



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2017 – 10:15 PM EDT

PDB ID : 2QEX
Title : Negamycin Binds to the Wall of the Nascent Chain Exit Tunnel of the 50S Ribosomal Subunit
Authors : Schroeder, S.J.; Blaha, G.
Deposited on : unknown
Resolution : 2.90 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 : rb-20030345
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) : rb-20030345

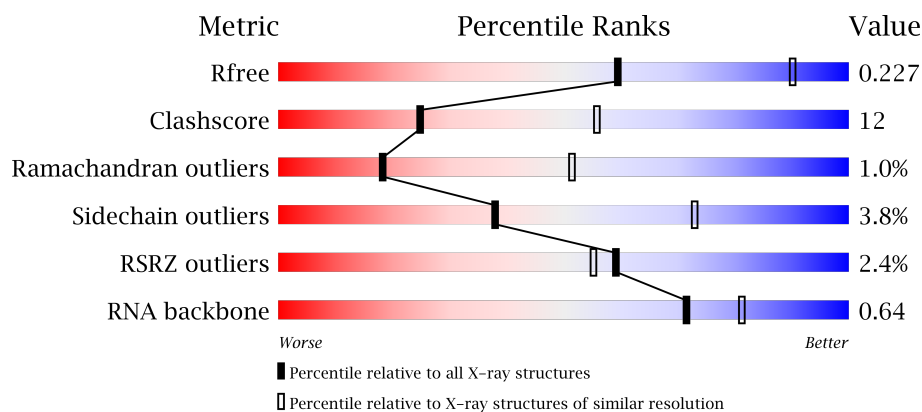
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.





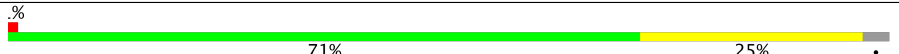
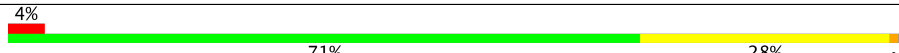

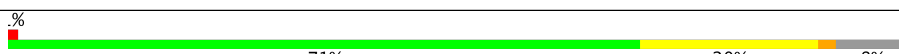
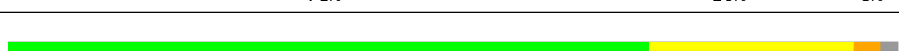

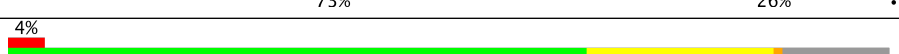
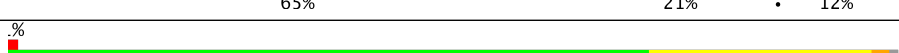
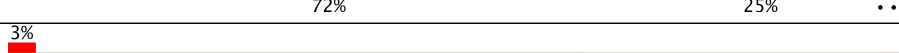
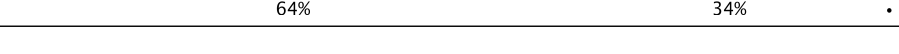
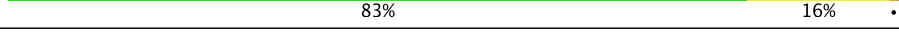

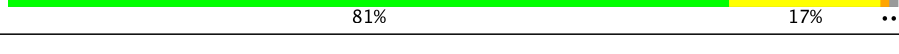



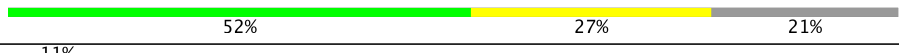
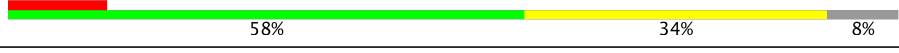
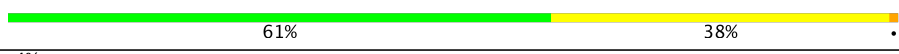

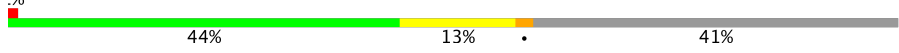


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1586 (2.90-2.90) |
| Clashscore | 112137 | 1807 (2.90-2.90) |
| Ramachandran outliers | 110173 | 1768 (2.90-2.90) |
| Sidechain outliers | 110143 | 1770 (2.90-2.90) |
| RSRZ outliers | 101464 | 1596 (2.90-2.90) |
| RNA backbone | 2435 | 1004 (3.20-2.60) |

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 | 0 | 2772 | <div> <div>0.1%</div> <div>61% 32% 6% .</div> </div> |
| 2 | 9 | 122 | <div> <div>2%</div> <div>38% 50% 11% .</div> </div> |
| 3 | A | 240 | <div> <div>0.1%</div> <div>71% 25% . .</div> </div> |
| 4 | B | 338 | <div> <div>66% 31% .</div> </div> |



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | C | 246 |  |
| 6 | D | 177 |  |
| 7 | E | 178 |  |
| 8 | F | 120 |  |
| 9 | G | 348 |  |
| 10 | H | 174 |  |
| 11 | J | 145 |  |
| 12 | K | 132 |  |
| 13 | L | 165 |  |
| 14 | M | 196 |  |
| 15 | N | 187 |  |
| 16 | O | 116 |  |
| 17 | P | 149 |  |
| 18 | Q | 96 |  |
| 19 | R | 155 |  |
| 20 | S | 85 |  |
| 21 | T | 120 |  |
| 22 | U | 67 |  |
| 23 | V | 71 |  |
| 24 | W | 154 |  |
| 25 | X | 92 |  |
| 26 | Y | 241 |  |
| 27 | Z | 73 |  |
| 28 | 1 | 57 |  |
| 29 | 2 | 50 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 30 | 3 | 92 |  |
| 31 | I | 162 |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 32 | MG | 0 | 8018 | - | - | - | X |
| 32 | MG | 0 | 8052 | - | - | - | X |
| 32 | MG | 0 | 8060 | - | - | - | X |
| 32 | MG | 0 | 8062 | - | - | - | X |
| 32 | MG | 0 | 8080 | - | - | - | X |
| 32 | MG | 0 | 8096 | - | - | - | X |
| 33 | K | 0 | 8401 | - | - | - | X |
| 34 | NA | 0 | 8503 | - | - | - | X |
| 34 | NA | 0 | 8510 | - | - | - | X |
| 34 | NA | 0 | 8514 | - | - | - | X |
| 34 | NA | 0 | 8520 | - | - | - | X |
| 34 | NA | 0 | 8521 | - | - | - | X |
| 34 | NA | 0 | 8523 | - | - | - | X |
| 34 | NA | 0 | 8526 | - | - | - | X |
| 34 | NA | 0 | 8527 | - | - | - | X |
| 34 | NA | 0 | 8535 | - | - | - | X |
| 34 | NA | 0 | 8559 | - | - | - | X |
| 34 | NA | 0 | 8561 | - | - | - | X |
| 34 | NA | 0 | 8562 | - | - | - | X |
| 34 | NA | 0 | 8564 | - | - | - | X |
| 34 | NA | 0 | 8565 | - | - | - | X |
| 34 | NA | 0 | 8566 | - | - | - | X |
| 34 | NA | 0 | 8568 | - | - | - | X |
| 34 | NA | 0 | 8571 | - | - | - | X |
| 34 | NA | 0 | 8572 | - | - | - | X |
| 34 | NA | 0 | 8573 | - | - | - | X |
| 34 | NA | 0 | 8576 | - | - | - | X |
| 34 | NA | 0 | 8577 | - | - | - | X |
| 34 | NA | 0 | 8578 | - | - | - | X |
| 34 | NA | 0 | 8582 | - | - | - | X |
| 34 | NA | L | 8580 | - | - | - | X |
| 34 | NA | R | 8586 | - | - | - | X |
| 36 | NEG | 0 | 8823 | - | - | - | X |

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | 0 | 2754 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59021 | 26350 | 10878 | 19048 | 2745 | | | |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | 9 | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2600 | 1160 | 472 | 847 | 121 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 9 | 3073 | G | A | CONFLICT | GB 6468293 |
| 9 | 3106 | C | U | CONFLICT | GB 6468293 |

- Molecule 3 is a protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1072 | 352 | 324 | 5 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | B | 337 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2625 | 1616 | 493 | 511 | 5 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | C | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1859 | 1131 | 344 | 383 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C | 73 | LEU | GLN | CONFLICT | UNP P12735 |

- Molecule 6 is a protein called 50S ribosomal protein L5P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | D | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 685 | 195 | 210 | 4 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | E | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1357 | 840 | 224 | 289 | 4 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | F | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 551 | 141 | 197 | 1 | | | |

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | G | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| G | 248 | ASP | ALA | CONFLICT | UNP P15825 |

- Molecule 10 is a protein called 50S ribosomal protein L10e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | H | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1266 | 785 | 237 | 238 | 6 | | | |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| H | 164 | ASP | - | INSERTION | UNP P60617 |
| H | 165 | SER | LYS | CONFLICT | UNP P60617 |
| H | 166 | SER | VAL | CONFLICT | UNP P60617 |
| H | 167 | PRO | GLU | CONFLICT | UNP P60617 |
| H | 168 | ALA | ARG | CONFLICT | UNP P60617 |
| H | ? | - | GLU | DELETION | UNP P60617 |
| H | ? | - | GLU | DELETION | UNP P60617 |
| H | ? | - | LEU | DELETION | UNP P60617 |
| H | ? | - | LEU | DELETION | UNP P60617 |
| H | 170 | ASN | ILE | CONFLICT | UNP P60617 |

- Molecule 11 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | J | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1120 | 696 | 199 | 222 | 3 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | K | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 992 | 609 | 187 | 192 | 4 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| K | 44 | LEU | HIS | CONFLICT | UNP P22450 |

- Molecule 13 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 13 | L | 145 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1118 | 670 | 222 | 226 | | | | |

- Molecule 14 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | M | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 943 | 332 | 283 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| M | 13 | GLU | LYS | CONFLICT | UNP P60618 |
| M | 194 | ALA | GLY | CONFLICT | UNP P60618 |

- Molecule 15 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | N | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 895 | 262 | 286 | 2 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 16 | O | 115 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 865 | 529 | 161 | 175 | | | | |

- Molecule 17 is a protein called 50S ribosomal protein L19e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17 | P | 143 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1136 | 683 | 229 | 224 | | | | |

- Molecule 18 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 18 | Q | 95 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 735 | 450 | 141 | 144 | | | | |

- Molecule 19 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | R | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1149 | 713 | 209 | 223 | 4 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | S | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 641 | 389 | 111 | 138 | 3 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L24P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 21 | T | 119 | Total | C | N | O | | | |
| | | | 950 | 568 | 180 | 202 | 0 | 0 | 0 |

- Molecule 22 is a protein called 50S ribosomal protein L24e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 22 | U | 53 | Total | C | N | O | S | | | |
| | | | 410 | 244 | 75 | 86 | 5 | 0 | 0 | 0 |

- Molecule 23 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 23 | V | 65 | Total | C | N | O | S | | | |
| | | | 499 | 304 | 94 | 100 | 1 | 0 | 0 | 0 |

- Molecule 24 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | W | 154 | Total | C | N | O | S | | | |
| | | | 1196 | 737 | 209 | 244 | 6 | 0 | 0 | 0 |

- Molecule 25 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | X | 82 | Total | C | N | O | S | | | |
| | | | 654 | 402 | 129 | 122 | 1 | 0 | 0 | 0 |

- Molecule 26 is a protein called 50S ribosomal protein L32e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26 | Y | 142 | Total | C | N | O | | | |
| | | | 1130 | 686 | 228 | 216 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | Z | 73 | Total | C | N | O | S | | | |
| | | | 579 | 346 | 116 | 112 | 5 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Z | 10 | ARG | SER | CONFLICT | UNP P60619 |

- Molecule 28 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 431 | 258 | 86 | 83 | 4 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 396 | 239 | 89 | 67 | 1 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L44e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | 3 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L11P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 31 | I | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 519 | 323 | 81 | 114 | 1 | | | |

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32 | 0 | 108 | Total | Mg | 0 | 0 |
| | | | 108 | 108 | | |
| 32 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 32 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 32 | 3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 33 | 0 | 2 | Total | K | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 34 | 0 | 72 | Total | Na | 0 | 0 |
| | | | 72 | 72 | | |
| 34 | J | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | Q | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | H | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | C | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | R | 3 | Total | Na | 0 | 0 |
| | | | 3 | 3 | | |
| 34 | 9 | 3 | Total | Na | 0 | 0 |
| | | | 3 | 3 | | |
| 34 | L | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | S | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | M | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

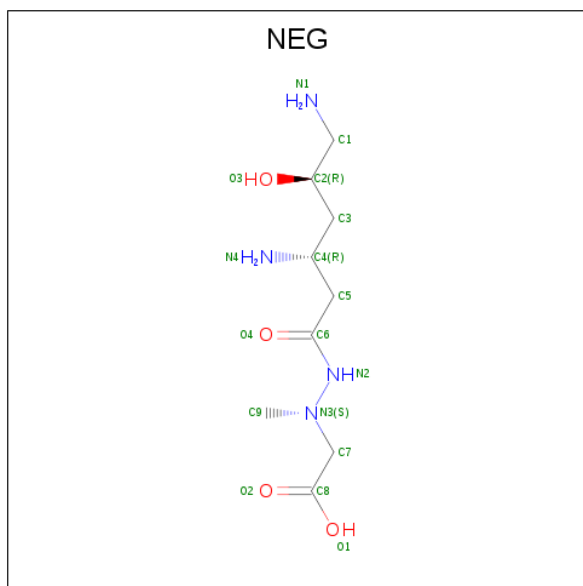
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 35 | 0 | 10 | Total | Cl | 0 | 0 |
| | | | 10 | 10 | | |
| 35 | J | 3 | Total | Cl | 0 | 0 |
| | | | 3 | 3 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 35 | Q | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | B | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | A | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | N | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | O | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | R | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | L | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | 3 | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | M | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 36 is NEGAMYCIN (three-letter code: NEG) (formula: $C_9H_{20}N_4O_4$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 36 | 0 | 1 | Total | C | N | O | 0 | 0 |
| | | | 17 | 9 | 4 | 4 | | |

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 37 | O | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | Z | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | 1 | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | 3 | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | U | 1 | Total Cd 1 1 | 0 | 0 |

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 38 | 0 | 5923 | Total O 5923 5923 | 0 | 0 |
| 38 | 9 | 142 | Total O 142 142 | 0 | 0 |
| 38 | A | 112 | Total O 112 112 | 0 | 0 |
| 38 | B | 137 | Total O 137 137 | 0 | 0 |
| 38 | C | 167 | Total O 167 167 | 0 | 0 |
| 38 | D | 44 | Total O 44 44 | 0 | 0 |
| 38 | E | 45 | Total O 45 45 | 0 | 0 |
| 38 | F | 27 | Total O 27 27 | 0 | 0 |
| 38 | G | 16 | Total O 16 16 | 0 | 0 |
| 38 | H | 70 | Total O 70 70 | 0 | 0 |
| 38 | J | 51 | Total O 51 51 | 0 | 0 |
| 38 | K | 57 | Total O 57 57 | 0 | 0 |
| 38 | L | 85 | Total O 85 85 | 0 | 0 |
| 38 | M | 122 | Total O 122 122 | 0 | 0 |
| 38 | N | 61 | Total O 61 61 | 0 | 0 |

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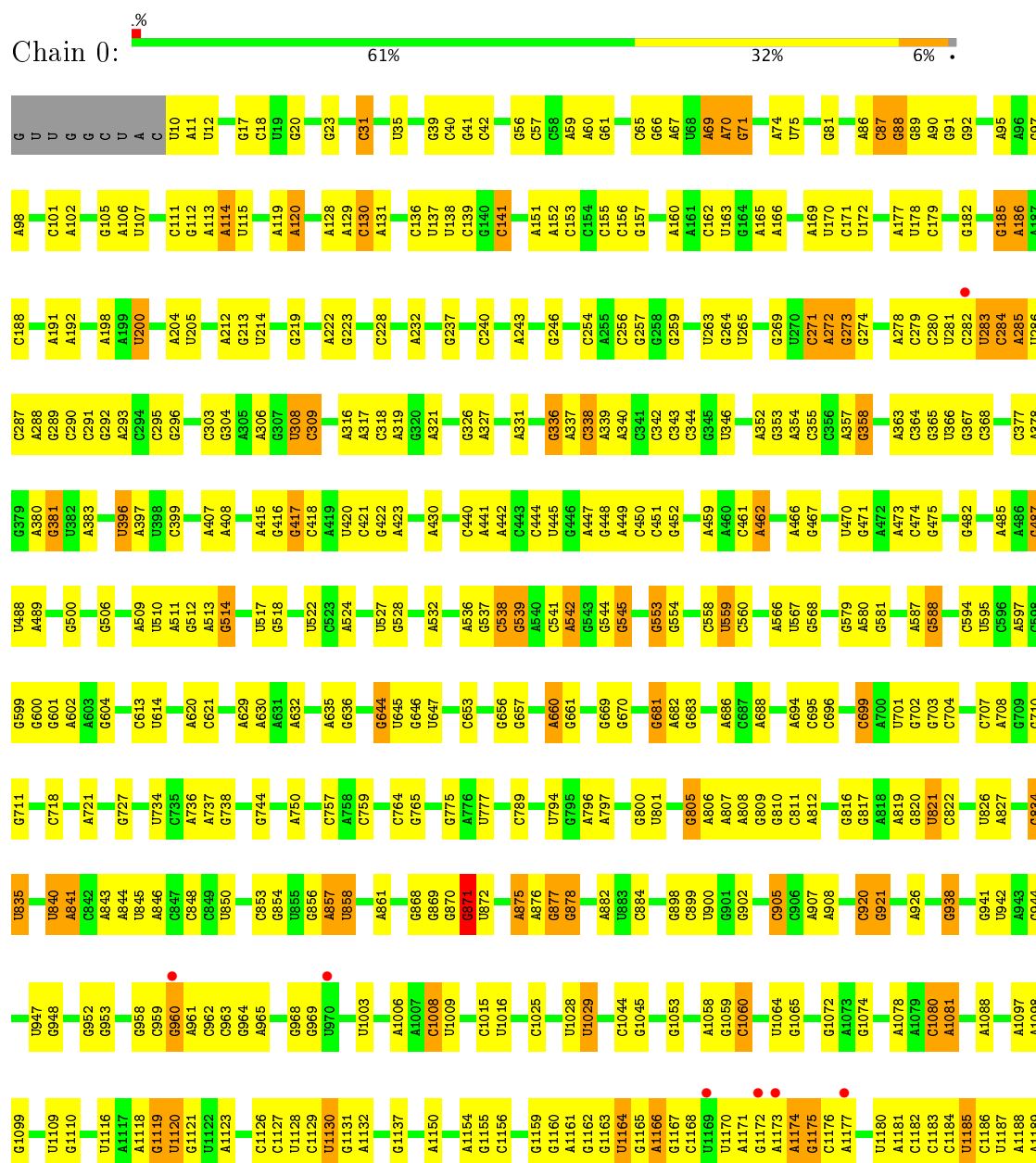
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 38 | O | 38 | Total 38 | O 38 | 0 | 0 |
| 38 | P | 63 | Total 63 | O 63 | 0 | 0 |
| 38 | Q | 50 | Total 50 | O 50 | 0 | 0 |
| 38 | R | 85 | Total 85 | O 85 | 0 | 0 |
| 38 | S | 39 | Total 39 | O 39 | 0 | 0 |
| 38 | T | 30 | Total 30 | O 30 | 0 | 0 |
| 38 | U | 28 | Total 28 | O 28 | 0 | 0 |
| 38 | V | 11 | Total 11 | O 11 | 0 | 0 |
| 38 | W | 69 | Total 69 | O 69 | 0 | 0 |
| 38 | X | 24 | Total 24 | O 24 | 0 | 0 |
| 38 | Y | 87 | Total 87 | O 87 | 0 | 0 |
| 38 | Z | 30 | Total 30 | O 30 | 0 | 0 |
| 38 | 1 | 60 | Total 60 | O 60 | 0 | 0 |
| 38 | 2 | 36 | Total 36 | O 36 | 0 | 0 |
| 38 | 3 | 74 | Total 74 | O 74 | 0 | 0 |
| 38 | I | 5 | Total 5 | O 5 | 0 | 0 |

3 Residue-property plots

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

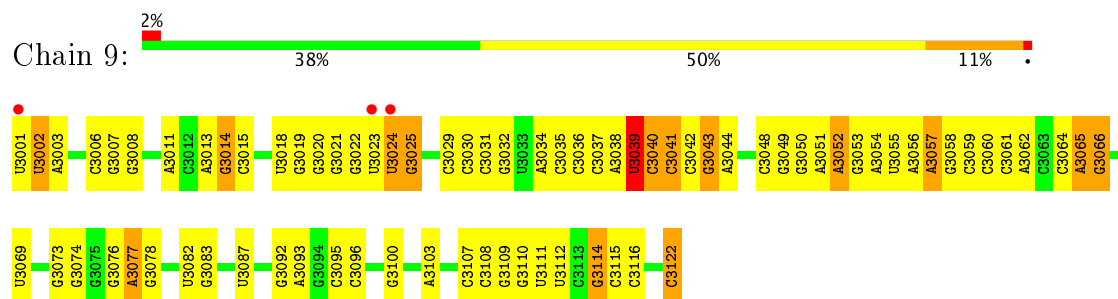
• Molecule 1: 23S ribosomal RNA



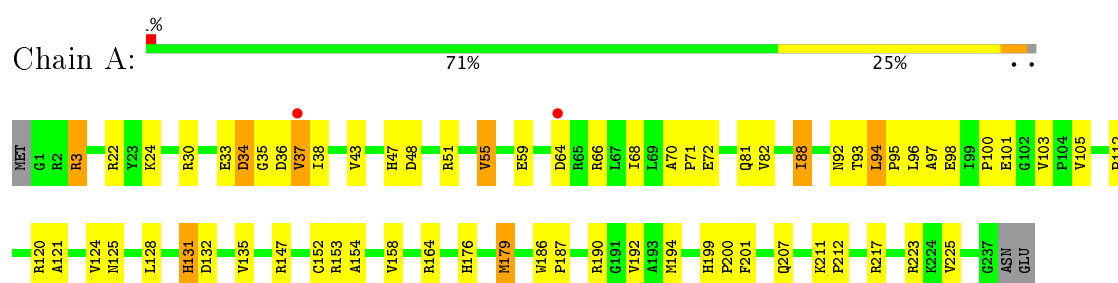




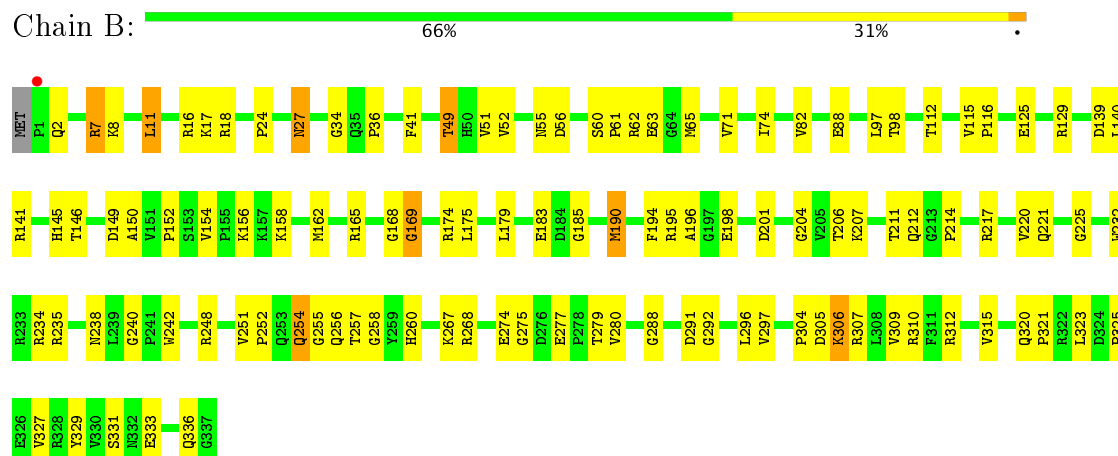
- Molecule 2: 5S ribosomal RNA



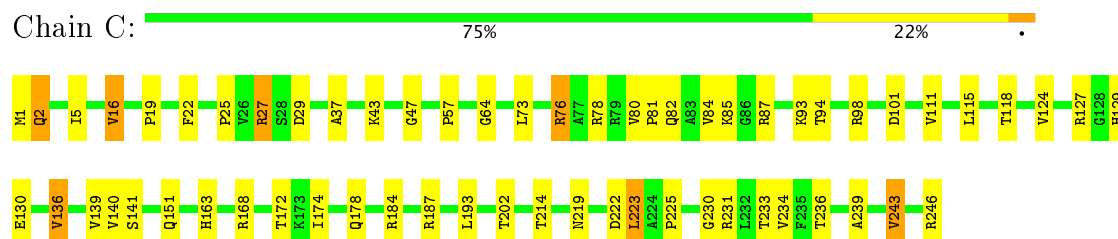
- Molecule 3: 50S ribosomal protein L2P



- Molecule 4: 50S ribosomal protein L3P



- Molecule 5: 50S ribosomal protein L4P



- Molecule 6: 50S ribosomal protein L5P

ALA THR GLU GLU PRO THR ASP ASP GLN ASP ASP THR ALA SER GLU ASP ASP ALA ASP ALA ASP ASP ALA ALA GLU GLU ALA ASP ASP ASP ASP ASP GLU ASP ALA GLY ASP ALA LEU GLY ALA MET PHE

- Molecule 10: 50S ribosomal protein L10e

Chain H:  71% 20% 8%

MET SER ASP K1 P2 A3 P12 R16 R17 E18 I23 S26 K32 K36 D39 Y43 P44 V45 Q46 I47 Q66 I57 R58 H59 G60 S61 L62 E63 R66 L67 E80 K84 P91 K99 GLN THR ALA GLY ALA ASP ARG VAL SER D111

G112 I120 R126 Q132 Y137 Y154 N155 R162 S165 S166 P167 A168 G169 N170 A171


- Molecule 11: 50S ribosomal protein L13P

Chain J:  72% 23% 5%

MET SER VAL A4 E5 I18 M19 V22 V26 D32 V39 V45 I46 T47 E51 Q52 E55 K56 Y57 G64 Y69 F70 Y71 R74 P75 D76 D77 I78 F79 R80 R81 T82 E99 L105 G106 N107 P108 Y109 I127 K128 F129 L132 I135 S136

L139 K143 T144 M145

- Molecule 12: 50S ribosomal protein L14P

Chain K:  73% 26% 1%

M1 L4 D7 Q10 K14 C20 N23 R27 E28 L29 I32 S33 V34 G39 M42 P45 K46 A47 G48 L49 V55 S56 V74 R75 K78 R81 R82 R87 V98 E102 T107 E108 L109 I113 A114 R115 E116 Q119

A125 S126 A127 A128 T129 M130 T131 V132


- Molecule 13: 50S ribosomal protein L15P

Chain L:  65% 21% 12%

MET T1 K4 K5 R6 S10 R11 R12 H13 H18 R21 R27 R30 R31 D32 A33 G34 R35 R38 E39 F40 H41 H42 H43 R53 P54 Q55 K56 V57 E60 D80 A82 E83 VAL ASP GLY F89 R90 Y91 D92 Y97 D101 D102 E117

I121 F125 A129 V133 A136 G137 G138 S139 V140 T143 D144 E148 R149 Q150 ALA GLU ALA GLU THR GLU ASP ALA ASP ASP GLU

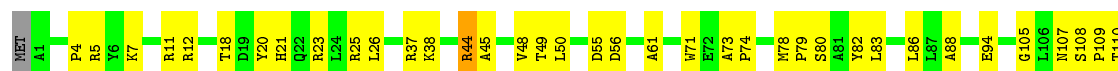
- Molecule 14: 50S ribosomal protein L15e

Chain M:  72% 25% 3%

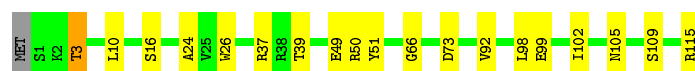
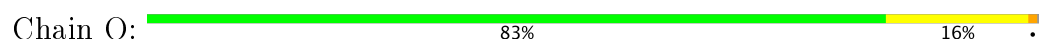
MET A1 I8 R9 D10 L23 Q24 R27 E30 E34 G35 A36 R42 P43 L46 D47 K48 Q52 K55 Q58 G59 Y60 I61 V62 A63 R64 V65 S66 Y67 R68 A72 G80 R81 R85 R93 R94 K95 R99 E102 E103 N116 R125



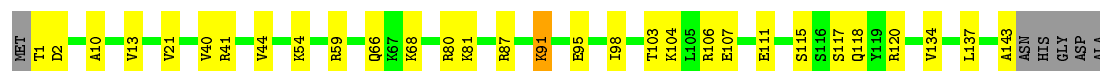
- Molecule 15: 50S ribosomal protein L18P



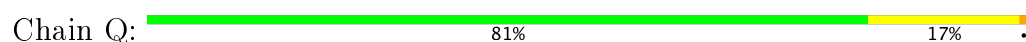
- Molecule 16: 50S ribosomal protein L18e



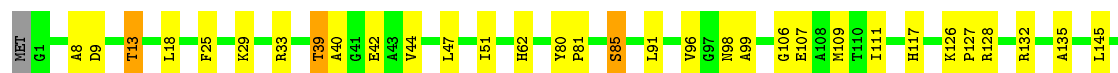
- Molecule 17: 50S ribosomal protein L19e



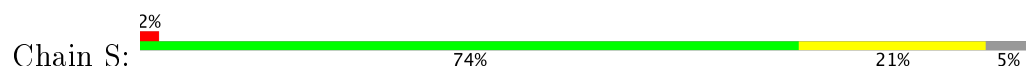
- Molecule 18: 50S ribosomal protein L21e



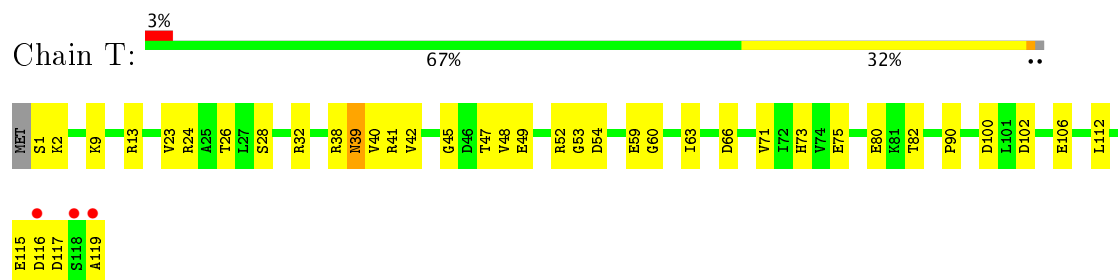
- Molecule 19: 50S ribosomal protein L22P



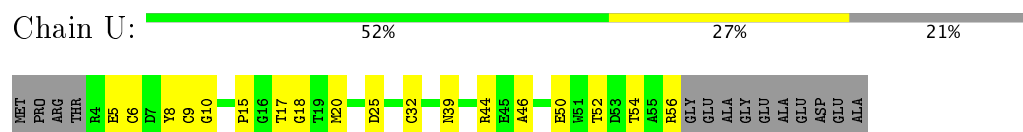
- Molecule 20: 50S ribosomal protein L23P



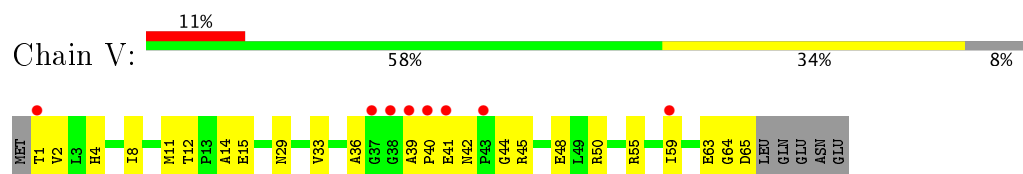
- Molecule 21: 50S ribosomal protein L24P



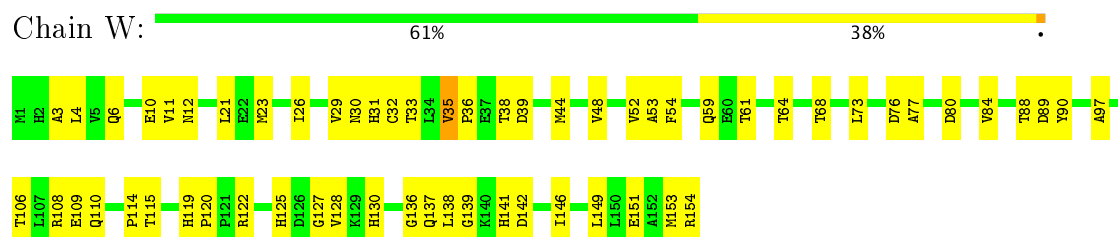
- Molecule 22: 50S ribosomal protein L24e



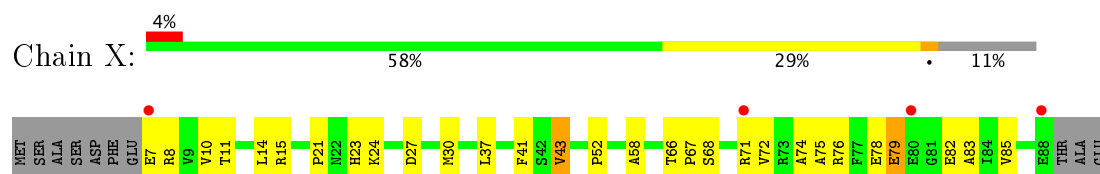
- Molecule 23: 50S ribosomal protein L29P



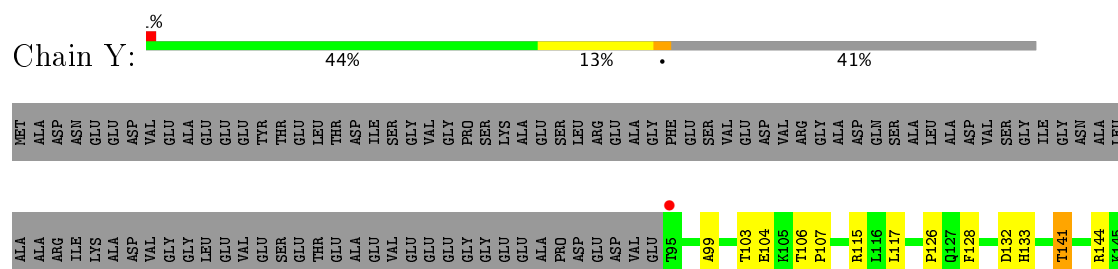
- Molecule 24: 50S ribosomal protein L30P



- Molecule 25: 50S ribosomal protein L31e



- Molecule 26: 50S ribosomal protein L32e



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 214.62Å 304.05Å 578.65Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.92 – 2.90 86.68 – 2.43 | Depositor EDS |
| % Data completeness (in resolution range) | 99.5 (49.92-2.90) 90.6 (86.68-2.43) | Depositor EDS |
| R_{merge} | 0.18 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.31 (at 2.77Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.204 , 0.241 0.194 , 0.227 | Depositor DCC |
| R_{free} test set | 4062 reflections (1.06%) | DCC |
| Wilson B-factor (Å ²) | 44.8 | Xtriage |
| Anisotropy | 0.223 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 68.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 99020 | wwPDB-VP |
| Average B, all atoms (Å ²) | 50.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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, OMG, CL, NEG, K, UR3, CD, OMU, NA, 1MA, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 0 | 0.38 | 0/65959 | 0.69 | 10/102870 (0.0%) |
| 2 | 9 | 0.35 | 0/2905 | 0.71 | 1/4528 (0.0%) |
| 3 | A | 0.34 | 0/1786 | 0.64 | 0/2408 |
| 4 | B | 0.32 | 0/2690 | 0.64 | 0/3652 |
| 5 | C | 0.36 | 0/1884 | 0.63 | 0/2551 |
| 6 | D | 0.33 | 0/1111 | 0.57 | 0/1498 |
| 7 | E | 0.33 | 0/1382 | 0.57 | 0/1880 |
| 8 | F | 0.35 | 0/901 | 0.58 | 0/1224 |
| 9 | G | 0.35 | 0/241 | 0.52 | 0/324 |
| 10 | H | 0.34 | 0/1287 | 0.65 | 1/1725 (0.1%) |
| 11 | J | 0.35 | 0/1136 | 0.60 | 0/1530 |
| 12 | K | 0.35 | 0/1001 | 0.65 | 0/1347 |
| 13 | L | 0.33 | 0/1130 | 0.65 | 0/1509 |
| 14 | M | 0.35 | 0/1583 | 0.61 | 0/2119 |
| 15 | N | 0.30 | 0/1474 | 0.65 | 0/1999 |
| 16 | O | 0.34 | 0/874 | 0.62 | 1/1181 (0.1%) |
| 17 | P | 0.35 | 0/1147 | 0.53 | 0/1528 |
| 18 | Q | 0.37 | 0/749 | 0.67 | 0/1005 |
| 19 | R | 0.40 | 0/1172 | 0.65 | 0/1578 |
| 20 | S | 0.34 | 0/648 | 0.57 | 0/875 |
| 21 | T | 0.32 | 0/958 | 0.62 | 0/1289 |
| 22 | U | 0.36 | 0/417 | 0.53 | 0/562 |
| 23 | V | 0.31 | 0/502 | 0.55 | 0/675 |
| 24 | W | 0.34 | 0/1219 | 0.63 | 0/1655 |
| 25 | X | 0.35 | 0/664 | 0.60 | 0/895 |
| 26 | Y | 0.35 | 0/1146 | 0.62 | 0/1536 |
| 27 | Z | 0.35 | 0/590 | 0.63 | 0/787 |
| 28 | 1 | 0.41 | 0/438 | 0.66 | 0/578 |
| 29 | 2 | 0.36 | 0/401 | 0.57 | 0/529 |
| 30 | 3 | 0.37 | 0/771 | 0.57 | 0/1024 |
| 31 | I | 0.34 | 0/526 | 0.53 | 0/716 |
| All | All | 0.37 | 0/98692 | 0.67 | 13/147577 (0.0%) |

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 | 0 | 1 | 37 |
| 2 | 9 | 0 | 2 |
| All | All | 1 | 39 |

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 0 | 805 | G | C2'-C3'-O3' | 7.33 | 125.62 | 109.50 |
| 1 | 0 | 1942 | A | C5'-C4'-C3' | 6.85 | 126.95 | 116.00 |
| 1 | 0 | 871 | G | C5'-C4'-O4' | -5.95 | 101.95 | 109.10 |
| 2 | 9 | 3039 | U | N1-C1'-C2' | 5.83 | 121.57 | 114.00 |
| 1 | 0 | 1942 | A | C5'-C4'-O4' | 5.80 | 116.06 | 109.10 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | 0 | 805 | G | C3' |

5 of 39 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | 0 | 23 | G | Sidechain |
| 1 | 0 | 246 | G | Sidechain |
| 1 | 0 | 396 | U | Sidechain |
| 1 | 0 | 462 | A | Sidechain |
| 1 | 0 | 471 | G | Sidechain |

5.2 Too-close contacts [i](#)

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 | 0 | 59021 | 0 | 29810 | 1019 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 9 | 2600 | 0 | 1326 | 87 | 0 |
| 3 | A | 1753 | 0 | 1766 | 61 | 0 |
| 4 | B | 2625 | 0 | 2533 | 85 | 0 |
| 5 | C | 1859 | 0 | 1816 | 53 | 0 |
| 6 | D | 1094 | 0 | 1085 | 39 | 0 |
| 7 | E | 1357 | 0 | 1266 | 32 | 0 |
| 8 | F | 890 | 0 | 843 | 24 | 0 |
| 9 | G | 240 | 0 | 231 | 12 | 0 |
| 10 | H | 1266 | 0 | 1268 | 31 | 0 |
| 11 | J | 1120 | 0 | 1098 | 36 | 0 |
| 12 | K | 992 | 0 | 1031 | 36 | 0 |
| 13 | L | 1118 | 0 | 1076 | 33 | 0 |
| 14 | M | 1559 | 0 | 1568 | 38 | 0 |
| 15 | N | 1445 | 0 | 1401 | 63 | 0 |
| 16 | O | 865 | 0 | 873 | 21 | 0 |
| 17 | P | 1136 | 0 | 1123 | 24 | 0 |
| 18 | Q | 735 | 0 | 729 | 12 | 0 |
| 19 | R | 1149 | 0 | 1122 | 29 | 0 |
| 20 | S | 641 | 0 | 605 | 15 | 0 |
| 21 | T | 950 | 0 | 923 | 27 | 0 |
| 22 | U | 410 | 0 | 364 | 19 | 0 |
| 23 | V | 499 | 0 | 511 | 17 | 0 |
| 24 | W | 1196 | 0 | 1137 | 54 | 0 |
| 25 | X | 654 | 0 | 653 | 22 | 0 |
| 26 | Y | 1130 | 0 | 1133 | 35 | 0 |
| 27 | Z | 579 | 0 | 539 | 19 | 0 |
| 28 | 1 | 431 | 0 | 426 | 19 | 0 |
| 29 | 2 | 396 | 0 | 413 | 18 | 0 |
| 30 | 3 | 755 | 0 | 730 | 19 | 0 |
| 31 | I | 519 | 0 | 500 | 30 | 0 |
| 32 | 0 | 108 | 0 | 0 | 0 | 0 |
| 32 | 3 | 1 | 0 | 0 | 0 | 0 |
| 32 | 9 | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 2 | 0 | 0 | 0 | 0 |
| 32 | B | 1 | 0 | 0 | 0 | 0 |
| 32 | K | 1 | 0 | 0 | 0 | 0 |
| 32 | T | 1 | 0 | 0 | 0 | 0 |
| 32 | Y | 1 | 0 | 0 | 0 | 0 |
| 33 | 0 | 2 | 0 | 0 | 0 | 0 |
| 34 | 0 | 72 | 0 | 0 | 1 | 0 |
| 34 | 9 | 3 | 0 | 0 | 0 | 0 |
| 34 | A | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34 | C | 1 | 0 | 0 | 0 | 0 |
| 34 | H | 1 | 0 | 0 | 0 | 0 |
| 34 | J | 1 | 0 | 0 | 0 | 0 |
| 34 | L | 1 | 0 | 0 | 1 | 0 |
| 34 | M | 1 | 0 | 0 | 0 | 0 |
| 34 | Q | 1 | 0 | 0 | 0 | 0 |
| 34 | R | 3 | 0 | 0 | 0 | 0 |
| 34 | S | 1 | 0 | 0 | 0 | 0 |
| 35 | 0 | 10 | 0 | 0 | 1 | 0 |
| 35 | 3 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 1 | 0 | 0 | 0 | 0 |
| 35 | B | 1 | 0 | 0 | 0 | 0 |
| 35 | J | 3 | 0 | 0 | 2 | 0 |
| 35 | L | 1 | 0 | 0 | 0 | 0 |
| 35 | M | 1 | 0 | 0 | 1 | 0 |
| 35 | N | 1 | 0 | 0 | 1 | 0 |
| 35 | O | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 1 | 0 | 0 | 0 | 0 |
| 35 | R | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 17 | 0 | 19 | 5 | 0 |
| 37 | 1 | 1 | 0 | 0 | 0 | 0 |
| 37 | 3 | 1 | 0 | 0 | 1 | 0 |
| 37 | O | 1 | 0 | 0 | 0 | 0 |
| 37 | U | 1 | 0 | 0 | 0 | 0 |
| 37 | Z | 1 | 0 | 0 | 0 | 0 |
| 38 | 0 | 5923 | 0 | 0 | 177 | 0 |
| 38 | 1 | 60 | 0 | 0 | 2 | 0 |
| 38 | 2 | 36 | 0 | 0 | 3 | 0 |
| 38 | 3 | 74 | 0 | 0 | 6 | 0 |
| 38 | 9 | 142 | 0 | 0 | 14 | 0 |
| 38 | A | 112 | 0 | 0 | 7 | 0 |
| 38 | B | 137 | 0 | 0 | 14 | 0 |
| 38 | C | 167 | 0 | 0 | 10 | 0 |
| 38 | D | 44 | 0 | 0 | 5 | 0 |
| 38 | E | 45 | 0 | 0 | 3 | 0 |
| 38 | F | 27 | 0 | 0 | 2 | 0 |
| 38 | G | 16 | 0 | 0 | 1 | 0 |
| 38 | H | 70 | 0 | 0 | 5 | 0 |
| 38 | I | 5 | 0 | 0 | 2 | 0 |
| 38 | J | 51 | 0 | 0 | 3 | 0 |
| 38 | K | 57 | 0 | 0 | 6 | 0 |
| 38 | L | 85 | 0 | 0 | 11 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38 | M | 122 | 0 | 0 | 2 | 0 |
| 38 | N | 61 | 0 | 0 | 7 | 0 |
| 38 | O | 38 | 0 | 0 | 5 | 0 |
| 38 | P | 63 | 0 | 0 | 1 | 0 |
| 38 | Q | 50 | 0 | 0 | 1 | 0 |
| 38 | R | 85 | 0 | 0 | 5 | 0 |
| 38 | S | 39 | 0 | 0 | 4 | 0 |
| 38 | T | 30 | 0 | 0 | 1 | 0 |
| 38 | U | 28 | 0 | 0 | 1 | 0 |
| 38 | V | 11 | 0 | 0 | 1 | 0 |
| 38 | W | 69 | 0 | 0 | 3 | 0 |
| 38 | X | 24 | 0 | 0 | 2 | 0 |
| 38 | Y | 87 | 0 | 0 | 7 | 0 |
| 38 | Z | 30 | 0 | 0 | 2 | 0 |
| All | All | 99020 | 0 | 59918 | 1837 | 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 1837 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:0:1160:G:C5' | 1:0:1161:A:H5' | 1.70 | 1.22 |
| 1:0:871:G:C8 | 1:0:871:G:H5' | 1.81 | 1.14 |
| 2:9:3006:C:H5'' | 15:N:37:ARG:NH1 | 1.63 | 1.12 |
| 1:0:871:G:H8 | 1:0:871:G:H5' | 1.10 | 1.11 |
| 1:0:656:G:H5' | 16:O:3:THR:HG22 | 1.18 | 1.10 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3 | A | 235/240 (98%) | 215 (92%) | 16 (7%) | 4 (2%) | 11 | 36 |
| 4 | B | 335/338 (99%) | 307 (92%) | 23 (7%) | 5 (2%) | 12 | 39 |
| 5 | C | 244/246 (99%) | 220 (90%) | 22 (9%) | 2 (1%) | 22 | 57 |
| 6 | D | 134/177 (76%) | 108 (81%) | 22 (16%) | 4 (3%) | 5 | 20 |
| 7 | E | 170/178 (96%) | 161 (95%) | 7 (4%) | 2 (1%) | 15 | 46 |
| 8 | F | 117/120 (98%) | 105 (90%) | 11 (9%) | 1 (1%) | 20 | 54 |
| 9 | G | 25/348 (7%) | 25 (100%) | 0 | 0 | 100 | 100 |
| 10 | H | 156/174 (90%) | 144 (92%) | 11 (7%) | 1 (1%) | 28 | 64 |
| 11 | J | 140/145 (97%) | 132 (94%) | 6 (4%) | 2 (1%) | 13 | 41 |
| 12 | K | 130/132 (98%) | 125 (96%) | 5 (4%) | 0 | 100 | 100 |
| 13 | L | 141/165 (86%) | 120 (85%) | 19 (14%) | 2 (1%) | 13 | 41 |
| 14 | M | 192/196 (98%) | 184 (96%) | 8 (4%) | 0 | 100 | 100 |
| 15 | N | 184/187 (98%) | 163 (89%) | 18 (10%) | 3 (2%) | 11 | 37 |
| 16 | O | 113/116 (97%) | 109 (96%) | 4 (4%) | 0 | 100 | 100 |
| 17 | P | 141/149 (95%) | 139 (99%) | 2 (1%) | 0 | 100 | 100 |
| 18 | Q | 93/96 (97%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 19 | R | 148/155 (96%) | 140 (95%) | 8 (5%) | 0 | 100 | 100 |
| 20 | S | 79/85 (93%) | 71 (90%) | 8 (10%) | 0 | 100 | 100 |
| 21 | T | 117/120 (98%) | 109 (93%) | 7 (6%) | 1 (1%) | 20 | 54 |
| 22 | U | 51/67 (76%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 23 | V | 63/71 (89%) | 59 (94%) | 4 (6%) | 0 | 100 | 100 |
| 24 | W | 152/154 (99%) | 147 (97%) | 3 (2%) | 2 (1%) | 14 | 43 |
| 25 | X | 80/92 (87%) | 71 (89%) | 7 (9%) | 2 (2%) | 6 | 25 |
| 26 | Y | 140/241 (58%) | 139 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | Z | 71/73 (97%) | 61 (86%) | 7 (10%) | 3 (4%) | 3 | 12 |
| 28 | 1 | 54/57 (95%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |
| 29 | 2 | 42/50 (84%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 30 | 3 | 90/92 (98%) | 85 (94%) | 4 (4%) | 1 (1%) | 17 | 48 |
| 31 | I | 68/162 (42%) | 50 (74%) | 17 (25%) | 1 (2%) | 12 | 39 |
| All | All | 3705/4426 (84%) | 3419 (92%) | 250 (7%) | 36 (1%) | 18 | 51 |

5 of 36 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 37 | VAL |
| 8 | F | 101 | ALA |
| 15 | N | 154 | LEU |
| 15 | N | 184 | ILE |
| 24 | W | 77 | ALA |

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 | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 3 | A | 179/182 (98%) | 171 (96%) | 8 (4%) | 32 | 66 |
| 4 | B | 282/283 (100%) | 271 (96%) | 11 (4%) | 37 | 72 |
| 5 | C | 193/193 (100%) | 179 (93%) | 14 (7%) | 16 | 43 |
| 6 | D | 117/148 (79%) | 109 (93%) | 8 (7%) | 18 | 47 |
| 7 | E | 152/156 (97%) | 150 (99%) | 2 (1%) | 73 | 93 |
| 8 | F | 93/94 (99%) | 92 (99%) | 1 (1%) | 78 | 94 |
| 9 | G | 27/283 (10%) | 26 (96%) | 1 (4%) | 39 | 74 |
| 10 | H | 132/141 (94%) | 125 (95%) | 7 (5%) | 26 | 60 |
| 11 | J | 118/121 (98%) | 112 (95%) | 6 (5%) | 28 | 62 |
| 12 | K | 106/106 (100%) | 102 (96%) | 4 (4%) | 38 | 73 |
| 13 | L | 113/127 (89%) | 108 (96%) | 5 (4%) | 33 | 67 |
| 14 | M | 158/160 (99%) | 149 (94%) | 9 (6%) | 24 | 56 |
| 15 | N | 149/150 (99%) | 142 (95%) | 7 (5%) | 30 | 65 |
| 16 | O | 93/94 (99%) | 92 (99%) | 1 (1%) | 78 | 94 |
| 17 | P | 113/117 (97%) | 110 (97%) | 3 (3%) | 50 | 82 |
| 18 | Q | 79/80 (99%) | 76 (96%) | 3 (4%) | 38 | 73 |
| 19 | R | 117/122 (96%) | 114 (97%) | 3 (3%) | 51 | 83 |
| 20 | S | 71/74 (96%) | 71 (100%) | 0 | 100 | 100 |
| 21 | T | 105/106 (99%) | 99 (94%) | 6 (6%) | 24 | 56 |
| 22 | U | 44/53 (83%) | 44 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 23 | V | 51/57 (90%) | 50 (98%) | 1 (2%) | 60 | 87 |
| 24 | W | 130/130 (100%) | 125 (96%) | 5 (4%) | 38 | 73 |
| 25 | X | 66/74 (89%) | 61 (92%) | 5 (8%) | 15 | 41 |
| 26 | Y | 120/196 (61%) | 116 (97%) | 4 (3%) | 43 | 77 |
| 27 | Z | 60/60 (100%) | 59 (98%) | 1 (2%) | 66 | 89 |
| 28 | 1 | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 29 | 2 | 42/46 (91%) | 41 (98%) | 1 (2%) | 54 | 84 |
| 30 | 3 | 79/79 (100%) | 77 (98%) | 2 (2%) | 53 | 83 |
| 31 | I | 58/130 (45%) | 58 (100%) | 0 | 100 | 100 |
| All | All | 3093/3609 (86%) | 2975 (96%) | 118 (4%) | 38 | 73 |

5 of 118 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | J | 39 | VAL |
| 13 | L | 140 | VAL |
| 25 | X | 79 | GLU |
| 11 | J | 46 | ILE |
| 12 | K | 10 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | M | 58 | GLN |
| 19 | R | 98 | ASN |
| 29 | 2 | 45 | ASN |
| 14 | M | 137 | ASN |
| 17 | P | 118 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 0 | 2745/2772 (99%) | 234 (8%) | 28 (1%) |
| 2 | 9 | 121/122 (99%) | 17 (14%) | 1 (0%) |
| All | All | 2866/2894 (99%) | 251 (8%) | 29 (1%) |

5 of 251 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 31 | C |
| 1 | 0 | 60 | A |
| 1 | 0 | 67 | A |
| 1 | 0 | 69 | A |
| 1 | 0 | 70 | A |

5 of 29 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1377 | C |
| 1 | 0 | 1506 | U |
| 1 | 0 | 2726 | U |
| 1 | 0 | 1450 | C |
| 1 | 0 | 1684 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 1 | OMU | 0 | 2587 | 1 | 14,22,23 | 1.01 | 1 (7%) | 18,31,34 | 3.66 | 2 (11%) |
| 1 | OMG | 0 | 2588 | 1 | 18,26,27 | 1.09 | 1 (5%) | 22,38,41 | 2.45 | 5 (22%) |
| 1 | UR3 | 0 | 2619 | 1 | 14,22,23 | 0.77 | 0 | 16,32,35 | 0.80 | 0 |
| 1 | PSU | 0 | 2621 | 1 | 16,21,22 | 1.55 | 3 (18%) | 20,30,33 | 6.07 | 4 (20%) |
| 1 | 1MA | 0 | 628 | 1 | 16,25,26 | 1.05 | 1 (6%) | 13,37,40 | 1.16 | 1 (7%) |

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 |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | OMU | 0 | 2587 | 1 | - | 0/5/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | OMG | 0 | 2588 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | UR3 | 0 | 2619 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | PSU | 0 | 2621 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 1MA | 0 | 628 | 1 | - | 0/3/25/26 | 0/3/3/3 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | 0 | 2621 | PSU | C5-C1' | -4.59 | 1.48 | 1.52 |
| 1 | 0 | 2621 | PSU | C2-N1 | 2.49 | 1.43 | 1.38 |
| 1 | 0 | 2621 | PSU | C4-N3 | 2.60 | 1.37 | 1.33 |
| 1 | 0 | 2587 | OMU | C4-N3 | 2.74 | 1.38 | 1.33 |
| 1 | 0 | 628 | 1MA | C6-N6 | 2.83 | 1.34 | 1.27 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 0 | 2621 | PSU | N1-C2-N3 | -19.05 | 114.70 | 128.40 |
| 1 | 0 | 2621 | PSU | C5-C4-N3 | -12.85 | 114.89 | 125.43 |
| 1 | 0 | 2588 | OMG | C5-C6-N1 | -8.37 | 111.57 | 123.48 |
| 1 | 0 | 628 | 1MA | C2-N3-C4 | -3.72 | 110.70 | 116.41 |
| 1 | 0 | 2587 | OMU | C5-C4-N3 | -3.61 | 114.51 | 123.12 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | 0 | 2587 | OMU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 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 | $\# Z > 2$ |
| 36 | NEG | 0 | 8823 | 32 | 11,16,16 | 1.38 | 1 (9%) | 11,20,20 | 1.41 | 1 (9%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 36 | NEG | 0 | 8823 | 32 | - | 0/15/18/18 | 0/0/0/0 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | 0 | 8823 | NEG | N2-N3 | -4.26 | 1.36 | 1.41 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | 0 | 8823 | NEG | C9-N3-C7 | -4.44 | 110.28 | 122.54 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 36 | 0 | 8823 | NEG | 5 | 0 |

5.7 Other polymers [i](#)

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 | 0 | 2749/2772 (99%) | -0.78 | 14 (0%) 90 90 | 19, 42, 86, 144 | 0 |
| 2 | 9 | 122/122 (100%) | -0.80 | 3 (2%) 58 53 | 35, 59, 83, 147 | 0 |
| 3 | A | 237/240 (98%) | -0.48 | 2 (0%) 86 85 | 25, 46, 78, 99 | 0 |
| 4 | B | 337/338 (99%) | -0.70 | 1 (0%) 93 93 | 26, 50, 75, 85 | 0 |
| 5 | C | 246/246 (100%) | -0.64 | 0 100 100 | 23, 44, 66, 75 | 0 |
| 6 | D | 140/177 (79%) | 1.01 | 27 (19%) 1 1 | 54, 94, 118, 126 | 0 |
| 7 | E | 172/178 (96%) | -0.52 | 1 (0%) 89 88 | 40, 63, 83, 88 | 0 |
| 8 | F | 119/120 (99%) | 0.16 | 5 (4%) 37 32 | 42, 67, 89, 100 | 0 |
| 9 | G | 29/348 (8%) | 1.08 | 9 (31%) 0 0 | 73, 89, 96, 98 | 0 |
| 10 | H | 160/174 (91%) | -0.16 | 1 (0%) 89 88 | 36, 56, 86, 95 | 0 |
| 11 | J | 142/145 (97%) | -0.69 | 0 100 100 | 32, 47, 68, 89 | 0 |
| 12 | K | 132/132 (100%) | -0.79 | 1 (0%) 86 85 | 29, 45, 67, 78 | 0 |
| 13 | L | 145/165 (87%) | -0.07 | 7 (4%) 31 27 | 23, 62, 102, 114 | 0 |
| 14 | M | 194/196 (98%) | -0.77 | 1 (0%) 90 90 | 30, 40, 55, 63 | 0 |
| 15 | N | 186/187 (99%) | -0.22 | 5 (2%) 55 50 | 37, 59, 103, 114 | 0 |
| 16 | O | 115/116 (99%) | -0.65 | 0 100 100 | 35, 51, 67, 76 | 0 |
| 17 | P | 143/149 (95%) | -0.61 | 0 100 100 | 36, 51, 63, 72 | 0 |
| 18 | Q | 95/96 (98%) | -0.65 | 0 100 100 | 33, 44, 56, 70 | 0 |
| 19 | R | 150/155 (96%) | -0.70 | 0 100 100 | 30, 43, 64, 79 | 0 |
| 20 | S | 81/85 (95%) | -0.11 | 2 (2%) 58 53 | 43, 58, 78, 80 | 0 |
| 21 | T | 119/120 (99%) | -0.34 | 3 (2%) 58 53 | 41, 54, 77, 95 | 0 |
| 22 | U | 53/67 (79%) | -0.60 | 0 100 100 | 37, 50, 70, 77 | 0 |
| 23 | V | 65/71 (91%) | 0.75 | 8 (12%) 5 3 | 51, 72, 106, 114 | 0 |
| 24 | W | 154/154 (100%) | -0.57 | 0 100 100 | 33, 47, 63, 73 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | X | 82/92 (89%) | -0.27 | 4 (4%) 30 26 | 43, 56, 81, 96 | 0 |
| 26 | Y | 142/241 (58%) | -0.72 | 2 (1%) 75 74 | 25, 42, 64, 84 | 0 |
| 27 | Z | 73/73 (100%) | -0.45 | 0 100 100 | 45, 57, 74, 93 | 0 |
| 28 | 1 | 56/57 (98%) | -0.80 | 0 100 100 | 28, 32, 39, 48 | 0 |
| 29 | 2 | 46/50 (92%) | -0.25 | 3 (6%) 20 15 | 34, 60, 93, 102 | 0 |
| 30 | 3 | 92/92 (100%) | -0.63 | 0 100 100 | 32, 51, 64, 75 | 0 |
| 31 | I | 70/162 (43%) | 3.75 | 58 (82%) 0 0 | 101, 115, 127, 129 | 0 |
| All | All | 6646/7320 (90%) | -0.53 | 157 (2%) 59 55 | 19, 48, 93, 147 | 0 |

The worst 5 of 157 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 23 | V | 1 | THR | 11.9 |
| 31 | I | 79 | ILE | 9.6 |
| 31 | I | 71 | GLY | 9.2 |
| 6 | D | 63 | ILE | 8.7 |
| 31 | I | 75 | THR | 7.6 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 1 | OMU | 0 | 2587 | 21/22 | 0.99 | 0.09 | - | 29,31,33,36 | 0 |
| 1 | UR3 | 0 | 2619 | 21/22 | 0.97 | 0.12 | - | 32,34,35,37 | 0 |
| 1 | 1MA | 0 | 628 | 23/24 | 0.98 | 0.14 | - | 26,29,30,31 | 0 |
| 1 | OMG | 0 | 2588 | 24/25 | 0.97 | 0.12 | - | 26,32,34,36 | 0 |
| 1 | PSU | 0 | 2621 | 20/21 | 0.98 | 0.11 | - | 23,27,32,33 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 34 | NA | 0 | 8577 | 1/1 | 0.57 | 0.53 | 29.60 | 70,70,70,70 | 0 |
| 34 | NA | 0 | 8520 | 1/1 | 0.96 | 0.34 | 24.90 | 35,35,35,35 | 0 |
| 34 | NA | 0 | 8571 | 1/1 | 0.81 | 0.28 | 24.19 | 46,46,46,46 | 0 |
| 34 | NA | 0 | 8573 | 1/1 | 0.90 | 0.32 | 22.85 | 56,56,56,56 | 0 |
| 33 | K | 0 | 8401 | 1/1 | 0.89 | 0.35 | 17.24 | 78,78,78,78 | 0 |
| 34 | NA | 0 | 8562 | 1/1 | 0.88 | 0.33 | 14.12 | 65,65,65,65 | 0 |
| 34 | NA | 0 | 8503 | 1/1 | 0.98 | 0.26 | 13.18 | 1,1,1,1 | 0 |
| 34 | NA | 0 | 8523 | 1/1 | 0.93 | 0.28 | 13.07 | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8062 | 1/1 | 0.92 | 0.21 | 12.76 | 5,5,5,5 | 0 |
| 34 | NA | 0 | 8559 | 1/1 | 0.88 | 0.30 | 11.80 | 48,48,48,48 | 0 |
| 34 | NA | 0 | 8582 | 1/1 | 0.57 | 0.26 | 10.72 | 88,88,88,88 | 0 |
| 34 | NA | 0 | 8578 | 1/1 | 0.89 | 0.37 | 9.19 | 49,49,49,49 | 0 |
| 36 | NEG | 0 | 8823 | 17/17 | 0.90 | 0.18 | 8.38 | 68,72,82,83 | 0 |
| 34 | NA | 0 | 8565 | 1/1 | 0.96 | 1.02 | 7.40 | 52,52,52,52 | 0 |
| 34 | NA | 0 | 8576 | 1/1 | 0.98 | 0.20 | 7.18 | 24,24,24,24 | 0 |
| 34 | NA | 0 | 8514 | 1/1 | 0.98 | 0.26 | 5.98 | 37,37,37,37 | 0 |
| 34 | NA | 0 | 8561 | 1/1 | 0.93 | 0.34 | 5.85 | 61,61,61,61 | 0 |
| 34 | NA | R | 8586 | 1/1 | 0.91 | 0.28 | 5.85 | 29,29,29,29 | 0 |
| 34 | NA | 0 | 8535 | 1/1 | 0.86 | 0.19 | 5.83 | 39,39,39,39 | 0 |
| 34 | NA | L | 8580 | 1/1 | 0.96 | 0.27 | 5.18 | 1,1,1,1 | 0 |
| 34 | NA | 0 | 8572 | 1/1 | 0.91 | 0.20 | 5.17 | 68,68,68,68 | 0 |
| 34 | NA | 0 | 8526 | 1/1 | 0.93 | 0.16 | 5.07 | 63,63,63,63 | 0 |
| 34 | NA | 0 | 8564 | 1/1 | 0.85 | 0.21 | 4.62 | 50,50,50,50 | 0 |
| 32 | MG | 0 | 8060 | 1/1 | 0.87 | 0.21 | 4.53 | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8096 | 1/1 | 0.89 | 0.12 | 3.19 | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8080 | 1/1 | 0.68 | 0.18 | 3.05 | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8018 | 1/1 | 0.98 | 0.17 | 2.94 | 26,26,26,26 | 0 |
| 34 | NA | 0 | 8568 | 1/1 | 0.82 | 0.12 | 2.79 | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8527 | 1/1 | 0.94 | 0.15 | 2.21 | 46,46,46,46 | 0 |
| 34 | NA | 0 | 8566 | 1/1 | 0.93 | 0.11 | 2.09 | 74,74,74,74 | 0 |
| 34 | NA | 0 | 8521 | 1/1 | 0.99 | 0.21 | 2.07 | 43,43,43,43 | 0 |
| 34 | NA | 0 | 8510 | 1/1 | 0.99 | 0.13 | 2.05 | 22,22,22,22 | 0 |
| 32 | MG | 0 | 8052 | 1/1 | 0.95 | 0.14 | 2.03 | 77,77,77,77 | 0 |
| 32 | MG | 0 | 8006 | 1/1 | 0.97 | 0.14 | 1.87 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 34 | NA | Q | 8548 | 1/1 | 0.78 | 0.19 | 1.82 | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8010 | 1/1 | 0.99 | 0.16 | 1.77 | 13,13,13,13 | 0 |
| 34 | NA | 0 | 8550 | 1/1 | 0.93 | 0.17 | 1.75 | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8553 | 1/1 | 0.97 | 0.16 | 1.53 | 32,32,32,32 | 0 |
| 32 | MG | 3 | 8078 | 1/1 | 0.99 | 0.15 | 1.35 | 11,11,11,11 | 0 |
| 32 | MG | 0 | 8004 | 1/1 | 0.92 | 0.15 | 1.11 | 23,23,23,23 | 0 |
| 32 | MG | 0 | 8002 | 1/1 | 0.99 | 0.14 | 0.91 | 27,27,27,27 | 0 |
| 32 | MG | 0 | 8057 | 1/1 | 0.91 | 0.10 | 0.82 | 29,29,29,29 | 0 |
| 32 | MG | 0 | 8038 | 1/1 | 0.98 | 0.14 | 0.80 | 21,21,21,21 | 0 |
| 32 | MG | 0 | 8091 | 1/1 | 0.96 | 0.12 | 0.45 | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8054 | 1/1 | 0.94 | 0.14 | 0.20 | 24,24,24,24 | 0 |
| 34 | NA | 0 | 8525 | 1/1 | 0.98 | 0.14 | 0.19 | 71,71,71,71 | 0 |
| 32 | MG | 0 | 8110 | 1/1 | 0.91 | 0.13 | -0.03 | 54,54,54,54 | 0 |
| 34 | NA | A | 8545 | 1/1 | 0.80 | 0.12 | -0.29 | 57,57,57,57 | 0 |
| 34 | NA | R | 8538 | 1/1 | 0.54 | 0.10 | -0.39 | 55,55,55,55 | 0 |
| 32 | MG | 0 | 8033 | 1/1 | 1.00 | 0.09 | -0.72 | 21,21,21,21 | 0 |
| 32 | MG | A | 8065 | 1/1 | 0.95 | 0.12 | -0.75 | 37,37,37,37 | 0 |
| 37 | CD | Z | 8703 | 1/1 | 1.00 | 0.09 | -0.78 | 63,63,63,63 | 0 |
| 35 | CL | J | 8821 | 1/1 | 0.89 | 0.11 | -0.81 | 60,60,60,60 | 0 |
| 32 | MG | 0 | 8067 | 1/1 | 0.98 | 0.11 | -0.81 | 52,52,52,52 | 0 |
| 32 | MG | Y | 8109 | 1/1 | 0.91 | 0.10 | -0.81 | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8543 | 1/1 | 0.94 | 0.09 | -0.91 | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8107 | 1/1 | 0.98 | 0.08 | -1.14 | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8013 | 1/1 | 0.97 | 0.10 | -1.15 | 26,26,26,26 | 0 |
| 34 | NA | 0 | 8532 | 1/1 | 0.92 | 0.09 | -1.16 | 34,34,34,34 | 0 |
| 35 | CL | O | 8808 | 1/1 | 0.88 | 0.09 | -1.30 | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8020 | 1/1 | 0.97 | 0.10 | -1.32 | 26,26,26,26 | 0 |
| 37 | CD | 3 | 8704 | 1/1 | 0.99 | 0.05 | -1.51 | 53,53,53,53 | 0 |
| 37 | CD | U | 8701 | 1/1 | 0.99 | 0.06 | -1.59 | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8017 | 1/1 | 0.94 | 0.12 | -1.69 | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8077 | 1/1 | 0.99 | 0.12 | -1.79 | 30,30,30,30 | 0 |
| 37 | CD | 1 | 8702 | 1/1 | 0.99 | 0.09 | -1.82 | 55,55,55,55 | 0 |
| 32 | MG | 0 | 8056 | 1/1 | 0.98 | 0.06 | -1.89 | 42,42,42,42 | 0 |
| 34 | NA | 0 | 8531 | 1/1 | 0.98 | 0.12 | -1.92 | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8014 | 1/1 | 1.00 | 0.10 | -1.99 | 34,34,34,34 | 0 |
| 35 | CL | 0 | 8805 | 1/1 | 0.84 | 0.07 | -2.00 | 58,58,58,58 | 0 |
| 32 | MG | T | 8073 | 1/1 | 0.91 | 0.04 | -2.00 | 63,63,63,63 | 0 |
| 34 | NA | 0 | 8509 | 1/1 | 0.96 | 0.08 | -2.04 | 23,23,23,23 | 0 |
| 32 | MG | 0 | 8074 | 1/1 | 0.99 | 0.04 | -2.05 | 28,28,28,28 | 0 |
| 34 | NA | J | 8546 | 1/1 | 0.94 | 0.05 | -2.06 | 27,27,27,27 | 0 |
| 35 | CL | M | 8818 | 1/1 | 0.99 | 0.09 | -2.12 | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8003 | 1/1 | 0.98 | 0.08 | -2.21 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 35 | CL | 0 | 8812 | 1/1 | 0.97 | 0.06 | -2.37 | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8517 | 1/1 | 0.93 | 0.08 | -2.42 | 24,24,24,24 | 0 |
| 32 | MG | 0 | 8112 | 1/1 | 0.94 | 0.07 | -2.82 | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8015 | 1/1 | 0.86 | 0.12 | -2.90 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8012 | 1/1 | 0.95 | 0.08 | -2.95 | 30,30,30,30 | 0 |
| 32 | MG | 0 | 8058 | 1/1 | 0.98 | 0.07 | -3.09 | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8001 | 1/1 | 0.97 | 0.09 | -3.30 | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8021 | 1/1 | 0.93 | 0.07 | -3.32 | 37,37,37,37 | 0 |
| 34 | NA | 0 | 8539 | 1/1 | 0.89 | 0.11 | -3.51 | 30,30,30,30 | 0 |
| 32 | MG | 0 | 8064 | 1/1 | 0.96 | 0.06 | -3.54 | 28,28,28,28 | 0 |
| 32 | MG | 0 | 8032 | 1/1 | 0.85 | 0.06 | -3.62 | 29,29,29,29 | 0 |
| 34 | NA | 0 | 8544 | 1/1 | 0.84 | 0.04 | -3.65 | 14,14,14,14 | 0 |
| 32 | MG | 0 | 8044 | 1/1 | 0.95 | 0.06 | -3.81 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8028 | 1/1 | 0.90 | 0.07 | -4.12 | 39,39,39,39 | 0 |
| 34 | NA | 0 | 8533 | 1/1 | 0.96 | 0.06 | -4.16 | 22,22,22,22 | 0 |
| 34 | NA | M | 8547 | 1/1 | 0.99 | 0.04 | -4.20 | 35,35,35,35 | 0 |
| 35 | CL | B | 8819 | 1/1 | 0.93 | 0.06 | -4.32 | 39,39,39,39 | 0 |
| 33 | K | 0 | 8402 | 1/1 | 0.95 | 0.10 | -4.33 | 49,49,49,49 | 0 |
| 35 | CL | 3 | 8804 | 1/1 | 1.00 | 0.04 | -4.49 | 42,42,42,42 | 0 |
| 32 | MG | 0 | 8108 | 1/1 | 0.91 | 0.04 | -4.98 | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8035 | 1/1 | 0.90 | 0.06 | -5.21 | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8019 | 1/1 | 0.92 | 0.04 | -5.40 | 26,26,26,26 | 0 |
| 32 | MG | 0 | 8008 | 1/1 | 0.95 | 0.08 | -5.50 | 27,27,27,27 | 0 |
| 32 | MG | 0 | 8084 | 1/1 | 0.99 | 0.03 | -6.13 | 42,42,42,42 | 0 |
| 32 | MG | 0 | 8088 | 1/1 | 0.88 | 0.07 | -6.56 | 22,22,22,22 | 0 |
| 34 | NA | 0 | 8556 | 1/1 | 0.96 | 0.08 | -7.51 | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8053 | 1/1 | 0.99 | 0.03 | -8.23 | 50,50,50,50 | 0 |
| 32 | MG | 0 | 8104 | 1/1 | 0.96 | 0.16 | - | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8040 | 1/1 | 0.85 | 0.12 | - | 46,46,46,46 | 0 |
| 34 | NA | 9 | 8552 | 1/1 | 0.85 | 0.15 | - | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8029 | 1/1 | 0.98 | 0.06 | - | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8116 | 1/1 | 0.94 | 0.10 | - | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8072 | 1/1 | 0.90 | 0.09 | - | 55,55,55,55 | 0 |
| 34 | NA | 0 | 8513 | 1/1 | 0.85 | 0.09 | - | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8102 | 1/1 | 0.85 | 0.14 | - | 70,70,70,70 | 0 |
| 34 | NA | 0 | 8511 | 1/1 | 0.93 | 0.09 | - | 46,46,46,46 | 0 |
| 34 | NA | 0 | 8560 | 1/1 | 0.96 | 0.08 | - | 44,44,44,44 | 0 |
| 34 | NA | 0 | 8541 | 1/1 | 0.98 | 0.11 | - | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8063 | 1/1 | 0.89 | 0.30 | - | 89,89,89,89 | 0 |
| 34 | NA | 0 | 8536 | 1/1 | 0.95 | 0.06 | - | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8016 | 1/1 | 0.99 | 0.13 | - | 19,19,19,19 | 0 |
| 32 | MG | K | 8069 | 1/1 | 0.98 | 0.07 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | 0 | 8009 | 1/1 | 0.94 | 0.15 | - | 31,31,31,31 | 0 |
| 32 | MG | 0 | 8039 | 1/1 | 0.99 | 0.11 | - | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8087 | 1/1 | 0.86 | 0.11 | - | 61,61,61,61 | 0 |
| 32 | MG | 0 | 8049 | 1/1 | 0.99 | 0.12 | - | 30,30,30,30 | 0 |
| 32 | MG | 0 | 8037 | 1/1 | 0.98 | 0.09 | - | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8100 | 1/1 | 0.94 | 0.21 | - | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8024 | 1/1 | 0.72 | 0.65 | - | 80,80,80,80 | 0 |
| 32 | MG | 0 | 8007 | 1/1 | 1.00 | 0.14 | - | 9,9,9,9 | 0 |
| 34 | NA | 0 | 8557 | 1/1 | 0.94 | 0.05 | - | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8081 | 1/1 | 0.97 | 0.11 | - | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8027 | 1/1 | 0.99 | 0.06 | - | 39,39,39,39 | 0 |
| 34 | NA | 0 | 8528 | 1/1 | 0.94 | 0.18 | - | 39,39,39,39 | 0 |
| 35 | CL | 0 | 8803 | 1/1 | 0.94 | 0.07 | - | 52,52,52,52 | 0 |
| 35 | CL | Q | 8811 | 1/1 | 0.97 | 0.08 | - | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8581 | 1/1 | 0.95 | 0.05 | - | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8071 | 1/1 | 0.76 | 0.12 | - | 62,62,62,62 | 0 |
| 34 | NA | 0 | 8516 | 1/1 | 0.96 | 0.26 | - | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8031 | 1/1 | 0.97 | 0.13 | - | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8061 | 1/1 | 0.96 | 0.10 | - | 30,30,30,30 | 0 |
| 34 | NA | 0 | 8524 | 1/1 | 0.94 | 0.11 | - | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8101 | 1/1 | 0.98 | 0.21 | - | 71,71,71,71 | 0 |
| 32 | MG | 0 | 8075 | 1/1 | 0.93 | 0.10 | - | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8103 | 1/1 | 0.96 | 0.21 | - | 77,77,77,77 | 0 |
| 34 | NA | 0 | 8505 | 1/1 | 0.91 | 0.13 | - | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8554 | 1/1 | 0.92 | 0.23 | - | 39,39,39,39 | 0 |
| 32 | MG | B | 8055 | 1/1 | 0.78 | 0.08 | - | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8023 | 1/1 | 0.98 | 0.15 | - | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8098 | 1/1 | 0.95 | 0.17 | - | 31,31,31,31 | 0 |
| 34 | NA | 9 | 8551 | 1/1 | 0.72 | 0.22 | - | 95,95,95,95 | 0 |
| 35 | CL | 0 | 8816 | 1/1 | 0.98 | 0.12 | - | 57,57,57,57 | 0 |
| 35 | CL | 0 | 8814 | 1/1 | 0.97 | 0.06 | - | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8094 | 1/1 | 0.80 | 0.10 | - | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8042 | 1/1 | 0.94 | 0.05 | - | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8111 | 1/1 | 0.94 | 0.13 | - | 50,50,50,50 | 0 |
| 32 | MG | 9 | 8095 | 1/1 | 0.92 | 0.05 | - | 55,55,55,55 | 0 |
| 32 | MG | 0 | 8041 | 1/1 | 0.86 | 0.07 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8079 | 1/1 | 0.99 | 0.14 | - | 27,27,27,27 | 0 |
| 34 | NA | 0 | 8575 | 1/1 | 0.96 | 0.28 | - | 52,52,52,52 | 0 |
| 35 | CL | J | 8801 | 1/1 | 0.94 | 0.08 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8093 | 1/1 | 0.97 | 0.05 | - | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8051 | 1/1 | 0.97 | 0.07 | - | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8508 | 1/1 | 0.78 | 0.22 | - | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | 0 | 8047 | 1/1 | 0.91 | 0.06 | - | 72,72,72,72 | 0 |
| 35 | CL | 0 | 8815 | 1/1 | 0.89 | 0.13 | - | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8563 | 1/1 | 0.98 | 0.19 | - | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8034 | 1/1 | 0.97 | 0.07 | - | 15,15,15,15 | 0 |
| 32 | MG | 0 | 8050 | 1/1 | 0.66 | 0.15 | - | 66,66,66,66 | 0 |
| 34 | NA | 0 | 8569 | 1/1 | 0.84 | 0.31 | - | 63,63,63,63 | 0 |
| 37 | CD | O | 8705 | 1/1 | 0.49 | 0.42 | - | 187,187,187,187 | 0 |
| 34 | NA | 0 | 8567 | 1/1 | 0.75 | 0.28 | - | 51,51,51,51 | 0 |
| 34 | NA | C | 8504 | 1/1 | 0.94 | 0.18 | - | 41,41,41,41 | 0 |
| 34 | NA | 0 | 8555 | 1/1 | 0.86 | 0.90 | - | 81,81,81,81 | 0 |
| 32 | MG | 0 | 8097 | 1/1 | 0.96 | 0.07 | - | 35,35,35,35 | 0 |
| 32 | MG | 0 | 8099 | 1/1 | 0.89 | 0.15 | - | 42,42,42,42 | 0 |
| 34 | NA | 9 | 8583 | 1/1 | 0.90 | 0.21 | - | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8059 | 1/1 | 0.85 | 0.09 | - | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8090 | 1/1 | 0.95 | 0.24 | - | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8026 | 1/1 | 0.97 | 0.15 | - | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8083 | 1/1 | 0.83 | 0.06 | - | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8530 | 1/1 | 0.94 | 0.08 | - | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8045 | 1/1 | 0.86 | 0.09 | - | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8089 | 1/1 | 0.99 | 0.12 | - | 32,32,32,32 | 0 |
| 34 | NA | 0 | 8502 | 1/1 | 0.91 | 0.11 | - | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8542 | 1/1 | 0.99 | 0.28 | - | 1,1,1,1 | 0 |
| 34 | NA | 0 | 8540 | 1/1 | 0.96 | 0.11 | - | 43,43,43,43 | 0 |
| 34 | NA | S | 8512 | 1/1 | 0.91 | 0.70 | - | 62,62,62,62 | 0 |
| 35 | CL | L | 8810 | 1/1 | 0.83 | 0.09 | - | 54,54,54,54 | 0 |
| 35 | CL | 0 | 8817 | 1/1 | 0.96 | 0.12 | - | 59,59,59,59 | 0 |
| 32 | MG | 0 | 8046 | 1/1 | 0.88 | 0.06 | - | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8558 | 1/1 | 0.70 | 0.41 | - | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8022 | 1/1 | 0.97 | 0.05 | - | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8534 | 1/1 | 0.96 | 0.06 | - | 41,41,41,41 | 0 |
| 32 | MG | 0 | 8082 | 1/1 | 0.86 | 0.22 | - | 65,65,65,65 | 0 |
| 32 | MG | 0 | 8106 | 1/1 | 0.51 | 0.17 | - | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8086 | 1/1 | 0.81 | 0.04 | - | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8115 | 1/1 | 0.98 | 0.03 | - | 41,41,41,41 | 0 |
| 34 | NA | 0 | 8585 | 1/1 | 0.81 | 0.32 | - | 59,59,59,59 | 0 |
| 32 | MG | 0 | 8092 | 1/1 | 0.82 | 0.11 | - | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8048 | 1/1 | 0.95 | 0.10 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8005 | 1/1 | 1.00 | 0.14 | - | 32,32,32,32 | 0 |
| 34 | NA | 0 | 8570 | 1/1 | 0.96 | 0.36 | - | 64,64,64,64 | 0 |
| 34 | NA | 0 | 8584 | 1/1 | 0.64 | 0.35 | - | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8085 | 1/1 | 0.80 | 0.14 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8068 | 1/1 | 0.96 | 0.06 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | 0 | 8070 | 1/1 | 0.88 | 0.10 | - | 34,34,34,34 | 0 |
| 34 | NA | 0 | 8506 | 1/1 | 0.84 | 0.37 | - | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8030 | 1/1 | 0.98 | 0.06 | - | 20,20,20,20 | 0 |
| 32 | MG | 0 | 8011 | 1/1 | 0.94 | 0.08 | - | 23,23,23,23 | 0 |
| 35 | CL | R | 8806 | 1/1 | 0.92 | 0.07 | - | 52,52,52,52 | 0 |
| 35 | CL | N | 8807 | 1/1 | 0.92 | 0.12 | - | 57,57,57,57 | 0 |
| 34 | NA | H | 8522 | 1/1 | 0.89 | 0.35 | - | 71,71,71,71 | 0 |
| 32 | MG | 0 | 8117 | 1/1 | 0.94 | 0.09 | - | 45,45,45,45 | 0 |
| 35 | CL | J | 8802 | 1/1 | 0.91 | 0.12 | - | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8501 | 1/1 | 0.94 | 0.04 | - | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8519 | 1/1 | 0.99 | 0.12 | - | 21,21,21,21 | 0 |
| 32 | MG | 0 | 8076 | 1/1 | 0.56 | 0.12 | - | 44,44,44,44 | 0 |
| 35 | CL | 0 | 8822 | 1/1 | 0.95 | 0.30 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 8066 | 1/1 | 0.96 | 0.14 | - | 47,47,47,47 | 0 |
| 35 | CL | A | 8809 | 1/1 | 0.97 | 0.13 | - | 71,71,71,71 | 0 |
| 34 | NA | 0 | 8549 | 1/1 | 0.87 | 0.19 | - | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8515 | 1/1 | 0.96 | 0.14 | - | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8036 | 1/1 | 0.98 | 0.04 | - | 29,29,29,29 | 0 |
| 34 | NA | 0 | 8529 | 1/1 | 0.91 | 0.15 | - | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8025 | 1/1 | 0.99 | 0.10 | - | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8043 | 1/1 | 0.84 | 0.19 | - | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8518 | 1/1 | 0.98 | 0.12 | - | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8507 | 1/1 | 0.81 | 0.12 | - | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8574 | 1/1 | 0.03 | 0.83 | - | 73,73,73,73 | 0 |
| 35 | CL | 0 | 8813 | 1/1 | 0.98 | 0.06 | - | 55,55,55,55 | 0 |
| 34 | NA | R | 8537 | 1/1 | 0.88 | 0.05 | - | 35,35,35,35 | 0 |
| 35 | CL | 0 | 8820 | 1/1 | 0.95 | 0.06 | - | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8113 | 1/1 | 0.77 | 0.13 | - | 49,49,49,49 | 0 |
| 34 | NA | 0 | 8579 | 1/1 | 0.95 | 0.08 | - | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8114 | 1/1 | 0.89 | 0.23 | - | 41,41,41,41 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.