



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:02 am GMT

PDB ID : 5HL7
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with lefamulin
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2016-01-14
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

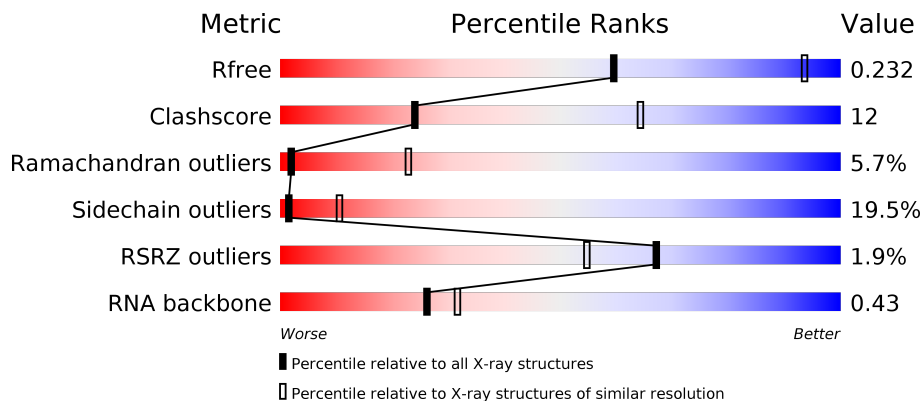
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 Å.

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








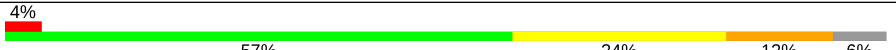
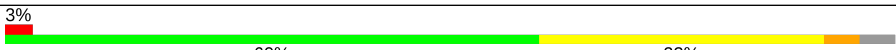

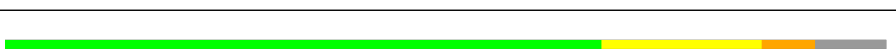



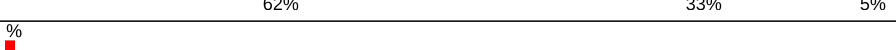




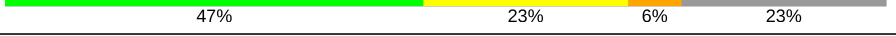




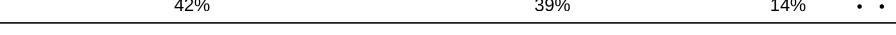

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1072 (3.70-3.42) |
| Clashscore | 112137 | 1003 (3.66-3.46) |
| Ramachandran outliers | 110173 | 1153 (3.70-3.42) |
| Sidechain outliers | 110143 | 1153 (3.70-3.42) |
| RSRZ outliers | 101464 | 1098 (3.70-3.42) |
| RNA backbone | 2435 | 1004 (4.22-2.88) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 277 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 24%, green 67%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 10% 10% 24% 67% </div> </div> |
| 2 | X | 2923 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 41%, green 32%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 10% 10% 41% 32% 7% </div> </div> |
| 3 | Y | 114 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 42%, green 34%, orange 23%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 42% 34% 23% </div> </div> |
| 4 | B | 220 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 34%, green 55%, orange 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 34% 55% 9% </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | C | 207 |  |
| 6 | D | 179 |  |
| 7 | E | 178 |  |
| 8 | G | 145 |  |
| 9 | H | 122 |  |
| 10 | I | 140 |  |
| 11 | J | 144 |  |
| 12 | K | 122 |  |
| 13 | L | 119 |  |
| 14 | M | 116 |  |
| 15 | N | 118 |  |
| 16 | O | 102 |  |
| 17 | P | 117 |  |
| 18 | Q | 91 |  |
| 19 | R | 105 |  |
| 20 | S | 217 |  |
| 21 | T | 94 |  |
| 22 | U | 62 |  |
| 23 | V | 69 |  |
| 24 | W | 59 |  |
| 25 | Z | 58 |  |
| 26 | 2 | 45 |  |
| 27 | 3 | 66 |  |
| 28 | 4 | 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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 29 | MN | A | 301 | - | - | - | X |
| 29 | MN | X | 3001 | - | - | - | X |
| 29 | MN | X | 3013 | - | - | - | X |
| 29 | MN | X | 3026 | - | - | - | X |
| 29 | MN | X | 3028 | - | - | - | X |
| 29 | MN | X | 3029 | - | - | - | X |
| 29 | MN | X | 3034 | - | - | - | X |
| 29 | MN | X | 3036 | - | - | - | X |
| 29 | MN | X | 3040 | - | - | - | X |
| 29 | MN | X | 3043 | - | - | - | X |
| 29 | MN | X | 3045 | - | - | - | X |
| 29 | MN | X | 3047 | - | - | - | X |
| 29 | MN | X | 3049 | - | - | - | X |
| 29 | MN | X | 3053 | - | - | - | X |
| 29 | MN | X | 3054 | - | - | - | X |
| 29 | MN | X | 3058 | - | - | - | X |
| 29 | MN | X | 3063 | - | - | - | X |
| 29 | MN | X | 3066 | - | - | - | X |
| 29 | MN | X | 3067 | - | - | - | X |
| 29 | MN | X | 3068 | - | - | - | X |
| 29 | MN | X | 3073 | - | - | - | X |
| 29 | MN | X | 3081 | - | - | - | X |
| 29 | MN | X | 3083 | - | - | - | X |
| 29 | MN | X | 3085 | - | - | - | X |
| 29 | MN | X | 3096 | - | - | - | X |
| 29 | MN | X | 3099 | - | - | - | X |
| 29 | MN | X | 3122 | - | - | - | X |
| 29 | MN | X | 3139 | - | - | - | X |
| 29 | MN | X | 3164 | - | - | - | X |
| 29 | MN | X | 3168 | - | - | - | X |
| 29 | MN | X | 3173 | - | - | - | X |
| 29 | MN | X | 3194 | - | - | - | X |
| 29 | MN | X | 3202 | - | - | - | X |
| 29 | MN | X | 3320 | - | - | - | X |
| 29 | MN | X | 3439 | - | - | - | X |
| 30 | MG | C | 301 | - | - | - | X |
| 30 | MG | I | 201 | - | - | - | X |
| 30 | MG | X | 3002 | - | - | - | X |
| 30 | MG | X | 3123 | - | - | - | X |
| 30 | MG | X | 3144 | - | - | - | X |
| 30 | MG | X | 3233 | - | - | - | X |
| 30 | MG | X | 3239 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 30 | MG | X | 3279 | - | - | - | X |
| 30 | MG | X | 3293 | - | - | - | X |
| 30 | MG | X | 3295 | - | - | - | X |
| 30 | MG | X | 3329 | - | - | - | X |
| 30 | MG | X | 3335 | - | - | - | X |
| 30 | MG | X | 3340 | - | - | - | X |
| 30 | MG | X | 3354 | - | - | - | X |
| 30 | MG | X | 3390 | - | - | - | X |
| 30 | MG | X | 3420 | - | - | - | X |
| 30 | MG | X | 3435 | - | - | - | X |
| 30 | MG | X | 3501 | - | - | - | X |
| 30 | MG | Y | 207 | - | - | - | X |
| 31 | 62B | X | 3003 | - | - | - | X |
| 32 | MPD | X | 3004 | - | - | - | X |
| 32 | MPD | X | 3005 | - | - | - | X |
| 32 | MPD | X | 3006 | - | - | - | X |
| 32 | MPD | X | 3007 | - | - | - | X |
| 32 | MPD | X | 3008 | - | - | - | X |
| 32 | MPD | X | 3009 | - | - | - | X |
| 32 | MPD | X | 3010 | - | - | - | X |
| 32 | MPD | X | 3011 | - | - | - | X |
| 33 | SPD | X | 3492 | - | - | - | X |
| 33 | SPD | X | 3494 | - | - | - | X |
| 33 | SPD | X | 3495 | - | - | - | X |
| 33 | SPD | X | 3496 | - | - | - | X |
| 33 | SPD | X | 3498 | - | - | - | X |
| 33 | SPD | Y | 213 | - | - | - | X |
| 35 | EPE | N | 201 | - | - | X | - |

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 81462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 269 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1667 | 1007 | 331 | 324 | 5 | | | |

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 2 | X | 2705 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 57983 | 25884 | 10620 | 18774 | 2705 | | | |

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 3 | Y | 114 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2430 | 1086 | 436 | 794 | 114 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | B | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1547 | 967 | 289 | 286 | 5 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | C | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1324 | 823 | 250 | 249 | 2 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | D | 165 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 853 | 512 | 165 | 174 | 2 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | E | 157 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 915 | 559 | 172 | 182 | 2 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| E | 174 | LYS | GLY | conflict | UNP Q2FW21 |

- Molecule 8 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | G | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1090 | 682 | 202 | 203 | 3 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | H | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 548 | 167 | 165 | 4 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | I | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 819 | 498 | 164 | 156 | 1 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | J | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1001 | 641 | 187 | 170 | 3 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | K | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 906 | 556 | 175 | 174 | 1 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 13 | L | 109 | Total | C | N | O | 0 | 0 | 0 |
| | | | 673 | 411 | 134 | 128 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14 | M | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 807 | 510 | 162 | 135 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | N | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 922 | 581 | 183 | 154 | 4 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | O | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 751 | 477 | 138 | 135 | 1 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | P | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 853 | 531 | 161 | 158 | 3 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | Q | 90 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 583 | 365 | 103 | 112 | 3 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | R | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 627 | 382 | 120 | 124 | 1 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | S | 167 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1087 | 682 | 191 | 212 | 2 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 21 | T | 75 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 559 | 349 | 110 | 100 | | | | |

- Molecule 22 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 22 | U | 42 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 242 | 149 | 48 | 45 | | | | |

- Molecule 23 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 23 | V | 65 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 486 | 299 | 89 | 98 | | | | |

- Molecule 24 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 24 | W | 57 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 437 | 271 | 82 | 84 | | | | |

- Molecule 25 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 25 | Z | 43 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 339 | 208 | 70 | 57 | 4 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | 2 | 43 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 350 | 213 | 85 | 51 | 1 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | 3 | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 405 | 248 | 81 | 74 | 2 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 4 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 181 | 107 | 36 | 36 | 2 | | | |

- Molecule 29 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 29 | Z | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |
| 29 | A | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |
| 29 | T | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |
| 29 | X | 268 | Total | Mn | 0 | 0 |
| | | | 268 | 268 | | |
| 29 | R | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |
| 29 | Y | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

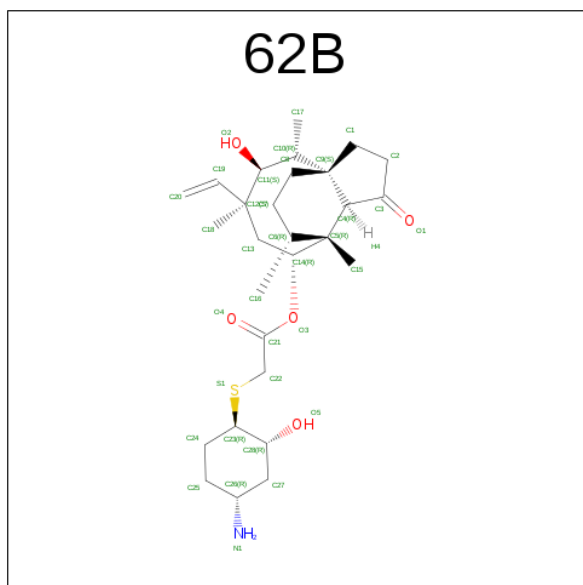
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 30 | P | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 30 | G | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 30 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 30 | I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 30 | C | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 30 | A | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 30 | X | 218 | Total | Mg | 0 | 0 |
| | | | 218 | 218 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 30 | O | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 30 | Y | 10 | Total | Mg | 0 | 0 |
| | | | 10 | 10 | | |
| 30 | M | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 31 is Lefamulin (three-letter code: 62B) (formula: $C_{28}H_{45}NO_5S$).



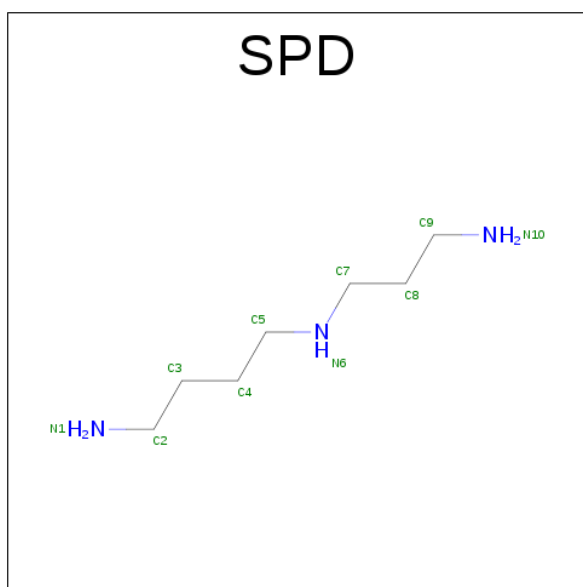
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 31 | X | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 35 | 28 | 1 | 5 | 1 | | |

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



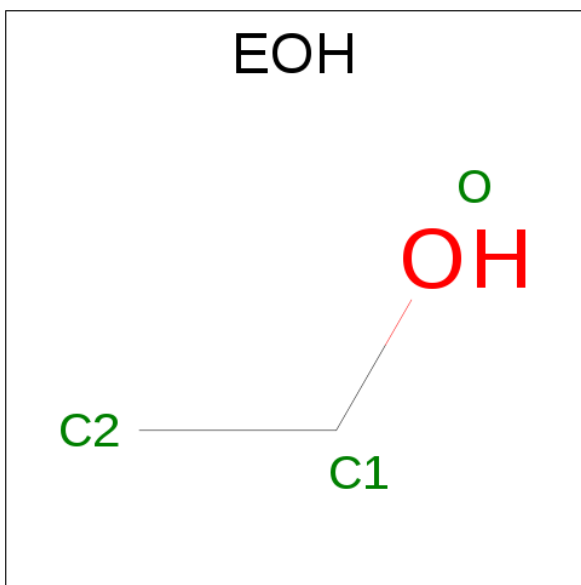
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 32 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | J | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | Q | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 32 | Z | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



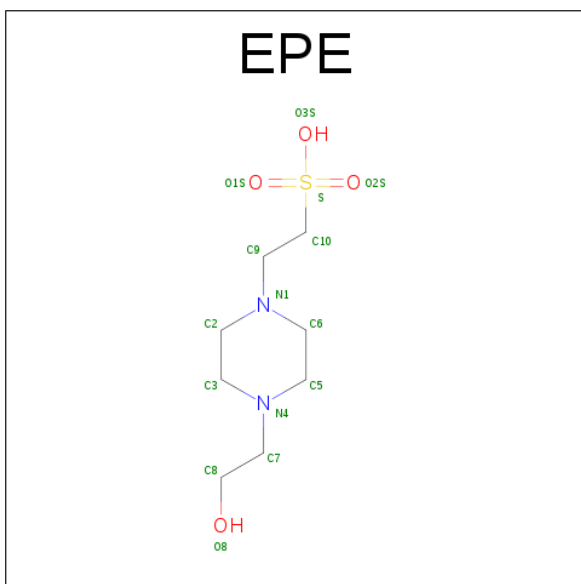
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 33 | X | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 33 | X | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 33 | X | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 33 | X | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 33 | X | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 33 | X | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 33 | Y | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 34 | X | 1 | Total | C | O | 0 | 0 |
| | | | 3 | 2 | 1 | | |
| 34 | X | 1 | Total | C | O | 0 | 0 |
| | | | 3 | 2 | 1 | | |
| 34 | S | 1 | Total | C | O | 0 | 0 |
| | | | 3 | 2 | 1 | | |

- Molecule 35 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).

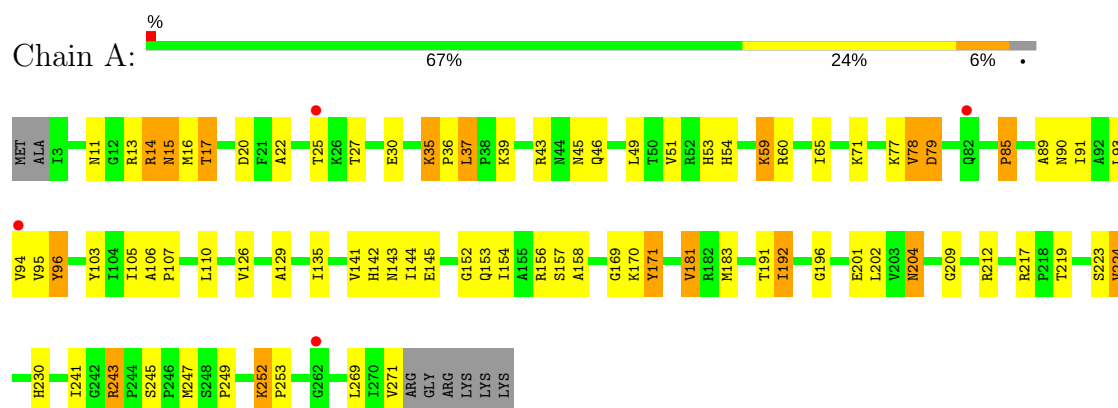


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 35 | N | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 15 | 8 | 2 | 4 | 1 | | |

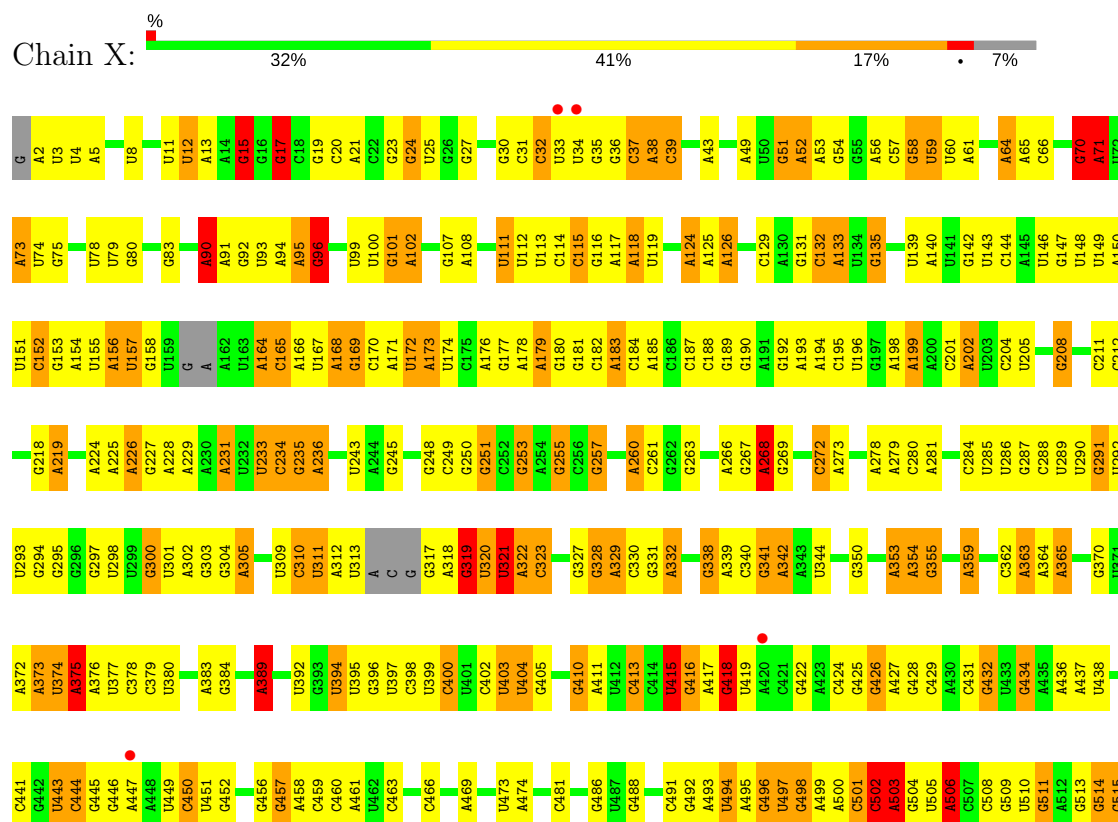
3 Residue-property plots

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

• Molecule 1: 50S ribosomal protein L2

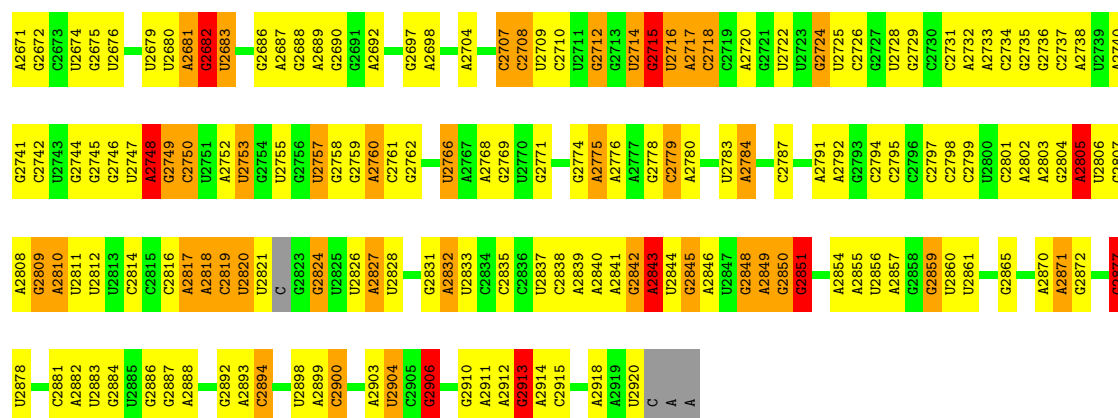


• Molecule 2: 23S ribosomal RNA



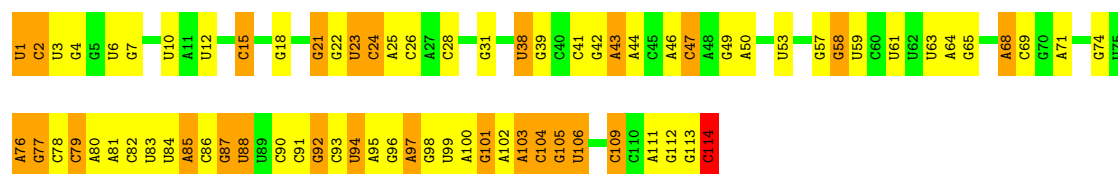
| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|
| C1541 | G1406 | U1338 | U1262 | A1195 | U1058 | G997 | C857 | U791 | C716 | C654 | U589 | A516 |
| C1542 | C1407 | U1339 | A1263 | C1196 | A1059 | G998 | U858 | U792 | C717 | A654 | U590 | A517 |
| G1543 | G1408 | G1340 | G1263 | C1197 | U1060 | U999 | C859 | G793 | G718 | G856 | A591 | A518 |
| G1544 | U1409 | A1341 | C1268 | U1198 | G1061 | G1000 | C | A794 | G719 | U657 | A592 | A519 |
| | A1410 | C1342 | A1269 | U1199 | U1062 | U1001 | C862 | A795 | A720 | A658 | U593 | G520 |
| G1547 | G1411 | | U1270 | U1200 | U1063 | A1002 | G863 | A796 | A721 | A659 | G594 | |
| U1548 | | A1345 | G1271 | A1201 | A1064 | A1003 | A864 | | A722 | A660 | | A523 |
| C1549 | G1414 | G1346 | U1272 | U1205 | A1065 | A1004 | A865 | U799 | | U661 | U597 | A524 |
| G1550 | A1415 | | G1273 | A1208 | U1066 | G1005 | A866 | G800 | G726 | G662 | G598 | A525 |
| U1551 | U1416 | U1349 | G1274 | A1209 | U1067 | U1006 | U867 | A801 | G727 | U663 | G599 | A526 |
| | G1417 | U1350 | | U1210 | G1068 | U1007 | A868 | G802 | U728 | G664 | U600 | G527 |
| A | G1418 | C1351 | C1277 | U1219 | G1069 | C1008 | G869 | C803 | G729 | G665 | | G528 |
| U1493 | | C1352 | G1278 | U1211 | A1070 | G1009 | C870 | G804 | A730 | A666 | | A529 |
| | A1422 | A1353 | C1279 | G1211 | A1071 | G1010 | U871 | G805 | U731 | G667 | G604 | G530 |
| C1495 | C1423 | G1354 | | U1212 | A1072 | U1011 | U872 | A906 | G732 | C668 | U605 | |
| G1496 | A1424 | A1355 | A1285 | C1213 | A1073 | G1012 | U873 | | U733 | C669 | U606 | C533 |
| A1497 | | G1356 | G1286 | U1215 | G1074 | U1013 | U874 | A810 | G735 | G670 | C607 | G534 |
| U1498 | G1429 | G1357 | U1287 | U1215 | G1075 | U1014 | G875 | C811 | C736 | U671 | C608 | A537 |
| U1499 | A1430 | A1358 | G1288 | U | A1076 | C1015 | G876 | U812 | C737 | A672 | U609 | G538 |
| G1500 | U1431 | A1359 | A1289 | U1217 | U1077 | G1016 | C877 | G813 | G738 | G673 | U610 | G539 |
| G1501 | A1432 | G1360 | G1290 | G1218 | G1078 | A1017 | C878 | G814 | U739 | G674 | U611 | U612 |
| A1502 | U1433 | G1361 | A1291 | G1219 | U1079 | A1018 | U879 | G815 | G740 | A676 | G613 | G541 |
| U1503 | U1434 | C1362 | A1292 | G1220 | G1080 | A1019 | A880 | | | A677 | U614 | A542 |
| U1504 | | U1293 | U1293 | C1221 | G1081 | G1020 | | G817 | C743 | A678 | A615 | G543 |
| G1505 | A1440 | G1363 | G1294 | U1224 | C1146 | G1021 | C883 | U818 | | G679 | G616 | |
| C1441 | C1441 | G1365 | C1295 | G1225 | A1147 | G1022 | U884 | G820 | G746 | C880 | A617 | U649 |
| | | U1366 | C1296 | G1226 | C1148 | A1023 | C885 | | U747 | G681 | A618 | A550 |
| A1447 | | C1367 | | G1226 | U1149 | A1024 | A886 | G823 | U748 | A682 | U619 | G551 |
| U | U | G1368 | U1300 | G1227 | C1149 | A1025 | A887 | A824 | | G683 | G620 | A552 |
| U1510 | | G1369 | G1301 | A1228 | G1151 | C1026 | G888 | G825 | | U684 | A621 | A553 |
| C1511 | C1370 | U1371 | G1302 | G1229 | U1152 | A1027 | U889 | A826 | G743 | C684 | | C554 |
| U1512 | A1303 | U1372 | A1303 | G1230 | C1153 | G1028 | C890 | A827 | U | C685 | C555 | |
| G1513 | C1372 | C1452 | G1304 | A1231 | G1154 | C1029 | A891 | A828 | A | U686 | G624 | C561 |
| A1514 | U1373 | G1453 | U1305 | A1232 | A1155 | C1030 | U892 | U829 | A | G687 | G626 | C562 |
| G1515 | U1454 | G1374 | G1306 | G1233 | G1156 | C1031 | | U830 | C | A688 | U631 | G563 |
| C1516 | U | | G1307 | G1234 | U1157 | A1032 | U896 | C831 | A | U689 | U632 | U564 |
| U1517 | U | | G1235 | G1235 | | G1033 | U897 | C832 | A | C695 | A633 | U565 |
| G1518 | U | U1377 | G1236 | G1236 | C1185 | A1034 | A897 | C833 | G764 | U697 | C634 | G567 |
| U1519 | A | U1378 | | | | | U898 | A833 | U765 | A691 | G635 | C568 |
| U | A | G1379 | A1310 | A1241 | G1099 | C1035 | | A834 | U766 | G692 | | |
| A | A | G1380 | A1311 | A1242 | G | C1036 | G901 | U835 | A768 | | | |
| U1521 | U1460 | U1381 | A1312 | G1243 | U | A1037 | A902 | C836 | | C696 | U637 | C572 |
| G1522 | C1461 | C1382 | G1313 | G1243 | G | C1038 | A903 | G837 | | U696 | U638 | A573 |
| G1523 | G1462 | G1383 | A1314 | G1244 | U | G1039 | G904 | A838 | G771 | U697 | U639 | A574 |
| C1524 | A1463 | | G1315 | G1245 | U | A1040 | G905 | A839 | | U698 | | G575 |
| U | U1464 | U1389 | G1316 | C1246 | G | G1041 | U980 | C840 | G774 | U699 | G643 | U576 |
| G1526 | G1465 | A1390 | G1317 | C1247 | G | C1042 | U981 | C841 | A775 | | G644 | A577 |
| U1527 | G1466 | A1391 | U1176 | U1248 | G | U1043 | G982 | U842 | | U702 | G645 | G578 |
| G1528 | G1467 | G1392 | U1177 | U1249 | C | U1044 | G983 | U843 | G778 | A703 | A646 | U579 |
| U1529 | G1468 | C1393 | C1178 | G1250 | U | A1045 | G984 | G844 | A779 | U704 | C580 | A581 |
| A1530 | G1469 | U1394 | C1179 | G1251 | A | G1046 | G985 | A845 | U790 | U705 | G647 | G582 |
| U | G1470 | G1395 | G1180 | A1252 | G | G1047 | U986 | G846 | | G706 | U649 | A583 |
| U1592 | A1471 | U1396 | U1185 | G1253 | A | | C921 | C847 | C761 | G707 | G643 | |
| G1593 | C1326 | G1397 | U1186 | G1253 | A | C1050 | G922 | A947 | G762 | U708 | G644 | A577 |
| U1594 | A1472 | C1327 | A1187 | C1254 | G | C1051 | A923 | G763 | G782 | G709 | A645 | U579 |
| C1595 | G1473 | A1255 | A1188 | A1255 | A | U1052 | G924 | A784 | A784 | U709 | A646 | C580 |
| G1596 | C1474 | C1399 | U1257 | G1256 | C | A1053 | G925 | C785 | G785 | C710 | G647 | A581 |
| U1597 | A1475 | C1400 | G1332 | G1257 | A | A1054 | G | U786 | U786 | G711 | G648 | G582 |
| U1598 | G1476 | G1401 | C1189 | A1258 | G | A1054 | C933 | U787 | U787 | U712 | U649 | A583 |
| G1599 | U1477 | A1402 | U1190 | C1259 | C | A1055 | G | A788 | A788 | A713 | U650 | |
| A1600 | U1478 | | A1191 | U1260 | C | U1056 | C | G789 | G789 | G714 | A651 | C587 |
| | | G1405 | G1261 | G1261 | A | A1057 | | G790 | | A715 | | G588 |





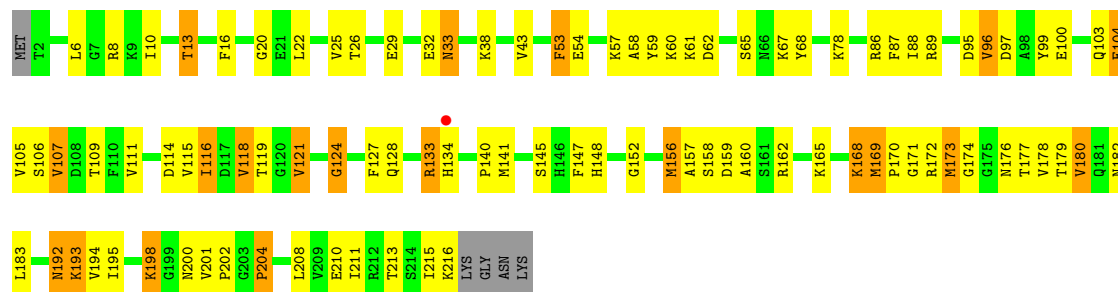
• Molecule 3: 5S ribosomal RNA

Chain Y: 34% 42% 23%



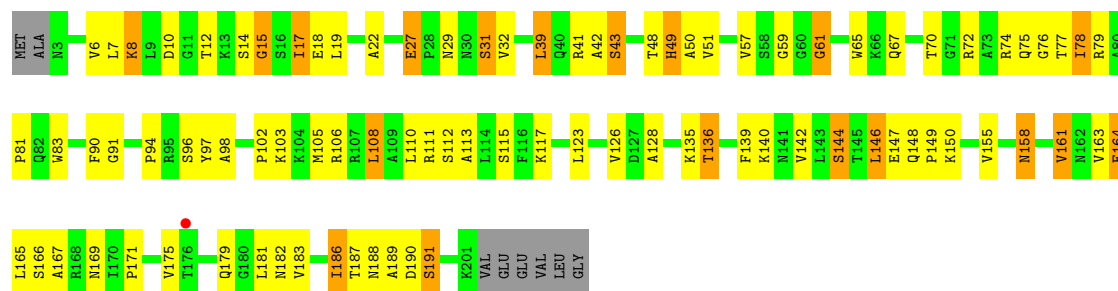
• Molecule 4: 50S ribosomal protein L3

Chain B: 55% 34% 9%

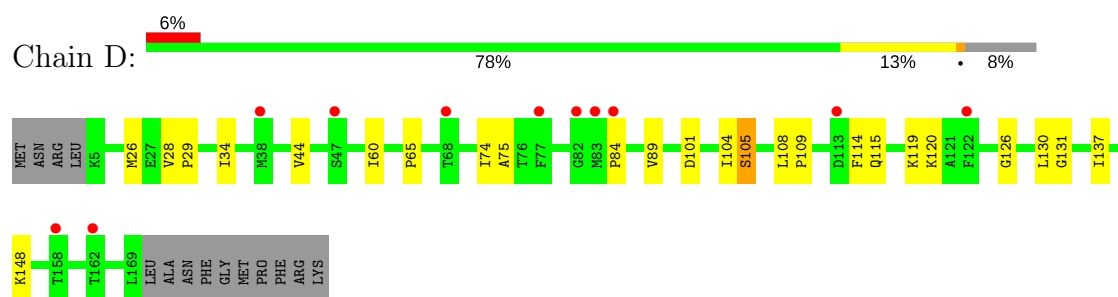


• Molecule 5: 50S ribosomal protein L4

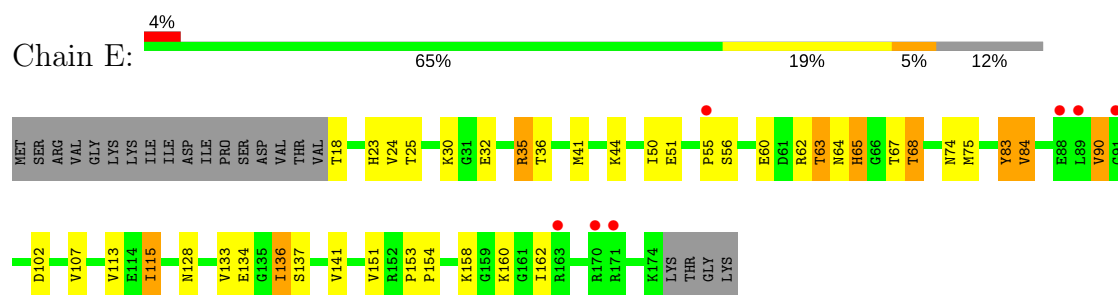
Chain C: 53% 34% 9%



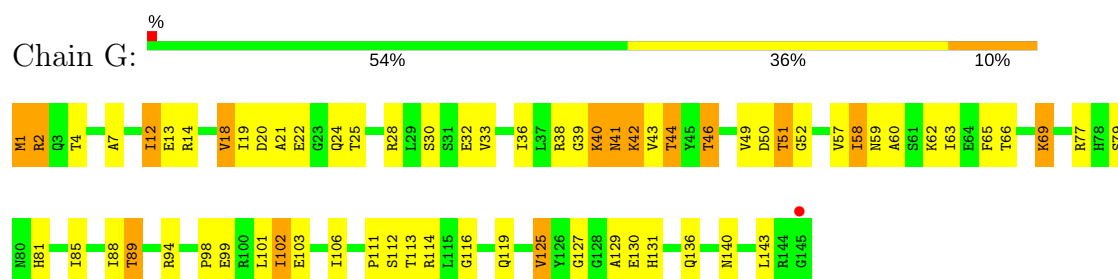
• Molecule 6: 50S ribosomal protein L5



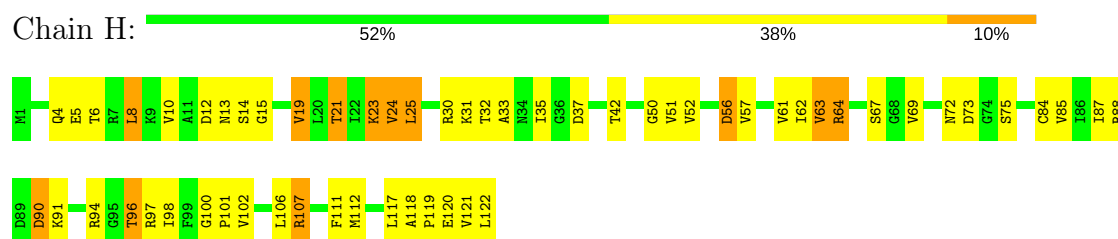
- Molecule 7: 50S ribosomal protein L6



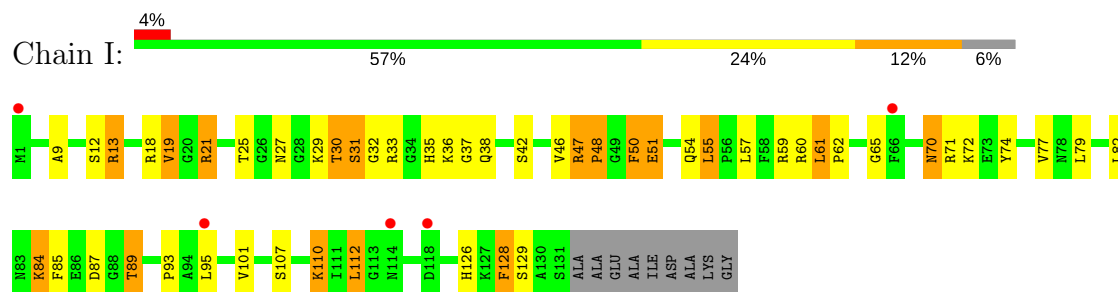
- Molecule 8: 50S ribosomal protein L13



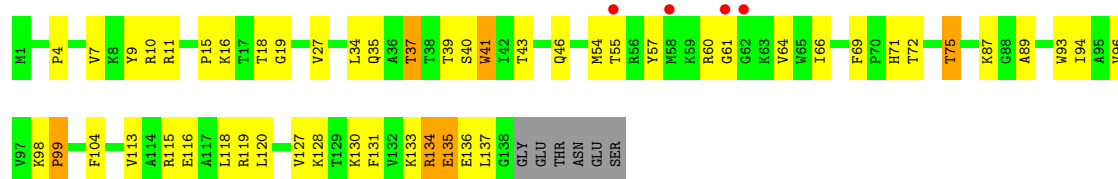
- Molecule 9: 50S ribosomal protein L14



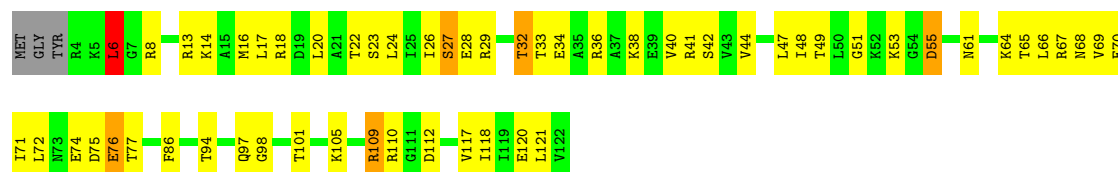
- Molecule 10: 50S ribosomal protein L15



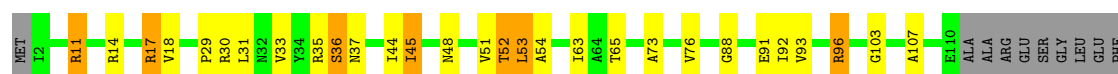
- Molecule 11: 50S ribosomal protein L16



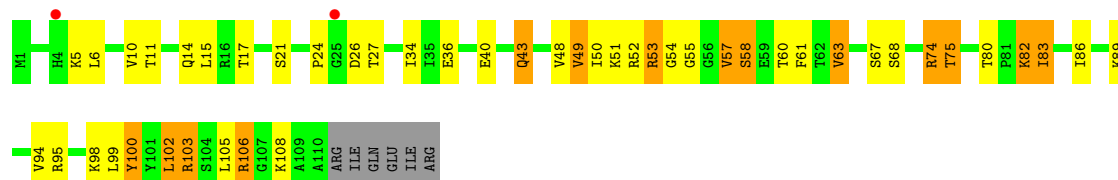
- Molecule 12: 50S ribosomal protein L17



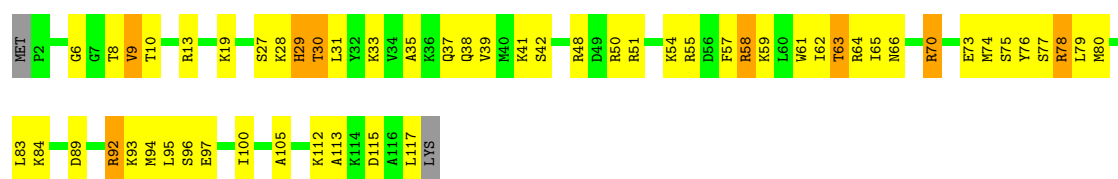
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19

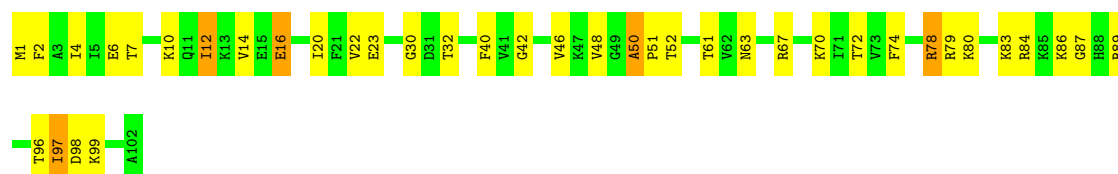


- Molecule 15: 50S ribosomal protein L20

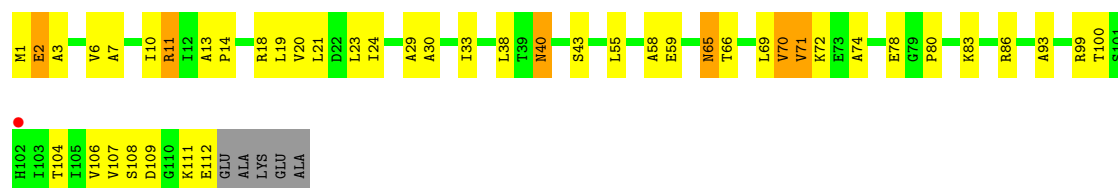


- Molecule 16: 50S ribosomal protein L21

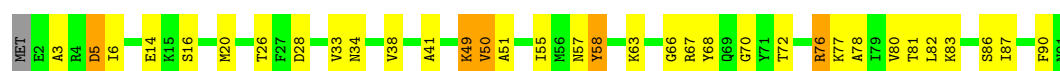




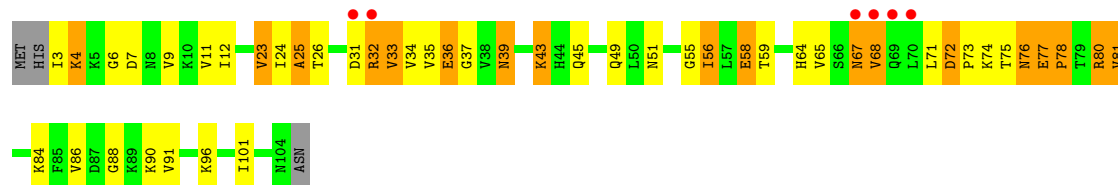
- Molecule 17: 50S ribosomal protein L22



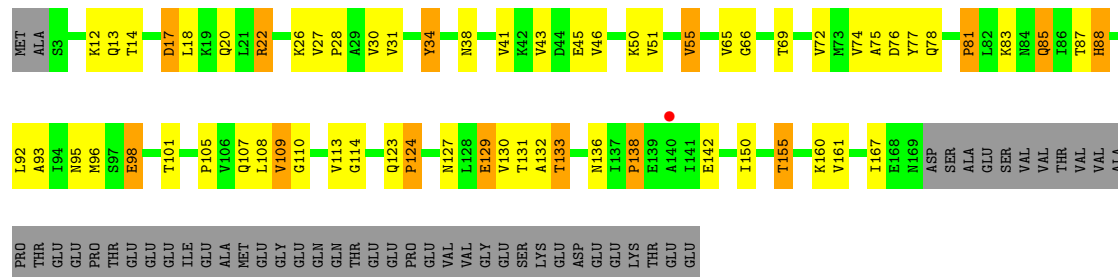
- Molecule 18: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L24

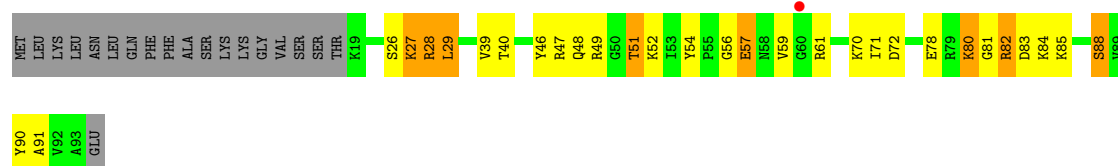


- Molecule 20: 50S ribosomal protein L25

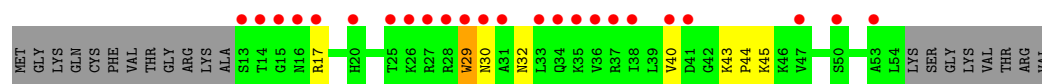
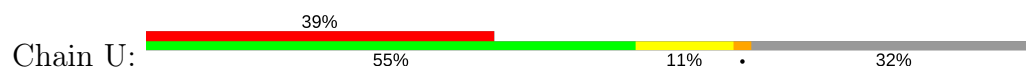


- Molecule 21: 50S ribosomal protein L27

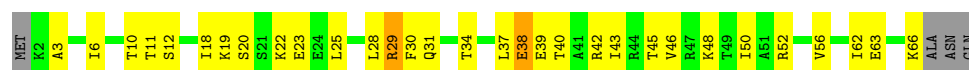




- Molecule 22: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32



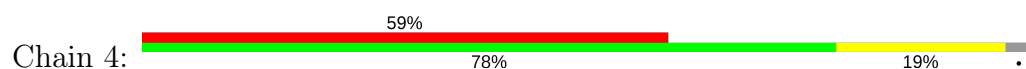
- Molecule 26: 50S ribosomal protein L34

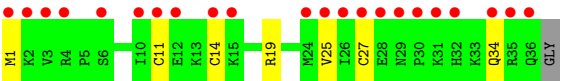


- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 65 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 282.11Å 282.11Å 875.34Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 49.93 – 3.55 49.93 – 3.55 | Depositor EDS |
| % Data completeness (in resolution range) | 95.4 (49.93-3.55) 95.4 (49.93-3.55) | Depositor EDS |
| R_{merge} | 0.21 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.53 (at 3.57Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.187 , 0.227 0.194 , 0.232 | Depositor DCC |
| R_{free} test set | 11840 reflections (5.29%) | DCC |
| Wilson B-factor (Å ²) | 105.6 | Xtriage |
| Anisotropy | 0.307 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.22 , 56.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 81462 | wwPDB-VP |
| Average B, all atoms (Å ²) | 110.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% 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: MG, MN, EOH, MPD, 62B, EPE, SPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.26 | 0/1697 | 0.56 | 0/2332 |
| 2 | X | 0.96 | 108/64923 (0.2%) | 1.63 | 1547/101215 (1.5%) |
| 3 | Y | 0.90 | 10/2717 (0.4%) | 1.73 | 90/4232 (2.1%) |
| 4 | B | 0.68 | 0/1570 | 0.90 | 2/2117 (0.1%) |
| 5 | C | 0.72 | 0/1343 | 0.98 | 1/1838 (0.1%) |
| 6 | D | 0.33 | 0/855 | 0.56 | 0/1185 |
| 7 | E | 0.44 | 0/925 | 0.61 | 0/1279 |
| 8 | G | 0.78 | 0/1112 | 0.87 | 0/1507 |
| 9 | H | 0.62 | 0/891 | 0.80 | 0/1203 |
| 10 | I | 0.75 | 0/827 | 1.02 | 2/1121 (0.2%) |
| 11 | J | 0.61 | 0/1023 | 0.80 | 0/1388 |
| 12 | K | 0.35 | 0/909 | 0.62 | 1/1217 (0.1%) |
| 13 | L | 0.50 | 0/678 | 0.69 | 0/927 |
| 14 | M | 0.72 | 0/819 | 0.94 | 2/1107 (0.2%) |
| 15 | N | 0.83 | 0/934 | 0.99 | 0/1241 |
| 16 | O | 0.84 | 1/761 (0.1%) | 0.97 | 3/1022 (0.3%) |
| 17 | P | 0.41 | 0/861 | 0.64 | 0/1160 |
| 18 | Q | 0.57 | 0/589 | 0.78 | 0/808 |
| 19 | R | 0.67 | 1/631 (0.2%) | 0.85 | 0/863 |
| 20 | S | 0.60 | 0/1099 | 0.84 | 0/1509 |
| 21 | T | 0.59 | 0/565 | 0.79 | 0/751 |
| 22 | U | 0.37 | 0/247 | 0.57 | 0/344 |
| 23 | V | 0.50 | 0/487 | 0.64 | 0/654 |
| 24 | W | 0.73 | 0/439 | 0.93 | 0/593 |
| 25 | Z | 0.80 | 0/345 | 0.90 | 0/460 |
| 26 | 2 | 0.72 | 0/353 | 0.94 | 0/463 |
| 27 | 3 | 0.75 | 0/409 | 1.07 | 1/550 (0.2%) |
| 28 | 4 | 0.41 | 0/180 | 0.66 | 0/249 |
| All | All | 0.89 | 120/88189 (0.1%) | 1.50 | 1649/133335 (1.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 4 | B | 0 | 2 |
| 5 | C | 0 | 2 |
| 10 | I | 0 | 1 |
| 16 | O | 0 | 1 |
| 17 | P | 0 | 1 |
| 20 | S | 0 | 1 |
| 27 | 3 | 0 | 2 |
| All | All | 0 | 11 |

The worst 5 of 120 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 2 | X | 1186 | A | N9-C4 | -12.81 | 1.30 | 1.37 |
| 2 | X | 1289 | A | N9-C4 | -11.75 | 1.30 | 1.37 |
| 2 | X | 2845 | G | N9-C4 | -9.65 | 1.30 | 1.38 |
| 2 | X | 1065 | A | N9-C4 | -9.16 | 1.32 | 1.37 |
| 2 | X | 2740 | A | N9-C4 | -8.95 | 1.32 | 1.37 |

The worst 5 of 1649 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 3 | Y | 93 | C | N3-C2-O2 | -20.18 | 107.77 | 121.90 |
| 2 | X | 2845 | G | N3-C4-C5 | 18.48 | 137.84 | 128.60 |
| 3 | Y | 93 | C | N1-C2-O2 | 16.73 | 128.94 | 118.90 |
| 2 | X | 1395 | G | N1-C6-O6 | -16.42 | 110.05 | 119.90 |
| 2 | X | 1289 | A | C2-N3-C4 | -16.32 | 102.44 | 110.60 |

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 77 | LYS | Peptide |
| 4 | B | 104 | GLU | Peptide |
| 4 | B | 57 | LYS | Peptide |
| 5 | C | 161 | VAL | Peptide |
| 5 | C | 27 | GLU | Peptide |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1667 | 0 | 1292 | 51 | 0 |
| 2 | X | 57983 | 0 | 29161 | 923 | 0 |
| 3 | Y | 2430 | 0 | 1229 | 58 | 0 |
| 4 | B | 1547 | 0 | 1514 | 66 | 0 |
| 5 | C | 1324 | 0 | 1175 | 57 | 0 |
| 6 | D | 853 | 0 | 444 | 6 | 0 |
| 7 | E | 915 | 0 | 648 | 22 | 0 |
| 8 | G | 1090 | 0 | 1034 | 48 | 0 |
| 9 | H | 884 | 0 | 902 | 45 | 0 |
| 10 | I | 819 | 0 | 687 | 43 | 0 |
| 11 | J | 1001 | 0 | 971 | 37 | 0 |
| 12 | K | 906 | 0 | 930 | 36 | 0 |
| 13 | L | 673 | 0 | 538 | 19 | 0 |
| 14 | M | 807 | 0 | 803 | 32 | 0 |
| 15 | N | 922 | 0 | 973 | 61 | 0 |
| 16 | O | 751 | 0 | 743 | 22 | 0 |
| 17 | P | 853 | 0 | 900 | 30 | 0 |
| 18 | Q | 583 | 0 | 472 | 21 | 0 |
| 19 | R | 627 | 0 | 510 | 24 | 0 |
| 20 | S | 1087 | 0 | 934 | 26 | 0 |
| 21 | T | 559 | 0 | 569 | 24 | 0 |
| 22 | U | 242 | 0 | 141 | 4 | 0 |
| 23 | V | 486 | 0 | 469 | 10 | 0 |
| 24 | W | 437 | 0 | 467 | 26 | 0 |
| 25 | Z | 339 | 0 | 350 | 23 | 0 |
| 26 | 2 | 350 | 0 | 383 | 12 | 0 |
| 27 | 3 | 405 | 0 | 363 | 19 | 0 |
| 28 | 4 | 181 | 0 | 76 | 5 | 0 |
| 29 | A | 1 | 0 | 0 | 0 | 0 |
| 29 | R | 1 | 0 | 0 | 0 | 0 |
| 29 | T | 1 | 0 | 0 | 0 | 0 |
| 29 | X | 268 | 0 | 0 | 0 | 0 |
| 29 | Y | 2 | 0 | 0 | 0 | 0 |
| 29 | Z | 1 | 0 | 0 | 0 | 0 |
| 30 | A | 3 | 0 | 0 | 0 | 0 |
| 30 | C | 2 | 0 | 0 | 0 | 0 |
| 30 | G | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30 | I | 1 | 0 | 0 | 0 | 0 |
| 30 | J | 1 | 0 | 0 | 0 | 0 |
| 30 | M | 1 | 0 | 0 | 0 | 0 |
| 30 | O | 1 | 0 | 0 | 0 | 0 |
| 30 | P | 1 | 0 | 0 | 0 | 0 |
| 30 | X | 218 | 0 | 0 | 0 | 0 |
| 30 | Y | 10 | 0 | 0 | 0 | 0 |
| 31 | X | 35 | 0 | 0 | 1 | 0 |
| 32 | J | 8 | 0 | 14 | 1 | 0 |
| 32 | Q | 8 | 0 | 14 | 0 | 0 |
| 32 | X | 64 | 0 | 112 | 7 | 0 |
| 32 | Z | 8 | 0 | 14 | 0 | 0 |
| 33 | X | 70 | 0 | 133 | 9 | 0 |
| 33 | Y | 10 | 0 | 19 | 1 | 0 |
| 34 | S | 3 | 0 | 6 | 0 | 0 |
| 34 | X | 6 | 0 | 12 | 0 | 0 |
| 35 | N | 15 | 0 | 17 | 17 | 0 |
| All | All | 81462 | 0 | 49019 | 1574 | 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 12.

The worst 5 of 1574 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) |
|-----------------|------------------|--------------------------|-------------------|
| 19:R:11:VAL:HA | 19:R:67:ASN:HB2 | 1.48 | 0.96 |
| 2:X:956:A:H2' | 11:J:11:ARG:HH11 | 1.30 | 0.96 |
| 2:X:83:G:H21 | 2:X:102:A:H2 | 1.15 | 0.93 |
| 4:B:124:GLY:HA2 | 4:B:174:GLY:HA3 | 1.53 | 0.91 |
| 3:Y:21:G:H1 | 3:Y:58:G:H1 | 1.08 | 0.91 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1 | A | 267/277 (96%) | 222 (83%) | 27 (10%) | 18 (7%) | 1 | 19 |
| 4 | B | 213/220 (97%) | 187 (88%) | 17 (8%) | 9 (4%) | 3 | 30 |
| 5 | C | 197/207 (95%) | 155 (79%) | 31 (16%) | 11 (6%) | 2 | 23 |
| 6 | D | 163/179 (91%) | 131 (80%) | 17 (10%) | 15 (9%) | 1 | 11 |
| 7 | E | 155/178 (87%) | 120 (77%) | 26 (17%) | 9 (6%) | 2 | 22 |
| 8 | G | 143/145 (99%) | 131 (92%) | 8 (6%) | 4 (3%) | 6 | 41 |
| 9 | H | 120/122 (98%) | 102 (85%) | 16 (13%) | 2 (2%) | 11 | 51 |
| 10 | I | 129/140 (92%) | 91 (70%) | 25 (19%) | 13 (10%) | 1 | 10 |
| 11 | J | 136/144 (94%) | 110 (81%) | 15 (11%) | 11 (8%) | 1 | 13 |
| 12 | K | 117/122 (96%) | 101 (86%) | 9 (8%) | 7 (6%) | 2 | 21 |
| 13 | L | 107/119 (90%) | 86 (80%) | 16 (15%) | 5 (5%) | 3 | 27 |
| 14 | M | 108/116 (93%) | 85 (79%) | 18 (17%) | 5 (5%) | 3 | 28 |
| 15 | N | 114/118 (97%) | 108 (95%) | 6 (5%) | 0 | 100 | 100 |
| 16 | O | 100/102 (98%) | 90 (90%) | 5 (5%) | 5 (5%) | 2 | 26 |
| 17 | P | 110/117 (94%) | 101 (92%) | 8 (7%) | 1 (1%) | 20 | 63 |
| 18 | Q | 88/91 (97%) | 74 (84%) | 9 (10%) | 5 (6%) | 2 | 23 |
| 19 | R | 100/105 (95%) | 71 (71%) | 17 (17%) | 12 (12%) | 0 | 7 |
| 20 | S | 165/217 (76%) | 121 (73%) | 23 (14%) | 21 (13%) | 0 | 6 |
| 21 | T | 73/94 (78%) | 63 (86%) | 10 (14%) | 0 | 100 | 100 |
| 22 | U | 40/62 (64%) | 32 (80%) | 6 (15%) | 2 (5%) | 2 | 26 |
| 23 | V | 63/69 (91%) | 55 (87%) | 5 (8%) | 3 (5%) | 2 | 27 |
| 24 | W | 55/59 (93%) | 51 (93%) | 3 (6%) | 1 (2%) | 10 | 50 |
| 25 | Z | 41/58 (71%) | 36 (88%) | 4 (10%) | 1 (2%) | 7 | 44 |
| 26 | 2 | 41/45 (91%) | 39 (95%) | 1 (2%) | 1 (2%) | 7 | 44 |
| 27 | 3 | 58/66 (88%) | 42 (72%) | 9 (16%) | 7 (12%) | 0 | 7 |
| 28 | 4 | 34/37 (92%) | 26 (76%) | 8 (24%) | 0 | 100 | 100 |
| All | All | 2937/3209 (92%) | 2430 (83%) | 339 (12%) | 168 (6%) | 2 | 23 |

5 of 168 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 27 | THR |
| 1 | A | 35 | LYS |
| 1 | A | 36 | PRO |
| 1 | A | 51 | VAL |
| 1 | A | 78 | 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 | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 112/224 (50%) | 97 (87%) | 15 (13%) | 4 | 27 |
| 4 | B | 150/177 (85%) | 121 (81%) | 29 (19%) | 1 | 10 |
| 5 | C | 106/169 (63%) | 84 (79%) | 22 (21%) | 1 | 9 |
| 6 | D | 15/158 (10%) | 13 (87%) | 2 (13%) | 4 | 27 |
| 7 | E | 51/156 (33%) | 39 (76%) | 12 (24%) | 1 | 6 |
| 8 | G | 106/123 (86%) | 87 (82%) | 19 (18%) | 2 | 13 |
| 9 | H | 91/100 (91%) | 74 (81%) | 17 (19%) | 2 | 11 |
| 10 | I | 56/108 (52%) | 39 (70%) | 17 (30%) | 0 | 3 |
| 11 | J | 90/119 (76%) | 80 (89%) | 10 (11%) | 7 | 35 |
| 12 | K | 91/102 (89%) | 77 (85%) | 14 (15%) | 3 | 21 |
| 13 | L | 40/95 (42%) | 30 (75%) | 10 (25%) | 1 | 5 |
| 14 | M | 75/102 (74%) | 53 (71%) | 22 (29%) | 0 | 3 |
| 15 | N | 91/98 (93%) | 70 (77%) | 21 (23%) | 1 | 6 |
| 16 | O | 71/86 (83%) | 63 (89%) | 8 (11%) | 7 | 34 |
| 17 | P | 89/94 (95%) | 77 (86%) | 12 (14%) | 4 | 27 |
| 18 | Q | 41/82 (50%) | 34 (83%) | 7 (17%) | 2 | 16 |
| 19 | R | 44/90 (49%) | 26 (59%) | 18 (41%) | 0 | 1 |
| 20 | S | 88/190 (46%) | 73 (83%) | 15 (17%) | 2 | 16 |
| 21 | T | 53/75 (71%) | 40 (76%) | 13 (24%) | 1 | 5 |
| 22 | U | 8/52 (15%) | 7 (88%) | 1 (12%) | 5 | 29 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 23 | V | 47/62 (76%) | 35 (74%) | 12 (26%) | 0 | 5 |
| 24 | W | 50/53 (94%) | 38 (76%) | 12 (24%) | 1 | 5 |
| 25 | Z | 38/51 (74%) | 32 (84%) | 6 (16%) | 3 | 20 |
| 26 | 2 | 35/40 (88%) | 29 (83%) | 6 (17%) | 2 | 16 |
| 27 | 3 | 33/57 (58%) | 27 (82%) | 6 (18%) | 2 | 12 |
| 28 | 4 | 2/35 (6%) | 1 (50%) | 1 (50%) | 0 | 0 |
| All | All | 1673/2698 (62%) | 1346 (80%) | 327 (20%) | 1 | 10 |

5 of 327 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | K | 36 | ARG |
| 14 | M | 82 | LYS |
| 24 | W | 40 | ASN |
| 12 | K | 94 | THR |
| 13 | L | 96 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | M | 14 | GLN |
| 16 | O | 63 | ASN |
| 17 | P | 40 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2 | X | 2684/2923 (91%) | 645 (24%) | 0 |
| 3 | Y | 113/114 (99%) | 18 (15%) | 0 |
| All | All | 2797/3037 (92%) | 663 (23%) | 0 |

5 of 663 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | X | 8 | U |
| 2 | X | 15 | G |
| 2 | X | 17 | G |
| 2 | X | 34 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | X | 38 | A |

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 538 ligands modelled in this entry, 514 are monoatomic - leaving 24 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 32 | MPD | J | 201 | - | 7,7,7 | 1.26 | 1 (14%) | 9,10,10 | 0.63 | 0 |
| 35 | EPE | N | 201 | - | 15,15,15 | 1.09 | 1 (6%) | 18,20,20 | 1.85 | 3 (16%) |
| 32 | MPD | Q | 101 | - | 7,7,7 | 0.71 | 0 | 9,10,10 | 0.24 | 0 |
| 34 | EOH | S | 301 | - | 2,2,2 | 0.70 | 0 | 1,1,1 | 0.29 | 0 |
| 31 | 62B | X | 3003 | - | 32,38,38 | 0.47 | 0 | 27,60,60 | 2.15 | 6 (22%) |
| 32 | MPD | X | 3004 | - | 7,7,7 | 1.12 | 1 (14%) | 9,10,10 | 0.65 | 0 |
| 32 | MPD | X | 3005 | - | 7,7,7 | 0.95 | 1 (14%) | 9,10,10 | 0.60 | 0 |
| 32 | MPD | X | 3006 | - | 7,7,7 | 0.97 | 1 (14%) | 9,10,10 | 0.51 | 0 |
| 32 | MPD | X | 3007 | - | 7,7,7 | 0.36 | 0 | 9,10,10 | 0.35 | 0 |
| 32 | MPD | X | 3008 | - | 7,7,7 | 1.13 | 1 (14%) | 9,10,10 | 0.63 | 0 |
| 32 | MPD | X | 3009 | - | 7,7,7 | 0.59 | 0 | 9,10,10 | 0.27 | 0 |
| 32 | MPD | X | 3010 | - | 7,7,7 | 0.91 | 1 (14%) | 9,10,10 | 0.37 | 0 |
| 32 | MPD | X | 3011 | - | 7,7,7 | 1.22 | 1 (14%) | 9,10,10 | 0.41 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 33 | SPD | X | 3492 | - | 9,9,9 | 0.39 | 0 | 8,8,8 | 0.43 | 0 |
| 33 | SPD | X | 3493 | - | 9,9,9 | 0.33 | 0 | 8,8,8 | 0.54 | 0 |
| 33 | SPD | X | 3494 | - | 9,9,9 | 0.22 | 0 | 8,8,8 | 0.29 | 0 |
| 33 | SPD | X | 3495 | - | 9,9,9 | 0.24 | 0 | 8,8,8 | 0.36 | 0 |
| 33 | SPD | X | 3496 | - | 9,9,9 | 0.27 | 0 | 8,8,8 | 0.20 | 0 |
| 33 | SPD | X | 3497 | - | 9,9,9 | 0.13 | 0 | 8,8,8 | 0.33 | 0 |
| 33 | SPD | X | 3498 | - | 9,9,9 | 0.38 | 0 | 8,8,8 | 0.62 | 0 |
| 34 | EOH | X | 3499 | - | 2,2,2 | 0.61 | 0 | 1,1,1 | 0.47 | 0 |
| 34 | EOH | X | 3500 | - | 2,2,2 | 0.62 | 0 | 1,1,1 | 0.49 | 0 |
| 33 | SPD | Y | 213 | - | 9,9,9 | 0.21 | 0 | 8,8,8 | 0.14 | 0 |
| 32 | MPD | Z | 101 | - | 7,7,7 | 0.59 | 0 | 9,10,10 | 0.20 | 0 |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 32 | MPD | J | 201 | - | - | 0/5/5/5 | 0/0/0/0 |
| 35 | EPE | N | 201 | - | - | 0/9/19/19 | 0/1/1/1 |
| 32 | MPD | Q | 101 | - | - | 0/5/5/5 | 0/0/0/0 |
| 34 | EOH | S | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 31 | 62B | X | 3003 | - | - | 0/11/86/86 | 0/2/4/4 |
| 32 | MPD | X | 3004 | - | - | 0/5/5/5 | 0/0/0/0 |
| 32 | MPD | X | 3005 | - | - | 0/5/5/5 | 0/0/0/0 |
| 32 | MPD | X | 3006 | - | - | 0/5/5/5 | 0/0/0/0 |
| 32 | MPD | X | 3007 | - | - | 0/5/5/5 | 0/0/0/0 |
| 32 | MPD | X | 3008 | - | - | 0/5/5/5 | 0/0/0/0 |
| 32 | MPD | X | 3009 | - | - | 0/5/5/5 | 0/0/0/0 |
| 32 | MPD | X | 3010 | - | - | 0/5/5/5 | 0/0/0/0 |
| 32 | MPD | X | 3011 | - | - | 0/5/5/5 | 0/0/0/0 |
| 33 | SPD | X | 3492 | - | - | 0/7/7/7 | 0/0/0/0 |
| 33 | SPD | X | 3493 | - | - | 0/7/7/7 | 0/0/0/0 |
| 33 | SPD | X | 3494 | - | - | 0/7/7/7 | 0/0/0/0 |
| 33 | SPD | X | 3495 | - | - | 0/7/7/7 | 0/0/0/0 |
| 33 | SPD | X | 3496 | - | - | 0/7/7/7 | 0/0/0/0 |
| 33 | SPD | X | 3497 | - | - | 0/7/7/7 | 0/0/0/0 |
| 33 | SPD | X | 3498 | - | - | 0/7/7/7 | 0/0/0/0 |
| 34 | EOH | X | 3499 | - | - | 0/0/0/0 | 0/0/0/0 |
| 34 | EOH | X | 3500 | - | - | 0/0/0/0 | 0/0/0/0 |
| 33 | SPD | Y | 213 | - | - | 0/7/7/7 | 0/0/0/0 |
| 32 | MPD | Z | 101 | - | - | 0/5/5/5 | 0/0/0/0 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 35 | N | 201 | EPE | C10-S | -3.56 | 1.72 | 1.77 |
| 32 | X | 3005 | MPD | C3-C2 | 2.03 | 1.59 | 1.53 |
| 32 | X | 3010 | MPD | C3-C2 | 2.06 | 1.59 | 1.53 |
| 32 | X | 3006 | MPD | C3-C2 | 2.37 | 1.60 | 1.53 |
| 32 | X | 3008 | MPD | C3-C2 | 2.67 | 1.61 | 1.53 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | X | 3003 | 62B | C24-C25-C26 | -7.05 | 103.25 | 111.52 |
| 35 | N | 201 | EPE | O3S-S-C10 | -5.81 | 98.92 | 106.06 |
| 31 | X | 3003 | 62B | C1-C9-C8 | -4.84 | 98.45 | 109.72 |
| 31 | X | 3003 | 62B | C28-C23-S1 | -4.46 | 103.18 | 111.02 |
| 31 | X | 3003 | 62B | C2-C3-C4 | -2.56 | 105.25 | 108.80 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 36 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32 | J | 201 | MPD | 1 | 0 |
| 35 | N | 201 | EPE | 17 | 0 |
| 31 | X | 3003 | 62B | 1 | 0 |
| 32 | X | 3004 | MPD | 2 | 0 |
| 32 | X | 3005 | MPD | 1 | 0 |
| 32 | X | 3006 | MPD | 2 | 0 |
| 32 | X | 3008 | MPD | 1 | 0 |
| 32 | X | 3010 | MPD | 1 | 0 |
| 33 | X | 3493 | SPD | 2 | 0 |
| 33 | X | 3494 | SPD | 1 | 0 |
| 33 | X | 3495 | SPD | 2 | 0 |
| 33 | X | 3497 | SPD | 3 | 0 |
| 33 | X | 3498 | SPD | 1 | 0 |
| 33 | Y | 213 | SPD | 1 | 0 |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 269/277 (97%) | -0.31 | 4 (1%) 74 62 | 92, 138, 160, 172 | 0 |
| 2 | X | 2705/2923 (92%) | -0.49 | 17 (0%) 89 82 | 53, 101, 188, 280 | 0 |
| 3 | Y | 114/114 (100%) | -0.63 | 0 100 100 | 76, 125, 175, 180 | 0 |
| 4 | B | 215/220 (97%) | -0.31 | 1 (0%) 90 84 | 62, 81, 99, 116 | 0 |
| 5 | C | 199/207 (96%) | -0.43 | 1 (0%) 90 84 | 64, 96, 113, 138 | 0 |
| 6 | D | 165/179 (92%) | 0.02 | 11 (6%) 19 14 | 166, 193, 231, 239 | 0 |
| 7 | E | 157/178 (88%) | -0.25 | 7 (4%) 34 25 | 133, 172, 206, 212 | 0 |
| 8 | G | 145/145 (100%) | -0.20 | 1 (0%) 87 79 | 64, 79, 91, 96 | 0 |
| 9 | H | 122/122 (100%) | -0.37 | 0 100 100 | 84, 102, 123, 128 | 0 |
| 10 | I | 131/140 (93%) | -0.01 | 5 (3%) 41 31 | 58, 116, 136, 142 | 0 |
| 11 | J | 138/144 (95%) | 0.24 | 4 (2%) 52 39 | 77, 103, 135, 152 | 0 |
| 12 | K | 119/122 (97%) | -0.54 | 0 100 100 | 67, 84, 108, 141 | 0 |
| 13 | L | 109/119 (91%) | -0.83 | 0 100 100 | 121, 130, 157, 189 | 0 |
| 14 | M | 110/116 (94%) | -0.39 | 2 (1%) 69 56 | 85, 99, 132, 156 | 0 |
| 15 | N | 116/118 (98%) | -0.43 | 0 100 100 | 54, 70, 90, 96 | 0 |
| 16 | O | 102/102 (100%) | -0.56 | 0 100 100 | 54, 88, 103, 109 | 0 |
| 17 | P | 112/117 (95%) | -0.01 | 1 (0%) 84 74 | 64, 75, 114, 139 | 0 |
| 18 | Q | 90/91 (98%) | -0.19 | 0 100 100 | 98, 122, 138, 170 | 0 |
| 19 | R | 102/105 (97%) | 0.30 | 6 (5%) 23 17 | 98, 121, 189, 206 | 0 |
| 20 | S | 167/217 (76%) | -0.27 | 1 (0%) 89 82 | 87, 109, 199, 218 | 0 |
| 21 | T | 75/94 (79%) | -0.00 | 1 (1%) 77 65 | 85, 97, 115, 129 | 0 |
| 22 | U | 42/62 (67%) | 2.37 | 24 (57%) 0 0 | 160, 172, 203, 213 | 0 |
| 23 | V | 65/69 (94%) | -0.06 | 0 100 100 | 134, 145, 159, 163 | 0 |
| 24 | W | 57/59 (96%) | 0.22 | 0 100 100 | 63, 77, 99, 101 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | Z | 43/58 (74%) | -0.26 | 0 100 100 | 54, 76, 131, 136 | 0 |
| 26 | 2 | 43/45 (95%) | 0.42 | 4 (9%) 9 8 | 83, 92, 102, 105 | 0 |
| 27 | 3 | 60/66 (90%) | -0.23 | 0 100 100 | 80, 89, 105, 109 | 0 |
| 28 | 4 | 36/37 (97%) | 2.41 | 22 (61%) 0 0 | 159, 164, 174, 178 | 0 |
| All | All | 5808/6246 (92%) | -0.32 | 112 (1%) 67 55 | 53, 103, 190, 280 | 0 |

The worst 5 of 112 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 22 | U | 16 | ASN | 5.6 |
| 22 | U | 30 | ASN | 5.4 |
| 28 | 4 | 32 | HIS | 5.1 |
| 22 | U | 27 | ARG | 5.1 |
| 28 | 4 | 30 | PRO | 5.0 |

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 30 | MG | X | 3354 | 1/1 | 0.82 | 0.72 | 70.70 | 75,75,75,75 | 0 |
| 32 | MPD | X | 3007 | 8/8 | 0.92 | 0.36 | 32.06 | 132,132,132,132 | 0 |
| 32 | MPD | X | 3011 | 8/8 | 0.92 | 0.30 | 30.74 | 75,75,75,75 | 0 |
| 30 | MG | X | 3335 | 1/1 | 0.63 | 0.70 | 23.54 | 61,61,61,61 | 0 |
| 29 | MN | X | 3034 | 1/1 | 0.90 | 0.26 | 21.37 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 29 | MN | X | 3058 | 1/1 | 0.87 | 0.40 | 17.49 | 101,101,101,101 | 0 |
| 30 | MG | X | 3002 | 1/1 | 0.85 | 1.01 | 17.41 | 100,100,100,100 | 0 |
| 30 | MG | X | 3293 | 1/1 | 0.72 | 0.46 | 16.47 | 117,117,117,117 | 0 |
| 30 | MG | X | 3420 | 1/1 | 0.88 | 0.47 | 15.89 | 75,75,75,75 | 0 |
| 30 | MG | X | 3390 | 1/1 | 0.94 | 0.57 | 15.78 | 63,63,63,63 | 0 |
| 33 | SPD | X | 3496 | 10/10 | 0.81 | 0.48 | 14.55 | 102,102,102,102 | 0 |
| 30 | MG | Y | 207 | 1/1 | 0.81 | 0.28 | 13.27 | 78,78,78,78 | 0 |
| 30 | MG | X | 3340 | 1/1 | 0.45 | 0.64 | 13.14 | 84,84,84,84 | 0 |
| 30 | MG | X | 3123 | 1/1 | 0.84 | 0.49 | 12.37 | 69,69,69,69 | 0 |
| 29 | MN | X | 3194 | 1/1 | 0.87 | 0.21 | 12.01 | 138,138,138,138 | 0 |
| 29 | MN | X | 3139 | 1/1 | 0.84 | 0.45 | 9.68 | 117,117,117,117 | 0 |
| 29 | MN | X | 3073 | 1/1 | 0.90 | 0.37 | 9.63 | 95,95,95,95 | 0 |
| 30 | MG | X | 3329 | 1/1 | 0.86 | 0.53 | 9.62 | 63,63,63,63 | 0 |
| 33 | SPD | X | 3494 | 10/10 | 0.86 | 0.27 | 9.35 | 87,87,87,87 | 0 |
| 29 | MN | X | 3096 | 1/1 | 0.95 | 0.38 | 9.23 | 100,100,100,100 | 0 |
| 33 | SPD | Y | 213 | 10/10 | 0.78 | 0.38 | 9.00 | 101,101,101,101 | 0 |
| 29 | MN | X | 3029 | 1/1 | 0.96 | 0.39 | 8.90 | 69,69,69,69 | 0 |
| 29 | MN | X | 3045 | 1/1 | 0.91 | 0.27 | 8.74 | 96,96,96,96 | 0 |
| 29 | MN | X | 3036 | 1/1 | 0.95 | 0.30 | 8.64 | 86,86,86,86 | 0 |
| 30 | MG | X | 3279 | 1/1 | 0.98 | 0.34 | 8.25 | 67,67,67,67 | 0 |
| 29 | MN | X | 3063 | 1/1 | 0.97 | 0.30 | 7.94 | 70,70,70,70 | 0 |
| 30 | MG | X | 3144 | 1/1 | 0.88 | 0.32 | 7.75 | 71,71,71,71 | 0 |
| 30 | MG | X | 3295 | 1/1 | 0.87 | 0.45 | 7.08 | 100,100,100,100 | 0 |
| 29 | MN | X | 3040 | 1/1 | 0.99 | 0.36 | 6.66 | 81,81,81,81 | 0 |
| 29 | MN | X | 3173 | 1/1 | 0.92 | 0.25 | 6.36 | 129,129,129,129 | 0 |
| 32 | MPD | X | 3009 | 8/8 | 0.93 | 0.39 | 5.99 | 129,129,129,129 | 0 |
| 29 | MN | X | 3043 | 1/1 | 0.99 | 0.34 | 5.88 | 81,81,81,81 | 0 |
| 33 | SPD | X | 3498 | 10/10 | 0.69 | 0.41 | 5.71 | 93,93,93,93 | 0 |
| 30 | MG | C | 301 | 1/1 | 0.97 | 0.40 | 5.69 | 64,64,64,64 | 0 |
| 29 | MN | X | 3320 | 1/1 | 0.88 | 0.31 | 5.67 | 107,107,107,107 | 0 |
| 30 | MG | X | 3501 | 1/1 | 0.95 | 0.83 | 5.59 | 64,64,64,64 | 0 |
| 33 | SPD | X | 3495 | 10/10 | 0.87 | 0.24 | 5.49 | 83,83,83,83 | 0 |
| 29 | MN | X | 3081 | 1/1 | 0.96 | 0.29 | 5.30 | 109,109,109,109 | 0 |
| 29 | MN | X | 3054 | 1/1 | 0.96 | 0.35 | 5.05 | 97,97,97,97 | 0 |
| 32 | MPD | X | 3004 | 8/8 | 0.78 | 0.30 | 4.81 | 135,135,135,135 | 0 |
| 30 | MG | I | 201 | 1/1 | 0.93 | 0.57 | 4.76 | 80,80,80,80 | 0 |
| 29 | MN | X | 3439 | 1/1 | 0.91 | 0.28 | 4.73 | 94,94,94,94 | 0 |
| 31 | 62B | X | 3003 | 35/35 | 0.95 | 0.29 | 4.69 | 65,65,65,65 | 0 |
| 29 | MN | X | 3085 | 1/1 | 1.00 | 0.27 | 4.62 | 59,59,59,59 | 0 |
| 29 | MN | X | 3067 | 1/1 | 0.97 | 0.42 | 4.36 | 104,104,104,104 | 0 |
| 29 | MN | X | 3066 | 1/1 | 0.99 | 0.24 | 4.31 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 29 | MN | X | 3068 | 1/1 | 0.96 | 0.35 | 4.26 | 94,94,94,94 | 0 |
| 29 | MN | X | 3099 | 1/1 | 0.98 | 0.28 | 4.21 | 82,82,82,82 | 0 |
| 29 | MN | X | 3028 | 1/1 | 0.98 | 0.26 | 4.14 | 53,53,53,53 | 0 |
| 29 | MN | X | 3001 | 1/1 | 0.97 | 0.38 | 3.89 | 97,97,97,97 | 0 |
| 29 | MN | X | 3202 | 1/1 | 0.66 | 0.22 | 3.79 | 173,173,173,173 | 0 |
| 29 | MN | X | 3026 | 1/1 | 0.97 | 0.29 | 3.77 | 66,66,66,66 | 0 |
| 30 | MG | X | 3239 | 1/1 | 0.94 | 0.38 | 3.76 | 91,91,91,91 | 0 |
| 29 | MN | X | 3049 | 1/1 | 0.96 | 0.30 | 3.75 | 93,93,93,93 | 0 |
| 29 | MN | X | 3164 | 1/1 | 0.99 | 0.28 | 3.55 | 111,111,111,111 | 0 |
| 29 | MN | X | 3168 | 1/1 | 0.84 | 0.29 | 3.55 | 115,115,115,115 | 0 |
| 29 | MN | A | 301 | 1/1 | 0.91 | 0.39 | 3.43 | 138,138,138,138 | 0 |
| 32 | MPD | X | 3006 | 8/8 | 0.92 | 0.22 | 3.39 | 82,82,82,82 | 0 |
| 32 | MPD | X | 3005 | 8/8 | 0.95 | 0.23 | 3.20 | 78,78,78,78 | 0 |
| 29 | MN | X | 3083 | 1/1 | 0.99 | 0.31 | 3.13 | 73,73,73,73 | 0 |
| 32 | MPD | X | 3010 | 8/8 | 0.88 | 0.22 | 2.99 | 113,113,113,113 | 0 |
| 29 | MN | X | 3013 | 1/1 | 0.95 | 0.25 | 2.94 | 70,70,70,70 | 0 |
| 33 | SPD | X | 3492 | 10/10 | 0.84 | 0.27 | 2.83 | 105,105,105,105 | 0 |
| 29 | MN | X | 3047 | 1/1 | 0.94 | 0.26 | 2.76 | 70,70,70,70 | 0 |
| 32 | MPD | X | 3008 | 8/8 | 0.85 | 0.26 | 2.52 | 94,94,94,94 | 0 |
| 30 | MG | X | 3233 | 1/1 | 0.86 | 0.34 | 2.48 | 68,68,68,68 | 0 |
| 30 | MG | X | 3435 | 1/1 | 0.68 | 0.28 | 2.44 | 153,153,153,153 | 0 |
| 29 | MN | X | 3122 | 1/1 | 0.93 | 0.23 | 2.41 | 99,99,99,99 | 0 |
| 29 | MN | X | 3053 | 1/1 | 0.98 | 0.22 | 2.22 | 58,58,58,58 | 0 |
| 29 | MN | X | 3097 | 1/1 | 0.96 | 0.26 | 1.99 | 109,109,109,109 | 0 |
| 29 | MN | X | 3095 | 1/1 | 0.95 | 0.20 | 1.99 | 79,79,79,79 | 0 |
| 30 | MG | X | 3299 | 1/1 | 0.95 | 0.22 | 1.87 | 149,149,149,149 | 0 |
| 29 | MN | X | 3075 | 1/1 | 0.98 | 0.23 | 1.81 | 71,71,71,71 | 0 |
| 29 | MN | X | 3199 | 1/1 | 0.92 | 0.20 | 1.63 | 143,143,143,143 | 0 |
| 29 | MN | X | 3126 | 1/1 | 0.99 | 0.21 | 1.63 | 74,74,74,74 | 0 |
| 29 | MN | X | 3463 | 1/1 | 0.84 | 0.17 | 1.59 | 134,134,134,134 | 0 |
| 30 | MG | X | 3434 | 1/1 | 0.93 | 0.20 | 1.56 | 64,64,64,64 | 0 |
| 29 | MN | X | 3263 | 1/1 | 0.66 | 0.35 | 1.47 | 166,166,166,166 | 0 |
| 29 | MN | X | 3503 | 1/1 | 0.98 | 0.25 | 1.34 | 68,68,68,68 | 0 |
| 30 | MG | A | 303 | 1/1 | 0.62 | 0.31 | 1.27 | 94,94,94,94 | 0 |
| 29 | MN | X | 3198 | 1/1 | 0.90 | 0.18 | 1.05 | 125,125,125,125 | 0 |
| 35 | EPE | N | 201 | 15/15 | 0.91 | 0.20 | 0.95 | 73,73,73,73 | 0 |
| 29 | MN | X | 3050 | 1/1 | 0.99 | 0.25 | 0.94 | 98,98,98,98 | 0 |
| 29 | MN | X | 3103 | 1/1 | 0.95 | 0.21 | 0.86 | 85,85,85,85 | 0 |
| 29 | MN | X | 3177 | 1/1 | 0.92 | 0.16 | 0.74 | 125,125,125,125 | 0 |
| 29 | MN | X | 3152 | 1/1 | 0.98 | 0.16 | 0.65 | 75,75,75,75 | 0 |
| 30 | MG | X | 3397 | 1/1 | 0.88 | 0.21 | 0.55 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 29 | MN | X | 3127 | 1/1 | 0.99 | 0.17 | 0.52 | 94,94,94,94 | 0 |
| 29 | MN | X | 3105 | 1/1 | 0.97 | 0.19 | 0.49 | 97,97,97,97 | 0 |
| 33 | SPD | X | 3493 | 10/10 | 0.89 | 0.28 | 0.34 | 83,83,83,83 | 0 |
| 32 | MPD | J | 201 | 8/8 | 0.78 | 0.30 | 0.31 | 125,125,125,125 | 0 |
| 29 | MN | X | 3181 | 1/1 | 0.70 | 0.12 | 0.30 | 142,142,142,142 | 0 |
| 29 | MN | X | 3109 | 1/1 | 0.92 | 0.14 | 0.17 | 92,92,92,92 | 0 |
| 29 | MN | X | 3146 | 1/1 | 0.81 | 0.20 | 0.14 | 122,122,122,122 | 0 |
| 30 | MG | X | 3356 | 1/1 | 0.83 | 0.13 | 0.01 | 83,83,83,83 | 0 |
| 29 | MN | X | 3409 | 1/1 | 0.97 | 0.17 | 0.00 | 87,87,87,87 | 0 |
| 29 | MN | X | 3160 | 1/1 | 0.96 | 0.15 | -0.07 | 100,100,100,100 | 0 |
| 29 | MN | X | 3200 | 1/1 | 0.97 | 0.19 | -0.22 | 123,123,123,123 | 0 |
| 30 | MG | X | 3353 | 1/1 | 0.93 | 0.17 | -0.30 | 79,79,79,79 | 0 |
| 29 | MN | X | 3091 | 1/1 | 0.98 | 0.16 | -0.30 | 92,92,92,92 | 0 |
| 29 | MN | X | 3219 | 1/1 | 0.99 | 0.15 | -0.38 | 85,85,85,85 | 0 |
| 29 | MN | T | 101 | 1/1 | 0.92 | 0.18 | -0.49 | 121,121,121,121 | 0 |
| 30 | MG | J | 202 | 1/1 | 0.88 | 0.18 | -0.65 | 92,92,92,92 | 0 |
| 29 | MN | X | 3185 | 1/1 | 0.81 | 0.16 | -0.70 | 101,101,101,101 | 0 |
| 29 | MN | X | 3217 | 1/1 | 0.99 | 0.14 | -0.88 | 86,86,86,86 | 0 |
| 29 | MN | X | 3104 | 1/1 | 0.93 | 0.14 | -1.04 | 94,94,94,94 | 0 |
| 29 | MN | X | 3270 | 1/1 | 0.99 | 0.12 | -1.06 | 110,110,110,110 | 0 |
| 29 | MN | X | 3106 | 1/1 | 0.98 | 0.14 | -1.15 | 100,100,100,100 | 0 |
| 29 | MN | X | 3022 | 1/1 | 0.98 | 0.11 | -1.30 | 92,92,92,92 | 0 |
| 30 | MG | X | 3218 | 1/1 | 0.96 | 0.17 | -2.03 | 75,75,75,75 | 0 |
| 29 | MN | X | 3234 | 1/1 | 0.97 | 0.05 | -2.25 | 144,144,144,144 | 0 |
| 29 | MN | X | 3215 | 1/1 | 0.99 | 0.14 | -2.32 | 87,87,87,87 | 0 |
| 29 | MN | X | 3220 | 1/1 | 0.96 | 0.08 | -2.70 | 103,103,103,103 | 0 |
| 29 | MN | X | 3318 | 1/1 | 0.94 | 0.08 | -2.77 | 128,128,128,128 | 0 |
| 29 | MN | X | 3192 | 1/1 | 0.95 | 0.09 | -3.77 | 138,138,138,138 | 0 |
| 29 | MN | X | 3015 | 1/1 | 0.96 | 0.09 | -4.76 | 80,80,80,80 | 0 |
| 29 | MN | X | 3016 | 1/1 | 0.96 | 0.12 | -6.29 | 75,75,75,75 | 0 |
| 30 | MG | X | 3221 | 1/1 | 0.97 | 0.12 | - | 89,89,89,89 | 0 |
| 30 | MG | X | 3429 | 1/1 | 0.83 | 0.22 | - | 102,102,102,102 | 0 |
| 29 | MN | X | 3118 | 1/1 | 0.98 | 0.19 | - | 65,65,65,65 | 0 |
| 29 | MN | X | 3322 | 1/1 | 0.92 | 0.15 | - | 137,137,137,137 | 0 |
| 29 | MN | X | 3059 | 1/1 | 0.90 | 0.24 | - | 111,111,111,111 | 0 |
| 29 | MN | Y | 202 | 1/1 | 0.95 | 0.15 | - | 105,105,105,105 | 0 |
| 29 | MN | X | 3115 | 1/1 | 0.94 | 0.32 | - | 116,116,116,116 | 0 |
| 30 | MG | X | 3430 | 1/1 | 0.98 | 0.40 | - | 74,74,74,74 | 0 |
| 30 | MG | X | 3204 | 1/1 | 0.95 | 0.14 | - | 100,100,100,100 | 0 |
| 30 | MG | Y | 201 | 1/1 | 0.97 | 0.28 | - | 66,66,66,66 | 0 |
| 30 | MG | X | 3438 | 1/1 | 0.95 | 0.20 | - | 84,84,84,84 | 0 |
| 32 | MPD | Q | 101 | 8/8 | 0.83 | 0.20 | - | 137,137,137,137 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 30 | MG | X | 3448 | 1/1 | 0.91 | 0.66 | - | 72,72,72,72 | 0 |
| 29 | MN | X | 3062 | 1/1 | 0.95 | 0.14 | - | 87,87,87,87 | 0 |
| 29 | MN | X | 3455 | 1/1 | 0.91 | 0.43 | - | 116,116,116,116 | 0 |
| 30 | MG | X | 3306 | 1/1 | 0.42 | 0.43 | - | 95,95,95,95 | 0 |
| 29 | MN | X | 3071 | 1/1 | 0.93 | 0.21 | - | 98,98,98,98 | 0 |
| 30 | MG | X | 3196 | 1/1 | 0.72 | 0.52 | - | 89,89,89,89 | 0 |
| 30 | MG | X | 3309 | 1/1 | 0.94 | 0.34 | - | 105,105,105,105 | 0 |
| 29 | MN | X | 3437 | 1/1 | 0.49 | 0.13 | - | 153,153,153,153 | 0 |
| 29 | MN | X | 3223 | 1/1 | 0.95 | 0.17 | - | 119,119,119,119 | 0 |
| 30 | MG | X | 3386 | 1/1 | 0.68 | 0.41 | - | 88,88,88,88 | 0 |
| 29 | MN | X | 3128 | 1/1 | 0.95 | 0.24 | - | 93,93,93,93 | 0 |
| 30 | MG | X | 3378 | 1/1 | 0.82 | 0.59 | - | 83,83,83,83 | 0 |
| 30 | MG | X | 3291 | 1/1 | 0.89 | 0.47 | - | 86,86,86,86 | 0 |
| 30 | MG | X | 3367 | 1/1 | 0.92 | 0.39 | - | 83,83,83,83 | 0 |
| 29 | MN | X | 3325 | 1/1 | 0.95 | 0.16 | - | 187,187,187,187 | 0 |
| 29 | MN | X | 3088 | 1/1 | 0.97 | 0.28 | - | 101,101,101,101 | 0 |
| 30 | MG | X | 3327 | 1/1 | 0.57 | 1.12 | - | 126,126,126,126 | 0 |
| 29 | MN | X | 3470 | 1/1 | 0.93 | 0.18 | - | 148,148,148,148 | 0 |
| 29 | MN | X | 3172 | 1/1 | 0.97 | 0.14 | - | 114,114,114,114 | 0 |
| 30 | MG | X | 3423 | 1/1 | 0.81 | 0.32 | - | 79,79,79,79 | 0 |
| 30 | MG | X | 3385 | 1/1 | 0.81 | 1.06 | - | 88,88,88,88 | 0 |
| 30 | MG | X | 3485 | 1/1 | 0.90 | 0.24 | - | 102,102,102,102 | 0 |
| 29 | MN | X | 3084 | 1/1 | 0.90 | 0.14 | - | 123,123,123,123 | 0 |
| 30 | MG | X | 3298 | 1/1 | 0.89 | 0.40 | - | 95,95,95,95 | 0 |
| 29 | MN | X | 3069 | 1/1 | 0.97 | 0.29 | - | 103,103,103,103 | 0 |
| 30 | MG | X | 3443 | 1/1 | 0.91 | 0.24 | - | 118,118,118,118 | 0 |
| 30 | MG | X | 3489 | 1/1 | 0.84 | 0.70 | - | 62,62,62,62 | 0 |
| 29 | MN | X | 3453 | 1/1 | 0.91 | 0.33 | - | 126,126,126,126 | 0 |
| 29 | MN | X | 3110 | 1/1 | 0.91 | 0.19 | - | 117,117,117,117 | 0 |
| 34 | EOH | X | 3499 | 3/3 | 0.93 | 0.40 | - | 80,80,80,80 | 0 |
| 30 | MG | Y | 211 | 1/1 | 0.90 | 0.42 | - | 115,115,115,115 | 0 |
| 30 | MG | X | 3408 | 1/1 | 0.82 | 1.49 | - | 97,97,97,97 | 0 |
| 30 | MG | X | 3249 | 1/1 | 0.89 | 0.98 | - | 109,109,109,109 | 0 |
| 29 | MN | X | 3197 | 1/1 | 0.96 | 0.26 | - | 138,138,138,138 | 0 |
| 30 | MG | X | 3282 | 1/1 | 0.88 | 0.25 | - | 85,85,85,85 | 0 |
| 30 | MG | X | 3285 | 1/1 | 0.91 | 0.21 | - | 75,75,75,75 | 0 |
| 29 | MN | X | 3446 | 1/1 | 0.66 | 0.46 | - | 142,142,142,142 | 0 |
| 30 | MG | X | 3389 | 1/1 | 0.96 | 0.38 | - | 94,94,94,94 | 0 |
| 30 | MG | X | 3334 | 1/1 | 0.87 | 0.72 | - | 89,89,89,89 | 0 |
| 29 | MN | X | 3132 | 1/1 | 0.99 | 0.20 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3076 | 1/1 | 0.98 | 0.30 | - | 90,90,90,90 | 0 |
| 29 | MN | X | 3112 | 1/1 | 0.77 | 0.25 | - | 124,124,124,124 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 29 | MN | X | 3042 | 1/1 | 0.99 | 0.23 | - | 74,74,74,74 | 0 |
| 30 | MG | G | 202 | 1/1 | 0.72 | 0.37 | - | 77,77,77,77 | 0 |
| 29 | MN | X | 3466 | 1/1 | 0.37 | 0.38 | - | 155,155,155,155 | 0 |
| 30 | MG | X | 3250 | 1/1 | 0.21 | 1.65 | - | 89,89,89,89 | 0 |
| 29 | MN | X | 3201 | 1/1 | 0.99 | 0.15 | - | 88,88,88,88 | 0 |
| 30 | MG | X | 3375 | 1/1 | 0.81 | 0.25 | - | 76,76,76,76 | 0 |
| 30 | MG | X | 3410 | 1/1 | 0.97 | 0.16 | - | 95,95,95,95 | 0 |
| 30 | MG | X | 3290 | 1/1 | 0.88 | 0.59 | - | 98,98,98,98 | 0 |
| 30 | MG | X | 3143 | 1/1 | 0.96 | 0.44 | - | 59,59,59,59 | 0 |
| 30 | MG | X | 3444 | 1/1 | 0.85 | 0.40 | - | 100,100,100,100 | 0 |
| 30 | MG | X | 3268 | 1/1 | 0.91 | 0.36 | - | 62,62,62,62 | 0 |
| 29 | MN | X | 3257 | 1/1 | 0.98 | 0.06 | - | 93,93,93,93 | 0 |
| 29 | MN | X | 3245 | 1/1 | 0.97 | 0.21 | - | 129,129,129,129 | 0 |
| 30 | MG | X | 3300 | 1/1 | 0.85 | 0.24 | - | 94,94,94,94 | 0 |
| 30 | MG | X | 3346 | 1/1 | 0.78 | 0.47 | - | 68,68,68,68 | 0 |
| 30 | MG | X | 3341 | 1/1 | 0.60 | 0.64 | - | 96,96,96,96 | 0 |
| 29 | MN | X | 3480 | 1/1 | 0.91 | 0.57 | - | 175,175,175,175 | 0 |
| 30 | MG | X | 3271 | 1/1 | 0.98 | 0.26 | - | 92,92,92,92 | 0 |
| 34 | EOH | S | 301 | 3/3 | 0.74 | 0.35 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3441 | 1/1 | 0.75 | 0.59 | - | 96,96,96,96 | 0 |
| 30 | MG | X | 3451 | 1/1 | 0.96 | 0.30 | - | 115,115,115,115 | 0 |
| 30 | MG | X | 3213 | 1/1 | 0.83 | 1.50 | - | 86,86,86,86 | 0 |
| 29 | MN | X | 3134 | 1/1 | 0.97 | 0.17 | - | 121,121,121,121 | 0 |
| 29 | MN | X | 3195 | 1/1 | 0.97 | 0.22 | - | 139,139,139,139 | 0 |
| 29 | MN | X | 3461 | 1/1 | 0.87 | 0.26 | - | 149,149,149,149 | 0 |
| 30 | MG | X | 3504 | 1/1 | 0.87 | 0.57 | - | 74,74,74,74 | 0 |
| 29 | MN | X | 3018 | 1/1 | 1.00 | 0.12 | - | 86,86,86,86 | 0 |
| 29 | MN | X | 3460 | 1/1 | 0.52 | 0.36 | - | 182,182,182,182 | 0 |
| 32 | MPD | Z | 101 | 8/8 | 0.87 | 0.20 | - | 145,145,145,145 | 0 |
| 30 | MG | X | 3266 | 1/1 | 0.76 | 0.34 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3297 | 1/1 | 0.93 | 0.19 | - | 81,81,81,81 | 0 |
| 29 | MN | X | 3502 | 1/1 | 0.97 | 0.26 | - | 88,88,88,88 | 0 |
| 29 | MN | X | 3237 | 1/1 | 0.94 | 0.07 | - | 167,167,167,167 | 0 |
| 29 | MN | X | 3188 | 1/1 | 0.99 | 0.25 | - | 114,114,114,114 | 0 |
| 29 | MN | X | 3169 | 1/1 | 0.98 | 0.19 | - | 107,107,107,107 | 0 |
| 29 | MN | X | 3312 | 1/1 | 0.96 | 0.26 | - | 115,115,115,115 | 0 |
| 30 | MG | X | 3332 | 1/1 | 0.79 | 0.44 | - | 81,81,81,81 | 0 |
| 29 | MN | X | 3321 | 1/1 | 0.93 | 0.07 | - | 159,159,159,159 | 0 |
| 29 | MN | X | 3131 | 1/1 | 0.96 | 0.23 | - | 126,126,126,126 | 0 |
| 29 | MN | X | 3360 | 1/1 | 0.84 | 0.11 | - | 146,146,146,146 | 0 |
| 30 | MG | X | 3224 | 1/1 | 0.86 | 0.79 | - | 66,66,66,66 | 0 |
| 30 | MG | X | 3229 | 1/1 | 0.81 | 0.20 | - | 98,98,98,98 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 29 | MN | X | 3469 | 1/1 | 0.81 | 0.17 | - | 140,140,140,140 | 0 |
| 30 | MG | X | 3344 | 1/1 | 0.66 | 0.85 | - | 91,91,91,91 | 0 |
| 30 | MG | X | 3419 | 1/1 | 0.84 | 0.71 | - | 107,107,107,107 | 0 |
| 30 | MG | X | 3387 | 1/1 | 0.84 | 0.34 | - | 175,175,175,175 | 0 |
| 29 | MN | X | 3317 | 1/1 | 0.93 | 0.14 | - | 137,137,137,137 | 0 |
| 33 | SPD | X | 3497 | 10/10 | 0.85 | 0.19 | - | 96,96,96,96 | 0 |
| 29 | MN | X | 3403 | 1/1 | 0.98 | 0.11 | - | 114,114,114,114 | 0 |
| 29 | MN | X | 3452 | 1/1 | 0.91 | 0.08 | - | 120,120,120,120 | 0 |
| 30 | MG | X | 3214 | 1/1 | 0.90 | 0.76 | - | 86,86,86,86 | 0 |
| 29 | MN | X | 3326 | 1/1 | 0.89 | 0.21 | - | 145,145,145,145 | 0 |
| 29 | MN | X | 3210 | 1/1 | 0.73 | 0.22 | - | 201,201,201,201 | 0 |
| 29 | MN | X | 3405 | 1/1 | 0.92 | 0.17 | - | 103,103,103,103 | 0 |
| 30 | MG | X | 3280 | 1/1 | 0.85 | 0.32 | - | 159,159,159,159 | 0 |
| 30 | MG | X | 3482 | 1/1 | 0.95 | 0.26 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3412 | 1/1 | 0.88 | 0.53 | - | 106,106,106,106 | 0 |
| 30 | MG | X | 3351 | 1/1 | 0.46 | 0.63 | - | 116,116,116,116 | 0 |
| 29 | MN | X | 3030 | 1/1 | 0.98 | 0.38 | - | 69,69,69,69 | 0 |
| 29 | MN | X | 3019 | 1/1 | 0.89 | 0.32 | - | 109,109,109,109 | 0 |
| 29 | MN | X | 3468 | 1/1 | 0.81 | 0.25 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3330 | 1/1 | 0.95 | 0.15 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3077 | 1/1 | 0.92 | 0.33 | - | 100,100,100,100 | 0 |
| 29 | MN | X | 3407 | 1/1 | 0.95 | 0.20 | - | 83,83,83,83 | 0 |
| 29 | MN | X | 3017 | 1/1 | 0.95 | 0.09 | - | 92,92,92,92 | 0 |
| 30 | MG | X | 3260 | 1/1 | 0.82 | 0.14 | - | 123,123,123,123 | 0 |
| 30 | MG | X | 3416 | 1/1 | 0.89 | 0.27 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3364 | 1/1 | 0.96 | 0.73 | - | 83,83,83,83 | 0 |
| 30 | MG | X | 3294 | 1/1 | 0.67 | 0.46 | - | 108,108,108,108 | 0 |
| 29 | MN | X | 3314 | 1/1 | 0.81 | 0.30 | - | 147,147,147,147 | 0 |
| 29 | MN | X | 3157 | 1/1 | 0.93 | 0.24 | - | 108,108,108,108 | 0 |
| 30 | MG | X | 3310 | 1/1 | 0.56 | 0.22 | - | 129,129,129,129 | 0 |
| 30 | MG | X | 3328 | 1/1 | 0.86 | 0.54 | - | 103,103,103,103 | 0 |
| 30 | MG | X | 3361 | 1/1 | 0.75 | 0.37 | - | 86,86,86,86 | 0 |
| 30 | MG | X | 3388 | 1/1 | 0.93 | 0.86 | - | 85,85,85,85 | 0 |
| 29 | MN | X | 3100 | 1/1 | 0.95 | 0.25 | - | 96,96,96,96 | 0 |
| 29 | MN | X | 3251 | 1/1 | 0.99 | 0.12 | - | 81,81,81,81 | 0 |
| 30 | MG | X | 3382 | 1/1 | 0.79 | 0.66 | - | 126,126,126,126 | 0 |
| 29 | MN | X | 3315 | 1/1 | 0.91 | 0.18 | - | 104,104,104,104 | 0 |
| 30 | MG | X | 3307 | 1/1 | 0.83 | 0.51 | - | 71,71,71,71 | 0 |
| 30 | MG | Y | 203 | 1/1 | 0.55 | 0.61 | - | 96,96,96,96 | 0 |
| 29 | MN | X | 3086 | 1/1 | 0.97 | 0.47 | - | 92,92,92,92 | 0 |
| 29 | MN | X | 3392 | 1/1 | 0.96 | 0.11 | - | 89,89,89,89 | 0 |
| 30 | MG | X | 3222 | 1/1 | 0.72 | 0.21 | - | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 30 | MG | X | 3395 | 1/1 | 0.72 | 0.37 | - | 79,79,79,79 | 0 |
| 29 | MN | X | 3216 | 1/1 | 0.98 | 0.04 | - | 94,94,94,94 | 0 |
| 30 | MG | X | 3484 | 1/1 | 0.89 | 0.17 | - | 77,77,77,77 | 0 |
| 29 | MN | X | 3163 | 1/1 | 0.93 | 0.13 | - | 124,124,124,124 | 0 |
| 30 | MG | X | 3287 | 1/1 | 0.89 | 1.56 | - | 102,102,102,102 | 0 |
| 29 | MN | X | 3156 | 1/1 | 0.98 | 0.21 | - | 77,77,77,77 | 0 |
| 30 | MG | X | 3289 | 1/1 | 0.96 | 0.24 | - | 110,110,110,110 | 0 |
| 30 | MG | X | 3343 | 1/1 | 0.89 | 0.64 | - | 73,73,73,73 | 0 |
| 29 | MN | X | 3376 | 1/1 | 0.87 | 0.10 | - | 119,119,119,119 | 0 |
| 29 | MN | X | 3166 | 1/1 | 0.76 | 0.21 | - | 92,92,92,92 | 0 |
| 29 | MN | X | 3436 | 1/1 | 0.95 | 0.17 | - | 119,119,119,119 | 0 |
| 29 | MN | X | 3262 | 1/1 | 0.87 | 0.12 | - | 143,143,143,143 | 0 |
| 29 | MN | X | 3057 | 1/1 | 0.97 | 0.23 | - | 68,68,68,68 | 0 |
| 29 | MN | X | 3119 | 1/1 | 0.90 | 0.20 | - | 140,140,140,140 | 0 |
| 29 | MN | X | 3089 | 1/1 | 0.96 | 0.14 | - | 113,113,113,113 | 0 |
| 29 | MN | X | 3184 | 1/1 | 0.91 | 0.13 | - | 128,128,128,128 | 0 |
| 30 | MG | X | 3253 | 1/1 | 0.68 | 1.55 | - | 112,112,112,112 | 0 |
| 30 | MG | Y | 209 | 1/1 | 0.96 | 0.91 | - | 153,153,153,153 | 0 |
| 29 | MN | X | 3471 | 1/1 | 0.66 | 1.22 | - | 130,130,130,130 | 0 |
| 30 | MG | X | 3474 | 1/1 | 0.52 | 0.23 | - | 106,106,106,106 | 0 |
| 29 | MN | X | 3174 | 1/1 | 0.84 | 0.18 | - | 121,121,121,121 | 0 |
| 29 | MN | X | 3074 | 1/1 | 0.95 | 0.52 | - | 113,113,113,113 | 0 |
| 29 | MN | X | 3098 | 1/1 | 0.99 | 0.19 | - | 92,92,92,92 | 0 |
| 30 | MG | X | 3252 | 1/1 | 0.75 | 1.35 | - | 114,114,114,114 | 0 |
| 30 | MG | X | 3486 | 1/1 | 0.90 | 0.60 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3398 | 1/1 | 0.72 | 0.58 | - | 99,99,99,99 | 0 |
| 30 | MG | X | 3255 | 1/1 | 0.74 | 0.62 | - | 94,94,94,94 | 0 |
| 29 | MN | X | 3079 | 1/1 | 0.99 | 0.27 | - | 58,58,58,58 | 0 |
| 30 | MG | X | 3449 | 1/1 | 0.47 | 0.42 | - | 86,86,86,86 | 0 |
| 30 | MG | X | 3370 | 1/1 | 0.71 | 1.19 | - | 113,113,113,113 | 0 |
| 29 | MN | X | 3425 | 1/1 | 0.73 | 0.30 | - | 101,101,101,101 | 0 |
| 30 | MG | X | 3415 | 1/1 | 0.93 | 0.25 | - | 81,81,81,81 | 0 |
| 29 | MN | X | 3459 | 1/1 | 0.98 | 0.34 | - | 161,161,161,161 | 0 |
| 30 | MG | X | 3244 | 1/1 | 0.76 | 0.51 | - | 109,109,109,109 | 0 |
| 29 | MN | X | 3186 | 1/1 | 0.79 | 0.46 | - | 143,143,143,143 | 0 |
| 30 | MG | X | 3258 | 1/1 | 0.93 | 0.26 | - | 80,80,80,80 | 0 |
| 30 | MG | M | 201 | 1/1 | 0.91 | 0.42 | - | 68,68,68,68 | 0 |
| 30 | MG | X | 3165 | 1/1 | 0.92 | 0.79 | - | 84,84,84,84 | 0 |
| 29 | MN | X | 3120 | 1/1 | 0.95 | 0.21 | - | 166,166,166,166 | 0 |
| 29 | MN | X | 3070 | 1/1 | 0.96 | 0.33 | - | 129,129,129,129 | 0 |
| 30 | MG | X | 3440 | 1/1 | 0.84 | 0.41 | - | 79,79,79,79 | 0 |
| 30 | MG | X | 3281 | 1/1 | 0.97 | 0.71 | - | 113,113,113,113 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 29 | MN | X | 3051 | 1/1 | 0.97 | 0.24 | - | 97,97,97,97 | 0 |
| 30 | MG | X | 3339 | 1/1 | 0.77 | 1.67 | - | 108,108,108,108 | 0 |
| 30 | MG | X | 3481 | 1/1 | 0.91 | 0.23 | - | 82,82,82,82 | 0 |
| 30 | MG | X | 3338 | 1/1 | 0.87 | 0.34 | - | 82,82,82,82 | 0 |
| 30 | MG | X | 3350 | 1/1 | 0.87 | 0.40 | - | 100,100,100,100 | 0 |
| 30 | MG | X | 3277 | 1/1 | 0.95 | 0.61 | - | 97,97,97,97 | 0 |
| 30 | MG | X | 3087 | 1/1 | 0.65 | 0.66 | - | 55,55,55,55 | 0 |
| 29 | MN | X | 3211 | 1/1 | 0.61 | 0.35 | - | 144,144,144,144 | 0 |
| 30 | MG | X | 3428 | 1/1 | 0.73 | 0.12 | - | 105,105,105,105 | 0 |
| 29 | MN | X | 3048 | 1/1 | 0.97 | 0.43 | - | 93,93,93,93 | 0 |
| 29 | MN | X | 3145 | 1/1 | 0.99 | 0.19 | - | 69,69,69,69 | 0 |
| 29 | MN | X | 3478 | 1/1 | 0.76 | 0.20 | - | 132,132,132,132 | 0 |
| 30 | MG | X | 3399 | 1/1 | 0.91 | 0.47 | - | 79,79,79,79 | 0 |
| 29 | MN | X | 3191 | 1/1 | 0.97 | 0.06 | - | 138,138,138,138 | 0 |
| 30 | MG | X | 3303 | 1/1 | 0.92 | 0.71 | - | 101,101,101,101 | 0 |
| 30 | MG | X | 3278 | 1/1 | 0.96 | 0.23 | - | 82,82,82,82 | 0 |
| 29 | MN | X | 3060 | 1/1 | 0.89 | 0.23 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3384 | 1/1 | 0.95 | 0.26 | - | 102,102,102,102 | 0 |
| 29 | MN | X | 3193 | 1/1 | 0.94 | 0.09 | - | 110,110,110,110 | 0 |
| 30 | MG | X | 3259 | 1/1 | 0.92 | 0.49 | - | 122,122,122,122 | 0 |
| 30 | MG | X | 3483 | 1/1 | 0.92 | 0.29 | - | 91,91,91,91 | 0 |
| 29 | MN | X | 3161 | 1/1 | 0.93 | 0.23 | - | 93,93,93,93 | 0 |
| 30 | MG | X | 3362 | 1/1 | 0.55 | 0.37 | - | 114,114,114,114 | 0 |
| 29 | MN | X | 3147 | 1/1 | 0.89 | 0.11 | - | 119,119,119,119 | 0 |
| 30 | MG | X | 3417 | 1/1 | 0.47 | 0.92 | - | 82,82,82,82 | 0 |
| 29 | MN | X | 3187 | 1/1 | 0.97 | 0.09 | - | 137,137,137,137 | 0 |
| 29 | MN | X | 3044 | 1/1 | 0.92 | 0.37 | - | 116,116,116,116 | 0 |
| 29 | MN | X | 3447 | 1/1 | 0.80 | 0.24 | - | 128,128,128,128 | 0 |
| 29 | MN | X | 3116 | 1/1 | 0.87 | 0.42 | - | 111,111,111,111 | 0 |
| 30 | MG | X | 3296 | 1/1 | 0.97 | 0.21 | - | 45,45,45,45 | 0 |
| 29 | MN | X | 3041 | 1/1 | 0.94 | 0.18 | - | 77,77,77,77 | 0 |
| 29 | MN | X | 3033 | 1/1 | 0.99 | 0.27 | - | 78,78,78,78 | 0 |
| 30 | MG | X | 3393 | 1/1 | 0.67 | 1.22 | - | 104,104,104,104 | 0 |
| 29 | MN | Y | 208 | 1/1 | 0.86 | 0.20 | - | 164,164,164,164 | 0 |
| 29 | MN | X | 3189 | 1/1 | 0.95 | 0.07 | - | 154,154,154,154 | 0 |
| 30 | MG | X | 3226 | 1/1 | 0.87 | 0.82 | - | 102,102,102,102 | 0 |
| 30 | MG | X | 3363 | 1/1 | 0.82 | 0.36 | - | 82,82,82,82 | 0 |
| 30 | MG | X | 3359 | 1/1 | 0.88 | 0.51 | - | 91,91,91,91 | 0 |
| 29 | MN | X | 3154 | 1/1 | 0.82 | 0.36 | - | 124,124,124,124 | 0 |
| 29 | MN | X | 3031 | 1/1 | 0.97 | 0.24 | - | 68,68,68,68 | 0 |
| 30 | MG | X | 3236 | 1/1 | 0.73 | 0.72 | - | 88,88,88,88 | 0 |
| 30 | MG | X | 3400 | 1/1 | 0.60 | 0.63 | - | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 30 | MG | X | 3261 | 1/1 | 0.95 | 0.22 | - | 91,91,91,91 | 0 |
| 30 | MG | X | 3366 | 1/1 | 0.94 | 0.67 | - | 99,99,99,99 | 0 |
| 29 | MN | X | 3231 | 1/1 | 0.80 | 0.26 | - | 161,161,161,161 | 0 |
| 30 | MG | X | 3488 | 1/1 | 0.57 | 0.68 | - | 100,100,100,100 | 0 |
| 30 | MG | X | 3394 | 1/1 | 0.80 | 0.19 | - | 98,98,98,98 | 0 |
| 29 | MN | X | 3078 | 1/1 | 0.97 | 0.44 | - | 111,111,111,111 | 0 |
| 29 | MN | X | 3020 | 1/1 | 0.97 | 0.28 | - | 107,107,107,107 | 0 |
| 29 | MN | X | 3323 | 1/1 | 0.81 | 0.26 | - | 141,141,141,141 | 0 |
| 30 | MG | X | 3358 | 1/1 | 0.71 | 1.38 | - | 88,88,88,88 | 0 |
| 30 | MG | X | 3442 | 1/1 | 0.96 | 0.16 | - | 71,71,71,71 | 0 |
| 34 | EOH | X | 3500 | 3/3 | 0.90 | 0.35 | - | 99,99,99,99 | 0 |
| 29 | MN | X | 3101 | 1/1 | 0.92 | 0.48 | - | 131,131,131,131 | 0 |
| 29 | MN | X | 3456 | 1/1 | 0.81 | 0.24 | - | 113,113,113,113 | 0 |
| 30 | MG | X | 3141 | 1/1 | 0.96 | 0.24 | - | 85,85,85,85 | 0 |
| 30 | MG | C | 302 | 1/1 | 0.83 | 0.29 | - | 78,78,78,78 | 0 |
| 29 | MN | X | 3401 | 1/1 | 0.96 | 0.13 | - | 104,104,104,104 | 0 |
| 30 | MG | Y | 212 | 1/1 | 0.64 | 0.63 | - | 95,95,95,95 | 0 |
| 30 | MG | X | 3372 | 1/1 | 0.85 | 0.51 | - | 78,78,78,78 | 0 |
| 30 | MG | X | 3269 | 1/1 | 0.98 | 0.17 | - | 132,132,132,132 | 0 |
| 30 | MG | X | 3383 | 1/1 | 0.92 | 0.46 | - | 75,75,75,75 | 0 |
| 29 | MN | X | 3404 | 1/1 | 0.95 | 0.15 | - | 131,131,131,131 | 0 |
| 29 | MN | X | 3182 | 1/1 | 0.88 | 0.14 | - | 133,133,133,133 | 0 |
| 30 | MG | X | 3308 | 1/1 | 0.63 | 0.44 | - | 77,77,77,77 | 0 |
| 30 | MG | X | 3413 | 1/1 | 0.80 | 0.55 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3205 | 1/1 | 0.89 | 0.15 | - | 98,98,98,98 | 0 |
| 29 | MN | X | 3124 | 1/1 | 0.89 | 0.13 | - | 147,147,147,147 | 0 |
| 29 | MN | X | 3148 | 1/1 | 0.86 | 0.25 | - | 144,144,144,144 | 0 |
| 30 | MG | X | 3490 | 1/1 | 0.91 | 0.29 | - | 100,100,100,100 | 0 |
| 29 | MN | X | 3061 | 1/1 | 0.98 | 0.13 | - | 92,92,92,92 | 0 |
| 29 | MN | X | 3133 | 1/1 | 0.83 | 0.27 | - | 133,133,133,133 | 0 |
| 29 | MN | X | 3179 | 1/1 | 0.94 | 0.12 | - | 106,106,106,106 | 0 |
| 29 | MN | X | 3140 | 1/1 | 0.96 | 0.12 | - | 105,105,105,105 | 0 |
| 29 | MN | X | 3159 | 1/1 | 0.91 | 0.17 | - | 118,118,118,118 | 0 |
| 30 | MG | X | 3238 | 1/1 | 0.89 | 0.87 | - | 85,85,85,85 | 0 |
| 29 | MN | X | 3117 | 1/1 | 0.90 | 0.26 | - | 107,107,107,107 | 0 |
| 29 | MN | X | 3136 | 1/1 | 0.99 | 0.25 | - | 55,55,55,55 | 0 |
| 29 | MN | X | 3094 | 1/1 | 0.94 | 0.15 | - | 124,124,124,124 | 0 |
| 29 | MN | X | 3149 | 1/1 | 0.94 | 0.26 | - | 109,109,109,109 | 0 |
| 29 | MN | X | 3056 | 1/1 | 0.97 | 0.18 | - | 88,88,88,88 | 0 |
| 29 | MN | X | 3209 | 1/1 | 0.43 | 0.19 | - | 150,150,150,150 | 0 |
| 30 | MG | X | 3348 | 1/1 | 0.76 | 0.62 | - | 72,72,72,72 | 0 |
| 29 | MN | X | 3380 | 1/1 | 0.86 | 0.26 | - | 151,151,151,151 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 30 | MG | X | 3424 | 1/1 | 0.88 | 1.45 | - | 89,89,89,89 | 0 |
| 29 | MN | X | 3151 | 1/1 | 0.88 | 0.25 | - | 97,97,97,97 | 0 |
| 30 | MG | X | 3274 | 1/1 | 0.94 | 0.34 | - | 99,99,99,99 | 0 |
| 30 | MG | X | 3286 | 1/1 | 0.79 | 0.46 | - | 77,77,77,77 | 0 |
| 30 | MG | X | 3305 | 1/1 | 0.82 | 0.44 | - | 123,123,123,123 | 0 |
| 30 | MG | X | 3377 | 1/1 | 0.96 | 0.43 | - | 121,121,121,121 | 0 |
| 30 | MG | X | 3129 | 1/1 | 0.87 | 0.60 | - | 79,79,79,79 | 0 |
| 30 | MG | X | 3138 | 1/1 | 0.90 | 0.53 | - | 72,72,72,72 | 0 |
| 30 | MG | X | 3227 | 1/1 | 0.96 | 0.72 | - | 95,95,95,95 | 0 |
| 29 | MN | X | 3037 | 1/1 | 0.94 | 0.27 | - | 90,90,90,90 | 0 |
| 29 | MN | X | 3102 | 1/1 | 0.96 | 0.57 | - | 124,124,124,124 | 0 |
| 29 | MN | X | 3162 | 1/1 | 0.82 | 0.24 | - | 118,118,118,118 | 0 |
| 29 | MN | X | 3316 | 1/1 | 0.84 | 0.10 | - | 173,173,173,173 | 0 |
| 29 | MN | X | 3176 | 1/1 | 0.88 | 0.31 | - | 128,128,128,128 | 0 |
| 29 | MN | X | 3418 | 1/1 | 0.95 | 0.13 | - | 124,124,124,124 | 0 |
| 30 | MG | X | 3391 | 1/1 | 0.58 | 1.00 | - | 107,107,107,107 | 0 |
| 30 | MG | X | 3288 | 1/1 | 0.83 | 0.32 | - | 81,81,81,81 | 0 |
| 30 | MG | X | 3342 | 1/1 | 0.78 | 0.53 | - | 80,80,80,80 | 0 |
| 29 | MN | X | 3203 | 1/1 | 0.71 | 0.19 | - | 145,145,145,145 | 0 |
| 30 | MG | X | 3373 | 1/1 | 0.93 | 0.33 | - | 97,97,97,97 | 0 |
| 30 | MG | X | 3355 | 1/1 | 0.89 | 0.19 | - | 91,91,91,91 | 0 |
| 29 | MN | X | 3243 | 1/1 | 0.93 | 0.18 | - | 114,114,114,114 | 0 |
| 29 | MN | X | 3190 | 1/1 | 0.93 | 0.20 | - | 124,124,124,124 | 0 |
| 30 | MG | X | 3473 | 1/1 | 0.89 | 0.19 | - | 82,82,82,82 | 0 |
| 29 | MN | X | 3111 | 1/1 | 0.93 | 0.32 | - | 130,130,130,130 | 0 |
| 30 | MG | X | 3167 | 1/1 | 0.83 | 0.34 | - | 62,62,62,62 | 0 |
| 29 | MN | X | 3454 | 1/1 | 0.79 | 0.49 | - | 126,126,126,126 | 0 |
| 30 | MG | X | 3301 | 1/1 | 0.94 | 0.19 | - | 72,72,72,72 | 0 |
| 30 | MG | Y | 206 | 1/1 | 0.91 | 0.87 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3080 | 1/1 | 0.98 | 0.23 | - | 78,78,78,78 | 0 |
| 29 | MN | X | 3072 | 1/1 | 0.74 | 0.21 | - | 123,123,123,123 | 0 |
| 30 | MG | X | 3411 | 1/1 | 0.87 | 0.42 | - | 82,82,82,82 | 0 |
| 29 | MN | X | 3479 | 1/1 | 0.82 | 0.23 | - | 171,171,171,171 | 0 |
| 29 | MN | X | 3158 | 1/1 | 0.79 | 0.30 | - | 117,117,117,117 | 0 |
| 29 | MN | X | 3462 | 1/1 | 0.91 | 0.28 | - | 152,152,152,152 | 0 |
| 30 | MG | X | 3477 | 1/1 | 0.82 | 0.32 | - | 80,80,80,80 | 0 |
| 29 | MN | X | 3225 | 1/1 | 0.73 | 0.52 | - | 157,157,157,157 | 0 |
| 30 | MG | X | 3241 | 1/1 | 0.87 | 1.24 | - | 78,78,78,78 | 0 |
| 29 | MN | X | 3027 | 1/1 | 0.90 | 0.36 | - | 68,68,68,68 | 0 |
| 30 | MG | X | 3242 | 1/1 | 0.86 | 0.69 | - | 65,65,65,65 | 0 |
| 30 | MG | X | 3371 | 1/1 | 0.85 | 0.50 | - | 88,88,88,88 | 0 |
| 30 | MG | X | 3347 | 1/1 | 0.88 | 1.25 | - | 108,108,108,108 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 29 | MN | X | 3422 | 1/1 | 0.87 | 0.24 | - | 154,154,154,154 | 0 |
| 30 | MG | X | 3304 | 1/1 | 0.91 | 0.46 | - | 117,117,117,117 | 0 |
| 30 | MG | X | 3267 | 1/1 | 0.97 | 0.26 | - | 72,72,72,72 | 0 |
| 30 | MG | X | 3247 | 1/1 | 0.95 | 0.54 | - | 85,85,85,85 | 0 |
| 30 | MG | X | 3381 | 1/1 | 0.90 | 0.72 | - | 97,97,97,97 | 0 |
| 29 | MN | X | 3374 | 1/1 | 0.97 | 0.12 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3171 | 1/1 | 0.95 | 0.22 | - | 114,114,114,114 | 0 |
| 30 | MG | X | 3137 | 1/1 | 0.93 | 1.14 | - | 63,63,63,63 | 0 |
| 30 | MG | X | 3406 | 1/1 | 0.82 | 0.29 | - | 71,71,71,71 | 0 |
| 30 | MG | X | 3396 | 1/1 | 0.91 | 0.60 | - | 108,108,108,108 | 0 |
| 29 | MN | X | 3038 | 1/1 | 0.98 | 0.31 | - | 106,106,106,106 | 0 |
| 30 | MG | X | 3368 | 1/1 | 0.88 | 0.54 | - | 87,87,87,87 | 0 |
| 29 | MN | X | 3457 | 1/1 | 0.99 | 0.46 | - | 135,135,135,135 | 0 |
| 30 | MG | X | 3180 | 1/1 | 0.56 | 1.16 | - | 78,78,78,78 | 0 |
| 30 | MG | X | 3207 | 1/1 | 0.90 | 0.28 | - | 66,66,66,66 | 0 |
| 30 | MG | X | 3333 | 1/1 | 0.92 | 0.77 | - | 97,97,97,97 | 0 |
| 29 | MN | X | 3046 | 1/1 | 0.96 | 0.29 | - | 91,91,91,91 | 0 |
| 30 | MG | X | 3254 | 1/1 | 0.73 | 0.77 | - | 66,66,66,66 | 0 |
| 29 | MN | X | 3012 | 1/1 | 0.97 | 0.38 | - | 79,79,79,79 | 0 |
| 30 | MG | X | 3228 | 1/1 | 0.81 | 0.30 | - | 150,150,150,150 | 0 |
| 30 | MG | X | 3275 | 1/1 | 0.99 | 0.16 | - | 71,71,71,71 | 0 |
| 30 | MG | Y | 204 | 1/1 | 0.92 | 0.38 | - | 78,78,78,78 | 0 |
| 30 | MG | X | 3450 | 1/1 | 0.95 | 0.74 | - | 132,132,132,132 | 0 |
| 29 | MN | X | 3311 | 1/1 | 0.93 | 0.17 | - | 124,124,124,124 | 0 |
| 29 | MN | X | 3125 | 1/1 | 0.95 | 0.13 | - | 123,123,123,123 | 0 |
| 29 | MN | X | 3032 | 1/1 | 0.99 | 0.33 | - | 64,64,64,64 | 0 |
| 29 | MN | X | 3052 | 1/1 | 0.96 | 0.31 | - | 90,90,90,90 | 0 |
| 30 | MG | X | 3283 | 1/1 | 0.84 | 0.22 | - | 129,129,129,129 | 0 |
| 29 | MN | X | 3235 | 1/1 | 0.97 | 0.11 | - | 155,155,155,155 | 0 |
| 30 | MG | X | 3142 | 1/1 | 0.94 | 0.51 | - | 72,72,72,72 | 0 |
| 30 | MG | X | 3433 | 1/1 | 0.60 | 0.34 | - | 124,124,124,124 | 0 |
| 29 | MN | X | 3107 | 1/1 | 0.98 | 0.29 | - | 73,73,73,73 | 0 |
| 30 | MG | P | 201 | 1/1 | 0.74 | 0.65 | - | 63,63,63,63 | 0 |
| 30 | MG | X | 3487 | 1/1 | 0.57 | 0.54 | - | 109,109,109,109 | 0 |
| 30 | MG | X | 3431 | 1/1 | 0.96 | 0.38 | - | 55,55,55,55 | 0 |
| 29 | MN | X | 3065 | 1/1 | 0.97 | 0.37 | - | 97,97,97,97 | 0 |
| 29 | MN | X | 3025 | 1/1 | 0.89 | 0.32 | - | 128,128,128,128 | 0 |
| 30 | MG | G | 201 | 1/1 | 0.76 | 0.57 | - | 89,89,89,89 | 0 |
| 30 | MG | X | 3276 | 1/1 | 0.97 | 0.23 | - | 67,67,67,67 | 0 |
| 29 | MN | X | 3324 | 1/1 | 0.62 | 0.16 | - | 164,164,164,164 | 0 |
| 30 | MG | X | 3491 | 1/1 | 0.98 | 0.15 | - | 86,86,86,86 | 0 |
| 29 | MN | X | 3082 | 1/1 | 0.94 | 0.20 | - | 112,112,112,112 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 29 | MN | X | 3113 | 1/1 | 0.88 | 0.23 | - | 96,96,96,96 | 0 |
| 29 | MN | X | 3035 | 1/1 | 0.97 | 0.23 | - | 74,74,74,74 | 0 |
| 30 | MG | X | 3426 | 1/1 | 0.97 | 0.26 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3021 | 1/1 | 0.96 | 0.21 | - | 91,91,91,91 | 0 |
| 29 | MN | X | 3465 | 1/1 | 0.90 | 0.24 | - | 117,117,117,117 | 0 |
| 29 | MN | X | 3064 | 1/1 | 0.97 | 0.18 | - | 84,84,84,84 | 0 |
| 29 | MN | X | 3114 | 1/1 | 0.71 | 0.57 | - | 122,122,122,122 | 0 |
| 30 | MG | X | 3273 | 1/1 | 0.98 | 0.47 | - | 124,124,124,124 | 0 |
| 29 | MN | X | 3206 | 1/1 | 0.97 | 0.07 | - | 95,95,95,95 | 0 |
| 30 | MG | X | 3331 | 1/1 | 0.95 | 0.36 | - | 86,86,86,86 | 0 |
| 29 | MN | X | 3023 | 1/1 | 0.99 | 0.27 | - | 92,92,92,92 | 0 |
| 30 | MG | Y | 205 | 1/1 | 0.85 | 0.82 | - | 94,94,94,94 | 0 |
| 30 | MG | X | 3427 | 1/1 | 0.94 | 0.15 | - | 59,59,59,59 | 0 |
| 30 | MG | X | 3256 | 1/1 | 0.98 | 0.37 | - | 69,69,69,69 | 0 |
| 29 | MN | X | 3175 | 1/1 | 0.77 | 0.28 | - | 122,122,122,122 | 0 |
| 30 | MG | O | 201 | 1/1 | 0.91 | 0.28 | - | 51,51,51,51 | 0 |
| 30 | MG | X | 3445 | 1/1 | 0.70 | 1.39 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3014 | 1/1 | 0.98 | 0.28 | - | 53,53,53,53 | 0 |
| 30 | MG | X | 3292 | 1/1 | 0.93 | 0.36 | - | 89,89,89,89 | 0 |
| 29 | MN | X | 3319 | 1/1 | 0.85 | 0.10 | - | 158,158,158,158 | 0 |
| 29 | MN | X | 3458 | 1/1 | 0.76 | 0.54 | - | 127,127,127,127 | 0 |
| 30 | MG | X | 3248 | 1/1 | 0.68 | 0.55 | - | 69,69,69,69 | 0 |
| 29 | MN | X | 3121 | 1/1 | 0.98 | 0.17 | - | 104,104,104,104 | 0 |
| 30 | MG | X | 3475 | 1/1 | 0.71 | 0.85 | - | 93,93,93,93 | 0 |
| 30 | MG | X | 3414 | 1/1 | 0.96 | 0.18 | - | 89,89,89,89 | 0 |
| 30 | MG | X | 3212 | 1/1 | 0.82 | 0.97 | - | 78,78,78,78 | 0 |
| 29 | MN | X | 3055 | 1/1 | 0.97 | 0.26 | - | 86,86,86,86 | 0 |
| 30 | MG | X | 3349 | 1/1 | 0.54 | 1.45 | - | 127,127,127,127 | 0 |
| 29 | MN | R | 201 | 1/1 | 0.90 | 0.28 | - | 123,123,123,123 | 0 |
| 29 | MN | X | 3135 | 1/1 | 0.96 | 0.15 | - | 115,115,115,115 | 0 |
| 29 | MN | X | 3464 | 1/1 | 0.95 | 0.56 | - | 149,149,149,149 | 0 |
| 30 | MG | X | 3365 | 1/1 | 0.78 | 0.69 | - | 76,76,76,76 | 0 |
| 30 | MG | X | 3246 | 1/1 | 0.84 | 0.91 | - | 72,72,72,72 | 0 |
| 30 | MG | X | 3272 | 1/1 | 0.92 | 0.45 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3402 | 1/1 | 0.97 | 0.13 | - | 108,108,108,108 | 0 |
| 29 | MN | X | 3170 | 1/1 | 0.99 | 0.17 | - | 104,104,104,104 | 0 |
| 29 | MN | X | 3092 | 1/1 | 0.99 | 0.22 | - | 90,90,90,90 | 0 |
| 29 | MN | X | 3379 | 1/1 | 0.79 | 0.19 | - | 158,158,158,158 | 0 |
| 30 | MG | X | 3240 | 1/1 | 0.94 | 0.67 | - | 78,78,78,78 | 0 |
| 30 | MG | X | 3130 | 1/1 | 0.79 | 0.37 | - | 72,72,72,72 | 0 |
| 29 | MN | X | 3093 | 1/1 | 0.96 | 0.22 | - | 81,81,81,81 | 0 |
| 30 | MG | X | 3345 | 1/1 | 0.84 | 0.29 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 30 | MG | Y | 210 | 1/1 | 0.17 | 1.31 | - | 105,105,105,105 | 0 |
| 30 | MG | X | 3284 | 1/1 | 0.96 | 0.17 | - | 72,72,72,72 | 0 |
| 30 | MG | X | 3336 | 1/1 | 0.79 | 0.93 | - | 99,99,99,99 | 0 |
| 30 | MG | X | 3352 | 1/1 | 0.76 | 0.52 | - | 94,94,94,94 | 0 |
| 30 | MG | X | 3337 | 1/1 | 0.55 | 0.47 | - | 89,89,89,89 | 0 |
| 29 | MN | X | 3313 | 1/1 | 0.96 | 0.10 | - | 117,117,117,117 | 0 |
| 30 | MG | X | 3432 | 1/1 | 0.95 | 0.23 | - | 71,71,71,71 | 0 |
| 30 | MG | X | 3476 | 1/1 | 0.95 | 0.15 | - | 64,64,64,64 | 0 |
| 30 | MG | A | 304 | 1/1 | 0.90 | 0.49 | - | 105,105,105,105 | 0 |
| 30 | MG | X | 3230 | 1/1 | 0.74 | 0.54 | - | 80,80,80,80 | 0 |
| 29 | MN | X | 3472 | 1/1 | 0.98 | 0.21 | - | 110,110,110,110 | 0 |
| 29 | MN | X | 3024 | 1/1 | 0.93 | 0.17 | - | 120,120,120,120 | 0 |
| 30 | MG | X | 3302 | 1/1 | 0.92 | 0.16 | - | 100,100,100,100 | 0 |
| 30 | MG | X | 3232 | 1/1 | 0.90 | 1.01 | - | 74,74,74,74 | 0 |
| 29 | MN | X | 3108 | 1/1 | 0.97 | 0.19 | - | 89,89,89,89 | 0 |
| 29 | MN | X | 3039 | 1/1 | 0.98 | 0.34 | - | 79,79,79,79 | 0 |
| 29 | MN | X | 3153 | 1/1 | 0.89 | 0.08 | - | 123,123,123,123 | 0 |
| 29 | MN | Z | 102 | 1/1 | 0.80 | 0.36 | - | 112,112,112,112 | 0 |
| 29 | MN | X | 3178 | 1/1 | 0.86 | 0.11 | - | 126,126,126,126 | 0 |
| 30 | MG | X | 3369 | 1/1 | 0.91 | 0.74 | - | 70,70,70,70 | 0 |
| 29 | MN | X | 3264 | 1/1 | 0.94 | 0.12 | - | 117,117,117,117 | 0 |
| 29 | MN | X | 3090 | 1/1 | 0.95 | 0.26 | - | 97,97,97,97 | 0 |
| 29 | MN | X | 3183 | 1/1 | 0.71 | 0.14 | - | 125,125,125,125 | 0 |
| 29 | MN | X | 3208 | 1/1 | 0.84 | 0.29 | - | 141,141,141,141 | 0 |
| 29 | MN | X | 3150 | 1/1 | 0.85 | 0.18 | - | 110,110,110,110 | 0 |
| 30 | MG | X | 3357 | 1/1 | 0.69 | 0.28 | - | 95,95,95,95 | 0 |
| 29 | MN | X | 3467 | 1/1 | 0.98 | 0.38 | - | 72,72,72,72 | 0 |
| 29 | MN | X | 3155 | 1/1 | 0.75 | 0.40 | - | 110,110,110,110 | 0 |
| 29 | MN | X | 3421 | 1/1 | 0.67 | 0.45 | - | 111,111,111,111 | 0 |
| 30 | MG | A | 302 | 1/1 | 0.79 | 0.58 | - | 92,92,92,92 | 0 |
| 30 | MG | X | 3265 | 1/1 | 0.75 | 0.64 | - | 96,96,96,96 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.