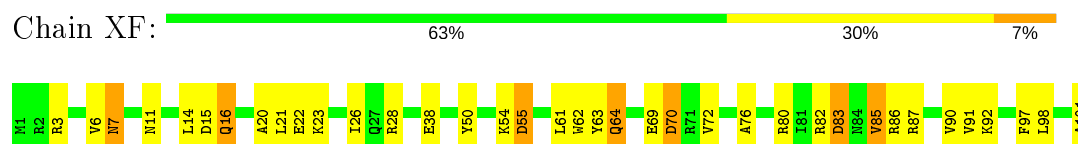


- Molecule 5: 30S ribosomal protein S5

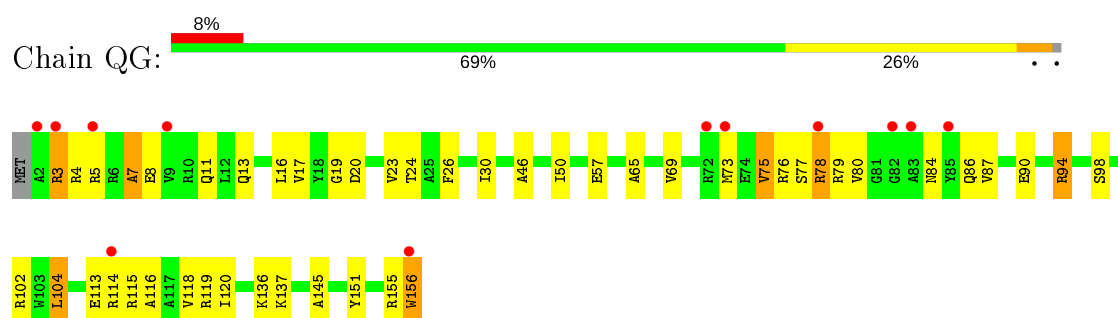




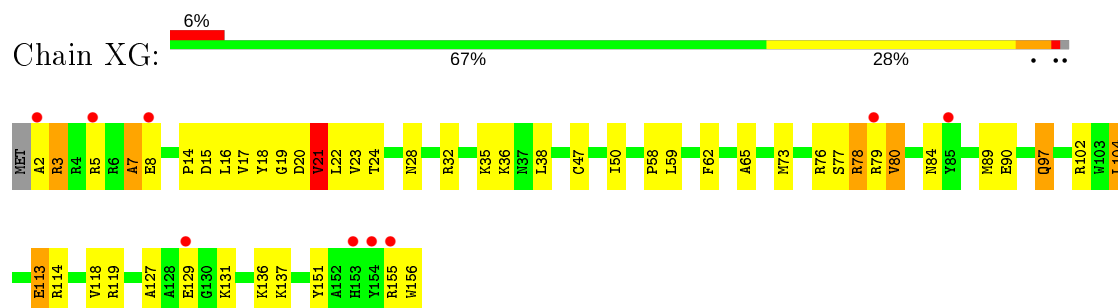
- Molecule 6: 30S ribosomal protein S6



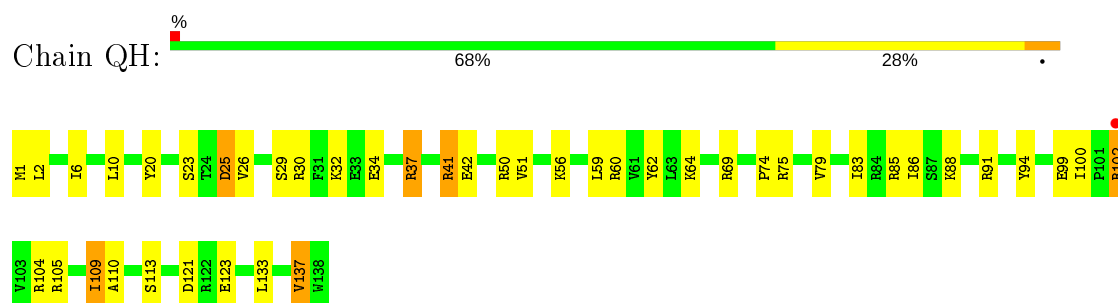
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

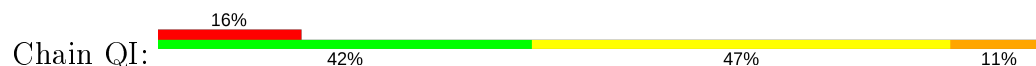


- Molecule 8: 30S ribosomal protein S8

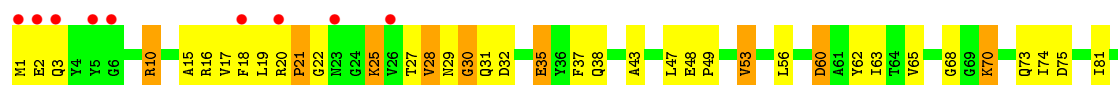




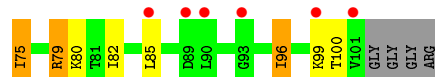
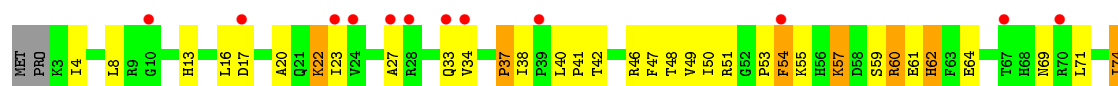
• Molecule 9: 30S ribosomal protein S9



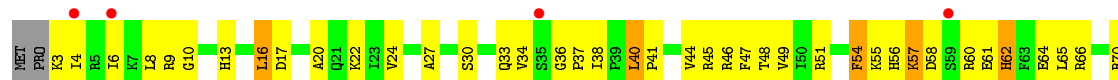
• Molecule 9: 30S ribosomal protein S9



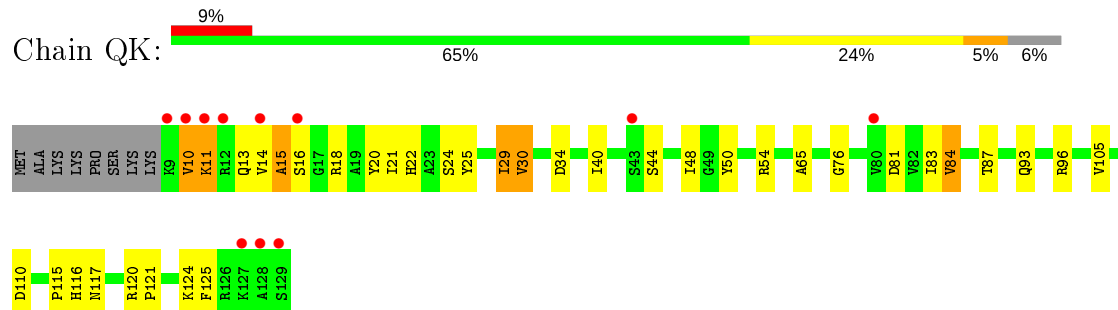
• Molecule 10: 30S ribosomal protein S10



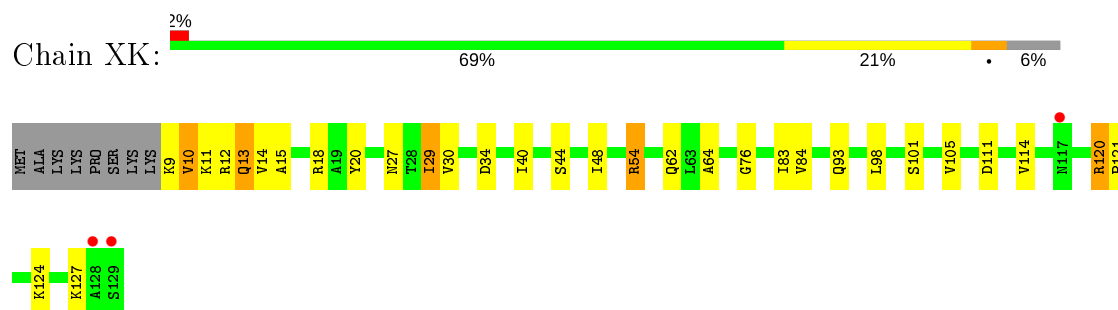
• Molecule 10: 30S ribosomal protein S10



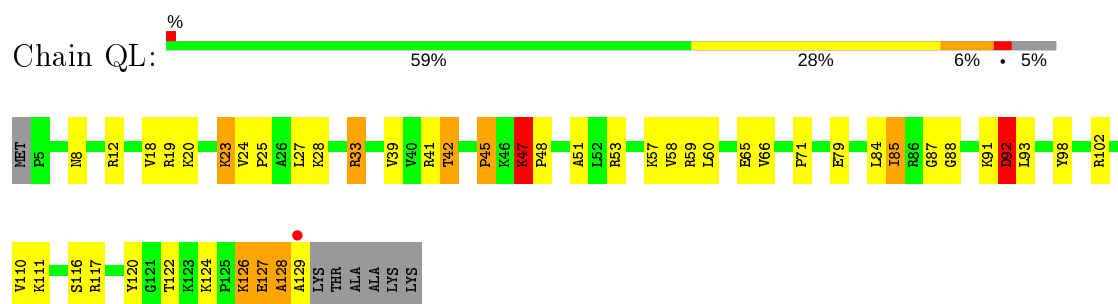
- Molecule 11: 30S ribosomal protein S11



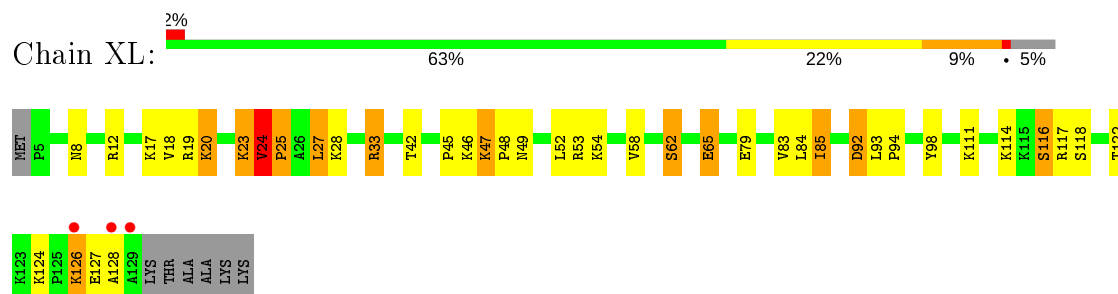
- Molecule 11: 30S ribosomal protein S11



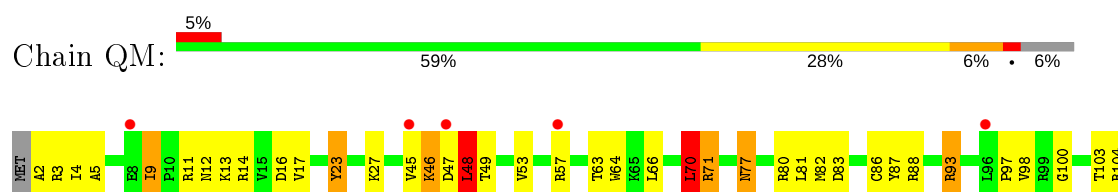
- Molecule 12: 30S ribosomal protein S12

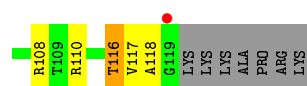


- Molecule 12: 30S ribosomal protein S12

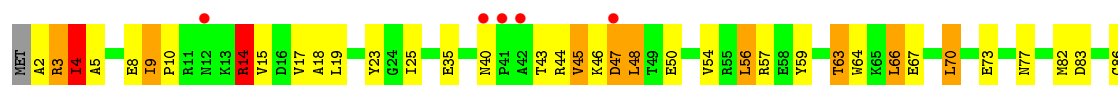


- Molecule 13: 30S ribosomal protein S13

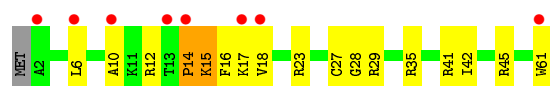
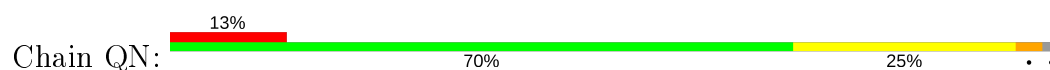




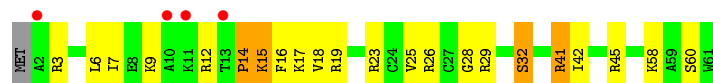
- Molecule 13: 30S ribosomal protein S13



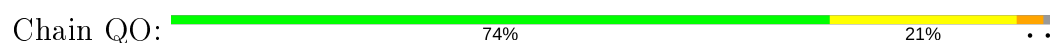
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

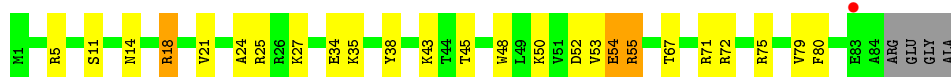


- Molecule 15: 30S ribosomal protein S15

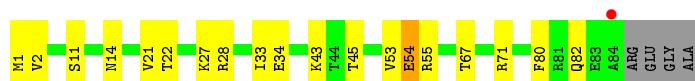
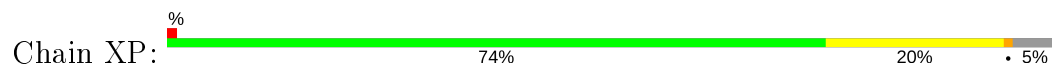


- Molecule 16: 30S ribosomal protein S16

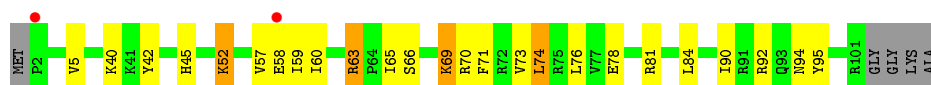
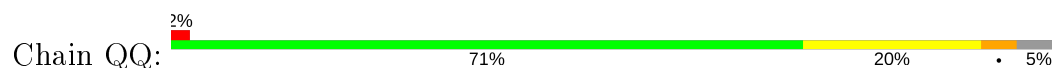




- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



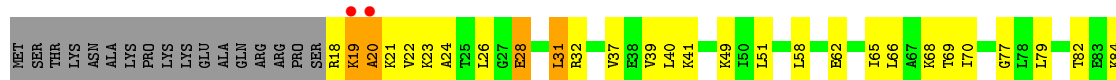
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

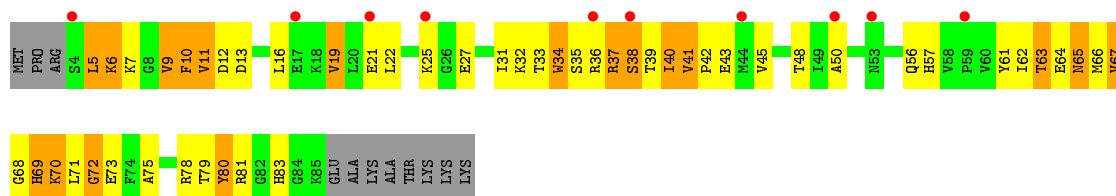


- Molecule 18: 30S ribosomal protein S18

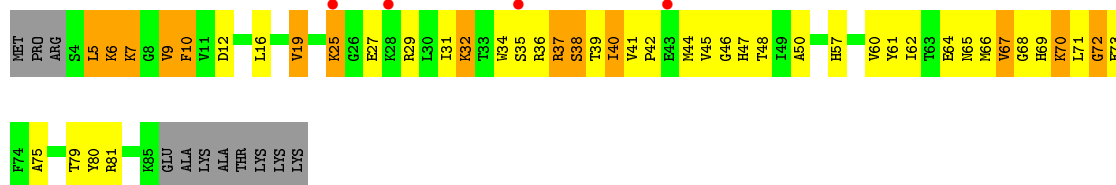
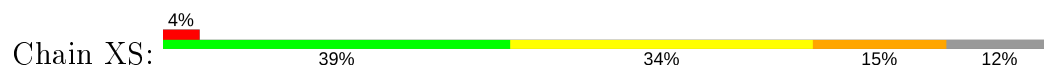


- Molecule 19: 30S ribosomal protein S19

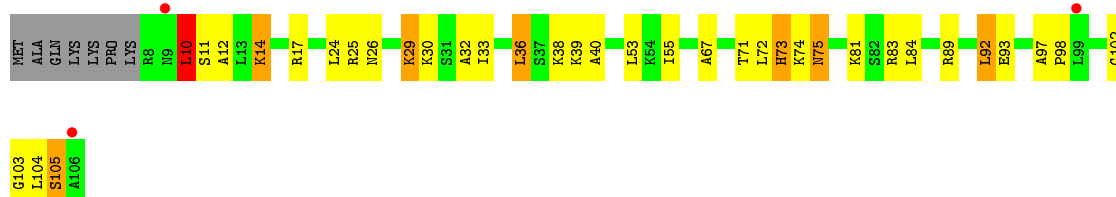




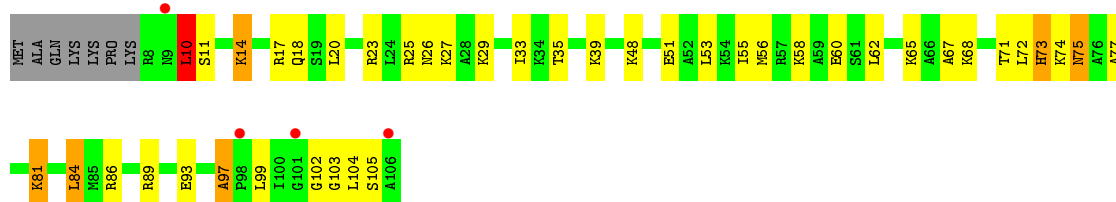
- Molecule 19: 30S ribosomal protein S19



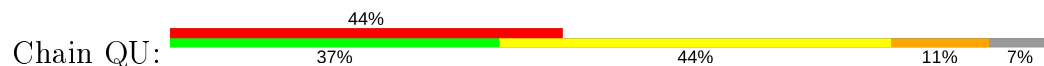
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20

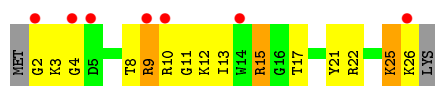


- Molecule 21: 30S ribosomal protein Thx

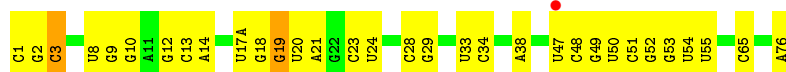


- Molecule 21: 30S ribosomal protein Thx

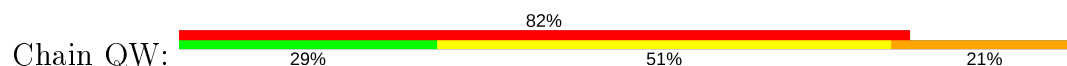




- Molecule 22: tRNA fMet



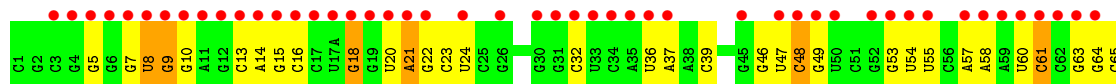
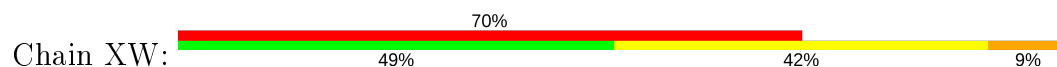
- Molecule 22: tRNA fMet



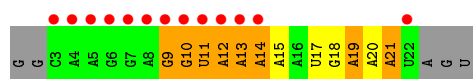
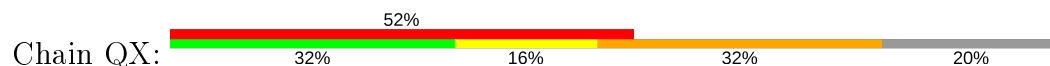
- Molecule 22: tRNA fMet



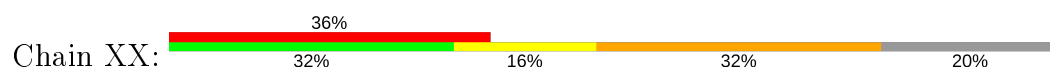
- Molecule 22: tRNA fMet

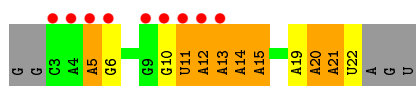


- Molecule 23: messenger RNA

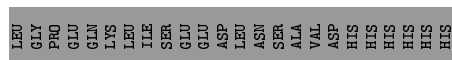
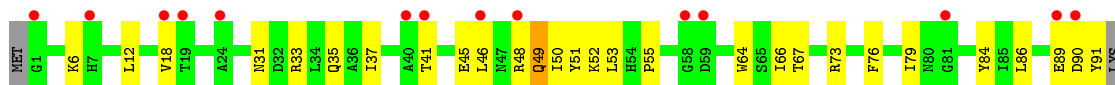


- Molecule 23: messenger RNA

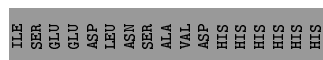
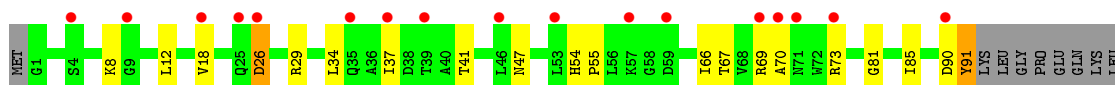




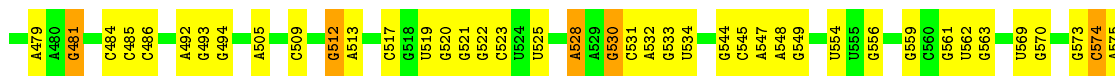
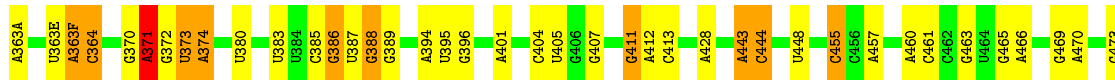
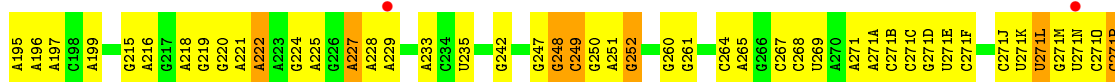
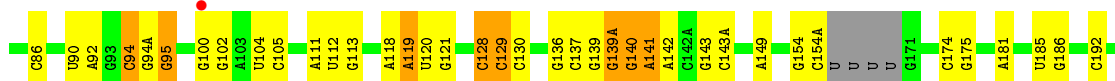
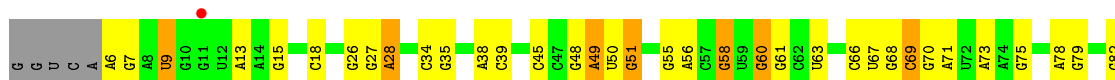
- Molecule 24: Host inhibition of growth B



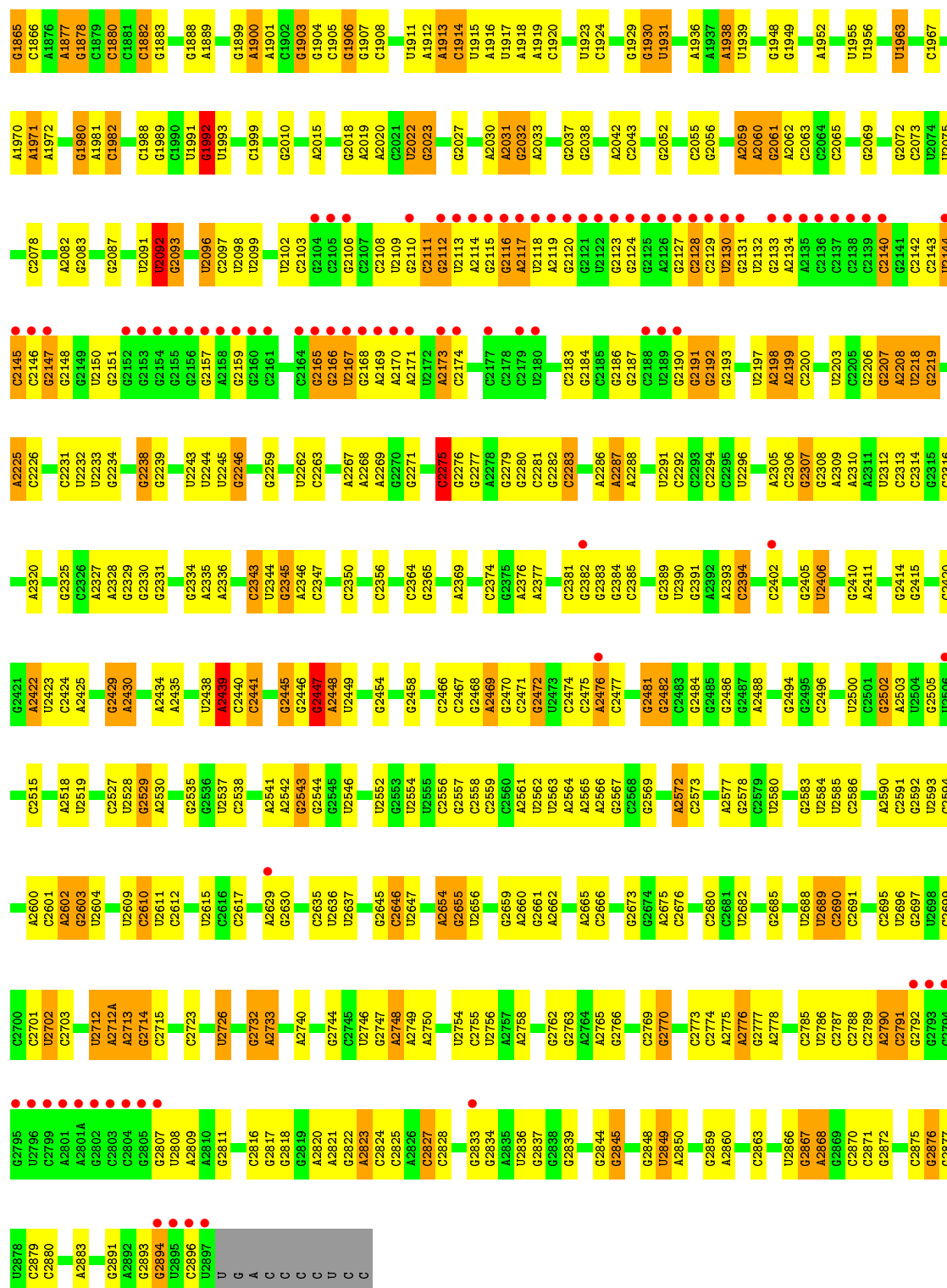
- Molecule 24: Host inhibition of growth B



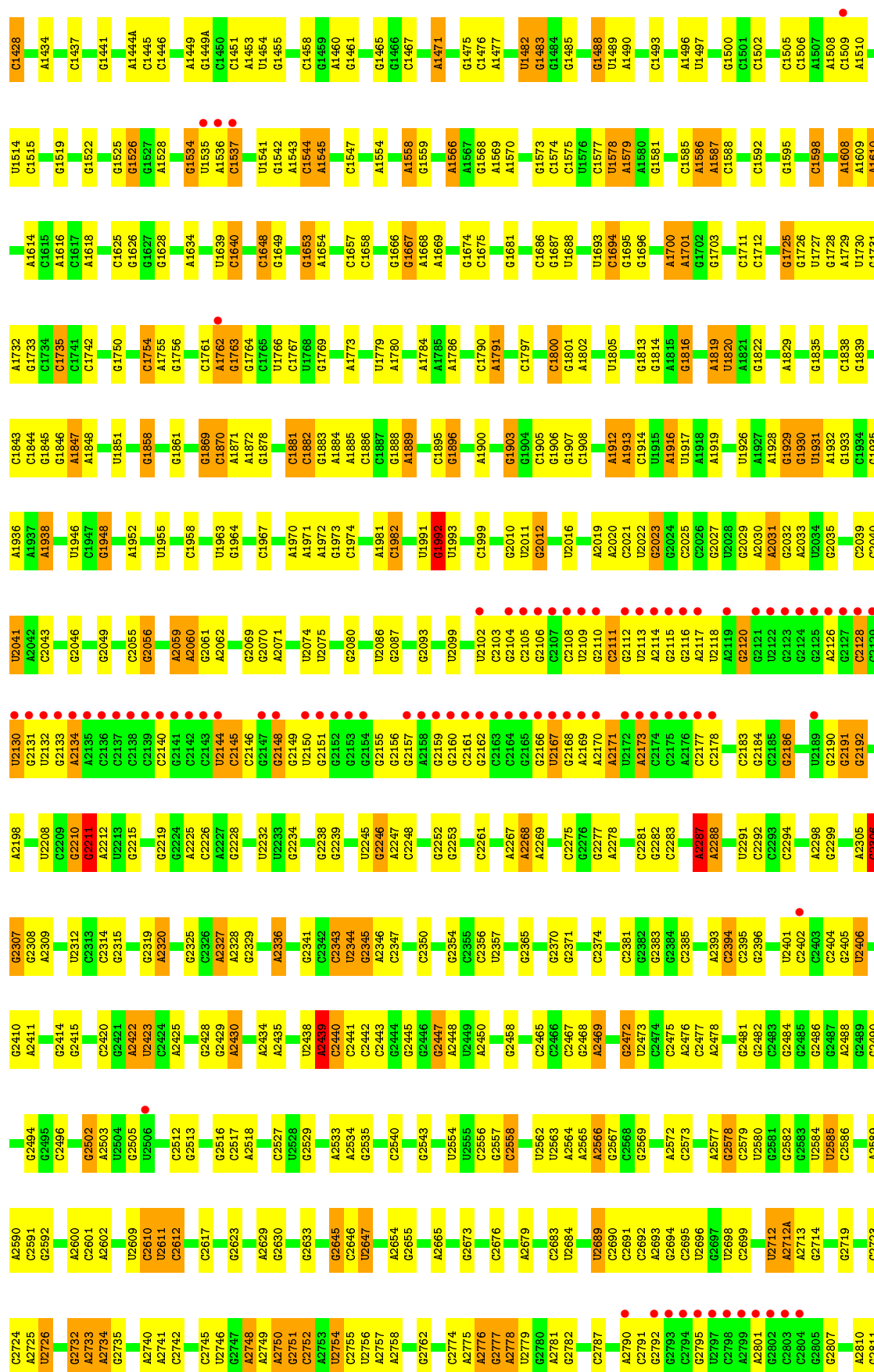
- Molecule 25: 23S rRNA

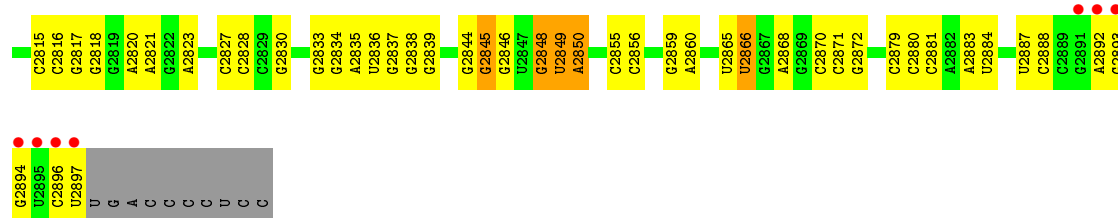


| | | | | | | | | | | | | | |
|-------|-------|-------|--------|-------|-------|--------|--------|-------|-------|------|------|-------|-------|
| C1774 | A1854 | C1547 | C1445A | G1358 | A1268 | G1173 | A1085 | G1017 | U930 | G854 | G746 | A654 | U576 |
| U1775 | C1657 | C1548 | A1449 | A1359 | A1269 | A1174 | A1086 | C1018 | G931 | G855 | G749 | G654A | G577 |
| A1780 | C1658 | C1549 | G1450 | G1360 | G1270 | U1175 | G1087 | U1019 | G932 | G856 | C749 | G654B | C580 |
| A1786 | G1667 | C1550 | A1452 | C1362 | G1271 | G1176 | A1088 | A1020 | A933 | C857 | A751 | G654C | C581 |
| C1790 | A1668 | A1554 | U1453 | G1363 | U1272 | A1177 | G1089 | A1021 | G934 | U958 | A752 | G654D | G582 |
| A1791 | G1674 | C1557 | G1455 | G1364 | A1274 | C1179 | G1090 | U1022 | A941 | G859 | C753 | G654E | G583 |
| G1792 | A1675 | A1558 | G1456 | A1365 | A1275 | C1180 | G1091 | U1023 | G942 | U860 | C754 | G654F | A586 |
| C1793 | A1676 | G1367 | A1460 | G1368 | A1278 | G1184 | U1094 | G1025 | U943 | A961 | C755 | A | C587 |
| U1794 | G1461 | G1374 | G1281 | G1369 | U1282 | G1186 | A1095 | A1027 | G944 | A863 | C756 | C | U588 |
| C1795 | G1681 | C1375 | U1282 | C1376 | U1282 | G1187 | A1096 | A1028 | G946 | C865 | A764 | C | C589 |
| U1796 | U1688 | C1376 | G1465 | C1377 | U1188 | U1188 | A1097 | U1033 | G947 | C866 | A774 | C | A590 |
| C1797 | A1689 | A1567 | G1466 | C1378 | A1189 | G1190 | G1099 | G1034 | A953 | U871 | G775 | G654G | G593 |
| G1799 | G1693 | G1568 | C1467 | A1379 | A1286 | G1191 | U1101 | G1035 | G956 | A872 | G776 | G654H | C601 |
| C1800 | U1693 | A1569 | A1471 | G1379 | G1289 | G1195 | U1102 | G1036 | A957 | G873 | U779 | C654I | G602 |
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| G1811 | C1577 | U1578 | G1482 | U1396 | A1307 | A1220 | G1111 | A1047 | C971 | G881 | G786 | A655 | G613 |
| A1812 | U1578 | U1578 | G1484 | U1397 | A1308 | G1221 | G1112 | A1048 | C972 | G882 | A787 | G656 | U614 |
| G1813 | G1581 | G1581 | G1485 | C1403 | G1309 | C1221A | G1113 | A1049 | G973 | G883 | A788 | U657 | U615 |
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| A1815 | G1584 | U1405 | G1311 | U1405 | G1312 | G1223 | G1115 | C1052 | G974 | C885 | G792 | C659 | U617A |
| G1816 | U1406 | U1406 | U1313 | U1407 | U1314 | C1224 | G1122 | A1054 | C974A | C888 | G793 | G660 | A614C |
| A1819 | C1587 | C1587 | G1493 | C1408 | G1315 | G1227 | G1125 | G1055 | G978 | C889 | G794 | G661 | G615 |
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| C1827 | G1595 | G1595 | A1496 | G1414 | A1317 | G1229 | A1129 | A1057 | A986 | G892 | C797 | G674 | G623 |
| G1828 | C1598 | C1598 | U1503 | G1415 | G1318 | U1234 | U1130 | C893 | C986 | C894 | A802 | G686 | G624 |
| A1829 | C1599 | C1599 | C1504 | G1416 | G1319 | G1235 | G1135 | U1061 | G987 | U895 | G805 | A706 | G625 |
| C1830 | C1600 | C1600 | G1505 | C1417 | G1320 | G1236 | G1136 | G1062 | G989 | A896 | C806 | G707 | A827 |
| G1831 | U1602 | U1602 | A1509A | G1418 | A1321 | G1239 | G1137 | G1063 | A990 | C897 | U807 | C708 | G628 |
| C1832 | A1608 | A1608 | U1518 | U1420 | A1322 | U1240 | G1138 | C1064 | C991 | C898 | U808 | U709 | G629 |
| G1835 | A1614 | A1614 | G1519 | G1421 | G1323 | A1241 | G1140 | U1065 | G992 | A899 | C812 | G710 | G630 |
| C1839 | A1618 | A1618 | U1520 | G1422 | U1329 | A1246 | U1141 | U1066 | G993 | A901 | U813 | A632 | A631 |
| A1847 | C1625 | C1625 | G1524 | G1423 | A1330 | A1246 | U1142 | G1067 | C994 | C904 | C814 | A716 | A633 |
| G1853 | G1626 | G1626 | A1528 | G1424 | A1331 | U1249 | A1142A | A1069 | A986 | G997 | A819 | G717 | C634 |
| A1854 | G1627 | G1627 | G1534 | A1427 | U1341 | G1250 | G1149 | G1071 | G997 | U907 | A819 | A722 | G635 |
| G1857 | U1629 | U1629 | U1535 | C1428 | A1342 | A1253 | C1150 | A1073 | A1000 | A910 | U826 | G723 | G636 |
| G1858 | A1536 | A1536 | G1537 | G1429 | A1345 | A1254 | G1151 | G1074 | A1001 | U827 | U724 | G730 | A637 |
| A1859 | C1537 | C1537 | G1538 | U1430 | G1346 | U1255 | G1154 | G1075 | G1002 | U828 | G725 | U639 | G638 |
| G1860 | U1766 | U1766 | G1538 | C1432 | G1347 | G1256 | A1155 | C1076 | G1003 | A917 | G726 | C640 | U639 |
| G1861 | C1640 | C1640 | A1353 | C1437 | G1348 | G1259 | U1165 | A1077 | C1006 | A918 | G729 | C641 | C641 |
| C1862 | U1768 | U1768 | A1354 | G1441 | A1353 | G1260 | U1167 | U1078 | G921 | G921 | C840 | G642 | A643 |
| G1863 | C1648 | C1648 | G1442 | G1442 | A1354 | G1264 | G1168 | C1080 | A1010 | U922 | C840 | A644 | A644 |
| U1864 | G1663 | G1663 | G1443 | G1443 | G1355 | A1265 | G1169 | U1081 | G1011 | C923 | C845 | G739 | C645 |
| | | | A1543 | G1444 | G1356 | G1266 | G1170 | U1082 | G1012 | C924 | C846 | U740 | A646 |
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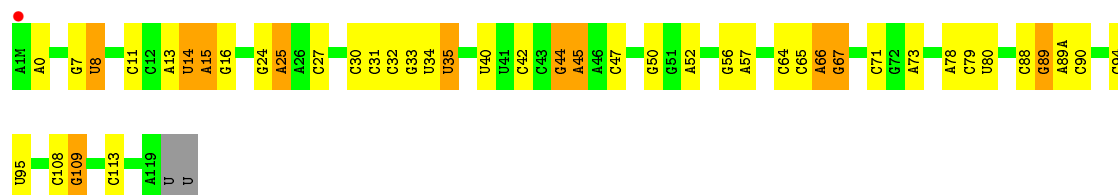


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| C1314 | G1219 | A1054 | A980 | G892 | C806 | G686 | U626 | U524 | A428 | A283 | A233 | G98 |
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| G1357 | U1241 | U1065 | G989 | C908 | A819 | G723 | G642 | C546 | C451 | A320 | G252 | A127 |
| G1358 | A1247 | U1066 | G993 | A909 | A820 | U724 | C645 | C546 | G452 | G321 | C253 | A127 |
| A1359 | G1248 | G1067 | C994 | A910 | A821 | G725 | C646 | C546 | G452 | G321 | G254 | G137A |
| A1360 | U1249 | A1068 | A996 | A911 | C825 | A646 | G647 | G561 | C453 | A322 | A255 | G137A |
| U1365 | U1250 | A1069 | G997 | U913 | C826 | U648 | G648 | U562 | A454 | G323 | A256 | G138 |
| G1365 | G1251 | G1070 | C998 | C914 | U827 | G730 | G649 | G563 | C455 | A324 | A257 | G139 |
| G1368 | G1252 | G1071 | U999 | C914 | U828 | G738 | G649 | G563 | C456 | G329 | G258 | A140 |
| A1368 | A1251 | C1072 | A1000 | A917 | U829 | G739 | G650 | U569 | A457 | A330 | G259 | A141 |
| G1368 | A1252 | A1073 | U999 | A918 | A828 | G739 | G651 | G570 | G458 | A331 | G260 | C141A |
| A1369 | A1253 | G1074 | G999 | G919 | G831 | A746 | C652 | A571 | G463 | A332 | A262 | G142 |
| A1369 | U1254 | G1075 | C1006 | G919 | G832 | U747 | A653 | G572 | C263 | C335 | C264 | A149 |
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| A1384 | G1266 | G1083 | C1013 | G932 | C837 | C755 | G | G577 | A470 | A346 | C270C | C155 |
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| G1385 | G1271 | A1084 | G934 | G934 | C838 | G760 | C | G579 | A472 | G356 | G270E | U |
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| C1402 | A1276 | C1092 | G1025 | G944 | U859 | G768 | C | A586 | A483 | A363A | C270J | A181 |
| C1403 | G1277 | G1093 | U1026 | G945 | U860 | A774 | G | C587 | A483 | A363B | U270K | A182 |
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| C1403 | G1279 | A1095 | G947 | G947 | G862 | G776 | C | C589 | G491 | G363D | U270M | C184 |
| C1404 | C1180 | A1096 | G950 | G950 | G862 | A777 | C | A590 | A492 | U363E | U270N | U185 |
| U1405 | G1280 | U1097 | C951 | C951 | A866 | G777 | C | C591 | G493 | A363F | U270O | G186 |
| U1406 | G1281 | A1098 | G952 | G952 | A866 | G777 | C | G592 | G494 | C364 | C270P | A191 |
| C1407 | U1283 | G1099 | A953 | A953 | C876 | G785 | C | G593 | G494 | C364 | C270Q | C192 |
| C1408 | G1285 | G1103 | G956 | G956 | U877 | G785 | A | A603 | G498 | G372 | G270T | A196 |
| G1416 | C1289 | A1104 | A957 | A957 | U878 | G785 | A | U606 | U499 | G372 | G270T | A196 |
| G1417 | G1297 | U1105 | U958 | U958 | G879 | A788 | G655 | U607 | G500 | U384 | C270U | A197 |
| G1418 | C1297 | G1106 | A959 | A959 | G880 | C790 | G656 | A501 | A502 | C385 | U270Z | G198 |
| A1419 | C1201 | C1109 | G1043 | G1043 | G881 | C791 | U657 | A503 | A503 | G386 | U271C | A199 |
| U1420 | G1202 | A1045 | G1044 | G1044 | G882 | G792 | C558 | U504 | U504 | G389 | G271 | G215 |
| G1421 | U1300 | G1110 | C961 | C961 | G883 | G792 | C559 | A505 | A505 | A394 | C273D | A216 |
| G1422 | A1204 | A1111 | A1046 | A1046 | G884 | G796 | C661 | C509 | C509 | U395 | U273E | G217 |
| A1423 | U1205 | G1112 | U969 | U969 | C885 | C797 | G662 | G617 | G617 | G396 | C273F | A218 |
| G1424 | G1206 | U1113 | C970 | C970 | C886 | C797 | G662 | G620 | G512 | G407 | G274 | A221 |
| G1425 | C1207 | G1114 | A973 | A973 | C887 | G798 | A670 | A821 | G512 | G407 | G275 | A222 |
| G1426 | G1309 | G1114 | G974 | G974 | C888 | A800 | G674 | G622 | A515 | G411 | A276 | A227 |
| A1427 | C1217 | G1122 | C974A | C974A | C889 | A800 | A675 | G623 | G518 | G411 | A278 | A228 |

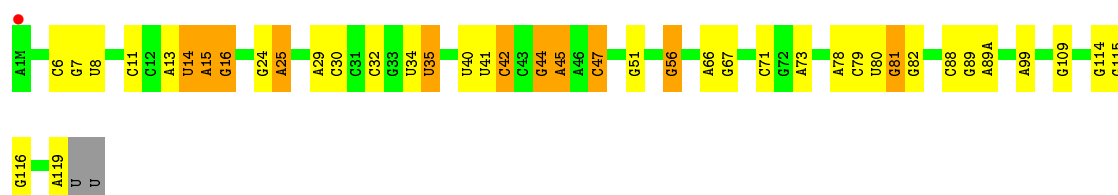




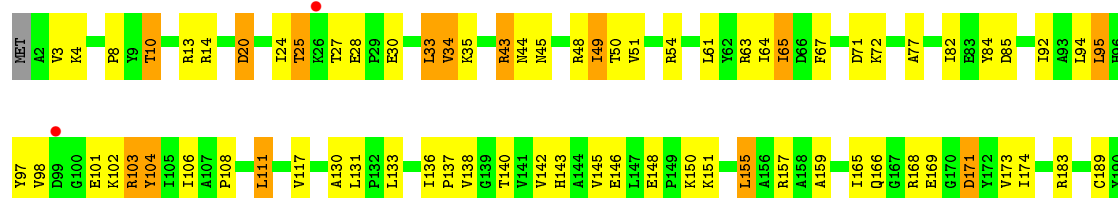
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

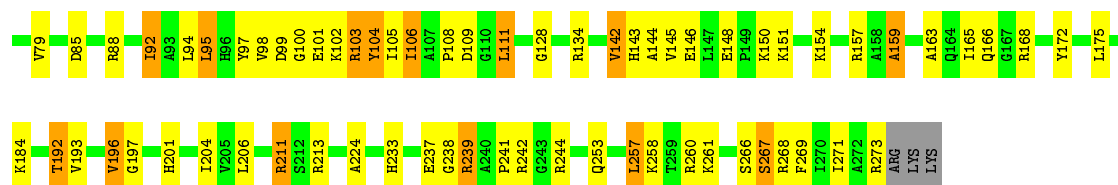


• Molecule 27: 50S ribosomal protein L2

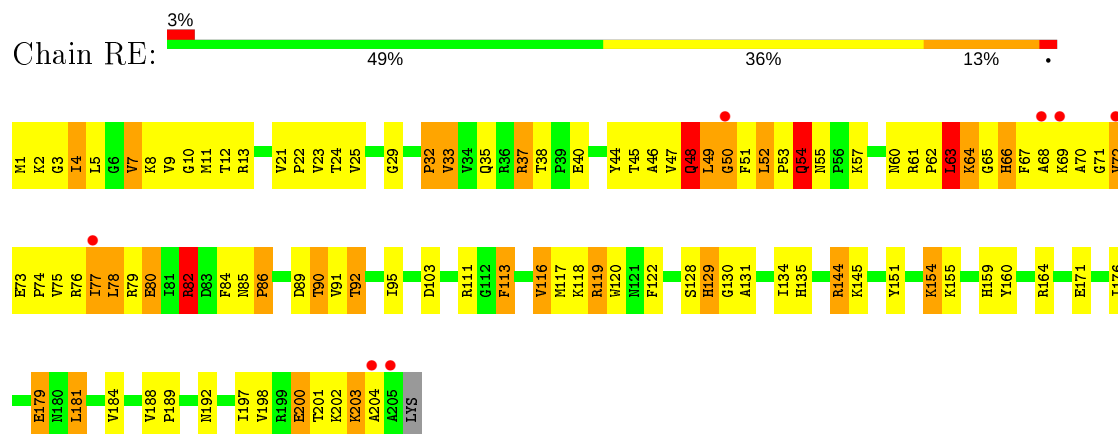


• Molecule 27: 50S ribosomal protein L2

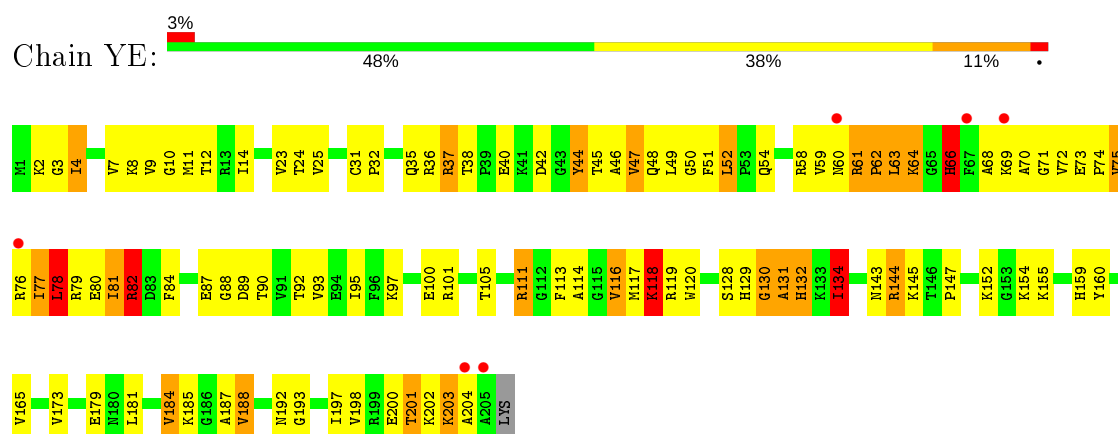




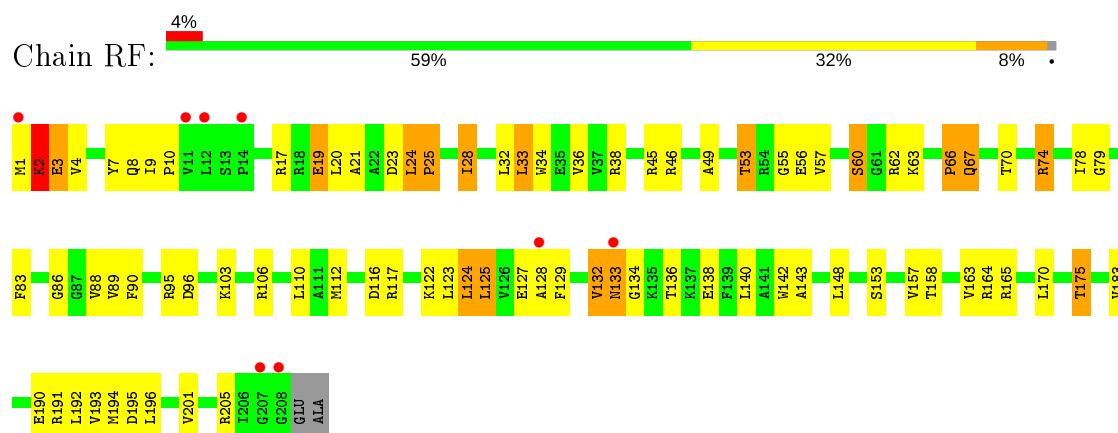
• Molecule 28: 50S ribosomal protein L3



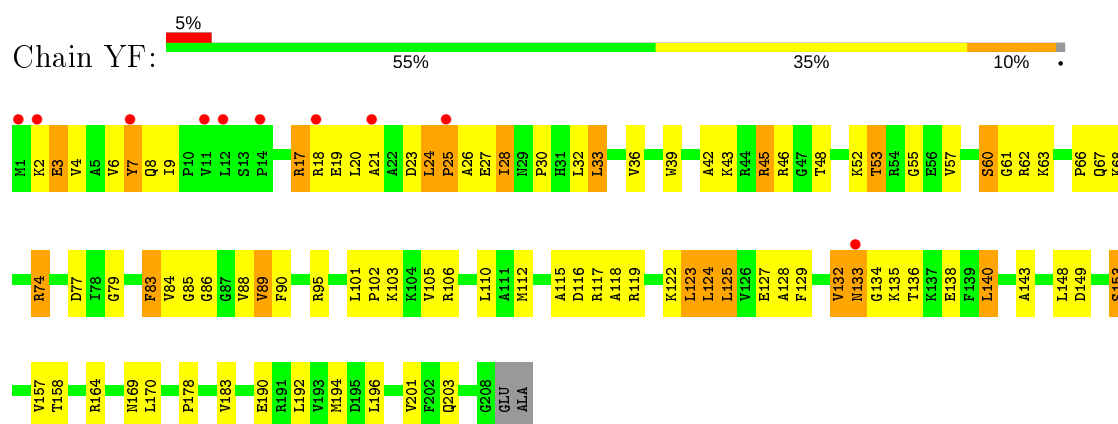
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4



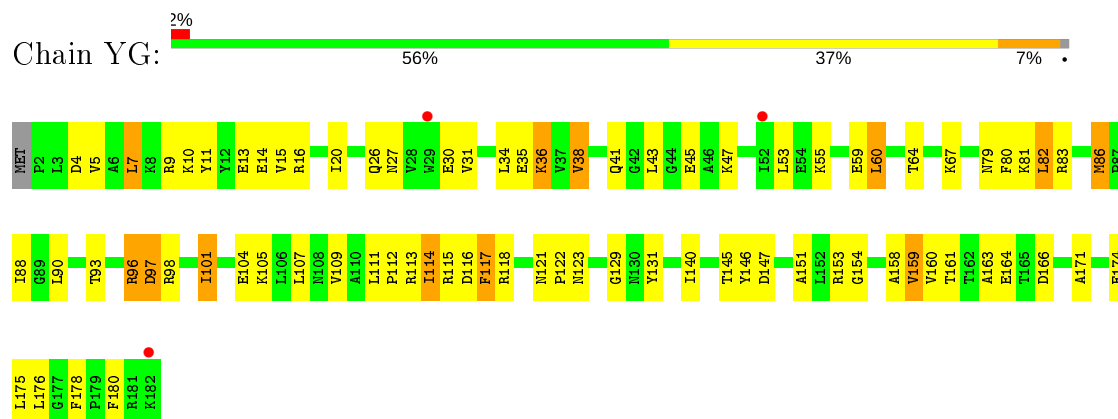
• Molecule 29: 50S ribosomal protein L4



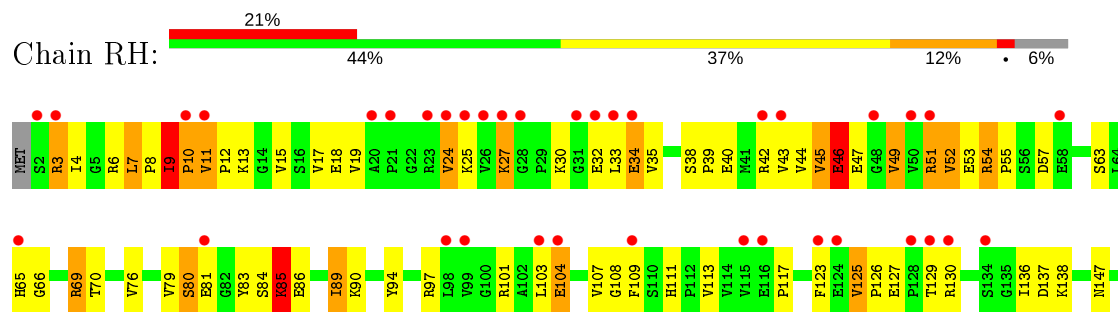
• Molecule 30: 50S ribosomal protein L5

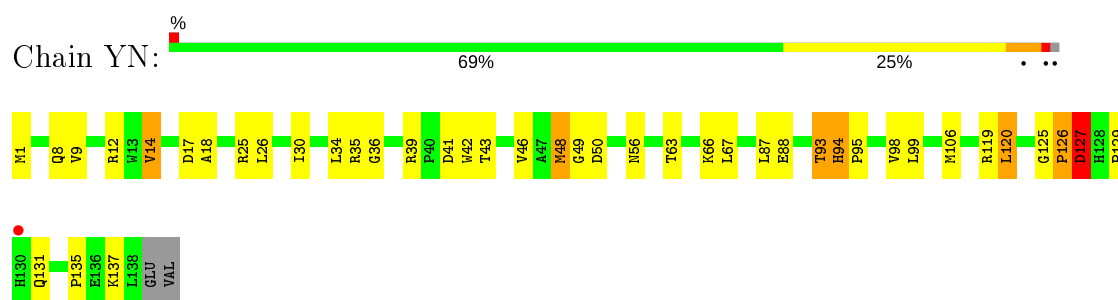


• Molecule 30: 50S ribosomal protein L5

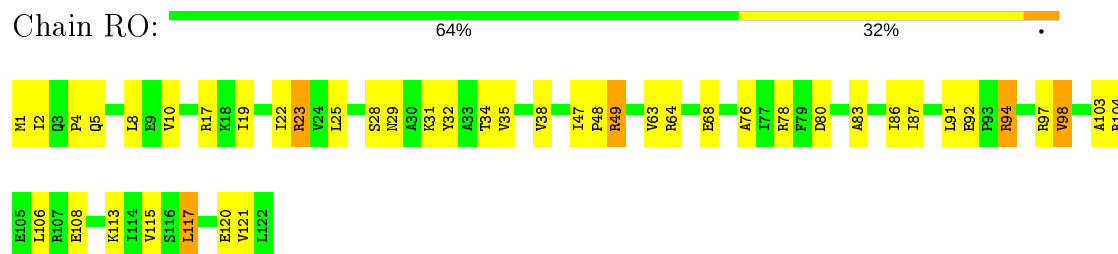


• Molecule 31: 50S ribosomal protein L6

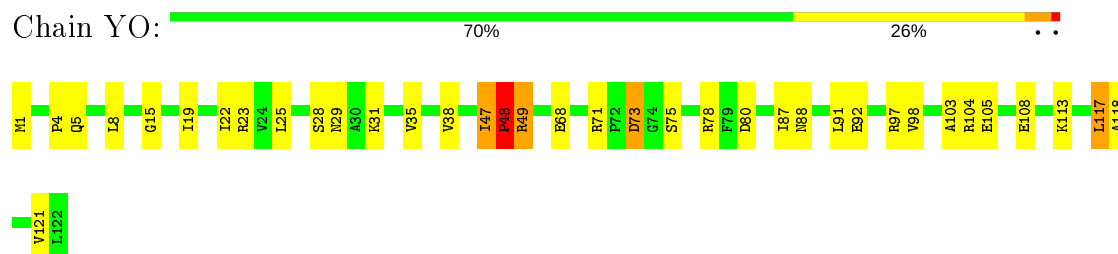




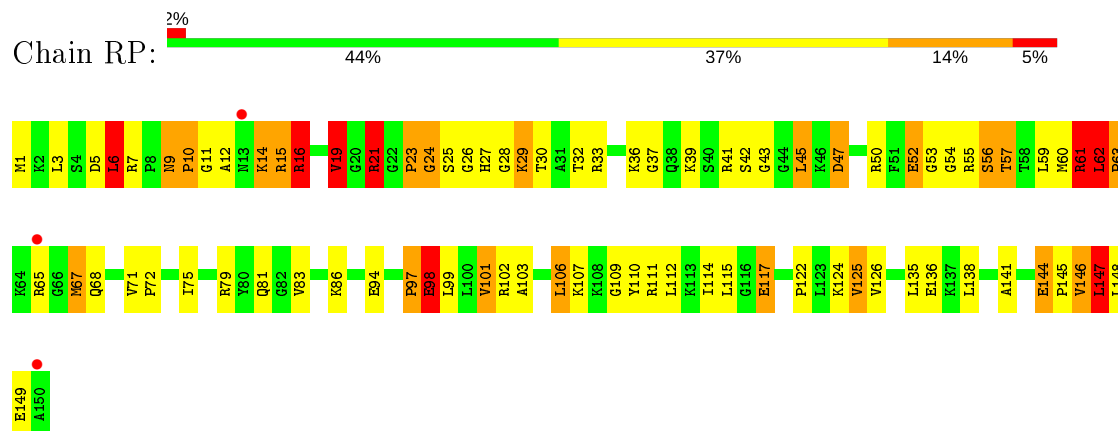
- Molecule 34: 50S ribosomal protein L14



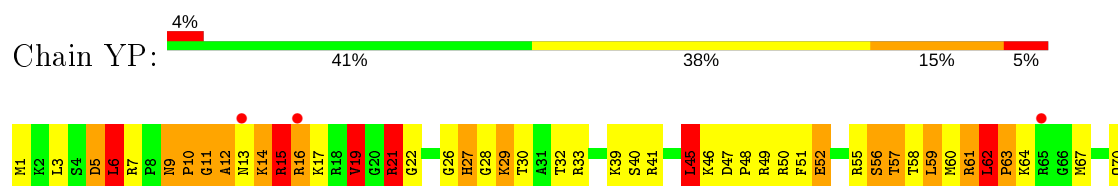
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L15





- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16



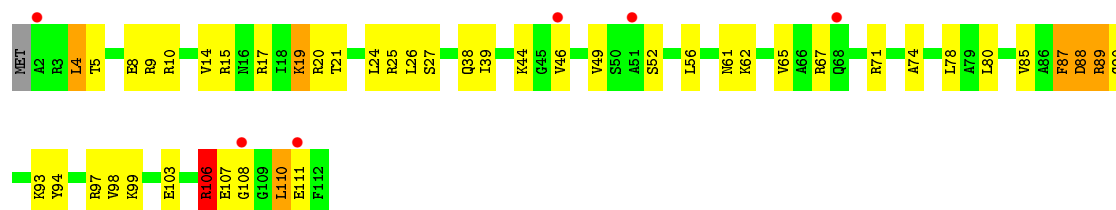
- Molecule 37: 50S ribosomal protein L17



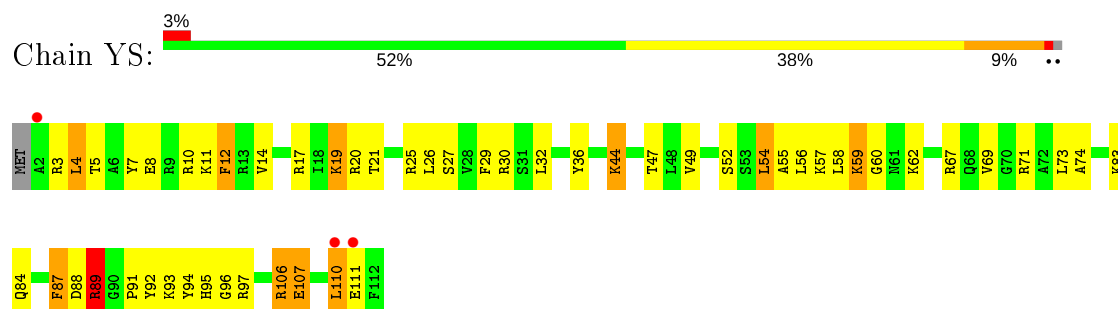
- Molecule 37: 50S ribosomal protein L17



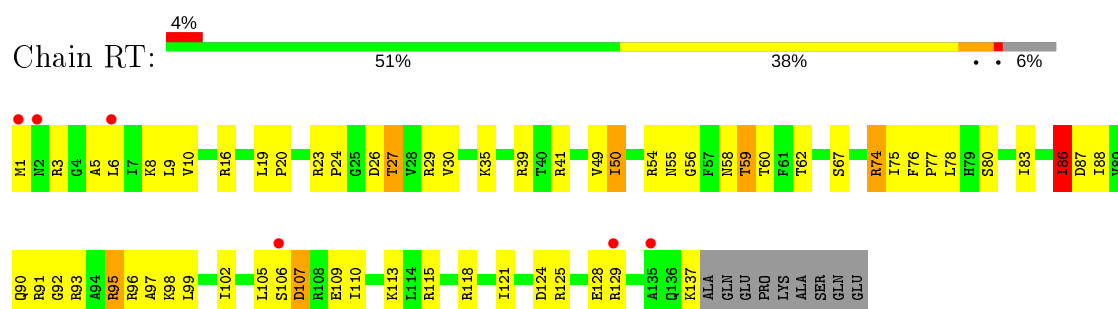
- Molecule 38: 50S ribosomal protein L18



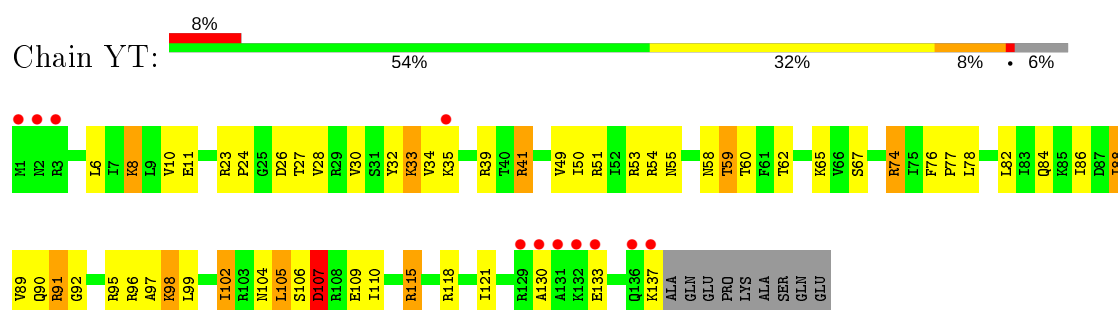
- Molecule 38: 50S ribosomal protein L18



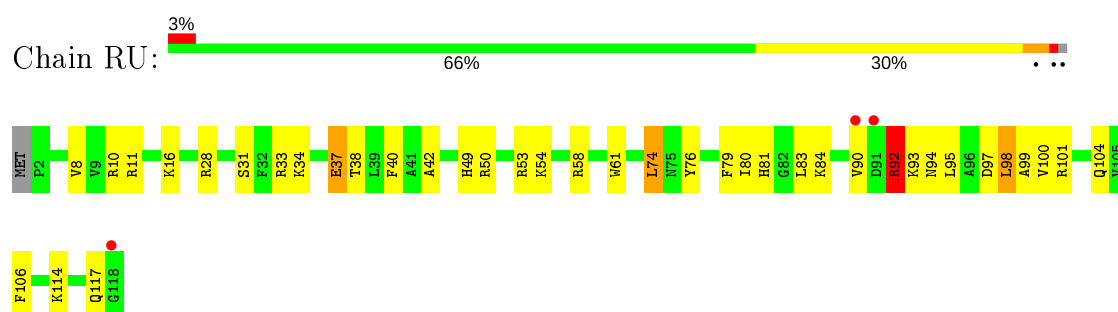
- Molecule 39: 50S ribosomal protein L19



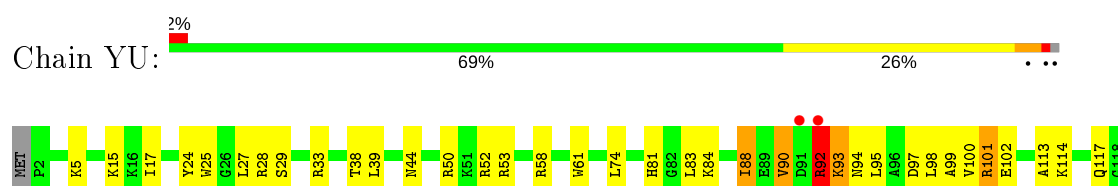
- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20

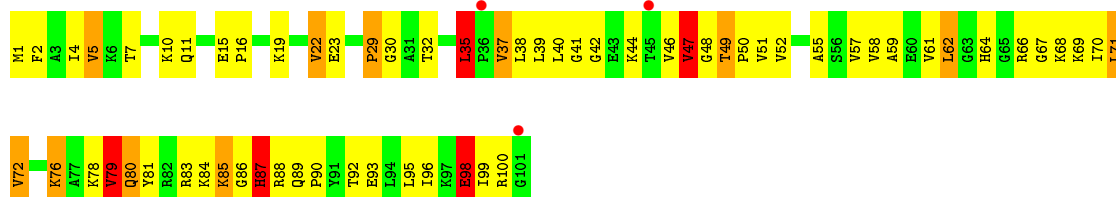


- Molecule 40: 50S ribosomal protein L20




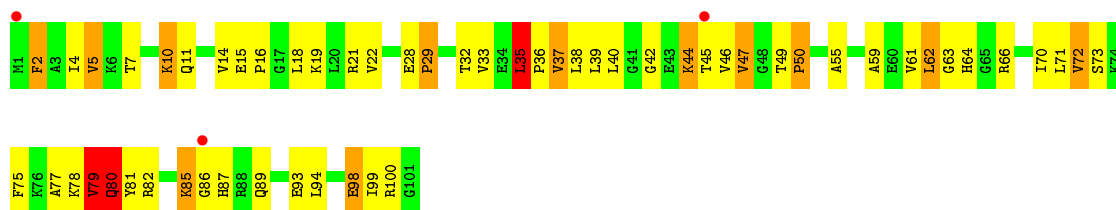
- Molecule 41: 50S ribosomal protein L21

Chain RV: 



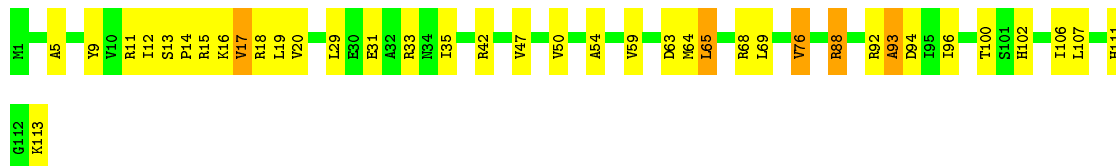
- Molecule 41: 50S ribosomal protein L21

Chain YV: 



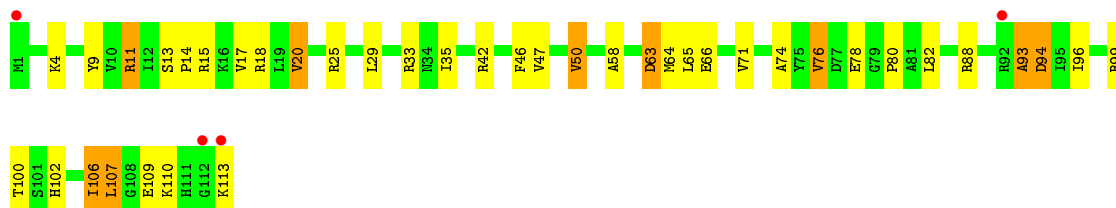
- Molecule 42: 50S ribosomal protein L22

Chain RW: 




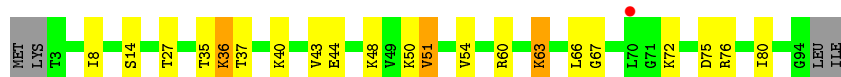
- Molecule 42: 50S ribosomal protein L22

Chain YW: 

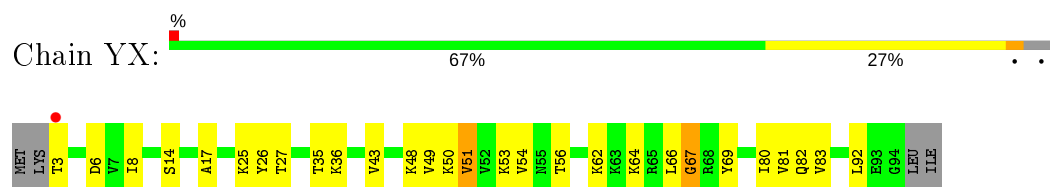


- Molecule 43: 50S ribosomal protein L23

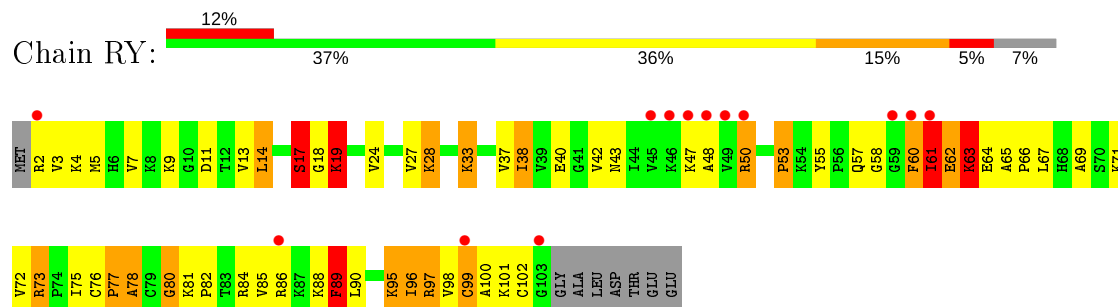
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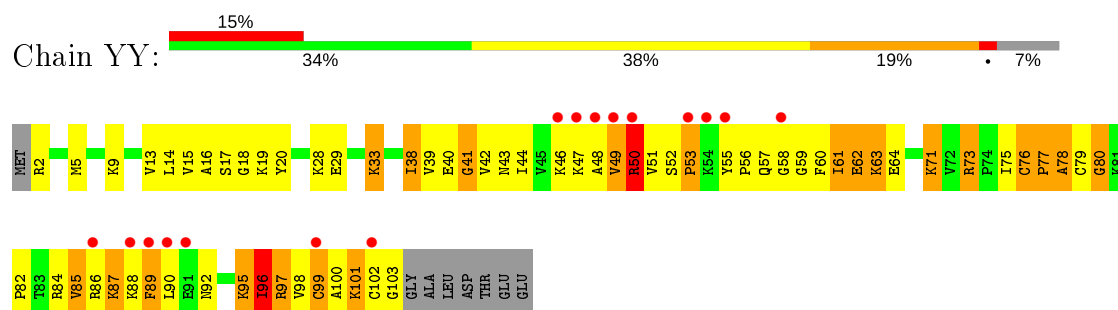
- Molecule 43: 50S ribosomal protein L23



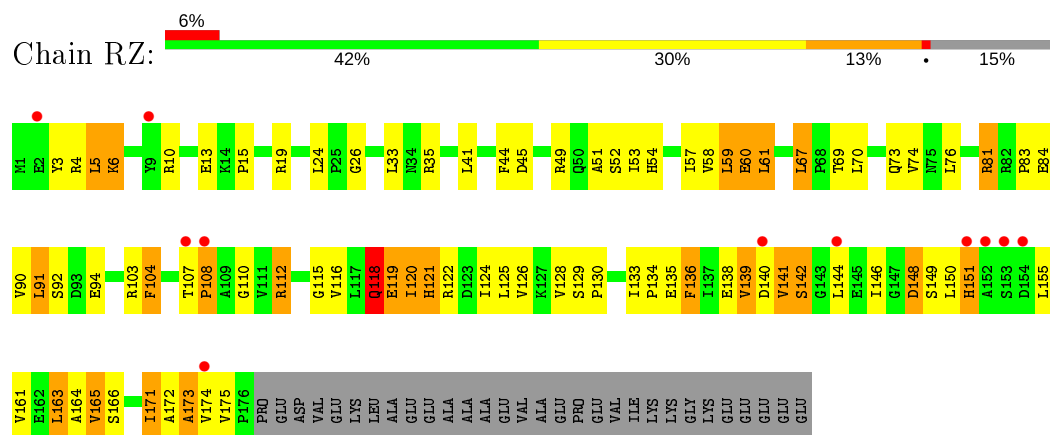
- Molecule 44: 50S ribosomal protein L24



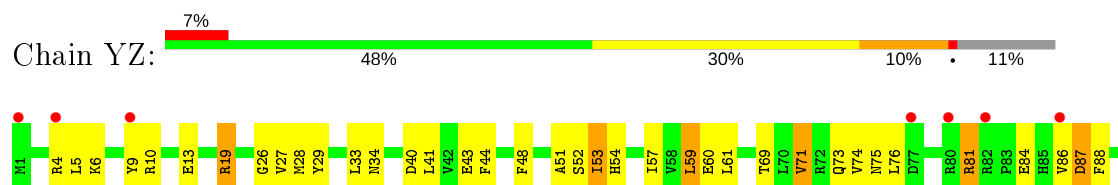
- Molecule 44: 50S ribosomal protein L24

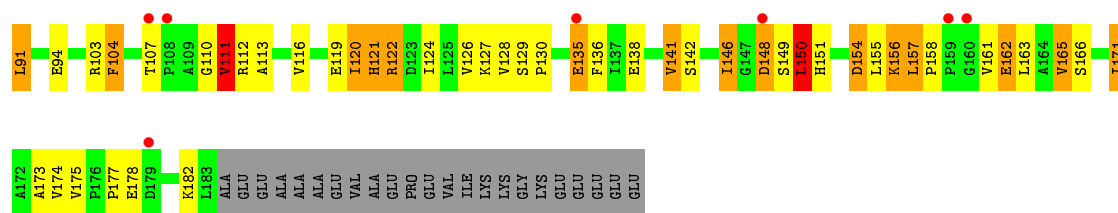


- Molecule 45: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L25





- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



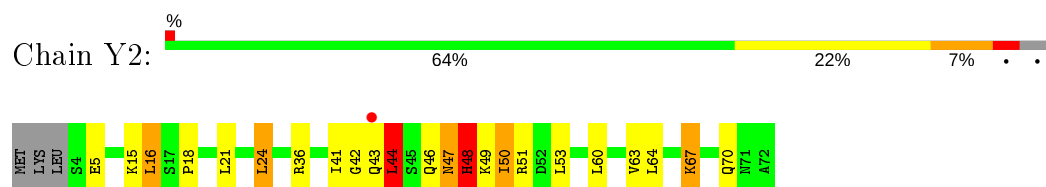
- Molecule 47: 50S ribosomal protein L28



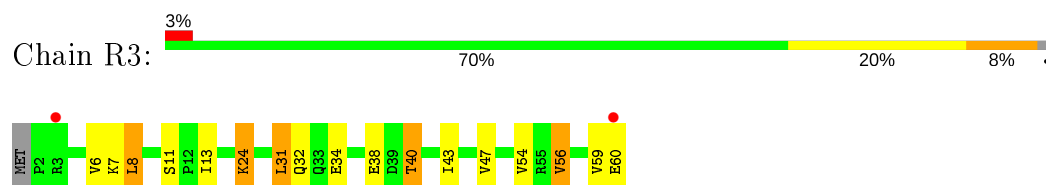
- Molecule 48: 50S ribosomal protein L29



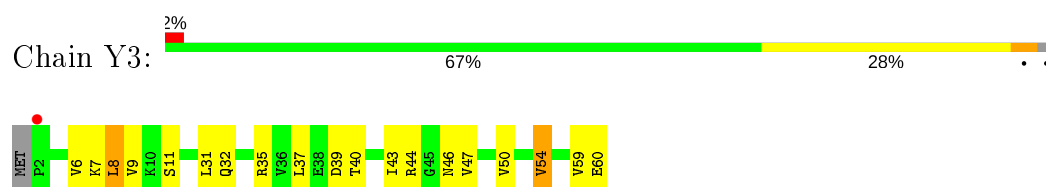
- Molecule 48: 50S ribosomal protein L29



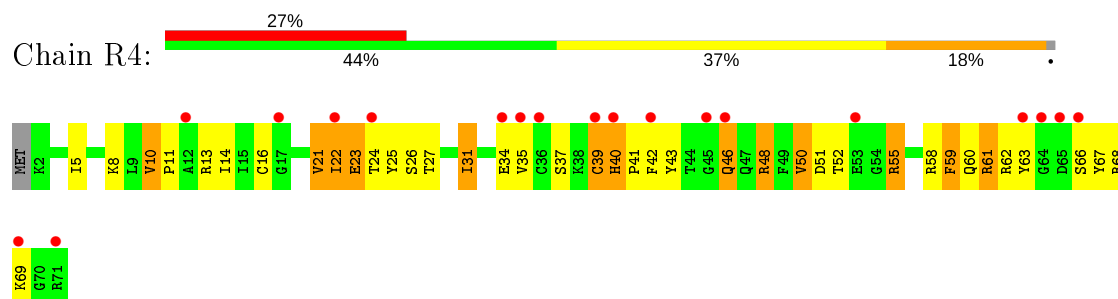
- Molecule 49: 50S ribosomal protein L30



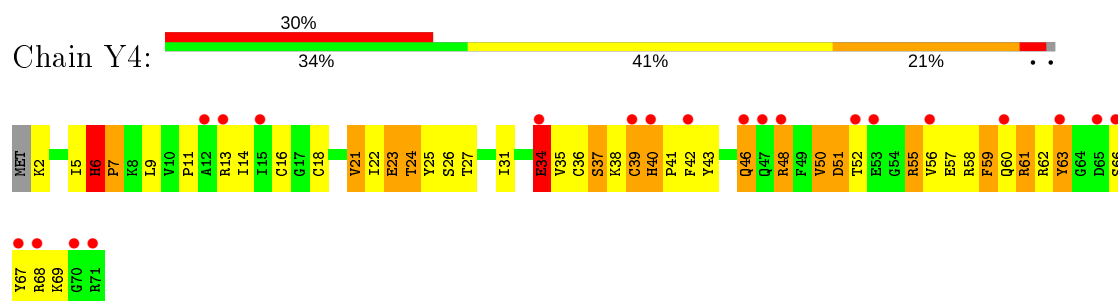
- Molecule 49: 50S ribosomal protein L30



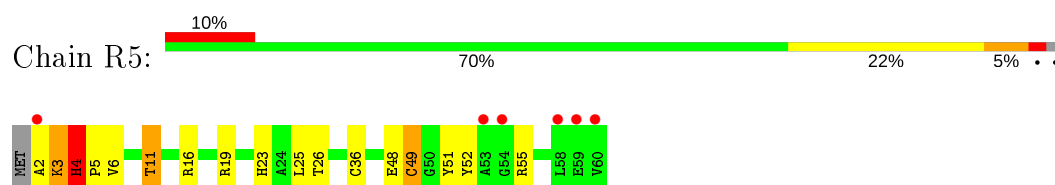
- Molecule 50: 50S ribosomal protein L31



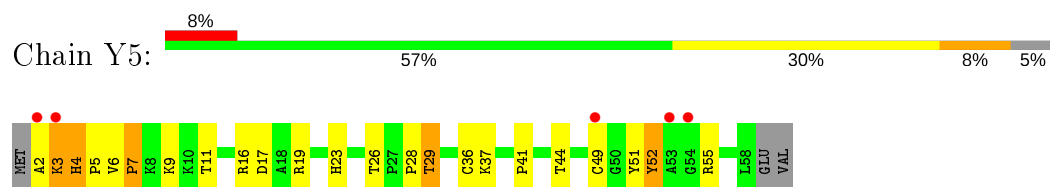
- Molecule 50: 50S ribosomal protein L31



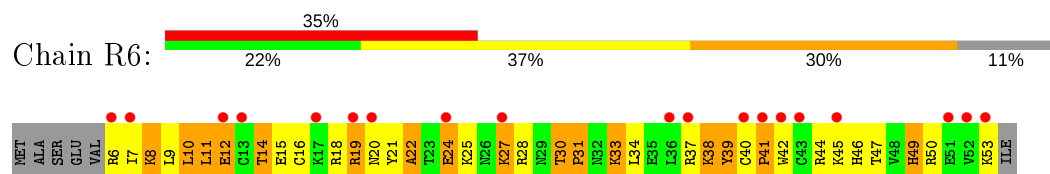
- Molecule 51: 50S ribosomal protein L32



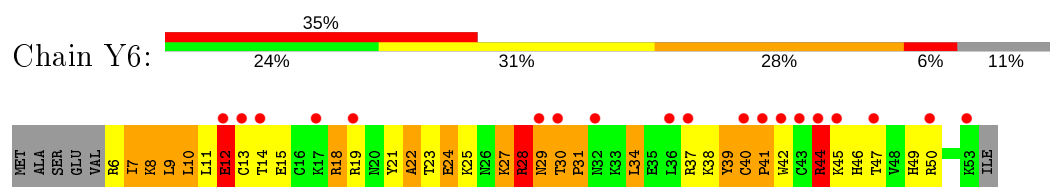
- Molecule 51: 50S ribosomal protein L32



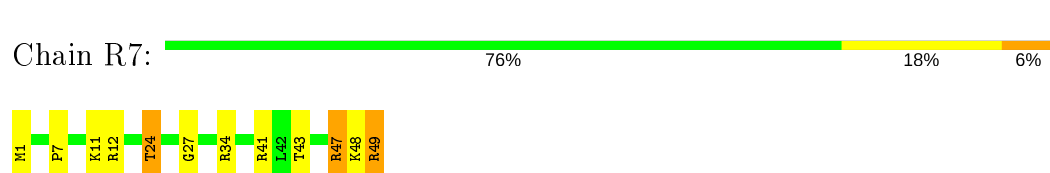
- Molecule 52: 50S ribosomal protein L33



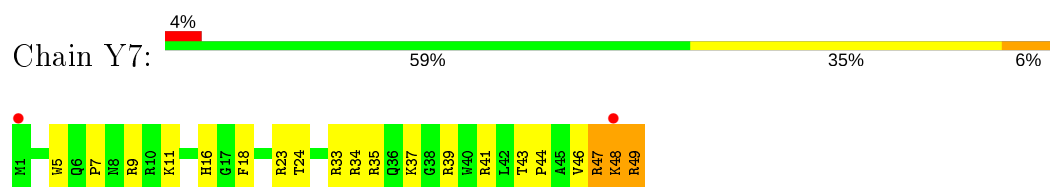
- Molecule 52: 50S ribosomal protein L33



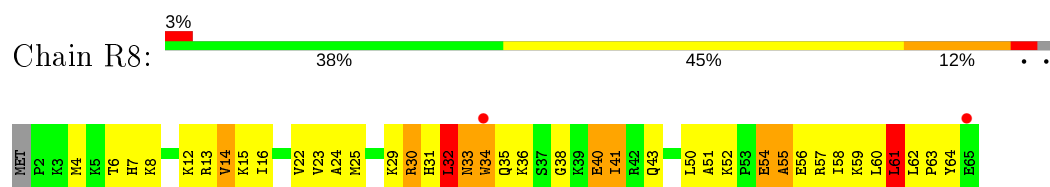
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35





• Molecule 55: 50S ribosomal protein L36



• Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 214.11Å 453.88Å 607.59Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 34.93 – 3.40 34.99 – 3.20 | Depositor EDS |
| % Data completeness (in resolution range) | 99.3 (34.93-3.40) 98.9 (34.99-3.20) | Depositor EDS |
| R_{merge} | 0.21 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.55 (at 3.18Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.2_1309) | Depositor |
| R, R_{free} | 0.202 , 0.234 0.215 , 0.248 | Depositor DCC |
| R_{free} test set | 44426 reflections (4.67%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 72.8 | Xtriage |
| Anisotropy | 0.176 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 76.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 297549 | wwPDB-VP |
| Average B, all atoms (Å ²) | 91.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: ZN, MG, A2M

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 | QA | 0.30 | 1/36346 (0.0%) | 0.79 | 15/56724 (0.0%) |
| 1 | XA | 0.31 | 0/36276 | 0.80 | 19/56615 (0.0%) |
| 2 | QB | 0.25 | 0/1950 | 0.49 | 0/2630 |
| 2 | XB | 0.26 | 0/1950 | 0.49 | 1/2630 (0.0%) |
| 3 | QC | 0.24 | 0/1636 | 0.47 | 0/2205 |
| 3 | XC | 0.27 | 0/1636 | 0.48 | 0/2205 |
| 4 | QD | 0.28 | 0/1733 | 0.50 | 0/2318 |
| 4 | XD | 0.28 | 0/1733 | 0.50 | 0/2318 |
| 5 | QE | 0.28 | 0/1195 | 0.48 | 0/1609 |
| 5 | XE | 0.29 | 0/1195 | 0.48 | 0/1609 |
| 6 | QF | 0.25 | 0/856 | 0.45 | 0/1154 |
| 6 | XF | 0.28 | 0/856 | 0.45 | 0/1154 |
| 7 | QG | 0.24 | 0/1276 | 0.45 | 0/1709 |
| 7 | XG | 0.26 | 0/1276 | 0.45 | 0/1709 |
| 8 | QH | 0.25 | 0/1136 | 0.47 | 0/1527 |
| 8 | XH | 0.27 | 0/1136 | 0.45 | 0/1527 |
| 9 | QI | 0.25 | 0/1037 | 0.48 | 0/1389 |
| 9 | XI | 0.26 | 0/1037 | 0.48 | 0/1389 |
| 10 | QJ | 0.24 | 0/814 | 0.45 | 0/1095 |
| 10 | XJ | 0.24 | 0/814 | 0.46 | 0/1095 |
| 11 | QK | 0.27 | 0/916 | 0.44 | 0/1234 |
| 11 | XK | 0.28 | 0/916 | 0.48 | 0/1234 |
| 12 | QL | 0.31 | 0/991 | 0.52 | 1/1327 (0.1%) |
| 12 | XL | 0.36 | 1/991 (0.1%) | 0.56 | 1/1327 (0.1%) |
| 13 | QM | 0.26 | 0/947 | 0.53 | 1/1270 (0.1%) |
| 13 | XM | 0.25 | 0/947 | 0.52 | 0/1270 |
| 14 | QN | 0.25 | 0/501 | 0.47 | 0/664 |
| 14 | XN | 0.29 | 0/501 | 0.49 | 0/664 |
| 15 | QO | 0.24 | 0/745 | 0.39 | 0/992 |
| 15 | XO | 0.27 | 0/745 | 0.43 | 0/992 |
| 16 | QP | 0.27 | 0/721 | 0.46 | 0/970 |
| 16 | XP | 0.25 | 0/721 | 0.45 | 0/970 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | QQ | 0.26 | 0/847 | 0.46 | 0/1131 |
| 17 | XQ | 0.30 | 0/847 | 0.47 | 0/1131 |
| 18 | QR | 0.25 | 0/590 | 0.48 | 0/782 |
| 18 | XR | 0.27 | 0/590 | 0.51 | 0/782 |
| 19 | QS | 0.27 | 0/670 | 0.53 | 0/901 |
| 19 | XS | 0.29 | 0/670 | 0.52 | 0/901 |
| 20 | QT | 0.25 | 0/765 | 0.49 | 1/1007 (0.1%) |
| 20 | XT | 0.25 | 0/765 | 0.48 | 0/1007 |
| 21 | QU | 0.23 | 0/221 | 0.46 | 0/288 |
| 21 | XU | 0.25 | 0/221 | 0.44 | 0/288 |
| 22 | QV | 0.28 | 0/1832 | 0.77 | 0/2855 |
| 22 | QW | 0.20 | 0/1832 | 0.75 | 0/2855 |
| 22 | XV | 0.31 | 0/1832 | 0.80 | 0/2855 |
| 22 | XW | 0.19 | 0/1832 | 0.77 | 0/2855 |
| 23 | QX | 0.44 | 0/417 | 0.87 | 0/649 |
| 23 | XX | 0.43 | 0/417 | 0.96 | 0/649 |
| 24 | QY | 0.31 | 0/762 | 0.45 | 0/1028 |
| 24 | XY | 0.26 | 0/762 | 0.42 | 0/1028 |
| 25 | RA | 0.39 | 4/69742 (0.0%) | 0.85 | 22/108874 (0.0%) |
| 25 | YA | 0.39 | 1/69356 (0.0%) | 0.86 | 21/108271 (0.0%) |
| 26 | RB | 0.28 | 0/2928 | 0.79 | 0/4568 |
| 26 | YB | 0.30 | 0/2928 | 0.80 | 0/4568 |
| 27 | RD | 0.34 | 0/2165 | 0.56 | 0/2919 |
| 27 | YD | 0.37 | 0/2165 | 0.60 | 0/2919 |
| 28 | RE | 0.33 | 0/1601 | 0.58 | 0/2160 |
| 28 | YE | 0.33 | 0/1601 | 0.58 | 0/2160 |
| 29 | RF | 0.35 | 0/1662 | 0.58 | 0/2249 |
| 29 | YF | 0.31 | 0/1662 | 0.58 | 0/2249 |
| 30 | RG | 0.25 | 0/1499 | 0.46 | 0/2016 |
| 30 | YG | 0.25 | 0/1499 | 0.46 | 0/2016 |
| 31 | RH | 0.25 | 0/1332 | 0.60 | 1/1802 (0.1%) |
| 31 | YH | 0.29 | 0/1332 | 0.67 | 1/1802 (0.1%) |
| 32 | RI | 0.24 | 0/1151 | 0.54 | 0/1558 |
| 32 | YI | 0.28 | 0/1151 | 0.58 | 0/1558 |
| 33 | RN | 0.28 | 0/1131 | 0.50 | 0/1525 |
| 33 | YN | 0.29 | 0/1131 | 0.51 | 0/1525 |
| 34 | RO | 0.32 | 0/943 | 0.51 | 0/1269 |
| 34 | YO | 0.33 | 0/943 | 0.53 | 0/1269 |
| 35 | RP | 0.34 | 0/1162 | 0.66 | 0/1544 |
| 35 | YP | 0.35 | 0/1162 | 0.70 | 2/1544 (0.1%) |
| 36 | RQ | 0.34 | 0/1133 | 0.57 | 0/1515 |
| 36 | YQ | 0.35 | 0/1128 | 0.58 | 1/1508 (0.1%) |
| 37 | RR | 0.27 | 0/974 | 0.51 | 0/1302 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 37 | YR | 0.30 | 0/974 | 0.53 | 0/1302 |
| 38 | RS | 0.25 | 0/892 | 0.48 | 0/1187 |
| 38 | YS | 0.29 | 0/892 | 0.54 | 0/1187 |
| 39 | RT | 0.27 | 0/1155 | 0.46 | 0/1542 |
| 39 | YT | 0.30 | 0/1155 | 0.47 | 0/1542 |
| 40 | RU | 0.32 | 0/982 | 0.53 | 0/1306 |
| 40 | YU | 0.33 | 0/982 | 0.52 | 0/1306 |
| 41 | RV | 0.37 | 0/790 | 0.69 | 1/1057 (0.1%) |
| 41 | YV | 0.35 | 0/790 | 0.68 | 1/1057 (0.1%) |
| 42 | RW | 0.30 | 0/911 | 0.51 | 0/1220 |
| 42 | YW | 0.31 | 0/911 | 0.52 | 0/1220 |
| 43 | RX | 0.32 | 0/739 | 0.51 | 0/993 |
| 43 | YX | 0.35 | 0/739 | 0.52 | 0/993 |
| 44 | RY | 0.33 | 0/798 | 0.61 | 0/1064 |
| 44 | YY | 0.31 | 0/798 | 0.59 | 0/1064 |
| 45 | RZ | 0.33 | 0/1435 | 0.58 | 1/1947 (0.1%) |
| 45 | YZ | 0.30 | 0/1493 | 0.60 | 0/2026 |
| 46 | R0 | 0.32 | 0/666 | 0.52 | 0/885 |
| 46 | Y0 | 0.32 | 0/666 | 0.58 | 0/885 |
| 47 | R1 | 0.31 | 0/770 | 0.57 | 0/1022 |
| 47 | Y1 | 0.36 | 0/770 | 0.59 | 0/1022 |
| 48 | R2 | 0.28 | 0/583 | 0.58 | 0/771 |
| 48 | Y2 | 0.33 | 0/583 | 0.59 | 1/771 (0.1%) |
| 49 | R3 | 0.29 | 0/474 | 0.44 | 0/635 |
| 49 | Y3 | 0.28 | 0/474 | 0.47 | 0/635 |
| 50 | R4 | 0.24 | 0/586 | 0.46 | 0/785 |
| 50 | Y4 | 0.30 | 0/586 | 0.50 | 0/785 |
| 51 | R5 | 0.30 | 0/473 | 0.58 | 1/639 (0.2%) |
| 51 | Y5 | 0.30 | 0/456 | 0.57 | 0/617 |
| 52 | R6 | 0.29 | 0/424 | 0.67 | 0/565 |
| 52 | Y6 | 0.46 | 0/424 | 0.80 | 0/565 |
| 53 | R7 | 0.33 | 0/438 | 0.49 | 0/575 |
| 53 | Y7 | 0.35 | 0/438 | 0.53 | 0/575 |
| 54 | R8 | 0.42 | 0/525 | 0.75 | 0/691 |
| 54 | Y8 | 0.39 | 0/525 | 0.66 | 0/691 |
| 55 | R9 | 0.26 | 0/310 | 0.43 | 0/407 |
| 55 | Y9 | 0.24 | 0/302 | 0.41 | 0/397 |
| All | All | 0.34 | 7/321792 (0.0%) | 0.76 | 92/481138 (0.0%) |

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

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 25 | RA | 1035 | U | O3'-P | -5.77 | 1.54 | 1.61 |
| 25 | RA | 1034 | G | O3'-P | -5.46 | 1.54 | 1.61 |
| 25 | YA | 1545 | A | O3'-P | 5.37 | 1.67 | 1.61 |
| 25 | RA | 371 | A | O3'-P | -5.36 | 1.54 | 1.61 |
| 25 | RA | 2092 | U | O3'-P | -5.31 | 1.54 | 1.61 |

The worst 5 of 92 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|--------|-------------|----------|
| 31 | YH | 9 | ILE | C-N-CD | -11.87 | 94.49 | 120.60 |
| 1 | XA | 315 | A | P-O3'-C3' | 7.69 | 128.93 | 119.70 |
| 25 | RA | 614(A) | U | P-O3'-C3' | 7.53 | 128.74 | 119.70 |
| 1 | QA | 345 | C | C2-N1-C1' | 7.50 | 127.05 | 118.80 |
| 1 | QA | 328 | C | P-O3'-C3' | 6.46 | 127.45 | 119.70 |

There are no chirality outliers.

There are no planarity outliers.

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 | QA | 32472 | 0 | 16393 | 490 | 0 |
| 1 | XA | 32409 | 0 | 16361 | 449 | 0 |
| 2 | QB | 1915 | 0 | 1969 | 56 | 0 |
| 2 | XB | 1915 | 0 | 1969 | 60 | 0 |
| 3 | QC | 1612 | 0 | 1677 | 51 | 0 |
| 3 | XC | 1612 | 0 | 1677 | 50 | 0 |
| 4 | QD | 1703 | 0 | 1765 | 47 | 0 |
| 4 | XD | 1703 | 0 | 1765 | 43 | 0 |
| 5 | QE | 1178 | 0 | 1234 | 29 | 0 |
| 5 | XE | 1178 | 0 | 1234 | 22 | 0 |
| 6 | QF | 843 | 0 | 857 | 18 | 0 |
| 6 | XF | 843 | 0 | 857 | 22 | 0 |
| 7 | QG | 1257 | 0 | 1296 | 30 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7 | XG | 1257 | 0 | 1296 | 35 | 0 |
| 8 | QH | 1116 | 0 | 1177 | 30 | 0 |
| 8 | XH | 1116 | 0 | 1177 | 27 | 0 |
| 9 | QI | 1018 | 0 | 1049 | 52 | 0 |
| 9 | XI | 1018 | 0 | 1049 | 45 | 0 |
| 10 | QJ | 801 | 0 | 849 | 35 | 0 |
| 10 | XJ | 801 | 0 | 849 | 46 | 0 |
| 11 | QK | 901 | 0 | 926 | 27 | 0 |
| 11 | XK | 901 | 0 | 926 | 23 | 0 |
| 12 | QL | 975 | 0 | 1062 | 27 | 0 |
| 12 | XL | 975 | 0 | 1062 | 24 | 0 |
| 13 | QM | 937 | 0 | 995 | 27 | 0 |
| 13 | XM | 937 | 0 | 995 | 56 | 0 |
| 14 | QN | 492 | 0 | 528 | 15 | 0 |
| 14 | XN | 492 | 0 | 528 | 20 | 0 |
| 15 | QO | 734 | 0 | 771 | 14 | 0 |
| 15 | XO | 734 | 0 | 771 | 14 | 0 |
| 16 | QP | 705 | 0 | 725 | 15 | 0 |
| 16 | XP | 705 | 0 | 725 | 9 | 0 |
| 17 | QQ | 834 | 0 | 904 | 16 | 0 |
| 17 | XQ | 834 | 0 | 904 | 19 | 0 |
| 18 | QR | 585 | 0 | 657 | 11 | 0 |
| 18 | XR | 585 | 0 | 657 | 19 | 0 |
| 19 | QS | 656 | 0 | 678 | 47 | 0 |
| 19 | XS | 656 | 0 | 678 | 42 | 0 |
| 20 | QT | 763 | 0 | 861 | 23 | 0 |
| 20 | XT | 763 | 0 | 861 | 28 | 0 |
| 21 | QU | 217 | 0 | 234 | 12 | 0 |
| 21 | XU | 217 | 0 | 234 | 16 | 0 |
| 22 | QV | 1640 | 0 | 837 | 29 | 0 |
| 22 | QW | 1640 | 0 | 837 | 46 | 0 |
| 22 | XV | 1640 | 0 | 837 | 18 | 0 |
| 22 | XW | 1640 | 0 | 837 | 23 | 0 |
| 23 | QX | 440 | 9 | 224 | 18 | 0 |
| 23 | XX | 440 | 9 | 224 | 15 | 0 |
| 24 | QY | 746 | 0 | 742 | 16 | 0 |
| 24 | XY | 746 | 0 | 742 | 17 | 0 |
| 25 | RA | 62269 | 0 | 31392 | 818 | 0 |
| 25 | YA | 61924 | 0 | 31213 | 687 | 0 |
| 26 | RB | 2617 | 0 | 1328 | 29 | 0 |
| 26 | YB | 2617 | 0 | 1328 | 33 | 0 |
| 27 | RD | 2115 | 0 | 2195 | 66 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27 | YD | 2115 | 0 | 2195 | 83 | 0 |
| 28 | RE | 1568 | 0 | 1634 | 123 | 0 |
| 28 | YE | 1568 | 0 | 1634 | 79 | 0 |
| 29 | RF | 1627 | 0 | 1680 | 50 | 0 |
| 29 | YF | 1627 | 0 | 1680 | 58 | 0 |
| 30 | RG | 1474 | 0 | 1535 | 49 | 0 |
| 30 | YG | 1474 | 0 | 1535 | 51 | 0 |
| 31 | RH | 1307 | 0 | 1382 | 89 | 0 |
| 31 | YH | 1307 | 0 | 1382 | 66 | 0 |
| 32 | RI | 1136 | 0 | 1223 | 32 | 0 |
| 32 | YI | 1136 | 0 | 1223 | 62 | 0 |
| 33 | RN | 1104 | 0 | 1180 | 14 | 0 |
| 33 | YN | 1104 | 0 | 1180 | 24 | 0 |
| 34 | RO | 933 | 0 | 996 | 32 | 0 |
| 34 | YO | 933 | 0 | 996 | 26 | 0 |
| 35 | RP | 1145 | 0 | 1228 | 91 | 0 |
| 35 | YP | 1145 | 0 | 1228 | 97 | 0 |
| 36 | RQ | 1112 | 0 | 1170 | 33 | 0 |
| 36 | YQ | 1107 | 0 | 1166 | 40 | 0 |
| 37 | RR | 960 | 0 | 1021 | 17 | 0 |
| 37 | YR | 960 | 0 | 1021 | 23 | 0 |
| 38 | RS | 882 | 0 | 943 | 30 | 0 |
| 38 | YS | 882 | 0 | 943 | 35 | 0 |
| 39 | RT | 1141 | 0 | 1202 | 46 | 0 |
| 39 | YT | 1141 | 0 | 1202 | 36 | 0 |
| 40 | RU | 964 | 0 | 1022 | 41 | 0 |
| 40 | YU | 964 | 0 | 1022 | 30 | 0 |
| 41 | RV | 779 | 0 | 852 | 63 | 0 |
| 41 | YV | 779 | 0 | 852 | 54 | 0 |
| 42 | RW | 900 | 0 | 964 | 24 | 0 |
| 42 | YW | 900 | 0 | 964 | 21 | 0 |
| 43 | RX | 725 | 0 | 778 | 14 | 0 |
| 43 | YX | 725 | 0 | 778 | 16 | 0 |
| 44 | RY | 785 | 0 | 878 | 54 | 0 |
| 44 | YY | 785 | 0 | 878 | 54 | 0 |
| 45 | RZ | 1404 | 0 | 1437 | 80 | 0 |
| 45 | YZ | 1461 | 0 | 1493 | 47 | 0 |
| 46 | R0 | 657 | 0 | 683 | 17 | 0 |
| 46 | Y0 | 657 | 0 | 683 | 25 | 0 |
| 47 | R1 | 763 | 0 | 848 | 31 | 0 |
| 47 | Y1 | 763 | 0 | 848 | 23 | 0 |
| 48 | R2 | 581 | 0 | 629 | 17 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48 | Y2 | 581 | 0 | 629 | 14 | 0 |
| 49 | R3 | 469 | 0 | 518 | 10 | 0 |
| 49 | Y3 | 469 | 0 | 518 | 9 | 0 |
| 50 | R4 | 573 | 0 | 565 | 25 | 0 |
| 50 | Y4 | 573 | 0 | 565 | 45 | 0 |
| 51 | R5 | 459 | 0 | 480 | 10 | 0 |
| 51 | Y5 | 442 | 0 | 465 | 24 | 0 |
| 52 | R6 | 417 | 0 | 441 | 27 | 0 |
| 52 | Y6 | 417 | 0 | 441 | 46 | 0 |
| 53 | R7 | 430 | 0 | 480 | 6 | 0 |
| 53 | Y7 | 430 | 0 | 480 | 12 | 0 |
| 54 | R8 | 517 | 0 | 582 | 42 | 0 |
| 54 | Y8 | 517 | 0 | 582 | 37 | 0 |
| 55 | R9 | 307 | 0 | 338 | 11 | 0 |
| 55 | Y9 | 299 | 0 | 326 | 6 | 0 |
| 56 | QA | 150 | 0 | 0 | 0 | 0 |
| 56 | QD | 2 | 0 | 0 | 0 | 0 |
| 56 | QL | 1 | 0 | 0 | 0 | 0 |
| 56 | QV | 4 | 0 | 0 | 0 | 0 |
| 56 | QX | 1 | 0 | 0 | 0 | 0 |
| 56 | R0 | 3 | 0 | 0 | 0 | 0 |
| 56 | R1 | 1 | 0 | 0 | 0 | 0 |
| 56 | R2 | 1 | 0 | 0 | 0 | 0 |
| 56 | R5 | 3 | 0 | 0 | 0 | 0 |
| 56 | RA | 441 | 0 | 0 | 0 | 0 |
| 56 | RB | 4 | 0 | 0 | 0 | 0 |
| 56 | RD | 2 | 0 | 0 | 0 | 0 |
| 56 | RE | 1 | 0 | 0 | 0 | 0 |
| 56 | RF | 1 | 0 | 0 | 0 | 0 |
| 56 | RP | 3 | 0 | 0 | 0 | 0 |
| 56 | RQ | 2 | 0 | 0 | 0 | 0 |
| 56 | RR | 1 | 0 | 0 | 0 | 0 |
| 56 | RT | 1 | 0 | 0 | 0 | 0 |
| 56 | RV | 1 | 0 | 0 | 0 | 0 |
| 56 | RY | 1 | 0 | 0 | 0 | 0 |
| 56 | XA | 163 | 0 | 0 | 0 | 0 |
| 56 | XD | 1 | 0 | 0 | 0 | 0 |
| 56 | XF | 1 | 0 | 0 | 0 | 0 |
| 56 | XL | 1 | 0 | 0 | 0 | 0 |
| 56 | XS | 1 | 0 | 0 | 0 | 0 |
| 56 | XV | 3 | 0 | 0 | 0 | 0 |
| 56 | Y0 | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56 | Y1 | 1 | 0 | 0 | 0 | 0 |
| 56 | Y5 | 3 | 0 | 0 | 0 | 0 |
| 56 | Y7 | 1 | 0 | 0 | 0 | 0 |
| 56 | YA | 487 | 0 | 0 | 0 | 0 |
| 56 | YB | 6 | 0 | 0 | 0 | 0 |
| 56 | YD | 1 | 0 | 0 | 0 | 0 |
| 56 | YE | 1 | 0 | 0 | 0 | 0 |
| 56 | YF | 1 | 0 | 0 | 0 | 0 |
| 56 | YG | 1 | 0 | 0 | 0 | 0 |
| 56 | YH | 1 | 0 | 0 | 0 | 0 |
| 56 | YN | 1 | 0 | 0 | 0 | 0 |
| 56 | YO | 1 | 0 | 0 | 0 | 0 |
| 56 | YP | 1 | 0 | 0 | 0 | 0 |
| 56 | YQ | 2 | 0 | 0 | 0 | 0 |
| 56 | YV | 1 | 0 | 0 | 0 | 0 |
| 56 | YW | 1 | 0 | 0 | 0 | 0 |
| 56 | YY | 1 | 0 | 0 | 0 | 0 |
| 57 | QD | 1 | 0 | 0 | 0 | 0 |
| 57 | QN | 1 | 0 | 0 | 0 | 0 |
| 57 | XD | 1 | 0 | 0 | 0 | 0 |
| 57 | XN | 1 | 0 | 0 | 0 | 0 |
| All | All | 297531 | 18 | 201516 | 5344 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5344 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) |
|------------------|-------------------|--------------------------|-------------------|
| 41:YV:49:THR:CG2 | 41:YV:50:PRO:HD3 | 1.35 | 1.56 |
| 44:RY:76:CYS:SG | 44:RY:77:PRO:HD2 | 1.44 | 1.55 |
| 31:RH:9:ILE:CG2 | 31:RH:10:PRO:HA | 1.36 | 1.51 |
| 41:RV:49:THR:CG2 | 41:RV:50:PRO:HD3 | 1.50 | 1.41 |
| 32:YI:77:LEU:HB2 | 32:YI:142:VAL:CG2 | 1.54 | 1.37 |

There are no symmetry-related clashes.

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 | QB | 234/256 (91%) | 186 (80%) | 29 (12%) | 19 (8%) | 1 | 5 |
| 2 | XB | 234/256 (91%) | 189 (81%) | 27 (12%) | 18 (8%) | 1 | 6 |
| 3 | QC | 204/239 (85%) | 162 (79%) | 26 (13%) | 16 (8%) | 1 | 6 |
| 3 | XC | 204/239 (85%) | 159 (78%) | 33 (16%) | 12 (6%) | 1 | 11 |
| 4 | QD | 206/209 (99%) | 169 (82%) | 26 (13%) | 11 (5%) | 2 | 13 |
| 4 | XD | 206/209 (99%) | 168 (82%) | 24 (12%) | 14 (7%) | 1 | 8 |
| 5 | QE | 152/162 (94%) | 136 (90%) | 12 (8%) | 4 (3%) | 5 | 26 |
| 5 | XE | 152/162 (94%) | 137 (90%) | 10 (7%) | 5 (3%) | 4 | 22 |
| 6 | QF | 99/101 (98%) | 89 (90%) | 10 (10%) | 0 | 100 | 100 |
| 6 | XF | 99/101 (98%) | 95 (96%) | 4 (4%) | 0 | 100 | 100 |
| 7 | QG | 153/156 (98%) | 136 (89%) | 13 (8%) | 4 (3%) | 5 | 26 |
| 7 | XG | 153/156 (98%) | 134 (88%) | 15 (10%) | 4 (3%) | 5 | 26 |
| 8 | QH | 136/138 (99%) | 126 (93%) | 7 (5%) | 3 (2%) | 6 | 29 |
| 8 | XH | 136/138 (99%) | 123 (90%) | 10 (7%) | 3 (2%) | 6 | 29 |
| 9 | QI | 126/128 (98%) | 94 (75%) | 24 (19%) | 8 (6%) | 1 | 9 |
| 9 | XI | 126/128 (98%) | 96 (76%) | 23 (18%) | 7 (6%) | 2 | 12 |
| 10 | QJ | 97/105 (92%) | 80 (82%) | 13 (13%) | 4 (4%) | 3 | 18 |
| 10 | XJ | 97/105 (92%) | 81 (84%) | 11 (11%) | 5 (5%) | 2 | 13 |
| 11 | QK | 119/129 (92%) | 100 (84%) | 14 (12%) | 5 (4%) | 3 | 18 |
| 11 | XK | 119/129 (92%) | 105 (88%) | 10 (8%) | 4 (3%) | 3 | 21 |
| 12 | QL | 123/132 (93%) | 99 (80%) | 16 (13%) | 8 (6%) | 1 | 8 |
| 12 | XL | 123/132 (93%) | 97 (79%) | 18 (15%) | 8 (6%) | 1 | 8 |
| 13 | QM | 116/126 (92%) | 88 (76%) | 17 (15%) | 11 (10%) | 0 | 4 |
| 13 | XM | 116/126 (92%) | 88 (76%) | 17 (15%) | 11 (10%) | 0 | 4 |
| 14 | QN | 58/61 (95%) | 51 (88%) | 4 (7%) | 3 (5%) | 2 | 13 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14 | XN | 58/61 (95%) | 50 (86%) | 5 (9%) | 3 (5%) | 2 | 13 |
| 15 | QO | 86/89 (97%) | 81 (94%) | 5 (6%) | 0 | 100 | 100 |
| 15 | XO | 86/89 (97%) | 79 (92%) | 7 (8%) | 0 | 100 | 100 |
| 16 | QP | 82/88 (93%) | 72 (88%) | 10 (12%) | 0 | 100 | 100 |
| 16 | XP | 82/88 (93%) | 76 (93%) | 6 (7%) | 0 | 100 | 100 |
| 17 | QQ | 98/105 (93%) | 90 (92%) | 7 (7%) | 1 (1%) | 15 | 46 |
| 17 | XQ | 98/105 (93%) | 89 (91%) | 7 (7%) | 2 (2%) | 7 | 30 |
| 18 | QR | 69/88 (78%) | 61 (88%) | 8 (12%) | 0 | 100 | 100 |
| 18 | XR | 69/88 (78%) | 62 (90%) | 6 (9%) | 1 (1%) | 11 | 37 |
| 19 | QS | 80/93 (86%) | 52 (65%) | 18 (22%) | 10 (12%) | 0 | 2 |
| 19 | XS | 80/93 (86%) | 52 (65%) | 18 (22%) | 10 (12%) | 0 | 2 |
| 20 | QT | 97/106 (92%) | 79 (81%) | 15 (16%) | 3 (3%) | 4 | 23 |
| 20 | XT | 97/106 (92%) | 80 (82%) | 14 (14%) | 3 (3%) | 4 | 23 |
| 21 | QU | 23/27 (85%) | 17 (74%) | 5 (22%) | 1 (4%) | 2 | 17 |
| 21 | XU | 23/27 (85%) | 18 (78%) | 3 (13%) | 2 (9%) | 1 | 5 |
| 24 | QY | 89/117 (76%) | 80 (90%) | 9 (10%) | 0 | 100 | 100 |
| 24 | XY | 89/117 (76%) | 84 (94%) | 5 (6%) | 0 | 100 | 100 |
| 27 | RD | 270/276 (98%) | 224 (83%) | 38 (14%) | 8 (3%) | 4 | 23 |
| 27 | YD | 270/276 (98%) | 229 (85%) | 31 (12%) | 10 (4%) | 3 | 20 |
| 28 | RE | 203/206 (98%) | 141 (70%) | 36 (18%) | 26 (13%) | 0 | 2 |
| 28 | YE | 203/206 (98%) | 133 (66%) | 37 (18%) | 33 (16%) | 0 | 0 |
| 29 | RF | 206/210 (98%) | 167 (81%) | 26 (13%) | 13 (6%) | 1 | 9 |
| 29 | YF | 206/210 (98%) | 168 (82%) | 22 (11%) | 16 (8%) | 1 | 6 |
| 30 | RG | 179/182 (98%) | 141 (79%) | 26 (14%) | 12 (7%) | 1 | 8 |
| 30 | YG | 179/182 (98%) | 147 (82%) | 21 (12%) | 11 (6%) | 1 | 10 |
| 31 | RH | 168/180 (93%) | 104 (62%) | 37 (22%) | 27 (16%) | 0 | 0 |
| 31 | YH | 168/180 (93%) | 98 (58%) | 42 (25%) | 28 (17%) | 0 | 0 |
| 32 | RI | 144/148 (97%) | 110 (76%) | 28 (19%) | 6 (4%) | 3 | 18 |
| 32 | YI | 144/148 (97%) | 116 (81%) | 22 (15%) | 6 (4%) | 3 | 18 |
| 33 | RN | 136/140 (97%) | 116 (85%) | 13 (10%) | 7 (5%) | 2 | 14 |
| 33 | YN | 136/140 (97%) | 110 (81%) | 19 (14%) | 7 (5%) | 2 | 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 34 | RO | 120/122 (98%) | 111 (92%) | 8 (7%) | 1 (1%) | 19 | 51 |
| 34 | YO | 120/122 (98%) | 109 (91%) | 10 (8%) | 1 (1%) | 19 | 51 |
| 35 | RP | 148/150 (99%) | 99 (67%) | 23 (16%) | 26 (18%) | 0 | 0 |
| 35 | YP | 148/150 (99%) | 103 (70%) | 22 (15%) | 23 (16%) | 0 | 0 |
| 36 | RQ | 138/141 (98%) | 110 (80%) | 17 (12%) | 11 (8%) | 1 | 6 |
| 36 | YQ | 137/141 (97%) | 111 (81%) | 15 (11%) | 11 (8%) | 1 | 6 |
| 37 | RR | 115/118 (98%) | 107 (93%) | 4 (4%) | 4 (4%) | 3 | 21 |
| 37 | YR | 115/118 (98%) | 109 (95%) | 3 (3%) | 3 (3%) | 5 | 26 |
| 38 | RS | 109/112 (97%) | 84 (77%) | 17 (16%) | 8 (7%) | 1 | 7 |
| 38 | YS | 109/112 (97%) | 85 (78%) | 13 (12%) | 11 (10%) | 0 | 4 |
| 39 | RT | 135/146 (92%) | 108 (80%) | 25 (18%) | 2 (2%) | 10 | 36 |
| 39 | YT | 135/146 (92%) | 113 (84%) | 17 (13%) | 5 (4%) | 3 | 20 |
| 40 | RU | 115/118 (98%) | 107 (93%) | 6 (5%) | 2 (2%) | 9 | 34 |
| 40 | YU | 115/118 (98%) | 103 (90%) | 9 (8%) | 3 (3%) | 5 | 26 |
| 41 | RV | 99/101 (98%) | 71 (72%) | 13 (13%) | 15 (15%) | 0 | 0 |
| 41 | YV | 99/101 (98%) | 70 (71%) | 15 (15%) | 14 (14%) | 0 | 1 |
| 42 | RW | 111/113 (98%) | 107 (96%) | 1 (1%) | 3 (3%) | 5 | 26 |
| 42 | YW | 111/113 (98%) | 104 (94%) | 3 (3%) | 4 (4%) | 3 | 21 |
| 43 | RX | 90/96 (94%) | 77 (86%) | 11 (12%) | 2 (2%) | 6 | 29 |
| 43 | YX | 90/96 (94%) | 77 (86%) | 11 (12%) | 2 (2%) | 6 | 29 |
| 44 | RY | 100/110 (91%) | 57 (57%) | 28 (28%) | 15 (15%) | 0 | 0 |
| 44 | YY | 100/110 (91%) | 58 (58%) | 26 (26%) | 16 (16%) | 0 | 0 |
| 45 | RZ | 174/206 (84%) | 119 (68%) | 33 (19%) | 22 (13%) | 0 | 2 |
| 45 | YZ | 181/206 (88%) | 122 (67%) | 42 (23%) | 17 (9%) | 0 | 4 |
| 46 | R0 | 81/85 (95%) | 73 (90%) | 5 (6%) | 3 (4%) | 3 | 20 |
| 46 | Y0 | 81/85 (95%) | 67 (83%) | 11 (14%) | 3 (4%) | 3 | 20 |
| 47 | R1 | 95/98 (97%) | 71 (75%) | 12 (13%) | 12 (13%) | 0 | 2 |
| 47 | Y1 | 95/98 (97%) | 76 (80%) | 13 (14%) | 6 (6%) | 1 | 9 |
| 48 | R2 | 67/72 (93%) | 54 (81%) | 8 (12%) | 5 (8%) | 1 | 7 |
| 48 | Y2 | 67/72 (93%) | 56 (84%) | 5 (8%) | 6 (9%) | 1 | 4 |
| 49 | R3 | 57/60 (95%) | 51 (90%) | 6 (10%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 49 | Y3 | 57/60 (95%) | 51 (90%) | 6 (10%) | 0 | 100 | 100 |
| 50 | R4 | 68/71 (96%) | 43 (63%) | 12 (18%) | 13 (19%) | 0 | 0 |
| 50 | Y4 | 68/71 (96%) | 37 (54%) | 15 (22%) | 16 (24%) | 0 | 0 |
| 51 | R5 | 57/60 (95%) | 46 (81%) | 9 (16%) | 2 (4%) | 3 | 21 |
| 51 | Y5 | 55/60 (92%) | 48 (87%) | 3 (6%) | 4 (7%) | 1 | 7 |
| 52 | R6 | 46/54 (85%) | 22 (48%) | 15 (33%) | 9 (20%) | 0 | 0 |
| 52 | Y6 | 46/54 (85%) | 16 (35%) | 17 (37%) | 13 (28%) | 0 | 0 |
| 53 | R7 | 47/49 (96%) | 47 (100%) | 0 | 0 | 100 | 100 |
| 53 | Y7 | 47/49 (96%) | 44 (94%) | 3 (6%) | 0 | 100 | 100 |
| 54 | R8 | 62/65 (95%) | 48 (77%) | 7 (11%) | 7 (11%) | 0 | 3 |
| 54 | Y8 | 62/65 (95%) | 48 (77%) | 7 (11%) | 7 (11%) | 0 | 3 |
| 55 | R9 | 35/37 (95%) | 34 (97%) | 0 | 1 (3%) | 4 | 24 |
| 55 | Y9 | 34/37 (92%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| All | All | 11647/12362 (94%) | 9400 (81%) | 1486 (13%) | 761 (6%) | 1 | 8 |

5 of 761 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 29 | ALA |
| 2 | QB | 165 | VAL |
| 2 | QB | 195 | ASP |
| 2 | QB | 238 | LEU |
| 3 | QC | 64 | VAL |

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 | QB | 204/220 (93%) | 174 (85%) | 30 (15%) | 3 | 12 |
| 2 | XB | 204/220 (93%) | 176 (86%) | 28 (14%) | 3 | 14 |
| 3 | QC | 160/188 (85%) | 142 (89%) | 18 (11%) | 6 | 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | XC | 160/188 (85%) | 142 (89%) | 18 (11%) | 6 | 21 |
| 4 | QD | 180/181 (99%) | 156 (87%) | 24 (13%) | 4 | 15 |
| 4 | XD | 180/181 (99%) | 157 (87%) | 23 (13%) | 4 | 16 |
| 5 | QE | 119/123 (97%) | 103 (87%) | 16 (13%) | 4 | 15 |
| 5 | XE | 119/123 (97%) | 106 (89%) | 13 (11%) | 6 | 23 |
| 6 | QF | 90/90 (100%) | 85 (94%) | 5 (6%) | 21 | 51 |
| 6 | XF | 90/90 (100%) | 76 (84%) | 14 (16%) | 2 | 11 |
| 7 | QG | 126/127 (99%) | 112 (89%) | 14 (11%) | 6 | 22 |
| 7 | XG | 126/127 (99%) | 109 (86%) | 17 (14%) | 4 | 14 |
| 8 | QH | 119/119 (100%) | 109 (92%) | 10 (8%) | 11 | 36 |
| 8 | XH | 119/119 (100%) | 106 (89%) | 13 (11%) | 6 | 23 |
| 9 | QI | 99/99 (100%) | 79 (80%) | 20 (20%) | 1 | 3 |
| 9 | XI | 99/99 (100%) | 80 (81%) | 19 (19%) | 1 | 4 |
| 10 | QJ | 89/92 (97%) | 77 (86%) | 12 (14%) | 4 | 14 |
| 10 | XJ | 89/92 (97%) | 75 (84%) | 14 (16%) | 2 | 10 |
| 11 | QK | 92/99 (93%) | 82 (89%) | 10 (11%) | 6 | 23 |
| 11 | XK | 92/99 (93%) | 83 (90%) | 9 (10%) | 8 | 28 |
| 12 | QL | 104/109 (95%) | 89 (86%) | 15 (14%) | 3 | 13 |
| 12 | XL | 104/109 (95%) | 87 (84%) | 17 (16%) | 2 | 9 |
| 13 | QM | 94/101 (93%) | 80 (85%) | 14 (15%) | 3 | 12 |
| 13 | XM | 94/101 (93%) | 82 (87%) | 12 (13%) | 4 | 16 |
| 14 | QN | 49/50 (98%) | 48 (98%) | 1 (2%) | 55 | 77 |
| 14 | XN | 49/50 (98%) | 43 (88%) | 6 (12%) | 5 | 18 |
| 15 | QO | 79/80 (99%) | 74 (94%) | 5 (6%) | 18 | 47 |
| 15 | XO | 79/80 (99%) | 74 (94%) | 5 (6%) | 18 | 47 |
| 16 | QP | 72/74 (97%) | 64 (89%) | 8 (11%) | 6 | 22 |
| 16 | XP | 72/74 (97%) | 64 (89%) | 8 (11%) | 6 | 22 |
| 17 | QQ | 95/97 (98%) | 90 (95%) | 5 (5%) | 22 | 52 |
| 17 | XQ | 95/97 (98%) | 88 (93%) | 7 (7%) | 13 | 42 |
| 18 | QR | 62/77 (80%) | 56 (90%) | 6 (10%) | 8 | 28 |
| 18 | XR | 62/77 (80%) | 54 (87%) | 8 (13%) | 4 | 16 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 19 | QS | 71/80 (89%) | 54 (76%) | 17 (24%) | 0 | 2 |
| 19 | XS | 71/80 (89%) | 58 (82%) | 13 (18%) | 1 | 5 |
| 20 | QT | 76/82 (93%) | 62 (82%) | 14 (18%) | 1 | 5 |
| 20 | XT | 76/82 (93%) | 66 (87%) | 10 (13%) | 4 | 15 |
| 21 | QU | 20/22 (91%) | 18 (90%) | 2 (10%) | 7 | 27 |
| 21 | XU | 20/22 (91%) | 18 (90%) | 2 (10%) | 7 | 27 |
| 24 | QY | 78/102 (76%) | 75 (96%) | 3 (4%) | 33 | 61 |
| 24 | XY | 78/102 (76%) | 74 (95%) | 4 (5%) | 24 | 54 |
| 27 | RD | 214/218 (98%) | 178 (83%) | 36 (17%) | 2 | 8 |
| 27 | YD | 214/218 (98%) | 180 (84%) | 34 (16%) | 2 | 10 |
| 28 | RE | 165/166 (99%) | 137 (83%) | 28 (17%) | 2 | 8 |
| 28 | YE | 165/166 (99%) | 138 (84%) | 27 (16%) | 2 | 9 |
| 29 | RF | 165/166 (99%) | 139 (84%) | 26 (16%) | 2 | 10 |
| 29 | YF | 165/166 (99%) | 142 (86%) | 23 (14%) | 3 | 13 |
| 30 | RG | 155/156 (99%) | 148 (96%) | 7 (4%) | 27 | 58 |
| 30 | YG | 155/156 (99%) | 138 (89%) | 17 (11%) | 6 | 23 |
| 31 | RH | 142/148 (96%) | 123 (87%) | 19 (13%) | 4 | 15 |
| 31 | YH | 142/148 (96%) | 117 (82%) | 25 (18%) | 2 | 6 |
| 32 | RI | 122/124 (98%) | 98 (80%) | 24 (20%) | 1 | 4 |
| 32 | YI | 122/124 (98%) | 99 (81%) | 23 (19%) | 1 | 4 |
| 33 | RN | 117/119 (98%) | 107 (92%) | 10 (8%) | 10 | 35 |
| 33 | YN | 117/119 (98%) | 104 (89%) | 13 (11%) | 6 | 22 |
| 34 | RO | 100/100 (100%) | 91 (91%) | 9 (9%) | 9 | 32 |
| 34 | YO | 100/100 (100%) | 90 (90%) | 10 (10%) | 7 | 27 |
| 35 | RP | 116/116 (100%) | 83 (72%) | 33 (28%) | 0 | 1 |
| 35 | YP | 116/116 (100%) | 84 (72%) | 32 (28%) | 0 | 1 |
| 36 | RQ | 110/111 (99%) | 93 (84%) | 17 (16%) | 2 | 11 |
| 36 | YQ | 110/111 (99%) | 93 (84%) | 17 (16%) | 2 | 11 |
| 37 | RR | 100/101 (99%) | 82 (82%) | 18 (18%) | 1 | 6 |
| 37 | YR | 100/101 (99%) | 87 (87%) | 13 (13%) | 4 | 16 |
| 38 | RS | 87/88 (99%) | 80 (92%) | 7 (8%) | 12 | 38 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 38 | YS | 87/88 (99%) | 73 (84%) | 14 (16%) | 2 | 10 |
| 39 | RT | 120/127 (94%) | 99 (82%) | 21 (18%) | 2 | 7 |
| 39 | YT | 120/127 (94%) | 98 (82%) | 22 (18%) | 1 | 5 |
| 40 | RU | 93/94 (99%) | 85 (91%) | 8 (9%) | 10 | 35 |
| 40 | YU | 93/94 (99%) | 85 (91%) | 8 (9%) | 10 | 35 |
| 41 | RV | 82/82 (100%) | 65 (79%) | 17 (21%) | 1 | 3 |
| 41 | YV | 82/82 (100%) | 64 (78%) | 18 (22%) | 1 | 3 |
| 42 | RW | 92/92 (100%) | 82 (89%) | 10 (11%) | 6 | 23 |
| 42 | YW | 92/92 (100%) | 79 (86%) | 13 (14%) | 3 | 13 |
| 43 | RX | 74/78 (95%) | 65 (88%) | 9 (12%) | 5 | 18 |
| 43 | YX | 74/78 (95%) | 68 (92%) | 6 (8%) | 11 | 38 |
| 44 | RY | 85/91 (93%) | 65 (76%) | 20 (24%) | 1 | 2 |
| 44 | YY | 85/91 (93%) | 61 (72%) | 24 (28%) | 0 | 1 |
| 45 | RZ | 155/179 (87%) | 127 (82%) | 28 (18%) | 1 | 6 |
| 45 | YZ | 162/179 (90%) | 134 (83%) | 28 (17%) | 2 | 7 |
| 46 | R0 | 66/67 (98%) | 62 (94%) | 4 (6%) | 18 | 48 |
| 46 | Y0 | 66/67 (98%) | 58 (88%) | 8 (12%) | 5 | 18 |
| 47 | R1 | 82/83 (99%) | 68 (83%) | 14 (17%) | 2 | 8 |
| 47 | Y1 | 82/83 (99%) | 72 (88%) | 10 (12%) | 5 | 18 |
| 48 | R2 | 64/67 (96%) | 52 (81%) | 12 (19%) | 1 | 4 |
| 48 | Y2 | 64/67 (96%) | 57 (89%) | 7 (11%) | 6 | 23 |
| 49 | R3 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 | 14 |
| 49 | Y3 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 39 |
| 50 | R4 | 62/63 (98%) | 47 (76%) | 15 (24%) | 0 | 2 |
| 50 | Y4 | 62/63 (98%) | 44 (71%) | 18 (29%) | 0 | 1 |
| 51 | R5 | 51/52 (98%) | 40 (78%) | 11 (22%) | 1 | 3 |
| 51 | Y5 | 49/52 (94%) | 43 (88%) | 6 (12%) | 5 | 18 |
| 52 | R6 | 47/52 (90%) | 32 (68%) | 15 (32%) | 0 | 1 |
| 52 | Y6 | 47/52 (90%) | 30 (64%) | 17 (36%) | 0 | 0 |
| 53 | R7 | 42/42 (100%) | 35 (83%) | 7 (17%) | 2 | 8 |
| 53 | Y7 | 42/42 (100%) | 35 (83%) | 7 (17%) | 2 | 8 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|-----|
| 54 | R8 | 54/55 (98%) | 44 (82%) | 10 (18%) | 1 | 5 |
| 54 | Y8 | 54/55 (98%) | 44 (82%) | 10 (18%) | 1 | 5 |
| 55 | R9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 19 | 49 |
| 55 | Y9 | 33/34 (97%) | 33 (100%) | 0 | 100 | 100 |
| All | All | 9854/10270 (96%) | 8447 (86%) | 1407 (14%) | 3 | 13 |

5 of 1407 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | R4 | 21 | VAL |
| 6 | XF | 85 | VAL |
| 45 | YZ | 71 | VAL |
| 51 | R5 | 48 | GLU |
| 2 | XB | 185 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | RZ | 118 | GLN |
| 3 | XC | 3 | ASN |
| 37 | YR | 3 | HIS |
| 40 | RU | 81 | HIS |
| 50 | Y4 | 6 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | QA | 1509/1522 (99%) | 295 (19%) | 46 (3%) |
| 1 | XA | 1506/1522 (98%) | 290 (19%) | 38 (2%) |
| 22 | QV | 76/77 (98%) | 13 (17%) | 0 |
| 22 | QW | 76/77 (98%) | 20 (26%) | 2 (2%) |
| 22 | XV | 76/77 (98%) | 12 (15%) | 1 (1%) |
| 22 | XW | 76/77 (98%) | 18 (23%) | 0 |
| 23 | QX | 19/25 (76%) | 8 (42%) | 2 (10%) |
| 23 | XX | 19/25 (76%) | 9 (47%) | 1 (5%) |
| 25 | RA | 2888/2916 (99%) | 590 (20%) | 42 (1%) |
| 25 | YA | 2872/2916 (98%) | 567 (19%) | 41 (1%) |
| 26 | RB | 121/124 (97%) | 20 (16%) | 1 (0%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 26 | YB | 121/124 (97%) | 21 (17%) | 1 (0%) |
| All | All | 9359/9482 (98%) | 1863 (19%) | 175 (1%) |

5 of 1863 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 4 | U |
| 1 | QA | 5 | U |
| 1 | QA | 6 | G |
| 1 | QA | 9 | G |
| 1 | QA | 22 | G |

5 of 175 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 2191 | G |
| 1 | XA | 115 | G |
| 25 | YA | 2191 | G |
| 25 | RA | 2275 | C |
| 25 | RA | 2776 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | A2M | QX | 19 | 23 | 18,25,26 | 0.99 | 1 (5%) | 18,36,39 | 1.55 | 4 (22%) |
| 23 | A2M | XX | 20 | 23 | 18,25,26 | 1.08 | 2 (11%) | 18,36,39 | 1.35 | 2 (11%) |
| 23 | A2M | QX | 21 | 1,23 | 18,25,26 | 1.04 | 2 (11%) | 18,36,39 | 1.51 | 2 (11%) |
| 23 | A2M | QX | 20 | 23 | 18,25,26 | 1.11 | 1 (5%) | 18,36,39 | 1.38 | 2 (11%) |
| 23 | A2M | XX | 21 | 1,23 | 18,25,26 | 0.99 | 1 (5%) | 18,36,39 | 1.49 | 3 (16%) |
| 23 | A2M | XX | 19 | 56,23 | 18,25,26 | 1.01 | 1 (5%) | 18,36,39 | 1.45 | 3 (16%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 23 | A2M | QX | 19 | 23 | - | 1/5/27/28 | 0/3/3/3 |
| 23 | A2M | XX | 20 | 23 | - | 0/5/27/28 | 0/3/3/3 |
| 23 | A2M | QX | 21 | 1,23 | - | 5/5/27/28 | 0/3/3/3 |
| 23 | A2M | QX | 20 | 23 | - | 2/5/27/28 | 0/3/3/3 |
| 23 | A2M | XX | 21 | 1,23 | - | 4/5/27/28 | 0/3/3/3 |
| 23 | A2M | XX | 19 | 56,23 | - | 2/5/27/28 | 0/3/3/3 |

The worst 5 of 8 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 23 | QX | 20 | A2M | C5-C4 | 2.72 | 1.48 | 1.40 |
| 23 | XX | 20 | A2M | O4'-C1' | 2.51 | 1.44 | 1.41 |
| 23 | XX | 19 | A2M | C5-C4 | 2.45 | 1.47 | 1.40 |
| 23 | QX | 21 | A2M | C5-C4 | 2.39 | 1.47 | 1.40 |
| 23 | XX | 21 | A2M | C5-C4 | 2.33 | 1.47 | 1.40 |

The worst 5 of 16 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 23 | QX | 20 | A2M | C4-C5-N7 | -3.64 | 105.61 | 109.40 |
| 23 | QX | 19 | A2M | N3-C2-N1 | -3.61 | 123.04 | 128.68 |
| 23 | QX | 21 | A2M | N3-C2-N1 | -3.40 | 123.37 | 128.68 |
| 23 | XX | 20 | A2M | N3-C2-N1 | -3.30 | 123.52 | 128.68 |
| 23 | XX | 21 | A2M | N3-C2-N1 | -3.23 | 123.63 | 128.68 |

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | QX | 21 | A2M | C1'-C2'-O2'-CM' |
| 23 | QX | 20 | A2M | O4'-C4'-C5'-O5' |
| 23 | QX | 20 | A2M | C3'-C4'-C5'-O5' |
| 23 | XX | 21 | A2M | C3'-C4'-C5'-O5' |
| 23 | XX | 21 | A2M | C1'-C2'-O2'-CM' |

There are no ring outliers.

4 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | QX | 19 | A2M | 1 | 0 |
| 23 | XX | 20 | A2M | 2 | 0 |
| 23 | QX | 21 | A2M | 2 | 0 |
| 23 | XX | 21 | A2M | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1312 ligands modelled in this entry, 1312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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 | QA | 1511/1522 (99%) | -0.00 | 42 (2%) | 53 | 51 | 39, 80, 190, 435 | 0 |
| 1 | XA | 1508/1522 (99%) | -0.01 | 40 (2%) | 54 | 53 | 27, 78, 175, 487 | 0 |
| 2 | QB | 236/256 (92%) | 0.55 | 27 (11%) | 5 | 6 | 58, 138, 241, 336 | 0 |
| 2 | XB | 236/256 (92%) | 0.31 | 20 (8%) | 10 | 12 | 52, 119, 215, 332 | 0 |
| 3 | QC | 206/239 (86%) | 0.41 | 15 (7%) | 15 | 17 | 61, 111, 200, 469 | 0 |
| 3 | XC | 206/239 (86%) | 0.25 | 12 (5%) | 23 | 24 | 44, 103, 197, 564 | 0 |
| 4 | QD | 208/209 (99%) | -0.18 | 3 (1%) | 75 | 74 | 35, 66, 119, 173 | 0 |
| 4 | XD | 208/209 (99%) | 0.04 | 6 (2%) | 51 | 50 | 41, 82, 132, 198 | 0 |
| 5 | QE | 154/162 (95%) | -0.08 | 2 (1%) | 77 | 76 | 34, 74, 138, 244 | 0 |
| 5 | XE | 154/162 (95%) | -0.02 | 5 (3%) | 47 | 46 | 31, 68, 144, 340 | 0 |
| 6 | QF | 101/101 (100%) | 0.35 | 4 (3%) | 38 | 37 | 58, 117, 161, 183 | 0 |
| 6 | XF | 101/101 (100%) | -0.14 | 0 | 100 | 100 | 29, 68, 110, 175 | 0 |
| 7 | QG | 155/156 (99%) | 0.31 | 12 (7%) | 13 | 15 | 80, 130, 214, 347 | 0 |
| 7 | XG | 155/156 (99%) | 0.16 | 9 (5%) | 23 | 24 | 54, 101, 179, 252 | 0 |
| 8 | QH | 138/138 (100%) | -0.20 | 1 (0%) | 87 | 87 | 41, 81, 119, 179 | 0 |
| 8 | XH | 138/138 (100%) | -0.08 | 1 (0%) | 87 | 87 | 48, 79, 128, 182 | 0 |
| 9 | QI | 128/128 (100%) | 0.89 | 21 (16%) | 1 | 2 | 78, 156, 267, 359 | 0 |
| 9 | XI | 128/128 (100%) | 0.53 | 12 (9%) | 8 | 10 | 61, 115, 202, 350 | 0 |
| 10 | QJ | 99/105 (94%) | 1.01 | 18 (18%) | 1 | 1 | 74, 149, 278, 339 | 0 |
| 10 | XJ | 99/105 (94%) | 0.64 | 8 (8%) | 12 | 13 | 63, 133, 253, 371 | 0 |
| 11 | QK | 121/129 (93%) | 0.53 | 11 (9%) | 9 | 10 | 43, 102, 182, 301 | 0 |
| 11 | XK | 121/129 (93%) | 0.06 | 3 (2%) | 57 | 55 | 32, 71, 159, 258 | 0 |
| 12 | QL | 125/132 (94%) | -0.06 | 1 (0%) | 86 | 85 | 27, 62, 103, 271 | 0 |
| 12 | XL | 125/132 (94%) | -0.04 | 3 (2%) | 59 | 57 | 30, 64, 103, 263 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | QM | 118/126 (93%) | 0.55 | 6 (5%) 28 28 | 75, 133, 248, 348 | 0 |
| 13 | XM | 118/126 (93%) | 0.36 | 7 (5%) 22 23 | 64, 114, 183, 467 | 0 |
| 14 | QN | 60/61 (98%) | 0.80 | 8 (13%) 3 4 | 79, 110, 169, 205 | 0 |
| 14 | XN | 60/61 (98%) | 0.55 | 4 (6%) 17 19 | 60, 93, 133, 240 | 0 |
| 15 | QO | 88/89 (98%) | 0.05 | 0 100 100 | 37, 86, 136, 170 | 0 |
| 15 | XO | 88/89 (98%) | -0.11 | 0 100 100 | 34, 74, 110, 161 | 0 |
| 16 | QP | 84/88 (95%) | -0.22 | 1 (1%) 79 77 | 38, 68, 111, 260 | 0 |
| 16 | XP | 84/88 (95%) | 0.26 | 1 (1%) 79 77 | 63, 90, 138, 347 | 0 |
| 17 | QQ | 100/105 (95%) | 0.01 | 2 (2%) 65 64 | 33, 79, 110, 133 | 0 |
| 17 | XQ | 100/105 (95%) | 0.12 | 1 (1%) 82 81 | 35, 82, 118, 188 | 0 |
| 18 | QR | 71/88 (80%) | 0.33 | 4 (5%) 24 25 | 64, 114, 191, 248 | 0 |
| 18 | XR | 71/88 (80%) | 0.13 | 3 (4%) 36 35 | 33, 66, 181, 270 | 0 |
| 19 | QS | 82/93 (88%) | 0.74 | 10 (12%) 4 5 | 78, 148, 306, 418 | 0 |
| 19 | XS | 82/93 (88%) | 0.63 | 4 (4%) 29 29 | 57, 126, 215, 401 | 0 |
| 20 | QT | 99/106 (93%) | 0.15 | 3 (3%) 50 49 | 54, 85, 160, 222 | 0 |
| 20 | XT | 99/106 (93%) | 0.29 | 4 (4%) 38 37 | 61, 107, 176, 212 | 0 |
| 21 | QU | 25/27 (92%) | 1.99 | 12 (48%) 0 0 | 94, 130, 197, 278 | 0 |
| 21 | XU | 25/27 (92%) | 1.37 | 7 (28%) 0 0 | 74, 113, 170, 194 | 0 |
| 22 | QV | 77/77 (100%) | 0.28 | 1 (1%) 77 76 | 46, 83, 132, 187 | 0 |
| 22 | QW | 77/77 (100%) | 3.43 | 63 (81%) 0 0 | 86, 279, 383, 409 | 0 |
| 22 | XV | 77/77 (100%) | -0.13 | 1 (1%) 77 76 | 42, 79, 123, 172 | 0 |
| 22 | XW | 77/77 (100%) | 3.19 | 54 (70%) 0 0 | 115, 271, 335, 411 | 0 |
| 23 | QX | 17/25 (68%) | 2.51 | 13 (76%) 0 0 | 53, 218, 306, 334 | 0 |
| 23 | XX | 17/25 (68%) | 2.29 | 9 (52%) 0 0 | 45, 237, 354, 390 | 0 |
| 24 | QY | 91/117 (77%) | 1.07 | 14 (15%) 2 2 | 83, 126, 163, 188 | 0 |
| 24 | XY | 91/117 (77%) | 1.25 | 17 (18%) 1 1 | 82, 127, 165, 185 | 0 |
| 25 | RA | 2891/2916 (99%) | 0.11 | 159 (5%) 25 25 | 20, 56, 239, 588 | 0 |
| 25 | YA | 2875/2916 (98%) | 0.05 | 150 (5%) 27 27 | 20, 54, 248, 583 | 0 |
| 26 | RB | 122/124 (98%) | 0.05 | 1 (0%) 86 85 | 46, 96, 148, 214 | 0 |
| 26 | YB | 122/124 (98%) | -0.01 | 1 (0%) 86 85 | 55, 86, 136, 215 | 0 |
| 27 | RD | 272/276 (98%) | -0.11 | 4 (1%) 73 72 | 17, 54, 102, 322 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 27 | YD | 272/276 (98%) | -0.27 | 1 (0%) 92 92 | 12, 35, 83, 212 | 0 |
| 28 | RE | 205/206 (99%) | 0.12 | 7 (3%) 45 44 | 25, 73, 159, 362 | 0 |
| 28 | YE | 205/206 (99%) | 0.11 | 6 (2%) 51 50 | 26, 73, 168, 563 | 0 |
| 29 | RF | 208/210 (99%) | -0.11 | 8 (3%) 40 39 | 13, 44, 168, 316 | 0 |
| 29 | YF | 208/210 (99%) | 0.03 | 10 (4%) 30 31 | 22, 67, 240, 535 | 0 |
| 30 | RG | 181/182 (99%) | 0.26 | 5 (2%) 53 51 | 62, 110, 161, 194 | 0 |
| 30 | YG | 181/182 (99%) | 0.13 | 3 (1%) 70 68 | 42, 97, 165, 199 | 0 |
| 31 | RH | 170/180 (94%) | 1.34 | 37 (21%) 0 1 | 59, 182, 468, 582 | 0 |
| 31 | YH | 170/180 (94%) | 0.95 | 36 (21%) 0 1 | 58, 146, 370, 574 | 0 |
| 32 | RI | 146/148 (98%) | 0.47 | 7 (4%) 30 31 | 51, 113, 183, 290 | 0 |
| 32 | YI | 146/148 (98%) | 0.35 | 6 (4%) 37 36 | 36, 92, 188, 341 | 0 |
| 33 | RN | 138/140 (98%) | -0.15 | 0 100 100 | 25, 75, 121, 188 | 0 |
| 33 | YN | 138/140 (98%) | -0.05 | 1 (0%) 87 87 | 26, 81, 141, 196 | 0 |
| 34 | RO | 122/122 (100%) | -0.38 | 0 100 100 | 26, 58, 90, 120 | 0 |
| 34 | YO | 122/122 (100%) | -0.37 | 0 100 100 | 27, 58, 91, 116 | 0 |
| 35 | RP | 150/150 (100%) | 0.03 | 3 (2%) 65 64 | 19, 68, 152, 324 | 0 |
| 35 | YP | 150/150 (100%) | 0.14 | 6 (4%) 38 37 | 27, 66, 149, 278 | 0 |
| 36 | RQ | 140/141 (99%) | 0.02 | 4 (2%) 51 50 | 30, 70, 115, 294 | 0 |
| 36 | YQ | 139/141 (98%) | 0.04 | 2 (1%) 75 74 | 35, 70, 127, 273 | 0 |
| 37 | RR | 117/118 (99%) | -0.19 | 0 100 100 | 26, 65, 100, 156 | 0 |
| 37 | YR | 117/118 (99%) | -0.12 | 0 100 100 | 33, 65, 115, 161 | 0 |
| 38 | RS | 111/112 (99%) | 0.28 | 6 (5%) 25 26 | 59, 112, 201, 486 | 0 |
| 38 | YS | 111/112 (99%) | 0.28 | 3 (2%) 54 53 | 54, 93, 171, 315 | 0 |
| 39 | RT | 137/146 (93%) | -0.10 | 6 (4%) 34 34 | 36, 78, 172, 561 | 0 |
| 39 | YT | 137/146 (93%) | 0.28 | 11 (8%) 12 13 | 29, 80, 263, 460 | 0 |
| 40 | RU | 117/118 (99%) | -0.18 | 3 (2%) 56 54 | 20, 56, 126, 223 | 0 |
| 40 | YU | 117/118 (99%) | 0.06 | 2 (1%) 70 68 | 32, 74, 147, 342 | 0 |
| 41 | RV | 101/101 (100%) | -0.08 | 3 (2%) 50 49 | 23, 79, 142, 406 | 0 |
| 41 | YV | 101/101 (100%) | 0.33 | 3 (2%) 50 49 | 27, 102, 149, 576 | 0 |
| 42 | RW | 113/113 (100%) | -0.15 | 0 100 100 | 23, 53, 113, 248 | 0 |
| 42 | YW | 113/113 (100%) | -0.00 | 4 (3%) 44 43 | 26, 61, 118, 368 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 43 | RX | 92/96 (95%) | -0.04 | 1 (1%) 80 79 | 37, 69, 114, 140 | 0 |
| 43 | YX | 92/96 (95%) | -0.18 | 1 (1%) 80 79 | 26, 55, 107, 126 | 0 |
| 44 | RY | 102/110 (92%) | 0.77 | 13 (12%) 3 4 | 33, 78, 230, 539 | 0 |
| 44 | YY | 102/110 (92%) | 0.77 | 16 (15%) 2 2 | 40, 95, 248, 579 | 0 |
| 45 | RZ | 176/206 (85%) | 0.46 | 13 (7%) 14 16 | 54, 109, 230, 333 | 0 |
| 45 | YZ | 183/206 (88%) | 0.37 | 14 (7%) 13 15 | 55, 111, 190, 333 | 0 |
| 46 | R0 | 83/85 (97%) | 0.26 | 6 (7%) 15 17 | 30, 69, 179, 363 | 0 |
| 46 | Y0 | 83/85 (97%) | 0.28 | 4 (4%) 30 31 | 29, 70, 166, 209 | 0 |
| 47 | R1 | 97/98 (98%) | 0.39 | 5 (5%) 27 27 | 27, 64, 206, 399 | 0 |
| 47 | Y1 | 97/98 (98%) | 0.20 | 8 (8%) 11 13 | 17, 46, 207, 422 | 0 |
| 48 | R2 | 69/72 (95%) | 0.11 | 2 (2%) 51 50 | 35, 87, 189, 288 | 0 |
| 48 | Y2 | 69/72 (95%) | -0.20 | 1 (1%) 75 74 | 28, 69, 119, 233 | 0 |
| 49 | R3 | 59/60 (98%) | 0.15 | 2 (3%) 45 44 | 36, 63, 116, 167 | 0 |
| 49 | Y3 | 59/60 (98%) | 0.05 | 1 (1%) 70 68 | 39, 80, 135, 184 | 0 |
| 50 | R4 | 70/71 (98%) | 1.29 | 19 (27%) 0 0 | 105, 280, 598, 608 | 0 |
| 50 | Y4 | 70/71 (98%) | 1.53 | 21 (30%) 0 0 | 92, 189, 571, 588 | 0 |
| 51 | R5 | 59/60 (98%) | 0.36 | 6 (10%) 6 8 | 21, 60, 201, 299 | 0 |
| 51 | Y5 | 57/60 (95%) | 0.36 | 5 (8%) 10 11 | 15, 71, 193, 303 | 0 |
| 52 | R6 | 48/54 (88%) | 1.83 | 19 (39%) 0 0 | 71, 128, 199, 285 | 0 |
| 52 | Y6 | 48/54 (88%) | 1.66 | 19 (39%) 0 0 | 60, 111, 181, 219 | 0 |
| 53 | R7 | 49/49 (100%) | -0.19 | 0 100 100 | 15, 36, 127, 208 | 0 |
| 53 | Y7 | 49/49 (100%) | -0.14 | 2 (4%) 37 36 | 10, 29, 97, 215 | 0 |
| 54 | R8 | 64/65 (98%) | 0.10 | 2 (3%) 49 48 | 22, 50, 116, 225 | 0 |
| 54 | Y8 | 64/65 (98%) | 0.30 | 3 (4%) 31 31 | 22, 52, 96, 236 | 0 |
| 55 | R9 | 37/37 (100%) | 3.11 | 26 (70%) 0 0 | 99, 140, 190, 246 | 0 |
| 55 | Y9 | 36/37 (97%) | 4.32 | 33 (91%) 0 0 | 88, 155, 219, 248 | 0 |
| All | All | 21218/21844 (97%) | 0.19 | 1265 (5%) 21 23 | 10, 78, 219, 608 | 0 |

The worst 5 of 1265 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 25 | RA | 2801(A) | A | 18.9 |
| 25 | RA | 1075 | C | 13.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | RA | 2801 | A | 13.7 |
| 25 | RA | 2169 | A | 13.5 |
| 25 | RA | 1076 | C | 13.3 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 23 | A2M | QX | 21 | 23/24 | 0.84 | 0.31 | 108,155,155,155 | 0 |
| 23 | A2M | XX | 21 | 23/24 | 0.84 | 0.30 | 108,164,164,164 | 0 |
| 23 | A2M | QX | 19 | 23/24 | 0.85 | 0.36 | 108,108,108,108 | 0 |
| 23 | A2M | XX | 19 | 23/24 | 0.88 | 0.26 | 99,99,108,108 | 0 |
| 23 | A2M | XX | 20 | 23/24 | 0.90 | 0.25 | 107,107,108,108 | 0 |
| 23 | A2M | QX | 20 | 23/24 | 0.90 | 0.26 | 108,114,114,114 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56 | MG | QD | 303 | 1/1 | 0.13 | 0.16 | 69,69,69,69 | 0 |
| 56 | MG | YH | 201 | 1/1 | 0.15 | 0.61 | 118,118,118,118 | 0 |
| 56 | MG | XA | 1625 | 1/1 | 0.24 | 0.29 | 80,80,80,80 | 0 |
| 56 | MG | RA | 3075 | 1/1 | 0.43 | 0.46 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3357 | 1/1 | 0.45 | 0.74 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3168 | 1/1 | 0.45 | 0.72 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3379 | 1/1 | 0.46 | 0.57 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3355 | 1/1 | 0.47 | 0.30 | 58,58,58,58 | 0 |
| 56 | MG | YA | 3416 | 1/1 | 0.48 | 0.27 | 9,9,9,9 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3415 | 1/1 | 0.49 | 0.51 | 68,68,68,68 | 0 |
| 56 | MG | RA | 3342 | 1/1 | 0.50 | 0.47 | 61,61,61,61 | 0 |
| 56 | MG | RA | 3134 | 1/1 | 0.50 | 0.78 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3171 | 1/1 | 0.51 | 0.40 | 51,51,51,51 | 0 |
| 56 | MG | RA | 3299 | 1/1 | 0.52 | 0.43 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3322 | 1/1 | 0.54 | 0.45 | 55,55,55,55 | 0 |
| 56 | MG | XA | 1755 | 1/1 | 0.54 | 0.30 | 68,68,68,68 | 0 |
| 56 | MG | Y5 | 102 | 1/1 | 0.57 | 0.55 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3391 | 1/1 | 0.57 | 0.43 | 19,19,19,19 | 0 |
| 56 | MG | RA | 3417 | 1/1 | 0.57 | 0.35 | 66,66,66,66 | 0 |
| 56 | MG | RA | 3220 | 1/1 | 0.58 | 0.47 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3215 | 1/1 | 0.58 | 0.29 | 79,79,79,79 | 0 |
| 56 | MG | RA | 3345 | 1/1 | 0.59 | 0.31 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3099 | 1/1 | 0.59 | 0.52 | 68,68,68,68 | 0 |
| 56 | MG | QA | 1627 | 1/1 | 0.60 | 0.80 | 72,72,72,72 | 0 |
| 56 | MG | QA | 1746 | 1/1 | 0.60 | 0.49 | 56,56,56,56 | 0 |
| 56 | MG | RA | 3360 | 1/1 | 0.60 | 0.51 | 51,51,51,51 | 0 |
| 56 | MG | RA | 3114 | 1/1 | 0.61 | 0.31 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3361 | 1/1 | 0.61 | 0.52 | 68,68,68,68 | 0 |
| 56 | MG | XA | 1696 | 1/1 | 0.61 | 0.34 | 71,71,71,71 | 0 |
| 56 | MG | QA | 1747 | 1/1 | 0.62 | 0.37 | 61,61,61,61 | 0 |
| 56 | MG | QA | 1724 | 1/1 | 0.62 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | YA | 3406 | 1/1 | 0.63 | 0.56 | 60,60,60,60 | 0 |
| 56 | MG | YA | 3163 | 1/1 | 0.64 | 0.55 | 40,40,40,40 | 0 |
| 56 | MG | XD | 302 | 1/1 | 0.65 | 0.13 | 85,85,85,85 | 0 |
| 56 | MG | QA | 1734 | 1/1 | 0.65 | 0.41 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3152 | 1/1 | 0.65 | 0.33 | 54,54,54,54 | 0 |
| 56 | MG | YG | 201 | 1/1 | 0.65 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | RA | 3380 | 1/1 | 0.67 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | RA | 3338 | 1/1 | 0.67 | 0.43 | 67,67,67,67 | 0 |
| 56 | MG | RA | 3426 | 1/1 | 0.68 | 0.93 | 65,65,65,65 | 0 |
| 56 | MG | YA | 3290 | 1/1 | 0.68 | 0.37 | 82,82,82,82 | 0 |
| 56 | MG | YA | 3196 | 1/1 | 0.68 | 0.27 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3396 | 1/1 | 0.68 | 0.27 | 54,54,54,54 | 0 |
| 56 | MG | RA | 3204 | 1/1 | 0.68 | 0.36 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3277 | 1/1 | 0.69 | 0.51 | 67,67,67,67 | 0 |
| 56 | MG | YA | 3432 | 1/1 | 0.69 | 0.58 | 78,78,78,78 | 0 |
| 56 | MG | Y7 | 101 | 1/1 | 0.69 | 0.40 | 45,45,45,45 | 0 |
| 56 | MG | QA | 1728 | 1/1 | 0.70 | 0.25 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3467 | 1/1 | 0.70 | 0.45 | 68,68,68,68 | 0 |
| 56 | MG | XA | 1656 | 1/1 | 0.70 | 0.17 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3448 | 1/1 | 0.70 | 0.40 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1721 | 1/1 | 0.70 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3001 | 1/1 | 0.70 | 0.95 | 73,73,73,73 | 0 |
| 56 | MG | XA | 1733 | 1/1 | 0.71 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3153 | 1/1 | 0.71 | 0.40 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3459 | 1/1 | 0.71 | 0.51 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3425 | 1/1 | 0.71 | 0.84 | 62,62,62,62 | 0 |
| 56 | MG | QA | 1750 | 1/1 | 0.71 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | RA | 3347 | 1/1 | 0.71 | 0.74 | 83,83,83,83 | 0 |
| 56 | MG | YA | 3223 | 1/1 | 0.71 | 0.37 | 60,60,60,60 | 0 |
| 56 | MG | RA | 3274 | 1/1 | 0.72 | 0.31 | 44,44,44,44 | 0 |
| 56 | MG | XA | 1630 | 1/1 | 0.72 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3227 | 1/1 | 0.72 | 0.38 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3343 | 1/1 | 0.72 | 0.40 | 61,61,61,61 | 0 |
| 56 | MG | XA | 1759 | 1/1 | 0.72 | 0.67 | 63,63,63,63 | 0 |
| 56 | MG | YA | 3068 | 1/1 | 0.72 | 0.46 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3233 | 1/1 | 0.72 | 0.41 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3344 | 1/1 | 0.72 | 0.51 | 35,35,35,35 | 0 |
| 56 | MG | QA | 1706 | 1/1 | 0.72 | 0.36 | 52,52,52,52 | 0 |
| 56 | MG | XA | 1750 | 1/1 | 0.72 | 0.27 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3326 | 1/1 | 0.72 | 0.42 | 56,56,56,56 | 0 |
| 56 | MG | YA | 3482 | 1/1 | 0.73 | 0.42 | 69,69,69,69 | 0 |
| 56 | MG | YA | 3182 | 1/1 | 0.73 | 0.28 | 58,58,58,58 | 0 |
| 56 | MG | RA | 3249 | 1/1 | 0.73 | 0.25 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3300 | 1/1 | 0.73 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3378 | 1/1 | 0.73 | 0.28 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3102 | 1/1 | 0.73 | 0.34 | 10,10,10,10 | 0 |
| 56 | MG | RA | 3245 | 1/1 | 0.73 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3422 | 1/1 | 0.73 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | YA | 3283 | 1/1 | 0.73 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | RA | 3320 | 1/1 | 0.73 | 0.61 | 63,63,63,63 | 0 |
| 56 | MG | RA | 3051 | 1/1 | 0.73 | 0.37 | 62,62,62,62 | 0 |
| 56 | MG | QA | 1719 | 1/1 | 0.74 | 0.48 | 70,70,70,70 | 0 |
| 56 | MG | QA | 1636 | 1/1 | 0.74 | 0.43 | 56,56,56,56 | 0 |
| 56 | MG | RA | 3332 | 1/1 | 0.74 | 0.31 | 40,40,40,40 | 0 |
| 56 | MG | RA | 3295 | 1/1 | 0.74 | 0.41 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3422 | 1/1 | 0.74 | 0.29 | 43,43,43,43 | 0 |
| 56 | MG | QA | 1701 | 1/1 | 0.74 | 0.18 | 42,42,42,42 | 0 |
| 56 | MG | RA | 3288 | 1/1 | 0.74 | 0.26 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3485 | 1/1 | 0.74 | 0.29 | 22,22,22,22 | 0 |
| 56 | MG | YA | 3341 | 1/1 | 0.74 | 0.75 | 71,71,71,71 | 0 |
| 56 | MG | YA | 3183 | 1/1 | 0.74 | 0.24 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3394 | 1/1 | 0.74 | 0.27 | 64,64,64,64 | 0 |
| 56 | MG | YA | 3401 | 1/1 | 0.74 | 0.59 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3037 | 1/1 | 0.74 | 0.67 | 24,24,24,24 | 0 |
| 56 | MG | QA | 1647 | 1/1 | 0.74 | 0.26 | 55,55,55,55 | 0 |
| 56 | MG | QA | 1630 | 1/1 | 0.75 | 0.33 | 64,64,64,64 | 0 |
| 56 | MG | RA | 3413 | 1/1 | 0.75 | 0.37 | 63,63,63,63 | 0 |
| 56 | MG | RY | 201 | 1/1 | 0.75 | 0.43 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3463 | 1/1 | 0.75 | 0.37 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3307 | 1/1 | 0.75 | 0.32 | 49,49,49,49 | 0 |
| 56 | MG | RQ | 202 | 1/1 | 0.75 | 0.52 | 48,48,48,48 | 0 |
| 56 | MG | QA | 1696 | 1/1 | 0.75 | 0.91 | 67,67,67,67 | 0 |
| 56 | MG | RA | 3357 | 1/1 | 0.75 | 0.29 | 51,51,51,51 | 0 |
| 56 | MG | RA | 3222 | 1/1 | 0.75 | 0.43 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3354 | 1/1 | 0.76 | 0.34 | 50,50,50,50 | 0 |
| 56 | MG | RA | 3083 | 1/1 | 0.76 | 0.26 | 5,5,5,5 | 0 |
| 56 | MG | YA | 3386 | 1/1 | 0.76 | 0.45 | 54,54,54,54 | 0 |
| 56 | MG | XA | 1658 | 1/1 | 0.76 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3402 | 1/1 | 0.76 | 0.24 | 70,70,70,70 | 0 |
| 56 | MG | RA | 3157 | 1/1 | 0.76 | 0.18 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3305 | 1/1 | 0.76 | 0.35 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3302 | 1/1 | 0.76 | 0.30 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1693 | 1/1 | 0.76 | 0.17 | 66,66,66,66 | 0 |
| 56 | MG | QA | 1702 | 1/1 | 0.76 | 0.30 | 81,81,81,81 | 0 |
| 56 | MG | YA | 3395 | 1/1 | 0.77 | 0.19 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3132 | 1/1 | 0.77 | 0.65 | 60,60,60,60 | 0 |
| 56 | MG | YA | 3317 | 1/1 | 0.77 | 0.56 | 48,48,48,48 | 0 |
| 56 | MG | RA | 3406 | 1/1 | 0.77 | 0.52 | 59,59,59,59 | 0 |
| 56 | MG | RA | 3166 | 1/1 | 0.77 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3225 | 1/1 | 0.77 | 0.23 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3263 | 1/1 | 0.77 | 0.34 | 41,41,41,41 | 0 |
| 56 | MG | QA | 1669 | 1/1 | 0.77 | 0.18 | 71,71,71,71 | 0 |
| 56 | MG | YA | 3155 | 1/1 | 0.78 | 0.24 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3472 | 1/1 | 0.78 | 0.54 | 69,69,69,69 | 0 |
| 56 | MG | RA | 3316 | 1/1 | 0.78 | 0.60 | 57,57,57,57 | 0 |
| 56 | MG | RA | 3253 | 1/1 | 0.78 | 0.59 | 59,59,59,59 | 0 |
| 56 | MG | RA | 3188 | 1/1 | 0.78 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | YA | 3384 | 1/1 | 0.78 | 0.39 | 64,64,64,64 | 0 |
| 56 | MG | QA | 1699 | 1/1 | 0.78 | 0.28 | 55,55,55,55 | 0 |
| 56 | MG | QA | 1603 | 1/1 | 0.78 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | XA | 1738 | 1/1 | 0.78 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3331 | 1/1 | 0.78 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | RA | 3108 | 1/1 | 0.78 | 0.61 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3149 | 1/1 | 0.78 | 0.41 | 54,54,54,54 | 0 |
| 56 | MG | RA | 3158 | 1/1 | 0.79 | 0.28 | 61,61,61,61 | 0 |
| 56 | MG | YA | 3398 | 1/1 | 0.79 | 0.28 | 55,55,55,55 | 0 |
| 56 | MG | QA | 1731 | 1/1 | 0.79 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | XA | 1727 | 1/1 | 0.79 | 1.22 | 78,78,78,78 | 0 |
| 56 | MG | RA | 3259 | 1/1 | 0.79 | 0.24 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3293 | 1/1 | 0.79 | 0.42 | 68,68,68,68 | 0 |
| 56 | MG | RA | 3298 | 1/1 | 0.79 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3002 | 1/1 | 0.79 | 0.63 | 42,42,42,42 | 0 |
| 56 | MG | XA | 1620 | 1/1 | 0.79 | 0.15 | 21,21,21,21 | 0 |
| 56 | MG | QA | 1665 | 1/1 | 0.79 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | YA | 3315 | 1/1 | 0.80 | 0.39 | 53,53,53,53 | 0 |
| 56 | MG | YA | 3188 | 1/1 | 0.80 | 0.36 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3484 | 1/1 | 0.80 | 0.30 | 24,24,24,24 | 0 |
| 56 | MG | QA | 1703 | 1/1 | 0.80 | 0.21 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3436 | 1/1 | 0.80 | 0.58 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1663 | 1/1 | 0.80 | 1.40 | 68,68,68,68 | 0 |
| 56 | MG | RA | 3175 | 1/1 | 0.80 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | QA | 1626 | 1/1 | 0.80 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3232 | 1/1 | 0.80 | 0.25 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3421 | 1/1 | 0.80 | 0.09 | 68,68,68,68 | 0 |
| 56 | MG | YA | 3121 | 1/1 | 0.81 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3141 | 1/1 | 0.81 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3355 | 1/1 | 0.81 | 0.49 | 63,63,63,63 | 0 |
| 56 | MG | XA | 1675 | 1/1 | 0.81 | 0.91 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3285 | 1/1 | 0.81 | 0.36 | 26,26,26,26 | 0 |
| 56 | MG | QA | 1733 | 1/1 | 0.81 | 0.29 | 86,86,86,86 | 0 |
| 56 | MG | RA | 3186 | 1/1 | 0.81 | 0.19 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3392 | 1/1 | 0.81 | 0.56 | 60,60,60,60 | 0 |
| 56 | MG | QA | 1677 | 1/1 | 0.81 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | YA | 3408 | 1/1 | 0.81 | 0.14 | 73,73,73,73 | 0 |
| 56 | MG | QA | 1720 | 1/1 | 0.81 | 0.28 | 53,53,53,53 | 0 |
| 56 | MG | QA | 1692 | 1/1 | 0.81 | 0.45 | 65,65,65,65 | 0 |
| 56 | MG | YA | 3456 | 1/1 | 0.81 | 0.21 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3260 | 1/1 | 0.81 | 0.27 | 32,32,32,32 | 0 |
| 56 | MG | RA | 3185 | 1/1 | 0.81 | 0.50 | 54,54,54,54 | 0 |
| 56 | MG | RA | 3191 | 1/1 | 0.81 | 0.15 | 15,15,15,15 | 0 |
| 56 | MG | RA | 3352 | 1/1 | 0.81 | 0.48 | 62,62,62,62 | 0 |
| 56 | MG | QA | 1745 | 1/1 | 0.81 | 0.27 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3096 | 1/1 | 0.82 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3146 | 1/1 | 0.82 | 0.21 | 26,26,26,26 | 0 |
| 56 | MG | QA | 1628 | 1/1 | 0.82 | 0.24 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3392 | 1/1 | 0.82 | 0.28 | 36,36,36,36 | 0 |
| 56 | MG | RA | 3328 | 1/1 | 0.82 | 0.37 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3082 | 1/1 | 0.82 | 0.27 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3206 | 1/1 | 0.82 | 0.24 | 18,18,18,18 | 0 |
| 56 | MG | XA | 1730 | 1/1 | 0.82 | 0.78 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3229 | 1/1 | 0.82 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3294 | 1/1 | 0.82 | 0.13 | 56,56,56,56 | 0 |
| 56 | MG | RB | 204 | 1/1 | 0.82 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | XA | 1758 | 1/1 | 0.82 | 0.76 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1695 | 1/1 | 0.82 | 0.54 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3268 | 1/1 | 0.82 | 0.58 | 48,48,48,48 | 0 |
| 56 | MG | XA | 1683 | 1/1 | 0.82 | 0.29 | 31,31,31,31 | 0 |
| 56 | MG | XA | 1719 | 1/1 | 0.82 | 0.24 | 50,50,50,50 | 0 |
| 56 | MG | XA | 1731 | 1/1 | 0.82 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3430 | 1/1 | 0.82 | 0.70 | 50,50,50,50 | 0 |
| 56 | MG | QA | 1662 | 1/1 | 0.82 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | RA | 3439 | 1/1 | 0.82 | 0.26 | 50,50,50,50 | 0 |
| 56 | MG | YA | 3278 | 1/1 | 0.82 | 0.46 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3031 | 1/1 | 0.82 | 0.46 | 26,26,26,26 | 0 |
| 56 | MG | QA | 1709 | 1/1 | 0.82 | 0.42 | 36,36,36,36 | 0 |
| 56 | MG | YA | 3342 | 1/1 | 0.82 | 0.52 | 66,66,66,66 | 0 |
| 56 | MG | XA | 1700 | 1/1 | 0.82 | 0.45 | 79,79,79,79 | 0 |
| 56 | MG | RQ | 201 | 1/1 | 0.82 | 0.40 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3397 | 1/1 | 0.82 | 0.22 | 49,49,49,49 | 0 |
| 56 | MG | RA | 3398 | 1/1 | 0.82 | 0.29 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3366 | 1/1 | 0.83 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | YA | 3140 | 1/1 | 0.83 | 0.21 | 58,58,58,58 | 0 |
| 56 | MG | XA | 1763 | 1/1 | 0.83 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3060 | 1/1 | 0.83 | 0.15 | 14,14,14,14 | 0 |
| 56 | MG | YO | 201 | 1/1 | 0.83 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3376 | 1/1 | 0.83 | 0.20 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3319 | 1/1 | 0.83 | 0.21 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3437 | 1/1 | 0.83 | 0.57 | 89,89,89,89 | 0 |
| 56 | MG | RA | 3128 | 1/1 | 0.83 | 0.41 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3323 | 1/1 | 0.83 | 0.34 | 37,37,37,37 | 0 |
| 56 | MG | YQ | 201 | 1/1 | 0.83 | 0.31 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3100 | 1/1 | 0.83 | 0.30 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3405 | 1/1 | 0.83 | 0.41 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3287 | 1/1 | 0.83 | 0.36 | 47,47,47,47 | 0 |
| 56 | MG | XA | 1691 | 1/1 | 0.83 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | XA | 1627 | 1/1 | 0.83 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | RA | 3290 | 1/1 | 0.83 | 0.31 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3324 | 1/1 | 0.83 | 0.24 | 45,45,45,45 | 0 |
| 56 | MG | QA | 1682 | 1/1 | 0.83 | 0.61 | 51,51,51,51 | 0 |
| 56 | MG | XA | 1713 | 1/1 | 0.83 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | XA | 1724 | 1/1 | 0.83 | 0.20 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3480 | 1/1 | 0.83 | 0.15 | 65,65,65,65 | 0 |
| 56 | MG | RA | 3265 | 1/1 | 0.83 | 0.23 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3148 | 1/1 | 0.83 | 0.23 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3318 | 1/1 | 0.83 | 0.54 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3345 | 1/1 | 0.83 | 0.42 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3151 | 1/1 | 0.83 | 0.35 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3336 | 1/1 | 0.83 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | RA | 3405 | 1/1 | 0.83 | 0.31 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3351 | 1/1 | 0.83 | 0.22 | 75,75,75,75 | 0 |
| 56 | MG | YA | 3231 | 1/1 | 0.83 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | XA | 1693 | 1/1 | 0.83 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | R0 | 101 | 1/1 | 0.84 | 0.44 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3111 | 1/1 | 0.84 | 0.21 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3162 | 1/1 | 0.84 | 0.45 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3239 | 1/1 | 0.84 | 0.33 | 40,40,40,40 | 0 |
| 56 | MG | QA | 1729 | 1/1 | 0.84 | 0.27 | 31,31,31,31 | 0 |
| 56 | MG | XL | 201 | 1/1 | 0.84 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3192 | 1/1 | 0.84 | 0.64 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3184 | 1/1 | 0.84 | 0.30 | 28,28,28,28 | 0 |
| 56 | MG | XA | 1688 | 1/1 | 0.84 | 0.59 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3453 | 1/1 | 0.84 | 0.19 | 35,35,35,35 | 0 |
| 56 | MG | XA | 1717 | 1/1 | 0.84 | 0.45 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3281 | 1/1 | 0.84 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | XA | 1739 | 1/1 | 0.84 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | RA | 3318 | 1/1 | 0.84 | 0.32 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3426 | 1/1 | 0.84 | 0.35 | 34,34,34,34 | 0 |
| 56 | MG | RA | 3368 | 1/1 | 0.84 | 0.36 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3373 | 1/1 | 0.84 | 0.47 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3356 | 1/1 | 0.84 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | RA | 3214 | 1/1 | 0.84 | 0.33 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3259 | 1/1 | 0.84 | 0.44 | 46,46,46,46 | 0 |
| 56 | MG | XA | 1757 | 1/1 | 0.84 | 0.61 | 60,60,60,60 | 0 |
| 56 | MG | YA | 3360 | 1/1 | 0.84 | 0.33 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3023 | 1/1 | 0.84 | 0.39 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3411 | 1/1 | 0.84 | 0.82 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3199 | 1/1 | 0.84 | 0.65 | 39,39,39,39 | 0 |
| 56 | MG | XA | 1646 | 1/1 | 0.84 | 0.49 | 64,64,64,64 | 0 |
| 56 | MG | YA | 3321 | 1/1 | 0.84 | 0.27 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3447 | 1/1 | 0.84 | 0.27 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3401 | 1/1 | 0.84 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | XA | 1714 | 1/1 | 0.84 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | RA | 3120 | 1/1 | 0.84 | 0.89 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3440 | 1/1 | 0.84 | 0.30 | 62,62,62,62 | 0 |
| 56 | MG | XA | 1706 | 1/1 | 0.85 | 0.26 | 37,37,37,37 | 0 |
| 56 | MG | RA | 3093 | 1/1 | 0.85 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | QA | 1743 | 1/1 | 0.85 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | XA | 1702 | 1/1 | 0.85 | 0.66 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3164 | 1/1 | 0.85 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | QA | 1683 | 1/1 | 0.85 | 0.50 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3441 | 1/1 | 0.85 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | XA | 1725 | 1/1 | 0.85 | 0.31 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3249 | 1/1 | 0.85 | 0.41 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3324 | 1/1 | 0.85 | 0.30 | 75,75,75,75 | 0 |
| 56 | MG | QA | 1707 | 1/1 | 0.85 | 0.61 | 57,57,57,57 | 0 |
| 56 | MG | YA | 3333 | 1/1 | 0.85 | 0.36 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3313 | 1/1 | 0.85 | 0.48 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3439 | 1/1 | 0.85 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3256 | 1/1 | 0.85 | 0.41 | 93,93,93,93 | 0 |
| 56 | MG | RA | 3416 | 1/1 | 0.85 | 0.72 | 58,58,58,58 | 0 |
| 56 | MG | YA | 3390 | 1/1 | 0.85 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | YB | 202 | 1/1 | 0.85 | 0.27 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3170 | 1/1 | 0.85 | 0.42 | 26,26,26,26 | 0 |
| 56 | MG | QA | 1686 | 1/1 | 0.85 | 0.70 | 72,72,72,72 | 0 |
| 56 | MG | QA | 1725 | 1/1 | 0.85 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | RA | 3184 | 1/1 | 0.85 | 0.21 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3329 | 1/1 | 0.85 | 0.48 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3051 | 1/1 | 0.85 | 0.69 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3389 | 1/1 | 0.85 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | XA | 1744 | 1/1 | 0.85 | 0.62 | 36,36,36,36 | 0 |
| 56 | MG | YA | 3301 | 1/1 | 0.85 | 0.27 | 34,34,34,34 | 0 |
| 56 | MG | RA | 3162 | 1/1 | 0.85 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | RA | 3276 | 1/1 | 0.85 | 0.25 | 50,50,50,50 | 0 |
| 56 | MG | XA | 1611 | 1/1 | 0.85 | 0.46 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3128 | 1/1 | 0.86 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | RA | 3325 | 1/1 | 0.86 | 0.28 | 46,46,46,46 | 0 |
| 56 | MG | QA | 1722 | 1/1 | 0.86 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3380 | 1/1 | 0.86 | 0.41 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3307 | 1/1 | 0.86 | 0.33 | 46,46,46,46 | 0 |
| 56 | MG | XA | 1726 | 1/1 | 0.86 | 0.99 | 59,59,59,59 | 0 |
| 56 | MG | YA | 3304 | 1/1 | 0.86 | 0.18 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | XA | 1629 | 1/1 | 0.86 | 0.25 | 53,53,53,53 | 0 |
| 56 | MG | YA | 3308 | 1/1 | 0.86 | 0.38 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3182 | 1/1 | 0.86 | 0.34 | 58,58,58,58 | 0 |
| 56 | MG | QA | 1680 | 1/1 | 0.86 | 0.31 | 48,48,48,48 | 0 |
| 56 | MG | RA | 3279 | 1/1 | 0.86 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3412 | 1/1 | 0.86 | 0.38 | 34,34,34,34 | 0 |
| 56 | MG | RA | 3258 | 1/1 | 0.86 | 0.33 | 51,51,51,51 | 0 |
| 56 | MG | YA | 3383 | 1/1 | 0.86 | 0.26 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3229 | 1/1 | 0.86 | 0.49 | 43,43,43,43 | 0 |
| 56 | MG | QA | 1681 | 1/1 | 0.86 | 0.42 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3452 | 1/1 | 0.86 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | XA | 1621 | 1/1 | 0.86 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3090 | 1/1 | 0.86 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3127 | 1/1 | 0.86 | 0.62 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3438 | 1/1 | 0.86 | 0.22 | 68,68,68,68 | 0 |
| 56 | MG | YA | 3013 | 1/1 | 0.86 | 0.27 | 0,0,0,0 | 0 |
| 56 | MG | YA | 3157 | 1/1 | 0.86 | 0.34 | 32,32,32,32 | 0 |
| 56 | MG | RA | 3264 | 1/1 | 0.86 | 0.33 | 42,42,42,42 | 0 |
| 56 | MG | XA | 1756 | 1/1 | 0.86 | 0.25 | 61,61,61,61 | 0 |
| 56 | MG | RA | 3421 | 1/1 | 0.86 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | XA | 1745 | 1/1 | 0.86 | 0.23 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3440 | 1/1 | 0.86 | 0.11 | 12,12,12,12 | 0 |
| 56 | MG | RA | 3349 | 1/1 | 0.86 | 0.59 | 55,55,55,55 | 0 |
| 56 | MG | YA | 3362 | 1/1 | 0.86 | 0.42 | 66,66,66,66 | 0 |
| 56 | MG | RA | 3427 | 1/1 | 0.86 | 0.39 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3478 | 1/1 | 0.86 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3211 | 1/1 | 0.86 | 0.14 | 11,11,11,11 | 0 |
| 56 | MG | YA | 3029 | 1/1 | 0.86 | 0.12 | 15,15,15,15 | 0 |
| 56 | MG | YA | 3454 | 1/1 | 0.86 | 0.37 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3292 | 1/1 | 0.86 | 0.49 | 35,35,35,35 | 0 |
| 56 | MG | XA | 1721 | 1/1 | 0.86 | 0.22 | 52,52,52,52 | 0 |
| 56 | MG | QV | 103 | 1/1 | 0.86 | 0.26 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3303 | 1/1 | 0.86 | 0.45 | 69,69,69,69 | 0 |
| 56 | MG | XF | 201 | 1/1 | 0.86 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | YA | 3351 | 1/1 | 0.86 | 0.24 | 42,42,42,42 | 0 |
| 56 | MG | QA | 1634 | 1/1 | 0.86 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3244 | 1/1 | 0.86 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | RA | 3340 | 1/1 | 0.86 | 0.43 | 72,72,72,72 | 0 |
| 56 | MG | QA | 1727 | 1/1 | 0.87 | 0.34 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3403 | 1/1 | 0.87 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | XA | 1741 | 1/1 | 0.87 | 0.23 | 55,55,55,55 | 0 |
| 56 | MG | QA | 1673 | 1/1 | 0.87 | 0.33 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3408 | 1/1 | 0.87 | 0.44 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3233 | 1/1 | 0.87 | 0.40 | 25,25,25,25 | 0 |
| 56 | MG | QA | 1671 | 1/1 | 0.87 | 0.39 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3412 | 1/1 | 0.87 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | XA | 1672 | 1/1 | 0.87 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3101 | 1/1 | 0.87 | 0.35 | 37,37,37,37 | 0 |
| 56 | MG | QA | 1613 | 1/1 | 0.87 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | RA | 3399 | 1/1 | 0.87 | 0.60 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3388 | 1/1 | 0.87 | 0.29 | 28,28,28,28 | 0 |
| 56 | MG | RA | 3215 | 1/1 | 0.87 | 0.39 | 41,41,41,41 | 0 |
| 56 | MG | QA | 1737 | 1/1 | 0.87 | 0.25 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3092 | 1/1 | 0.87 | 0.45 | 41,41,41,41 | 0 |
| 56 | MG | RB | 201 | 1/1 | 0.87 | 0.35 | 28,28,28,28 | 0 |
| 56 | MG | Y0 | 103 | 1/1 | 0.87 | 0.33 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3095 | 1/1 | 0.87 | 0.45 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3275 | 1/1 | 0.87 | 0.83 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3328 | 1/1 | 0.87 | 0.46 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3464 | 1/1 | 0.87 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | YA | 3400 | 1/1 | 0.87 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | YA | 3339 | 1/1 | 0.87 | 0.25 | 62,62,62,62 | 0 |
| 56 | MG | RA | 3402 | 1/1 | 0.87 | 0.53 | 57,57,57,57 | 0 |
| 56 | MG | RA | 3232 | 1/1 | 0.87 | 0.37 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3471 | 1/1 | 0.87 | 0.21 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3387 | 1/1 | 0.87 | 0.21 | 27,27,27,27 | 0 |
| 56 | MG | RA | 3131 | 1/1 | 0.87 | 0.24 | 78,78,78,78 | 0 |
| 56 | MG | YA | 3371 | 1/1 | 0.87 | 0.60 | 57,57,57,57 | 0 |
| 56 | MG | XA | 1715 | 1/1 | 0.87 | 0.43 | 52,52,52,52 | 0 |
| 56 | MG | XA | 1761 | 1/1 | 0.87 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3473 | 1/1 | 0.88 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3263 | 1/1 | 0.88 | 0.81 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3253 | 1/1 | 0.88 | 0.28 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3118 | 1/1 | 0.88 | 0.34 | 27,27,27,27 | 0 |
| 56 | MG | RA | 3365 | 1/1 | 0.88 | 0.34 | 21,21,21,21 | 0 |
| 56 | MG | RA | 3187 | 1/1 | 0.88 | 0.52 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3084 | 1/1 | 0.88 | 0.09 | 11,11,11,11 | 0 |
| 56 | MG | YA | 3381 | 1/1 | 0.88 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | XA | 1728 | 1/1 | 0.88 | 0.57 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3169 | 1/1 | 0.88 | 0.25 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3270 | 1/1 | 0.88 | 0.27 | 49,49,49,49 | 0 |
| 56 | MG | RA | 3354 | 1/1 | 0.88 | 0.31 | 34,34,34,34 | 0 |
| 56 | MG | RA | 3251 | 1/1 | 0.88 | 0.25 | 63,63,63,63 | 0 |
| 56 | MG | RA | 3180 | 1/1 | 0.88 | 0.26 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | XA | 1710 | 1/1 | 0.88 | 0.29 | 48,48,48,48 | 0 |
| 56 | MG | QA | 1742 | 1/1 | 0.88 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3364 | 1/1 | 0.88 | 0.27 | 39,39,39,39 | 0 |
| 56 | MG | XA | 1705 | 1/1 | 0.88 | 0.62 | 38,38,38,38 | 0 |
| 56 | MG | QA | 1650 | 1/1 | 0.88 | 0.44 | 19,19,19,19 | 0 |
| 56 | MG | YB | 206 | 1/1 | 0.88 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3220 | 1/1 | 0.88 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | YF | 301 | 1/1 | 0.88 | 0.65 | 37,37,37,37 | 0 |
| 56 | MG | RA | 3226 | 1/1 | 0.88 | 0.39 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3127 | 1/1 | 0.88 | 0.33 | 51,51,51,51 | 0 |
| 56 | MG | YA | 3110 | 1/1 | 0.88 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | QA | 1675 | 1/1 | 0.88 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3248 | 1/1 | 0.88 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3214 | 1/1 | 0.88 | 0.70 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3121 | 1/1 | 0.88 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3363 | 1/1 | 0.88 | 0.52 | 56,56,56,56 | 0 |
| 56 | MG | RV | 201 | 1/1 | 0.89 | 0.33 | 4,4,4,4 | 0 |
| 56 | MG | YA | 3271 | 1/1 | 0.89 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3460 | 1/1 | 0.89 | 0.61 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3173 | 1/1 | 0.89 | 0.38 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3303 | 1/1 | 0.89 | 0.24 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3368 | 1/1 | 0.89 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | RA | 3153 | 1/1 | 0.89 | 0.23 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3420 | 1/1 | 0.89 | 0.17 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3347 | 1/1 | 0.89 | 0.26 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3239 | 1/1 | 0.89 | 0.58 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3431 | 1/1 | 0.89 | 0.29 | 40,40,40,40 | 0 |
| 56 | MG | QL | 201 | 1/1 | 0.89 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3213 | 1/1 | 0.89 | 0.42 | 21,21,21,21 | 0 |
| 56 | MG | XV | 103 | 1/1 | 0.89 | 0.31 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3041 | 1/1 | 0.89 | 0.26 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3187 | 1/1 | 0.89 | 0.32 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3466 | 1/1 | 0.89 | 0.43 | 49,49,49,49 | 0 |
| 56 | MG | RA | 3172 | 1/1 | 0.89 | 0.18 | 28,28,28,28 | 0 |
| 56 | MG | R2 | 101 | 1/1 | 0.89 | 0.25 | 62,62,62,62 | 0 |
| 56 | MG | RR | 201 | 1/1 | 0.89 | 0.28 | 31,31,31,31 | 0 |
| 56 | MG | YV | 201 | 1/1 | 0.89 | 0.29 | 22,22,22,22 | 0 |
| 56 | MG | XA | 1607 | 1/1 | 0.89 | 0.52 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3147 | 1/1 | 0.89 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | RA | 3169 | 1/1 | 0.89 | 0.31 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3423 | 1/1 | 0.89 | 0.38 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3349 | 1/1 | 0.89 | 0.34 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3116 | 1/1 | 0.89 | 0.32 | 18,18,18,18 | 0 |
| 56 | MG | YA | 3268 | 1/1 | 0.89 | 0.74 | 49,49,49,49 | 0 |
| 56 | MG | RA | 3432 | 1/1 | 0.89 | 0.30 | 91,91,91,91 | 0 |
| 56 | MG | XA | 1654 | 1/1 | 0.89 | 0.48 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3141 | 1/1 | 0.89 | 0.26 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3311 | 1/1 | 0.89 | 0.27 | 74,74,74,74 | 0 |
| 56 | MG | YA | 3476 | 1/1 | 0.89 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3334 | 1/1 | 0.89 | 0.88 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3438 | 1/1 | 0.89 | 0.23 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3172 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | XA | 1687 | 1/1 | 0.89 | 0.26 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3244 | 1/1 | 0.89 | 0.45 | 16,16,16,16 | 0 |
| 56 | MG | QA | 1629 | 1/1 | 0.89 | 0.46 | 26,26,26,26 | 0 |
| 56 | MG | YA | 3091 | 1/1 | 0.89 | 0.20 | 19,19,19,19 | 0 |
| 57 | ZN | XD | 301 | 1/1 | 0.89 | 0.37 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3276 | 1/1 | 0.89 | 0.35 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3240 | 1/1 | 0.89 | 0.35 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3083 | 1/1 | 0.89 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | QA | 1710 | 1/1 | 0.89 | 0.32 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3252 | 1/1 | 0.89 | 0.26 | 21,21,21,21 | 0 |
| 56 | MG | XA | 1648 | 1/1 | 0.90 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3154 | 1/1 | 0.90 | 0.22 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3343 | 1/1 | 0.90 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | YA | 3332 | 1/1 | 0.90 | 0.47 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3132 | 1/1 | 0.90 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3481 | 1/1 | 0.90 | 0.50 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3391 | 1/1 | 0.90 | 0.35 | 44,44,44,44 | 0 |
| 56 | MG | XA | 1711 | 1/1 | 0.90 | 0.45 | 39,39,39,39 | 0 |
| 56 | MG | YA | 3280 | 1/1 | 0.90 | 0.73 | 40,40,40,40 | 0 |
| 56 | MG | RA | 3400 | 1/1 | 0.90 | 0.24 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3046 | 1/1 | 0.90 | 0.24 | 14,14,14,14 | 0 |
| 56 | MG | QA | 1712 | 1/1 | 0.90 | 0.32 | 46,46,46,46 | 0 |
| 56 | MG | XA | 1722 | 1/1 | 0.90 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | XA | 1747 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3250 | 1/1 | 0.90 | 0.23 | 22,22,22,22 | 0 |
| 56 | MG | XA | 1670 | 1/1 | 0.90 | 0.33 | 36,36,36,36 | 0 |
| 56 | MG | YA | 3059 | 1/1 | 0.90 | 0.14 | 15,15,15,15 | 0 |
| 56 | MG | RA | 3425 | 1/1 | 0.90 | 0.39 | 38,38,38,38 | 0 |
| 56 | MG | XA | 1754 | 1/1 | 0.90 | 0.36 | 55,55,55,55 | 0 |
| 56 | MG | RA | 3333 | 1/1 | 0.90 | 0.30 | 35,35,35,35 | 0 |
| 56 | MG | RA | 3358 | 1/1 | 0.90 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3225 | 1/1 | 0.90 | 0.33 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3230 | 1/1 | 0.90 | 0.43 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3014 | 1/1 | 0.90 | 0.27 | 3,3,3,3 | 0 |
| 56 | MG | QA | 1716 | 1/1 | 0.90 | 0.21 | 36,36,36,36 | 0 |
| 56 | MG | YA | 3411 | 1/1 | 0.90 | 0.49 | 63,63,63,63 | 0 |
| 56 | MG | XA | 1734 | 1/1 | 0.90 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | RB | 203 | 1/1 | 0.90 | 0.32 | 37,37,37,37 | 0 |
| 56 | MG | QV | 102 | 1/1 | 0.90 | 0.26 | 28,28,28,28 | 0 |
| 56 | MG | RA | 3089 | 1/1 | 0.90 | 0.29 | 18,18,18,18 | 0 |
| 56 | MG | RA | 3105 | 1/1 | 0.90 | 0.32 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3353 | 1/1 | 0.90 | 0.50 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3197 | 1/1 | 0.90 | 0.21 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3245 | 1/1 | 0.90 | 0.31 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3091 | 1/1 | 0.90 | 0.22 | 27,27,27,27 | 0 |
| 56 | MG | QA | 1643 | 1/1 | 0.90 | 0.27 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3242 | 1/1 | 0.90 | 0.53 | 42,42,42,42 | 0 |
| 56 | MG | RA | 3267 | 1/1 | 0.90 | 0.21 | 28,28,28,28 | 0 |
| 56 | MG | QA | 1606 | 1/1 | 0.90 | 0.30 | 18,18,18,18 | 0 |
| 56 | MG | RA | 3435 | 1/1 | 0.90 | 0.55 | 64,64,64,64 | 0 |
| 56 | MG | RA | 3152 | 1/1 | 0.90 | 0.44 | 19,19,19,19 | 0 |
| 56 | MG | Y0 | 102 | 1/1 | 0.90 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3098 | 1/1 | 0.90 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | XA | 1662 | 1/1 | 0.90 | 0.28 | 44,44,44,44 | 0 |
| 56 | MG | QA | 1648 | 1/1 | 0.90 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | RA | 3415 | 1/1 | 0.90 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | YA | 3277 | 1/1 | 0.90 | 0.31 | 38,38,38,38 | 0 |
| 56 | MG | XA | 1743 | 1/1 | 0.90 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | YA | 3427 | 1/1 | 0.90 | 0.26 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3195 | 1/1 | 0.90 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1735 | 1/1 | 0.90 | 0.56 | 66,66,66,66 | 0 |
| 56 | MG | YA | 3048 | 1/1 | 0.90 | 0.29 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3389 | 1/1 | 0.90 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | YA | 3069 | 1/1 | 0.90 | 0.18 | 14,14,14,14 | 0 |
| 56 | MG | YA | 3150 | 1/1 | 0.90 | 0.40 | 9,9,9,9 | 0 |
| 56 | MG | RA | 3428 | 1/1 | 0.91 | 0.19 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3234 | 1/1 | 0.91 | 0.25 | 30,30,30,30 | 0 |
| 56 | MG | QA | 1637 | 1/1 | 0.91 | 0.47 | 53,53,53,53 | 0 |
| 56 | MG | RA | 3285 | 1/1 | 0.91 | 0.33 | 28,28,28,28 | 0 |
| 56 | MG | XA | 1666 | 1/1 | 0.91 | 0.26 | 39,39,39,39 | 0 |
| 56 | MG | RA | 3135 | 1/1 | 0.91 | 0.31 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3199 | 1/1 | 0.91 | 0.30 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3174 | 1/1 | 0.91 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | YA | 3296 | 1/1 | 0.91 | 0.23 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | QA | 1668 | 1/1 | 0.91 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3296 | 1/1 | 0.91 | 0.20 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3265 | 1/1 | 0.91 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3295 | 1/1 | 0.91 | 0.39 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3362 | 1/1 | 0.91 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3094 | 1/1 | 0.91 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3309 | 1/1 | 0.91 | 0.16 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3394 | 1/1 | 0.91 | 0.63 | 36,36,36,36 | 0 |
| 56 | MG | XA | 1624 | 1/1 | 0.91 | 0.37 | 59,59,59,59 | 0 |
| 56 | MG | YA | 3130 | 1/1 | 0.91 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3256 | 1/1 | 0.91 | 0.17 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3226 | 1/1 | 0.91 | 0.19 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3430 | 1/1 | 0.91 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | RA | 3209 | 1/1 | 0.91 | 0.47 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3210 | 1/1 | 0.91 | 0.28 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3097 | 1/1 | 0.91 | 0.31 | 48,48,48,48 | 0 |
| 56 | MG | RA | 3383 | 1/1 | 0.91 | 0.77 | 44,44,44,44 | 0 |
| 56 | MG | QA | 1738 | 1/1 | 0.91 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | RA | 3095 | 1/1 | 0.91 | 0.52 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3047 | 1/1 | 0.91 | 0.42 | 10,10,10,10 | 0 |
| 56 | MG | XA | 1723 | 1/1 | 0.91 | 0.38 | 58,58,58,58 | 0 |
| 56 | MG | RA | 3410 | 1/1 | 0.91 | 0.36 | 70,70,70,70 | 0 |
| 56 | MG | YA | 3457 | 1/1 | 0.91 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3205 | 1/1 | 0.91 | 0.46 | 43,43,43,43 | 0 |
| 56 | MG | XA | 1729 | 1/1 | 0.91 | 0.34 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3235 | 1/1 | 0.91 | 0.63 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3151 | 1/1 | 0.91 | 0.22 | 26,26,26,26 | 0 |
| 56 | MG | QA | 1621 | 1/1 | 0.91 | 0.17 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3133 | 1/1 | 0.91 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | XA | 1634 | 1/1 | 0.91 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3396 | 1/1 | 0.91 | 0.24 | 37,37,37,37 | 0 |
| 56 | MG | R1 | 101 | 1/1 | 0.91 | 0.42 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3329 | 1/1 | 0.91 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | XA | 1686 | 1/1 | 0.91 | 1.10 | 64,64,64,64 | 0 |
| 56 | MG | XA | 1704 | 1/1 | 0.91 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3105 | 1/1 | 0.91 | 0.21 | 50,50,50,50 | 0 |
| 56 | MG | YA | 3375 | 1/1 | 0.91 | 0.51 | 51,51,51,51 | 0 |
| 56 | MG | RA | 3414 | 1/1 | 0.91 | 0.31 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3330 | 1/1 | 0.91 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | QA | 1652 | 1/1 | 0.91 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3350 | 1/1 | 0.91 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | XA | 1677 | 1/1 | 0.91 | 0.11 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3038 | 1/1 | 0.91 | 0.59 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3372 | 1/1 | 0.91 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | QA | 1711 | 1/1 | 0.91 | 0.36 | 53,53,53,53 | 0 |
| 56 | MG | XA | 1613 | 1/1 | 0.91 | 0.24 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3099 | 1/1 | 0.91 | 0.49 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3281 | 1/1 | 0.91 | 0.13 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3185 | 1/1 | 0.91 | 0.19 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3004 | 1/1 | 0.91 | 0.37 | 12,12,12,12 | 0 |
| 56 | MG | XA | 1622 | 1/1 | 0.91 | 0.76 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3190 | 1/1 | 0.91 | 0.74 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3125 | 1/1 | 0.91 | 0.31 | 26,26,26,26 | 0 |
| 56 | MG | QV | 101 | 1/1 | 0.91 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3424 | 1/1 | 0.91 | 0.24 | 46,46,46,46 | 0 |
| 56 | MG | YA | 3137 | 1/1 | 0.92 | 0.22 | 5,5,5,5 | 0 |
| 56 | MG | QA | 1614 | 1/1 | 0.92 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | QA | 1741 | 1/1 | 0.92 | 0.44 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3385 | 1/1 | 0.92 | 0.40 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3315 | 1/1 | 0.92 | 0.31 | 30,30,30,30 | 0 |
| 56 | MG | YB | 203 | 1/1 | 0.92 | 0.33 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3219 | 1/1 | 0.92 | 0.31 | 39,39,39,39 | 0 |
| 56 | MG | XA | 1749 | 1/1 | 0.92 | 0.23 | 39,39,39,39 | 0 |
| 56 | MG | RA | 3240 | 1/1 | 0.92 | 0.20 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3339 | 1/1 | 0.92 | 0.25 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3070 | 1/1 | 0.92 | 0.32 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3279 | 1/1 | 0.92 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3218 | 1/1 | 0.92 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | RA | 3235 | 1/1 | 0.92 | 0.20 | 28,28,28,28 | 0 |
| 56 | MG | RA | 3434 | 1/1 | 0.92 | 0.20 | 37,37,37,37 | 0 |
| 56 | MG | XA | 1746 | 1/1 | 0.92 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3106 | 1/1 | 0.92 | 0.27 | 15,15,15,15 | 0 |
| 56 | MG | YA | 3108 | 1/1 | 0.92 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3302 | 1/1 | 0.92 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3379 | 1/1 | 0.92 | 0.23 | 26,26,26,26 | 0 |
| 56 | MG | QA | 1748 | 1/1 | 0.92 | 0.37 | 47,47,47,47 | 0 |
| 56 | MG | QA | 1694 | 1/1 | 0.92 | 0.22 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3102 | 1/1 | 0.92 | 0.40 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3165 | 1/1 | 0.92 | 0.55 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3145 | 1/1 | 0.92 | 0.13 | 68,68,68,68 | 0 |
| 56 | MG | YA | 3262 | 1/1 | 0.92 | 0.33 | 36,36,36,36 | 0 |
| 56 | MG | XA | 1751 | 1/1 | 0.92 | 0.31 | 70,70,70,70 | 0 |
| 56 | MG | RA | 3418 | 1/1 | 0.92 | 0.35 | 28,28,28,28 | 0 |
| 56 | MG | XA | 1697 | 1/1 | 0.92 | 0.25 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | QA | 1608 | 1/1 | 0.92 | 0.55 | 25,25,25,25 | 0 |
| 56 | MG | YB | 204 | 1/1 | 0.92 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3443 | 1/1 | 0.92 | 0.14 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3246 | 1/1 | 0.92 | 0.44 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3181 | 1/1 | 0.92 | 0.35 | 33,33,33,33 | 0 |
| 56 | MG | QA | 1713 | 1/1 | 0.92 | 0.28 | 38,38,38,38 | 0 |
| 56 | MG | QA | 1670 | 1/1 | 0.92 | 0.37 | 48,48,48,48 | 0 |
| 56 | MG | XV | 102 | 1/1 | 0.92 | 0.22 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3178 | 1/1 | 0.92 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | RA | 3312 | 1/1 | 0.92 | 0.48 | 26,26,26,26 | 0 |
| 56 | MG | RD | 301 | 1/1 | 0.92 | 0.21 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3222 | 1/1 | 0.92 | 0.35 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3075 | 1/1 | 0.92 | 0.29 | 8,8,8,8 | 0 |
| 56 | MG | XA | 1617 | 1/1 | 0.92 | 0.39 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3479 | 1/1 | 0.92 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3247 | 1/1 | 0.92 | 0.34 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3017 | 1/1 | 0.92 | 0.12 | 17,17,17,17 | 0 |
| 56 | MG | XA | 1684 | 1/1 | 0.92 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3161 | 1/1 | 0.92 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | YA | 3364 | 1/1 | 0.92 | 0.80 | 50,50,50,50 | 0 |
| 56 | MG | YA | 3165 | 1/1 | 0.92 | 0.29 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3136 | 1/1 | 0.92 | 0.21 | 22,22,22,22 | 0 |
| 56 | MG | QA | 1623 | 1/1 | 0.92 | 0.74 | 35,35,35,35 | 0 |
| 56 | MG | RA | 3334 | 1/1 | 0.92 | 0.65 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3461 | 1/1 | 0.92 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3458 | 1/1 | 0.92 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | YA | 3410 | 1/1 | 0.92 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3211 | 1/1 | 0.92 | 0.19 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3190 | 1/1 | 0.92 | 0.37 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3326 | 1/1 | 0.92 | 0.60 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1678 | 1/1 | 0.92 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3306 | 1/1 | 0.92 | 0.67 | 63,63,63,63 | 0 |
| 56 | MG | XA | 1667 | 1/1 | 0.92 | 0.32 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3429 | 1/1 | 0.92 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | QA | 1708 | 1/1 | 0.92 | 0.61 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3358 | 1/1 | 0.92 | 0.32 | 27,27,27,27 | 0 |
| 56 | MG | RA | 3084 | 1/1 | 0.92 | 0.19 | 27,27,27,27 | 0 |
| 56 | MG | QA | 1685 | 1/1 | 0.92 | 0.10 | 11,11,11,11 | 0 |
| 56 | MG | RA | 3433 | 1/1 | 0.92 | 0.22 | 39,39,39,39 | 0 |
| 56 | MG | RA | 3143 | 1/1 | 0.92 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | RA | 3261 | 1/1 | 0.92 | 0.41 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3137 | 1/1 | 0.92 | 0.18 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3346 | 1/1 | 0.92 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3397 | 1/1 | 0.92 | 0.57 | 58,58,58,58 | 0 |
| 56 | MG | YA | 3216 | 1/1 | 0.92 | 0.28 | 13,13,13,13 | 0 |
| 56 | MG | QA | 1705 | 1/1 | 0.92 | 0.24 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3026 | 1/1 | 0.92 | 0.39 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3352 | 1/1 | 0.92 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | RA | 3370 | 1/1 | 0.92 | 0.52 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3246 | 1/1 | 0.92 | 0.24 | 25,25,25,25 | 0 |
| 56 | MG | XA | 1678 | 1/1 | 0.92 | 0.35 | 41,41,41,41 | 0 |
| 56 | MG | XA | 1718 | 1/1 | 0.92 | 0.18 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3166 | 1/1 | 0.92 | 0.40 | 24,24,24,24 | 0 |
| 56 | MG | QA | 1618 | 1/1 | 0.92 | 0.27 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3311 | 1/1 | 0.93 | 0.63 | 55,55,55,55 | 0 |
| 56 | MG | RA | 3237 | 1/1 | 0.93 | 0.18 | 23,23,23,23 | 0 |
| 56 | MG | QA | 1611 | 1/1 | 0.93 | 0.24 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3101 | 1/1 | 0.93 | 0.38 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3050 | 1/1 | 0.93 | 0.19 | 24,24,24,24 | 0 |
| 56 | MG | RA | 3161 | 1/1 | 0.93 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | YA | 3272 | 1/1 | 0.93 | 0.26 | 26,26,26,26 | 0 |
| 56 | MG | QA | 1679 | 1/1 | 0.93 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3019 | 1/1 | 0.93 | 0.36 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3117 | 1/1 | 0.93 | 0.31 | 28,28,28,28 | 0 |
| 56 | MG | RA | 3366 | 1/1 | 0.93 | 0.24 | 67,67,67,67 | 0 |
| 56 | MG | QA | 1639 | 1/1 | 0.93 | 0.30 | 48,48,48,48 | 0 |
| 56 | MG | RA | 3241 | 1/1 | 0.93 | 0.31 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3117 | 1/1 | 0.93 | 0.35 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3103 | 1/1 | 0.93 | 0.43 | 43,43,43,43 | 0 |
| 56 | MG | RA | 3164 | 1/1 | 0.93 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | XA | 1631 | 1/1 | 0.93 | 0.35 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3313 | 1/1 | 0.93 | 0.42 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3269 | 1/1 | 0.93 | 0.33 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3272 | 1/1 | 0.93 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | QD | 302 | 1/1 | 0.93 | 0.30 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3266 | 1/1 | 0.93 | 0.46 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3433 | 1/1 | 0.93 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3238 | 1/1 | 0.93 | 0.12 | 14,14,14,14 | 0 |
| 56 | MG | QA | 1697 | 1/1 | 0.93 | 0.53 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3282 | 1/1 | 0.93 | 0.55 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3159 | 1/1 | 0.93 | 0.27 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3291 | 1/1 | 0.93 | 0.28 | 33,33,33,33 | 0 |
| 56 | MG | XA | 1736 | 1/1 | 0.93 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3073 | 1/1 | 0.93 | 0.63 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | XA | 1645 | 1/1 | 0.93 | 0.31 | 35,35,35,35 | 0 |
| 56 | MG | YN | 201 | 1/1 | 0.93 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | RA | 3202 | 1/1 | 0.93 | 0.20 | 22,22,22,22 | 0 |
| 56 | MG | QA | 1718 | 1/1 | 0.93 | 0.34 | 47,47,47,47 | 0 |
| 56 | MG | XA | 1608 | 1/1 | 0.93 | 0.44 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3261 | 1/1 | 0.93 | 0.22 | 40,40,40,40 | 0 |
| 56 | MG | RF | 301 | 1/1 | 0.93 | 0.10 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3449 | 1/1 | 0.93 | 0.48 | 36,36,36,36 | 0 |
| 56 | MG | XA | 1652 | 1/1 | 0.93 | 0.73 | 48,48,48,48 | 0 |
| 57 | ZN | XN | 101 | 1/1 | 0.93 | 0.13 | 67,67,67,67 | 0 |
| 56 | MG | RA | 3167 | 1/1 | 0.93 | 0.21 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3359 | 1/1 | 0.93 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3251 | 1/1 | 0.93 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | QA | 1740 | 1/1 | 0.93 | 0.51 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3144 | 1/1 | 0.93 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3428 | 1/1 | 0.93 | 0.55 | 55,55,55,55 | 0 |
| 56 | MG | YA | 3255 | 1/1 | 0.93 | 0.61 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3377 | 1/1 | 0.93 | 0.50 | 24,24,24,24 | 0 |
| 56 | MG | QA | 1612 | 1/1 | 0.93 | 0.23 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3035 | 1/1 | 0.93 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | YQ | 202 | 1/1 | 0.93 | 0.29 | 27,27,27,27 | 0 |
| 56 | MG | RA | 3314 | 1/1 | 0.93 | 0.33 | 19,19,19,19 | 0 |
| 56 | MG | RB | 202 | 1/1 | 0.93 | 0.35 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3176 | 1/1 | 0.93 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | QA | 1689 | 1/1 | 0.93 | 0.45 | 42,42,42,42 | 0 |
| 56 | MG | QA | 1674 | 1/1 | 0.93 | 0.55 | 27,27,27,27 | 0 |
| 56 | MG | QA | 1659 | 1/1 | 0.93 | 0.28 | 25,25,25,25 | 0 |
| 56 | MG | QA | 1744 | 1/1 | 0.93 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | RA | 3322 | 1/1 | 0.93 | 0.12 | 15,15,15,15 | 0 |
| 56 | MG | XA | 1685 | 1/1 | 0.93 | 0.49 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3462 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | QA | 1749 | 1/1 | 0.93 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3221 | 1/1 | 0.93 | 0.22 | 16,16,16,16 | 0 |
| 56 | MG | YA | 3167 | 1/1 | 0.93 | 0.32 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3393 | 1/1 | 0.93 | 0.49 | 21,21,21,21 | 0 |
| 56 | MG | YA | 3111 | 1/1 | 0.93 | 0.25 | 53,53,53,53 | 0 |
| 56 | MG | YA | 3092 | 1/1 | 0.93 | 0.90 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3136 | 1/1 | 0.93 | 0.34 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3129 | 1/1 | 0.93 | 0.35 | 41,41,41,41 | 0 |
| 56 | MG | R5 | 103 | 1/1 | 0.93 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | R5 | 102 | 1/1 | 0.93 | 0.38 | 53,53,53,53 | 0 |
| 56 | MG | RP | 202 | 1/1 | 0.93 | 0.17 | 18,18,18,18 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3040 | 1/1 | 0.93 | 0.29 | 25,25,25,25 | 0 |
| 56 | MG | QA | 1615 | 1/1 | 0.93 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | YW | 201 | 1/1 | 0.93 | 0.52 | 52,52,52,52 | 0 |
| 56 | MG | XA | 1665 | 1/1 | 0.93 | 0.40 | 26,26,26,26 | 0 |
| 56 | MG | YA | 3258 | 1/1 | 0.93 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3346 | 1/1 | 0.93 | 0.34 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3097 | 1/1 | 0.93 | 0.32 | 21,21,21,21 | 0 |
| 56 | MG | RA | 3386 | 1/1 | 0.94 | 0.23 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3227 | 1/1 | 0.94 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | QA | 1661 | 1/1 | 0.94 | 0.11 | 23,23,23,23 | 0 |
| 56 | MG | QA | 1638 | 1/1 | 0.94 | 0.39 | 64,64,64,64 | 0 |
| 56 | MG | QA | 1610 | 1/1 | 0.94 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | YA | 3180 | 1/1 | 0.94 | 0.23 | 58,58,58,58 | 0 |
| 56 | MG | RA | 3375 | 1/1 | 0.94 | 0.32 | 25,25,25,25 | 0 |
| 56 | MG | QA | 1698 | 1/1 | 0.94 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | QA | 1688 | 1/1 | 0.94 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3330 | 1/1 | 0.94 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3310 | 1/1 | 0.94 | 0.44 | 28,28,28,28 | 0 |
| 56 | MG | RA | 3283 | 1/1 | 0.94 | 0.18 | 18,18,18,18 | 0 |
| 56 | MG | RA | 3098 | 1/1 | 0.94 | 0.37 | 44,44,44,44 | 0 |
| 56 | MG | XA | 1760 | 1/1 | 0.94 | 0.28 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3236 | 1/1 | 0.94 | 0.43 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3114 | 1/1 | 0.94 | 0.20 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3267 | 1/1 | 0.94 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | XA | 1641 | 1/1 | 0.94 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1732 | 1/1 | 0.94 | 0.08 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3247 | 1/1 | 0.94 | 0.29 | 41,41,41,41 | 0 |
| 56 | MG | QA | 1616 | 1/1 | 0.94 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3106 | 1/1 | 0.94 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | YY | 201 | 1/1 | 0.94 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3014 | 1/1 | 0.94 | 0.30 | 18,18,18,18 | 0 |
| 56 | MG | RA | 3319 | 1/1 | 0.94 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | YA | 3382 | 1/1 | 0.94 | 0.40 | 37,37,37,37 | 0 |
| 56 | MG | XA | 1695 | 1/1 | 0.94 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | YA | 3434 | 1/1 | 0.94 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | RA | 3050 | 1/1 | 0.94 | 0.37 | 6,6,6,6 | 0 |
| 56 | MG | YA | 3257 | 1/1 | 0.94 | 0.24 | 36,36,36,36 | 0 |
| 56 | MG | XA | 1647 | 1/1 | 0.94 | 0.20 | 47,47,47,47 | 0 |
| 56 | MG | QA | 1622 | 1/1 | 0.94 | 0.23 | 29,29,29,29 | 0 |
| 56 | MG | QA | 1658 | 1/1 | 0.94 | 0.91 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3323 | 1/1 | 0.94 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | QA | 1691 | 1/1 | 0.94 | 0.32 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | QA | 1666 | 1/1 | 0.94 | 0.13 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3213 | 1/1 | 0.94 | 0.38 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3254 | 1/1 | 0.94 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | XA | 1669 | 1/1 | 0.94 | 0.30 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3308 | 1/1 | 0.94 | 0.28 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3305 | 1/1 | 0.94 | 0.30 | 21,21,21,21 | 0 |
| 56 | MG | YA | 3142 | 1/1 | 0.94 | 0.33 | 14,14,14,14 | 0 |
| 56 | MG | XA | 1637 | 1/1 | 0.94 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | YA | 3224 | 1/1 | 0.94 | 0.47 | 22,22,22,22 | 0 |
| 56 | MG | XA | 1698 | 1/1 | 0.94 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3469 | 1/1 | 0.94 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | RA | 3069 | 1/1 | 0.94 | 0.46 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3177 | 1/1 | 0.94 | 0.35 | 35,35,35,35 | 0 |
| 56 | MG | XA | 1707 | 1/1 | 0.94 | 0.66 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3179 | 1/1 | 0.94 | 0.39 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3198 | 1/1 | 0.94 | 0.27 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3369 | 1/1 | 0.94 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | RA | 3076 | 1/1 | 0.94 | 0.38 | 15,15,15,15 | 0 |
| 56 | MG | XA | 1682 | 1/1 | 0.94 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3248 | 1/1 | 0.94 | 0.37 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3086 | 1/1 | 0.94 | 0.18 | 23,23,23,23 | 0 |
| 56 | MG | XA | 1612 | 1/1 | 0.94 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | YA | 3455 | 1/1 | 0.94 | 0.47 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3418 | 1/1 | 0.94 | 0.17 | 16,16,16,16 | 0 |
| 56 | MG | YA | 3340 | 1/1 | 0.94 | 0.53 | 29,29,29,29 | 0 |
| 56 | MG | XA | 1703 | 1/1 | 0.94 | 0.39 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3160 | 1/1 | 0.94 | 0.39 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3107 | 1/1 | 0.94 | 0.42 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3420 | 1/1 | 0.94 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | XA | 1636 | 1/1 | 0.94 | 0.26 | 57,57,57,57 | 0 |
| 56 | MG | RA | 3210 | 1/1 | 0.94 | 0.50 | 50,50,50,50 | 0 |
| 56 | MG | XA | 1748 | 1/1 | 0.94 | 0.23 | 66,66,66,66 | 0 |
| 56 | MG | YA | 3298 | 1/1 | 0.94 | 0.21 | 21,21,21,21 | 0 |
| 56 | MG | XA | 1663 | 1/1 | 0.94 | 0.24 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3348 | 1/1 | 0.94 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3156 | 1/1 | 0.94 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3022 | 1/1 | 0.94 | 0.36 | 17,17,17,17 | 0 |
| 56 | MG | XA | 1680 | 1/1 | 0.94 | 0.21 | 24,24,24,24 | 0 |
| 56 | MG | QA | 1717 | 1/1 | 0.94 | 0.77 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3331 | 1/1 | 0.94 | 0.19 | 24,24,24,24 | 0 |
| 56 | MG | XA | 1632 | 1/1 | 0.94 | 0.27 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3367 | 1/1 | 0.94 | 0.16 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3224 | 1/1 | 0.94 | 0.19 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3486 | 1/1 | 0.94 | 0.10 | 19,19,19,19 | 0 |
| 56 | MG | RA | 3371 | 1/1 | 0.94 | 0.40 | 51,51,51,51 | 0 |
| 56 | MG | RA | 3183 | 1/1 | 0.94 | 0.23 | 21,21,21,21 | 0 |
| 56 | MG | RA | 3429 | 1/1 | 0.94 | 0.25 | 50,50,50,50 | 0 |
| 56 | MG | RA | 3123 | 1/1 | 0.94 | 0.43 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3041 | 1/1 | 0.94 | 0.31 | 30,30,30,30 | 0 |
| 56 | MG | XA | 1618 | 1/1 | 0.94 | 0.31 | 15,15,15,15 | 0 |
| 56 | MG | XA | 1737 | 1/1 | 0.94 | 0.47 | 14,14,14,14 | 0 |
| 56 | MG | XA | 1644 | 1/1 | 0.94 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3289 | 1/1 | 0.94 | 0.25 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3252 | 1/1 | 0.94 | 0.50 | 47,47,47,47 | 0 |
| 56 | MG | QA | 1739 | 1/1 | 0.94 | 0.43 | 42,42,42,42 | 0 |
| 56 | MG | RA | 3359 | 1/1 | 0.94 | 0.16 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3286 | 1/1 | 0.94 | 0.33 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3072 | 1/1 | 0.94 | 0.34 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3193 | 1/1 | 0.94 | 0.17 | 18,18,18,18 | 0 |
| 56 | MG | QA | 1646 | 1/1 | 0.94 | 0.37 | 36,36,36,36 | 0 |
| 56 | MG | RA | 3335 | 1/1 | 0.94 | 0.35 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3403 | 1/1 | 0.94 | 0.28 | 43,43,43,43 | 0 |
| 56 | MG | XA | 1753 | 1/1 | 0.94 | 0.29 | 70,70,70,70 | 0 |
| 56 | MG | YA | 3275 | 1/1 | 0.94 | 0.34 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3417 | 1/1 | 0.95 | 0.47 | 22,22,22,22 | 0 |
| 56 | MG | YA | 3335 | 1/1 | 0.95 | 0.50 | 16,16,16,16 | 0 |
| 56 | MG | XS | 300 | 1/1 | 0.95 | 0.30 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3353 | 1/1 | 0.95 | 0.38 | 8,8,8,8 | 0 |
| 56 | MG | YA | 3297 | 1/1 | 0.95 | 0.45 | 35,35,35,35 | 0 |
| 56 | MG | RA | 3372 | 1/1 | 0.95 | 0.20 | 7,7,7,7 | 0 |
| 56 | MG | XA | 1638 | 1/1 | 0.95 | 0.33 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3314 | 1/1 | 0.95 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3043 | 1/1 | 0.95 | 0.35 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3338 | 1/1 | 0.95 | 0.47 | 15,15,15,15 | 0 |
| 56 | MG | QA | 1631 | 1/1 | 0.95 | 0.38 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3337 | 1/1 | 0.95 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3271 | 1/1 | 0.95 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3196 | 1/1 | 0.95 | 0.39 | 18,18,18,18 | 0 |
| 56 | MG | RA | 3142 | 1/1 | 0.95 | 0.23 | 24,24,24,24 | 0 |
| 56 | MG | RA | 3393 | 1/1 | 0.95 | 0.21 | 38,38,38,38 | 0 |
| 56 | MG | QA | 1620 | 1/1 | 0.95 | 0.15 | 13,13,13,13 | 0 |
| 56 | MG | YA | 3154 | 1/1 | 0.95 | 0.15 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3361 | 1/1 | 0.95 | 0.56 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3053 | 1/1 | 0.95 | 0.18 | 21,21,21,21 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | QA | 1602 | 1/1 | 0.95 | 0.47 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3470 | 1/1 | 0.95 | 0.28 | 35,35,35,35 | 0 |
| 57 | ZN | QN | 101 | 1/1 | 0.95 | 0.14 | 76,76,76,76 | 0 |
| 56 | MG | YA | 3146 | 1/1 | 0.95 | 0.38 | 24,24,24,24 | 0 |
| 56 | MG | YB | 205 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3465 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | QA | 1609 | 1/1 | 0.95 | 0.31 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3450 | 1/1 | 0.95 | 0.23 | 43,43,43,43 | 0 |
| 56 | MG | YA | 3080 | 1/1 | 0.95 | 0.49 | 15,15,15,15 | 0 |
| 56 | MG | RA | 3150 | 1/1 | 0.95 | 0.40 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3431 | 1/1 | 0.95 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | QA | 1649 | 1/1 | 0.95 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3414 | 1/1 | 0.95 | 0.68 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3241 | 1/1 | 0.95 | 0.26 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3045 | 1/1 | 0.95 | 0.23 | 3,3,3,3 | 0 |
| 56 | MG | QA | 1617 | 1/1 | 0.95 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3129 | 1/1 | 0.95 | 0.13 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3018 | 1/1 | 0.95 | 0.45 | 10,10,10,10 | 0 |
| 56 | MG | YA | 3002 | 1/1 | 0.95 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | XA | 1742 | 1/1 | 0.95 | 0.43 | 73,73,73,73 | 0 |
| 56 | MG | RA | 3437 | 1/1 | 0.95 | 0.18 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3116 | 1/1 | 0.95 | 0.27 | 16,16,16,16 | 0 |
| 56 | MG | YA | 3022 | 1/1 | 0.95 | 0.54 | 49,49,49,49 | 0 |
| 56 | MG | XA | 1643 | 1/1 | 0.95 | 0.35 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3218 | 1/1 | 0.95 | 0.21 | 13,13,13,13 | 0 |
| 56 | MG | RT | 201 | 1/1 | 0.95 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3147 | 1/1 | 0.95 | 0.59 | 1,1,1,1 | 0 |
| 56 | MG | RA | 3382 | 1/1 | 0.95 | 0.28 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3065 | 1/1 | 0.95 | 0.24 | 29,29,29,29 | 0 |
| 56 | MG | QA | 1687 | 1/1 | 0.95 | 0.25 | 52,52,52,52 | 0 |
| 56 | MG | RA | 3262 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | RA | 3205 | 1/1 | 0.95 | 0.23 | 19,19,19,19 | 0 |
| 56 | MG | RA | 3297 | 1/1 | 0.95 | 0.34 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3031 | 1/1 | 0.95 | 0.33 | 6,6,6,6 | 0 |
| 56 | MG | RA | 3138 | 1/1 | 0.95 | 0.29 | 10,10,10,10 | 0 |
| 56 | MG | YA | 3176 | 1/1 | 0.95 | 0.39 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3477 | 1/1 | 0.95 | 0.35 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3216 | 1/1 | 0.95 | 0.32 | 36,36,36,36 | 0 |
| 56 | MG | YA | 3088 | 1/1 | 0.95 | 0.21 | 5,5,5,5 | 0 |
| 56 | MG | YA | 3112 | 1/1 | 0.95 | 0.14 | 14,14,14,14 | 0 |
| 56 | MG | RP | 203 | 1/1 | 0.95 | 0.17 | 4,4,4,4 | 0 |
| 56 | MG | XA | 1655 | 1/1 | 0.95 | 0.18 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | R0 | 102 | 1/1 | 0.95 | 0.61 | 39,39,39,39 | 0 |
| 56 | MG | RA | 3278 | 1/1 | 0.95 | 0.42 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3292 | 1/1 | 0.95 | 0.71 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3269 | 1/1 | 0.95 | 0.40 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3008 | 1/1 | 0.95 | 0.96 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3212 | 1/1 | 0.95 | 0.34 | 18,18,18,18 | 0 |
| 56 | MG | RA | 3107 | 1/1 | 0.95 | 0.25 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3404 | 1/1 | 0.95 | 0.39 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3208 | 1/1 | 0.95 | 0.50 | 27,27,27,27 | 0 |
| 56 | MG | QA | 1672 | 1/1 | 0.95 | 0.66 | 54,54,54,54 | 0 |
| 56 | MG | RA | 3317 | 1/1 | 0.95 | 0.22 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3413 | 1/1 | 0.95 | 0.26 | 7,7,7,7 | 0 |
| 56 | MG | RA | 3126 | 1/1 | 0.95 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3144 | 1/1 | 0.95 | 0.21 | 10,10,10,10 | 0 |
| 56 | MG | RA | 3030 | 1/1 | 0.95 | 0.20 | 13,13,13,13 | 0 |
| 56 | MG | RA | 3341 | 1/1 | 0.95 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3115 | 1/1 | 0.95 | 0.36 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3071 | 1/1 | 0.95 | 0.20 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3068 | 1/1 | 0.95 | 0.40 | 13,13,13,13 | 0 |
| 56 | MG | YA | 3206 | 1/1 | 0.95 | 0.15 | 12,12,12,12 | 0 |
| 56 | MG | YA | 3266 | 1/1 | 0.95 | 0.25 | 42,42,42,42 | 0 |
| 56 | MG | RA | 3304 | 1/1 | 0.95 | 0.35 | 37,37,37,37 | 0 |
| 56 | MG | RA | 3282 | 1/1 | 0.95 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | R5 | 101 | 1/1 | 0.95 | 0.32 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3054 | 1/1 | 0.95 | 0.36 | 11,11,11,11 | 0 |
| 56 | MG | Y1 | 101 | 1/1 | 0.95 | 0.37 | 24,24,24,24 | 0 |
| 56 | MG | RA | 3436 | 1/1 | 0.95 | 0.30 | 8,8,8,8 | 0 |
| 56 | MG | RA | 3390 | 1/1 | 0.95 | 0.32 | 49,49,49,49 | 0 |
| 56 | MG | RA | 3294 | 1/1 | 0.95 | 0.12 | 10,10,10,10 | 0 |
| 56 | MG | YA | 3171 | 1/1 | 0.95 | 0.09 | 26,26,26,26 | 0 |
| 56 | MG | XA | 1660 | 1/1 | 0.95 | 0.38 | 37,37,37,37 | 0 |
| 56 | MG | XA | 1651 | 1/1 | 0.95 | 0.21 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3201 | 1/1 | 0.95 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | YA | 3254 | 1/1 | 0.95 | 0.40 | 26,26,26,26 | 0 |
| 56 | MG | XA | 1623 | 1/1 | 0.95 | 0.11 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3223 | 1/1 | 0.95 | 0.25 | 26,26,26,26 | 0 |
| 56 | MG | YA | 3204 | 1/1 | 0.95 | 0.20 | 10,10,10,10 | 0 |
| 56 | MG | RA | 3049 | 1/1 | 0.95 | 0.36 | 19,19,19,19 | 0 |
| 56 | MG | RA | 3284 | 1/1 | 0.95 | 0.33 | 48,48,48,48 | 0 |
| 56 | MG | RA | 3363 | 1/1 | 0.95 | 0.65 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3377 | 1/1 | 0.95 | 0.22 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3123 | 1/1 | 0.95 | 0.37 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3017 | 1/1 | 0.96 | 0.70 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3133 | 1/1 | 0.96 | 0.34 | 52,52,52,52 | 0 |
| 56 | MG | XA | 1614 | 1/1 | 0.96 | 0.22 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3483 | 1/1 | 0.96 | 0.96 | 58,58,58,58 | 0 |
| 56 | MG | RA | 3208 | 1/1 | 0.96 | 0.30 | 35,35,35,35 | 0 |
| 56 | MG | RA | 3270 | 1/1 | 0.96 | 0.32 | 51,51,51,51 | 0 |
| 56 | MG | QA | 1736 | 1/1 | 0.96 | 0.18 | 33,33,33,33 | 0 |
| 56 | MG | XA | 1615 | 1/1 | 0.96 | 0.32 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3243 | 1/1 | 0.96 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3367 | 1/1 | 0.96 | 0.29 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3365 | 1/1 | 0.96 | 0.39 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3441 | 1/1 | 0.96 | 0.28 | 14,14,14,14 | 0 |
| 56 | MG | YA | 3131 | 1/1 | 0.96 | 0.17 | 11,11,11,11 | 0 |
| 56 | MG | RA | 3203 | 1/1 | 0.96 | 0.25 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3219 | 1/1 | 0.96 | 0.16 | 9,9,9,9 | 0 |
| 56 | MG | XA | 1673 | 1/1 | 0.96 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | RP | 201 | 1/1 | 0.96 | 0.25 | 21,21,21,21 | 0 |
| 56 | MG | RA | 3257 | 1/1 | 0.96 | 0.13 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3001 | 1/1 | 0.96 | 0.33 | 41,41,41,41 | 0 |
| 56 | MG | YA | 3156 | 1/1 | 0.96 | 0.36 | 15,15,15,15 | 0 |
| 56 | MG | RA | 3090 | 1/1 | 0.96 | 0.42 | 4,4,4,4 | 0 |
| 56 | MG | YA | 3021 | 1/1 | 0.96 | 0.21 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3327 | 1/1 | 0.96 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | RA | 3301 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | QA | 1641 | 1/1 | 0.96 | 0.45 | 32,32,32,32 | 0 |
| 56 | MG | QA | 1632 | 1/1 | 0.96 | 0.46 | 57,57,57,57 | 0 |
| 56 | MG | YA | 3203 | 1/1 | 0.96 | 0.25 | 30,30,30,30 | 0 |
| 56 | MG | QA | 1676 | 1/1 | 0.96 | 0.31 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3234 | 1/1 | 0.96 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | XA | 1762 | 1/1 | 0.96 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | YA | 3042 | 1/1 | 0.96 | 0.38 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3475 | 1/1 | 0.96 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | RA | 3044 | 1/1 | 0.96 | 0.32 | 1,1,1,1 | 0 |
| 56 | MG | YA | 3139 | 1/1 | 0.96 | 0.28 | 36,36,36,36 | 0 |
| 56 | MG | RA | 3178 | 1/1 | 0.96 | 0.21 | 32,32,32,32 | 0 |
| 56 | MG | QV | 104 | 1/1 | 0.96 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | YA | 3143 | 1/1 | 0.96 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3120 | 1/1 | 0.96 | 0.54 | 33,33,33,33 | 0 |
| 56 | MG | YA | 3175 | 1/1 | 0.96 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | XA | 1626 | 1/1 | 0.96 | 0.34 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3094 | 1/1 | 0.96 | 0.66 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3168 | 1/1 | 0.96 | 0.30 | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3242 | 1/1 | 0.96 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | XA | 1692 | 1/1 | 0.96 | 0.25 | 36,36,36,36 | 0 |
| 56 | MG | YA | 3320 | 1/1 | 0.96 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3444 | 1/1 | 0.96 | 0.27 | 5,5,5,5 | 0 |
| 56 | MG | YA | 3374 | 1/1 | 0.96 | 0.18 | 28,28,28,28 | 0 |
| 56 | MG | YA | 3007 | 1/1 | 0.96 | 1.05 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3036 | 1/1 | 0.96 | 0.30 | 26,26,26,26 | 0 |
| 56 | MG | YA | 3474 | 1/1 | 0.96 | 0.13 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3122 | 1/1 | 0.96 | 0.49 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3309 | 1/1 | 0.96 | 0.74 | 45,45,45,45 | 0 |
| 56 | MG | RA | 3200 | 1/1 | 0.96 | 0.46 | 31,31,31,31 | 0 |
| 56 | MG | XA | 1671 | 1/1 | 0.96 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | XA | 1740 | 1/1 | 0.96 | 0.32 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3376 | 1/1 | 0.96 | 0.32 | 5,5,5,5 | 0 |
| 56 | MG | YA | 3197 | 1/1 | 0.96 | 0.38 | 22,22,22,22 | 0 |
| 56 | MG | YA | 3217 | 1/1 | 0.96 | 0.28 | 23,23,23,23 | 0 |
| 56 | MG | QA | 1704 | 1/1 | 0.96 | 0.56 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3399 | 1/1 | 0.96 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | YA | 3074 | 1/1 | 0.96 | 0.54 | 21,21,21,21 | 0 |
| 56 | MG | RA | 3344 | 1/1 | 0.96 | 0.13 | 15,15,15,15 | 0 |
| 56 | MG | YA | 3096 | 1/1 | 0.96 | 0.30 | 40,40,40,40 | 0 |
| 56 | MG | YA | 3119 | 1/1 | 0.96 | 0.15 | 10,10,10,10 | 0 |
| 56 | MG | YA | 3160 | 1/1 | 0.96 | 0.27 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3020 | 1/1 | 0.96 | 0.30 | 11,11,11,11 | 0 |
| 56 | MG | YA | 3250 | 1/1 | 0.96 | 0.44 | 27,27,27,27 | 0 |
| 56 | MG | RA | 3321 | 1/1 | 0.96 | 0.27 | 33,33,33,33 | 0 |
| 56 | MG | RA | 3374 | 1/1 | 0.96 | 0.31 | 51,51,51,51 | 0 |
| 56 | MG | XA | 1701 | 1/1 | 0.96 | 0.34 | 42,42,42,42 | 0 |
| 56 | MG | YA | 3016 | 1/1 | 0.96 | 0.07 | 2,2,2,2 | 0 |
| 56 | MG | RA | 3350 | 1/1 | 0.96 | 0.24 | 45,45,45,45 | 0 |
| 56 | MG | XA | 1633 | 1/1 | 0.96 | 0.33 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3273 | 1/1 | 0.96 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3015 | 1/1 | 0.96 | 0.28 | 9,9,9,9 | 0 |
| 56 | MG | XA | 1676 | 1/1 | 0.96 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | XA | 1694 | 1/1 | 0.96 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3198 | 1/1 | 0.96 | 0.28 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3124 | 1/1 | 0.96 | 0.24 | 32,32,32,32 | 0 |
| 56 | MG | RA | 3104 | 1/1 | 0.96 | 0.46 | 28,28,28,28 | 0 |
| 56 | MG | RA | 3409 | 1/1 | 0.96 | 0.21 | 69,69,69,69 | 0 |
| 56 | MG | RA | 3086 | 1/1 | 0.96 | 0.25 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3055 | 1/1 | 0.96 | 0.25 | 12,12,12,12 | 0 |
| 56 | MG | QA | 1645 | 1/1 | 0.96 | 0.25 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3369 | 1/1 | 0.96 | 0.54 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3004 | 1/1 | 0.96 | 0.43 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3255 | 1/1 | 0.96 | 0.27 | 38,38,38,38 | 0 |
| 56 | MG | RA | 3029 | 1/1 | 0.96 | 0.24 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3388 | 1/1 | 0.96 | 0.47 | 15,15,15,15 | 0 |
| 56 | MG | YA | 3373 | 1/1 | 0.96 | 0.26 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3005 | 1/1 | 0.96 | 0.23 | 1,1,1,1 | 0 |
| 56 | MG | YA | 3138 | 1/1 | 0.96 | 0.04 | 18,18,18,18 | 0 |
| 56 | MG | YA | 3070 | 1/1 | 0.96 | 0.34 | 3,3,3,3 | 0 |
| 56 | MG | YA | 3015 | 1/1 | 0.96 | 0.28 | 9,9,9,9 | 0 |
| 56 | MG | RA | 3012 | 1/1 | 0.96 | 0.76 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3079 | 1/1 | 0.96 | 0.24 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3407 | 1/1 | 0.96 | 0.34 | 4,4,4,4 | 0 |
| 56 | MG | YA | 3085 | 1/1 | 0.96 | 0.36 | 17,17,17,17 | 0 |
| 56 | MG | XA | 1674 | 1/1 | 0.96 | 0.23 | 32,32,32,32 | 0 |
| 56 | MG | RA | 3119 | 1/1 | 0.96 | 0.17 | 8,8,8,8 | 0 |
| 56 | MG | YA | 3012 | 1/1 | 0.96 | 0.28 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3424 | 1/1 | 0.96 | 0.16 | 26,26,26,26 | 0 |
| 56 | MG | YA | 3028 | 1/1 | 0.96 | 0.27 | 18,18,18,18 | 0 |
| 56 | MG | YA | 3063 | 1/1 | 0.96 | 0.18 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3299 | 1/1 | 0.96 | 0.29 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3179 | 1/1 | 0.96 | 0.40 | 30,30,30,30 | 0 |
| 56 | MG | YA | 3356 | 1/1 | 0.97 | 0.19 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3010 | 1/1 | 0.97 | 0.41 | 14,14,14,14 | 0 |
| 56 | MG | XA | 1639 | 1/1 | 0.97 | 0.39 | 48,48,48,48 | 0 |
| 56 | MG | YA | 3011 | 1/1 | 0.97 | 0.52 | 0,0,0,0 | 0 |
| 56 | MG | QA | 1642 | 1/1 | 0.97 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | YA | 3072 | 1/1 | 0.97 | 0.36 | 19,19,19,19 | 0 |
| 56 | MG | XV | 101 | 1/1 | 0.97 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | XA | 1628 | 1/1 | 0.97 | 0.49 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3065 | 1/1 | 0.97 | 0.41 | 10,10,10,10 | 0 |
| 56 | MG | YA | 3442 | 1/1 | 0.97 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | QA | 1625 | 1/1 | 0.97 | 0.32 | 66,66,66,66 | 0 |
| 56 | MG | YA | 3300 | 1/1 | 0.97 | 0.33 | 48,48,48,48 | 0 |
| 56 | MG | XA | 1708 | 1/1 | 0.97 | 0.27 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3286 | 1/1 | 0.97 | 0.18 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3053 | 1/1 | 0.97 | 0.49 | 27,27,27,27 | 0 |
| 56 | MG | RA | 3088 | 1/1 | 0.97 | 0.20 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3103 | 1/1 | 0.97 | 0.36 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3264 | 1/1 | 0.97 | 0.29 | 16,16,16,16 | 0 |
| 56 | MG | YA | 3200 | 1/1 | 0.97 | 0.11 | 1,1,1,1 | 0 |
| 56 | MG | RA | 3115 | 1/1 | 0.97 | 0.31 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3194 | 1/1 | 0.97 | 0.38 | 21,21,21,21 | 0 |
| 56 | MG | YA | 3027 | 1/1 | 0.97 | 0.42 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3231 | 1/1 | 0.97 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | RA | 3243 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | YA | 3194 | 1/1 | 0.97 | 0.28 | 17,17,17,17 | 0 |
| 56 | MG | XA | 1657 | 1/1 | 0.97 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | XA | 1602 | 1/1 | 0.97 | 0.44 | 8,8,8,8 | 0 |
| 56 | MG | RA | 3071 | 1/1 | 0.97 | 0.28 | 9,9,9,9 | 0 |
| 56 | MG | YA | 3003 | 1/1 | 0.97 | 0.44 | 4,4,4,4 | 0 |
| 56 | MG | RA | 3337 | 1/1 | 0.97 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | XA | 1752 | 1/1 | 0.97 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | RA | 3260 | 1/1 | 0.97 | 0.37 | 22,22,22,22 | 0 |
| 56 | MG | YA | 3043 | 1/1 | 0.97 | 0.24 | 9,9,9,9 | 0 |
| 56 | MG | YA | 3032 | 1/1 | 0.97 | 0.23 | 16,16,16,16 | 0 |
| 56 | MG | QA | 1651 | 1/1 | 0.97 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3395 | 1/1 | 0.97 | 0.40 | 27,27,27,27 | 0 |
| 56 | MG | QA | 1730 | 1/1 | 0.97 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | YA | 3451 | 1/1 | 0.97 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3170 | 1/1 | 0.97 | 0.41 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3073 | 1/1 | 0.97 | 0.34 | 15,15,15,15 | 0 |
| 56 | MG | Y5 | 103 | 1/1 | 0.97 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | QA | 1635 | 1/1 | 0.97 | 0.40 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3066 | 1/1 | 0.97 | 0.29 | 27,27,27,27 | 0 |
| 56 | MG | QX | 101 | 1/1 | 0.97 | 0.23 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3287 | 1/1 | 0.97 | 0.09 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3293 | 1/1 | 0.97 | 0.39 | 58,58,58,58 | 0 |
| 56 | MG | RA | 3078 | 1/1 | 0.97 | 0.41 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3181 | 1/1 | 0.97 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | QA | 1700 | 1/1 | 0.97 | 0.56 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3040 | 1/1 | 0.97 | 0.47 | 4,4,4,4 | 0 |
| 56 | MG | XA | 1616 | 1/1 | 0.97 | 0.24 | 25,25,25,25 | 0 |
| 56 | MG | YP | 201 | 1/1 | 0.97 | 0.13 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3125 | 1/1 | 0.97 | 0.23 | 13,13,13,13 | 0 |
| 57 | ZN | QD | 301 | 1/1 | 0.97 | 0.33 | 29,29,29,29 | 0 |
| 56 | MG | XA | 1681 | 1/1 | 0.97 | 0.34 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3110 | 1/1 | 0.97 | 0.44 | 8,8,8,8 | 0 |
| 56 | MG | QA | 1715 | 1/1 | 0.97 | 0.38 | 72,72,72,72 | 0 |
| 56 | MG | YA | 3212 | 1/1 | 0.97 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | XA | 1604 | 1/1 | 0.97 | 0.28 | 9,9,9,9 | 0 |
| 56 | MG | RA | 3021 | 1/1 | 0.97 | 0.21 | 4,4,4,4 | 0 |
| 56 | MG | YA | 3089 | 1/1 | 0.97 | 0.51 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3030 | 1/1 | 0.97 | 0.31 | 3,3,3,3 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | YA | 3327 | 1/1 | 0.97 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | YA | 3036 | 1/1 | 0.97 | 0.38 | 10,10,10,10 | 0 |
| 56 | MG | QA | 1644 | 1/1 | 0.97 | 0.24 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3310 | 1/1 | 0.97 | 0.39 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3487 | 1/1 | 0.97 | 0.34 | 18,18,18,18 | 0 |
| 56 | MG | Y5 | 101 | 1/1 | 0.97 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | YA | 3186 | 1/1 | 0.97 | 0.40 | 1,1,1,1 | 0 |
| 56 | MG | YA | 3236 | 1/1 | 0.97 | 0.33 | 14,14,14,14 | 0 |
| 56 | MG | XA | 1661 | 1/1 | 0.97 | 0.30 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3387 | 1/1 | 0.97 | 0.42 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3028 | 1/1 | 0.97 | 0.49 | 10,10,10,10 | 0 |
| 56 | MG | RA | 3145 | 1/1 | 0.97 | 0.24 | 9,9,9,9 | 0 |
| 56 | MG | RA | 3055 | 1/1 | 0.97 | 0.51 | 10,10,10,10 | 0 |
| 56 | MG | RA | 3221 | 1/1 | 0.97 | 0.28 | 22,22,22,22 | 0 |
| 56 | MG | XA | 1635 | 1/1 | 0.97 | 0.53 | 36,36,36,36 | 0 |
| 56 | MG | XA | 1679 | 1/1 | 0.97 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | RA | 3046 | 1/1 | 0.97 | 0.44 | 7,7,7,7 | 0 |
| 56 | MG | RA | 3027 | 1/1 | 0.97 | 0.42 | 2,2,2,2 | 0 |
| 56 | MG | RA | 3009 | 1/1 | 0.97 | 0.15 | 6,6,6,6 | 0 |
| 56 | MG | RA | 3139 | 1/1 | 0.97 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | RA | 3057 | 1/1 | 0.97 | 0.52 | 2,2,2,2 | 0 |
| 56 | MG | YA | 3124 | 1/1 | 0.97 | 0.23 | 8,8,8,8 | 0 |
| 56 | MG | YA | 3052 | 1/1 | 0.97 | 0.29 | 1,1,1,1 | 0 |
| 56 | MG | YA | 3273 | 1/1 | 0.97 | 0.18 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3228 | 1/1 | 0.97 | 0.17 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3074 | 1/1 | 0.97 | 0.44 | 27,27,27,27 | 0 |
| 56 | MG | RA | 3026 | 1/1 | 0.97 | 0.54 | 24,24,24,24 | 0 |
| 56 | MG | RA | 3006 | 1/1 | 0.97 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | RA | 3113 | 1/1 | 0.97 | 0.11 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3081 | 1/1 | 0.97 | 0.34 | 4,4,4,4 | 0 |
| 56 | MG | YA | 3109 | 1/1 | 0.97 | 0.44 | 14,14,14,14 | 0 |
| 56 | MG | YA | 3288 | 1/1 | 0.97 | 0.19 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3140 | 1/1 | 0.97 | 0.30 | 34,34,34,34 | 0 |
| 56 | MG | RA | 3122 | 1/1 | 0.97 | 0.39 | 8,8,8,8 | 0 |
| 56 | MG | XA | 1659 | 1/1 | 0.97 | 0.42 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3202 | 1/1 | 0.97 | 0.26 | 15,15,15,15 | 0 |
| 56 | MG | RA | 3419 | 1/1 | 0.97 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3468 | 1/1 | 0.97 | 0.76 | 47,47,47,47 | 0 |
| 56 | MG | RA | 3052 | 1/1 | 0.97 | 0.26 | 4,4,4,4 | 0 |
| 56 | MG | YA | 3445 | 1/1 | 0.97 | 0.10 | 19,19,19,19 | 0 |
| 56 | MG | YA | 3191 | 1/1 | 0.97 | 0.40 | 9,9,9,9 | 0 |
| 56 | MG | QA | 1726 | 1/1 | 0.97 | 0.09 | 23,23,23,23 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | XA | 1653 | 1/1 | 0.97 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | Y0 | 101 | 1/1 | 0.97 | 0.14 | 18,18,18,18 | 0 |
| 56 | MG | XA | 1732 | 1/1 | 0.97 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | XA | 1735 | 1/1 | 0.97 | 0.26 | 16,16,16,16 | 0 |
| 56 | MG | YA | 3077 | 1/1 | 0.97 | 0.42 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3109 | 1/1 | 0.97 | 0.62 | 18,18,18,18 | 0 |
| 56 | MG | YA | 3230 | 1/1 | 0.97 | 0.32 | 38,38,38,38 | 0 |
| 56 | MG | YA | 3312 | 1/1 | 0.97 | 0.39 | 63,63,63,63 | 0 |
| 56 | MG | YA | 3113 | 1/1 | 0.98 | 0.28 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3291 | 1/1 | 0.98 | 0.33 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3163 | 1/1 | 0.98 | 0.25 | 34,34,34,34 | 0 |
| 56 | MG | YA | 3284 | 1/1 | 0.98 | 0.17 | 14,14,14,14 | 0 |
| 56 | MG | QA | 1714 | 1/1 | 0.98 | 0.13 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3155 | 1/1 | 0.98 | 0.24 | 12,12,12,12 | 0 |
| 56 | MG | YA | 3024 | 1/1 | 0.98 | 0.28 | 13,13,13,13 | 0 |
| 56 | MG | YA | 3207 | 1/1 | 0.98 | 0.19 | 13,13,13,13 | 0 |
| 56 | MG | RA | 3228 | 1/1 | 0.98 | 0.42 | 18,18,18,18 | 0 |
| 56 | MG | YA | 3158 | 1/1 | 0.98 | 0.28 | 40,40,40,40 | 0 |
| 56 | MG | XA | 1605 | 1/1 | 0.98 | 0.26 | 6,6,6,6 | 0 |
| 56 | MG | RA | 3289 | 1/1 | 0.98 | 0.26 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3009 | 1/1 | 0.98 | 0.33 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3174 | 1/1 | 0.98 | 0.15 | 15,15,15,15 | 0 |
| 56 | MG | YA | 3033 | 1/1 | 0.98 | 0.25 | 10,10,10,10 | 0 |
| 56 | MG | YA | 3006 | 1/1 | 0.98 | 0.49 | 32,32,32,32 | 0 |
| 56 | MG | QA | 1653 | 1/1 | 0.98 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3325 | 1/1 | 0.98 | 0.37 | 14,14,14,14 | 0 |
| 56 | MG | YA | 3419 | 1/1 | 0.98 | 0.23 | 2,2,2,2 | 0 |
| 56 | MG | RA | 3077 | 1/1 | 0.98 | 0.35 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3130 | 1/1 | 0.98 | 0.29 | 12,12,12,12 | 0 |
| 56 | MG | YA | 3370 | 1/1 | 0.98 | 0.33 | 24,24,24,24 | 0 |
| 56 | MG | RA | 3238 | 1/1 | 0.98 | 0.10 | 11,11,11,11 | 0 |
| 56 | MG | YA | 3093 | 1/1 | 0.98 | 0.23 | 17,17,17,17 | 0 |
| 56 | MG | QA | 1664 | 1/1 | 0.98 | 0.20 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3067 | 1/1 | 0.98 | 0.38 | 19,19,19,19 | 0 |
| 56 | MG | RA | 3038 | 1/1 | 0.98 | 0.23 | 2,2,2,2 | 0 |
| 56 | MG | RA | 3063 | 1/1 | 0.98 | 0.63 | 29,29,29,29 | 0 |
| 56 | MG | YA | 3054 | 1/1 | 0.98 | 0.48 | 1,1,1,1 | 0 |
| 56 | MG | XA | 1699 | 1/1 | 0.98 | 0.17 | 78,78,78,78 | 0 |
| 56 | MG | XA | 1609 | 1/1 | 0.98 | 0.06 | 79,79,79,79 | 0 |
| 56 | MG | XA | 1603 | 1/1 | 0.98 | 0.20 | 24,24,24,24 | 0 |
| 56 | MG | RA | 3381 | 1/1 | 0.98 | 0.46 | 0,0,0,0 | 0 |
| 56 | MG | RA | 3385 | 1/1 | 0.98 | 0.35 | 2,2,2,2 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3378 | 1/1 | 0.98 | 0.37 | 2,2,2,2 | 0 |
| 56 | MG | XA | 1712 | 1/1 | 0.98 | 0.34 | 34,34,34,34 | 0 |
| 56 | MG | RA | 3016 | 1/1 | 0.98 | 0.30 | 6,6,6,6 | 0 |
| 56 | MG | YA | 3135 | 1/1 | 0.98 | 0.21 | 14,14,14,14 | 0 |
| 56 | MG | QA | 1684 | 1/1 | 0.98 | 0.25 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3020 | 1/1 | 0.98 | 0.22 | 18,18,18,18 | 0 |
| 56 | MG | YA | 3435 | 1/1 | 0.98 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | QA | 1619 | 1/1 | 0.98 | 0.41 | 12,12,12,12 | 0 |
| 56 | MG | QA | 1657 | 1/1 | 0.98 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3019 | 1/1 | 0.98 | 0.27 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3076 | 1/1 | 0.98 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3189 | 1/1 | 0.98 | 0.46 | 6,6,6,6 | 0 |
| 56 | MG | YD | 301 | 1/1 | 0.98 | 0.44 | 2,2,2,2 | 0 |
| 56 | MG | RA | 3118 | 1/1 | 0.98 | 0.32 | 31,31,31,31 | 0 |
| 56 | MG | QA | 1723 | 1/1 | 0.98 | 0.66 | 46,46,46,46 | 0 |
| 56 | MG | QA | 1633 | 1/1 | 0.98 | 0.42 | 23,23,23,23 | 0 |
| 56 | MG | RA | 3195 | 1/1 | 0.98 | 0.61 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3025 | 1/1 | 0.98 | 0.21 | 12,12,12,12 | 0 |
| 56 | MG | YA | 3201 | 1/1 | 0.98 | 0.42 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3237 | 1/1 | 0.98 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | QA | 1660 | 1/1 | 0.98 | 0.19 | 14,14,14,14 | 0 |
| 56 | MG | RA | 3112 | 1/1 | 0.98 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | XA | 1690 | 1/1 | 0.98 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | RA | 3193 | 1/1 | 0.98 | 0.33 | 0,0,0,0 | 0 |
| 56 | MG | QA | 1601 | 1/1 | 0.98 | 0.24 | 17,17,17,17 | 0 |
| 56 | MG | YE | 301 | 1/1 | 0.98 | 0.15 | 4,4,4,4 | 0 |
| 56 | MG | RE | 301 | 1/1 | 0.98 | 0.28 | 1,1,1,1 | 0 |
| 56 | MG | RA | 3207 | 1/1 | 0.98 | 0.21 | 18,18,18,18 | 0 |
| 56 | MG | QA | 1690 | 1/1 | 0.98 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3148 | 1/1 | 0.98 | 0.30 | 32,32,32,32 | 0 |
| 56 | MG | XA | 1664 | 1/1 | 0.98 | 0.40 | 30,30,30,30 | 0 |
| 56 | MG | QA | 1624 | 1/1 | 0.98 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | QA | 1604 | 1/1 | 0.98 | 0.27 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3045 | 1/1 | 0.98 | 0.37 | 4,4,4,4 | 0 |
| 56 | MG | RA | 3047 | 1/1 | 0.98 | 0.23 | 25,25,25,25 | 0 |
| 56 | MG | YA | 3134 | 1/1 | 0.98 | 0.33 | 32,32,32,32 | 0 |
| 56 | MG | RA | 3005 | 1/1 | 0.98 | 0.67 | 32,32,32,32 | 0 |
| 56 | MG | YA | 3060 | 1/1 | 0.98 | 0.27 | 3,3,3,3 | 0 |
| 56 | MG | YA | 3104 | 1/1 | 0.98 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | YA | 3087 | 1/1 | 0.98 | 0.20 | 14,14,14,14 | 0 |
| 56 | MG | QA | 1605 | 1/1 | 0.98 | 0.28 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3034 | 1/1 | 0.98 | 0.33 | 21,21,21,21 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3407 | 1/1 | 0.98 | 0.31 | 4,4,4,4 | 0 |
| 56 | MG | RA | 3042 | 1/1 | 0.98 | 0.25 | 7,7,7,7 | 0 |
| 56 | MG | YA | 3081 | 1/1 | 0.98 | 0.49 | 7,7,7,7 | 0 |
| 56 | MG | XA | 1610 | 1/1 | 0.98 | 0.22 | 15,15,15,15 | 0 |
| 56 | MG | QA | 1607 | 1/1 | 0.98 | 0.28 | 12,12,12,12 | 0 |
| 56 | MG | XA | 1668 | 1/1 | 0.98 | 0.44 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3024 | 1/1 | 0.98 | 0.47 | 7,7,7,7 | 0 |
| 56 | MG | XA | 1716 | 1/1 | 0.98 | 0.37 | 25,25,25,25 | 0 |
| 56 | MG | RA | 3067 | 1/1 | 0.98 | 0.41 | 28,28,28,28 | 0 |
| 56 | MG | R0 | 103 | 1/1 | 0.98 | 0.19 | 19,19,19,19 | 0 |
| 56 | MG | XA | 1619 | 1/1 | 0.98 | 0.14 | 12,12,12,12 | 0 |
| 56 | MG | XA | 1720 | 1/1 | 0.98 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | YA | 3126 | 1/1 | 0.98 | 0.27 | 10,10,10,10 | 0 |
| 56 | MG | RA | 3149 | 1/1 | 0.98 | 0.62 | 2,2,2,2 | 0 |
| 56 | MG | YA | 3056 | 1/1 | 0.98 | 0.47 | 1,1,1,1 | 0 |
| 56 | MG | RA | 3079 | 1/1 | 0.98 | 0.47 | 10,10,10,10 | 0 |
| 56 | MG | QA | 1654 | 1/1 | 0.98 | 0.21 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3100 | 1/1 | 0.98 | 0.28 | 3,3,3,3 | 0 |
| 56 | MG | XA | 1689 | 1/1 | 0.98 | 0.41 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3018 | 1/1 | 0.98 | 0.22 | 18,18,18,18 | 0 |
| 56 | MG | RA | 3217 | 1/1 | 0.98 | 0.19 | 27,27,27,27 | 0 |
| 56 | MG | YA | 3061 | 1/1 | 0.98 | 0.37 | 0,0,0,0 | 0 |
| 56 | MG | RA | 3348 | 1/1 | 0.98 | 0.34 | 45,45,45,45 | 0 |
| 56 | MG | YA | 3336 | 1/1 | 0.98 | 0.45 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3044 | 1/1 | 0.98 | 0.33 | 12,12,12,12 | 0 |
| 56 | MG | RA | 3033 | 1/1 | 0.98 | 0.35 | 8,8,8,8 | 0 |
| 56 | MG | RD | 302 | 1/1 | 0.98 | 0.35 | 9,9,9,9 | 0 |
| 56 | MG | XA | 1642 | 1/1 | 0.98 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | RA | 3056 | 1/1 | 0.98 | 0.20 | 14,14,14,14 | 0 |
| 56 | MG | XA | 1650 | 1/1 | 0.98 | 0.44 | 16,16,16,16 | 0 |
| 56 | MG | RA | 3061 | 1/1 | 0.98 | 0.24 | 17,17,17,17 | 0 |
| 56 | MG | YA | 3274 | 1/1 | 0.98 | 0.41 | 35,35,35,35 | 0 |
| 56 | MG | YA | 3010 | 1/1 | 0.98 | 0.26 | 4,4,4,4 | 0 |
| 56 | MG | YA | 3039 | 1/1 | 0.98 | 0.51 | 14,14,14,14 | 0 |
| 56 | MG | YA | 3025 | 1/1 | 0.98 | 0.63 | 16,16,16,16 | 0 |
| 56 | MG | QA | 1655 | 1/1 | 0.98 | 0.44 | 31,31,31,31 | 0 |
| 56 | MG | YA | 3316 | 1/1 | 0.98 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | RA | 3159 | 1/1 | 0.99 | 0.36 | 5,5,5,5 | 0 |
| 56 | MG | RA | 3048 | 1/1 | 0.99 | 0.49 | 5,5,5,5 | 0 |
| 56 | MG | YA | 3023 | 1/1 | 0.99 | 0.44 | 2,2,2,2 | 0 |
| 56 | MG | YA | 3409 | 1/1 | 0.99 | 0.39 | 10,10,10,10 | 0 |
| 56 | MG | RA | 3062 | 1/1 | 0.99 | 0.35 | 5,5,5,5 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3384 | 1/1 | 0.99 | 0.09 | 8,8,8,8 | 0 |
| 56 | MG | YA | 3057 | 1/1 | 0.99 | 0.33 | 3,3,3,3 | 0 |
| 56 | MG | YA | 3078 | 1/1 | 0.99 | 0.43 | 9,9,9,9 | 0 |
| 56 | MG | YA | 3058 | 1/1 | 0.99 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | QA | 1640 | 1/1 | 0.99 | 0.38 | 53,53,53,53 | 0 |
| 56 | MG | YA | 3446 | 1/1 | 0.99 | 0.26 | 20,20,20,20 | 0 |
| 56 | MG | YA | 3062 | 1/1 | 0.99 | 0.26 | 0,0,0,0 | 0 |
| 56 | MG | YA | 3209 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 0 |
| 56 | MG | XA | 1640 | 1/1 | 0.99 | 0.34 | 29,29,29,29 | 0 |
| 56 | MG | RA | 3058 | 1/1 | 0.99 | 0.29 | 1,1,1,1 | 0 |
| 56 | MG | XA | 1606 | 1/1 | 0.99 | 0.29 | 14,14,14,14 | 0 |
| 56 | MG | YA | 3404 | 1/1 | 0.99 | 0.35 | 20,20,20,20 | 0 |
| 56 | MG | YB | 201 | 1/1 | 0.99 | 0.36 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3173 | 1/1 | 0.99 | 0.44 | 5,5,5,5 | 0 |
| 56 | MG | RA | 3032 | 1/1 | 0.99 | 0.28 | 5,5,5,5 | 0 |
| 56 | MG | RA | 3082 | 1/1 | 0.99 | 0.45 | 0,0,0,0 | 0 |
| 56 | MG | RA | 3034 | 1/1 | 0.99 | 0.35 | 9,9,9,9 | 0 |
| 56 | MG | RA | 3064 | 1/1 | 0.99 | 0.23 | 18,18,18,18 | 0 |
| 56 | MG | YA | 3037 | 1/1 | 0.99 | 0.36 | 10,10,10,10 | 0 |
| 56 | MG | QA | 1667 | 1/1 | 0.99 | 0.22 | 27,27,27,27 | 0 |
| 56 | MG | XA | 1649 | 1/1 | 0.99 | 0.14 | 12,12,12,12 | 0 |
| 56 | MG | RA | 3003 | 1/1 | 0.99 | 0.26 | 8,8,8,8 | 0 |
| 56 | MG | RA | 3085 | 1/1 | 0.99 | 0.12 | 13,13,13,13 | 0 |
| 56 | MG | QA | 1656 | 1/1 | 0.99 | 0.46 | 26,26,26,26 | 0 |
| 56 | MG | RA | 3087 | 1/1 | 0.99 | 0.23 | 20,20,20,20 | 0 |
| 56 | MG | RA | 3192 | 1/1 | 0.99 | 0.47 | 15,15,15,15 | 0 |
| 56 | MG | XA | 1601 | 1/1 | 0.99 | 0.22 | 8,8,8,8 | 0 |
| 56 | MG | RA | 3039 | 1/1 | 0.99 | 0.29 | 21,21,21,21 | 0 |
| 56 | MG | XA | 1709 | 1/1 | 0.99 | 0.50 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3189 | 1/1 | 0.99 | 0.21 | 12,12,12,12 | 0 |
| 56 | MG | RA | 3035 | 1/1 | 0.99 | 0.16 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3059 | 1/1 | 0.99 | 0.20 | 24,24,24,24 | 0 |
| 56 | MG | YA | 3306 | 1/1 | 0.99 | 0.19 | 22,22,22,22 | 0 |
| 56 | MG | RA | 3013 | 1/1 | 0.99 | 0.31 | 0,0,0,0 | 0 |
| 56 | MG | RA | 3177 | 1/1 | 0.99 | 0.31 | 16,16,16,16 | 0 |
| 56 | MG | YA | 3049 | 1/1 | 0.99 | 0.47 | 12,12,12,12 | 0 |
| 56 | MG | RA | 3007 | 1/1 | 0.99 | 0.30 | 5,5,5,5 | 0 |
| 56 | MG | YA | 3423 | 1/1 | 0.99 | 0.24 | 23,23,23,23 | 0 |
| 56 | MG | YA | 3008 | 1/1 | 0.99 | 0.17 | 2,2,2,2 | 0 |
| 56 | MG | YA | 3064 | 1/1 | 0.99 | 0.33 | 5,5,5,5 | 0 |
| 56 | MG | RA | 3280 | 1/1 | 0.99 | 0.25 | 17,17,17,17 | 0 |
| 56 | MG | RA | 3011 | 1/1 | 0.99 | 0.19 | 1,1,1,1 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | RA | 3066 | 1/1 | 0.99 | 0.35 | 31,31,31,31 | 0 |
| 56 | MG | RA | 3080 | 1/1 | 1.00 | 0.27 | 17,17,17,17 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.