# wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:58 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1QVG |
| Title | : | Structure of CCA oligonucleotide bound to the tRNA binding sites of the large ribosomal subunit of Haloarcula marismortui |
| Authors | : | Schmeing, T.M.; Moore, P.B.; Steitz, T.A. |
| Deposited on | : | 2003-08-27 |
| 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

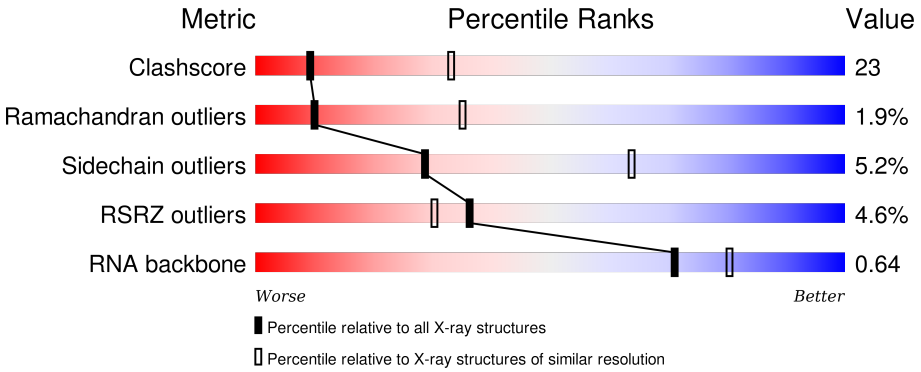
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | trunk26765 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

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)) |
|---|---|---|
| Clashscore | 102246 | 1668 (2.90-2.90) |
| Ramachandran outliers | 100387 | 1630 (2.90-2.90) |
| Sidechain outliers | 100360 | 1632 (2.90-2.90) |
| RSRZ outliers | 91569 | 1456 (2.90-2.90) |
| RNA backbone | 2183 | 1093 (3.30-2.50) |

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 <=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 | 2922 | 46% 41% 7% • 6% |
| 2 | 9 | 122 | 2% 44% 41% 12% • |
| 3 | 3 | 3 | 33% 33% 67% |
| 3 | 4 | 3 | 33% 33% 67% |
| 3 | 5 | 3 | 67% 33% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | A | 239 | 9% 56% 36% 7% |
| 5 | B | 337 | 47% 45% 7% |
| 6 | C | 246 | 55% 40% 5% |
| 7 | D | 176 | 27% 25% 47% 7% 20% |
| 8 | E | 177 | 4% 53% 41% |
| 9 | F | 119 | 16% 47% 51% |
| 10 | G | 348 | 5% 6% 92% |
| 11 | H | 167 | 2% 39% 46% 8% 7% |
| 12 | I | 145 | 48% 43% 7% |
| 13 | J | 132 | 52% 46% |
| 14 | K | 164 | 12% 52% 33% 12% |
| 15 | L | 194 | 2% 36% 61% |
| 16 | M | 186 | 16% 36% 58% 6% |
| 17 | N | 115 | 2% 59% 40% |
| 18 | O | 148 | 3% 61% 34% |
| 19 | P | 95 | 62% 37% |
| 20 | Q | 154 | % 60% 34% |
| 21 | R | 84 | 4% 60% 37% |
| 22 | S | 119 | 14% 46% 50% |
| 23 | T | 66 | 6% 39% 41% 20% |
| 24 | U | 70 | 27% 43% 44% 7% |
| 25 | V | 154 | 42% 53% 6% |
| 26 | W | 91 | 13% 44% 37% 9% 10% |
| 27 | X | 240 | 3% 33% 23% 41% |
| 28 | Y | 73 | 7% 36% 58% 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | Z | 56 | 57% 43% |
| 30 | 1 | 48 | 35% 48% 46% |
| 31 | 2 | 92 | 9% 63% 36% |

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 | 8049 | - | - | - | X |
| 32 | MG | 0 | 8054 | - | - | - | X |
| 34 | NA | 0 | 8310 | - | - | - | X |
| 34 | NA | 0 | 8320 | - | - | - | X |
| 34 | NA | 0 | 8321 | - | - | - | X |
| 34 | NA | 0 | 8325 | - | - | - | X |
| 34 | NA | 0 | 8326 | - | - | - | X |
| 34 | NA | 0 | 8328 | - | - | - | X |
| 34 | NA | 0 | 8335 | - | - | - | X |
| 34 | NA | 0 | 8350 | - | - | - | X |
| 34 | NA | 0 | 8355 | - | - | - | X |
| 34 | NA | 0 | 8356 | - | - | - | X |
| 34 | NA | 0 | 8359 | - | - | - | X |
| 34 | NA | 0 | 8361 | - | - | - | X |
| 34 | NA | 0 | 8362 | - | - | - | X |
| 34 | NA | 0 | 8365 | - | - | - | X |
| 34 | NA | 0 | 8367 | - | - | - | X |
| 34 | NA | 0 | 8371 | - | - | - | X |
| 34 | NA | 0 | 8372 | - | - | - | X |
| 34 | NA | 0 | 8373 | - | - | - | X |
| 34 | NA | 0 | 8374 | - | - | - | X |
| 34 | NA | 0 | 8376 | - | - | - | X |
| 34 | NA | 0 | 8378 | - | - | - | X |
| 34 | NA | 0 | 8379 | - | - | - | X |
| 34 | NA | 0 | 8382 | - | - | - | X |
| 34 | NA | 9 | 8383 | - | - | - | X |
| 34 | NA | C | 8304 | - | - | - | X |
| 34 | NA | K | 8380 | - | - | - | X |
| 34 | NA | Q | 8337 | - | - | - | X |
| 34 | NA | Q | 8386 | - | - | - | X |
| 35 | CL | 0 | 8505 | - | - | - | X |
| 35 | CL | 0 | 8515 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 35 | CL | B | 8519 | - | - | - | X |
| 35 | CL | I | 8502 | - | - | X | - |
| 35 | CL | N | 8508 | - | - | - | X |

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98494 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 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | 0 | 2754 | 59017 | 26346 | 10878 | 19048 | 2745 | 0 | 0 | 0 |

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

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

- Molecule 3 is a RNA chain called Oligonucleotide CCA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 3 | 3 | 3 | 59 | 28 | 11 | 18 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | P | | | |
| 3 | 4 | 3 | 59 | 28 | 11 | 18 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | P | | | |
| 3 | 5 | 3 | 59 | 28 | 11 | 18 | 2 | 0 | 0 | 0 |

- Molecule 4 is a protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | A | 237 | 1754 | 1072 | 352 | 325 | 5 | 0 | 0 | 0 |

- Molecule 5 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | B | 337 | 2624 | 1616 | 493 | 510 | 5 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | ? | - | PRO | DELETION | UNP P20279 |
| B | 310 | ARG | PHE | CONFLICT | UNP P20279 |

- Molecule 6 is a protein called 50S ribosomal protein L4E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | C | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1858 | 1131 | 344 | 382 | 1 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L5P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | D | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 685 | 195 | 210 | 4 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | E | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1357 | 840 | 224 | 289 | 4 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | F | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 552 | 141 | 191 | 1 | | | |

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | G | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

- Molecule 11 is a protein called L10 Ribosomal Protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | H | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1215 | 766 | 233 | 212 | 4 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | I | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1119 | 696 | 199 | 221 | 3 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | J | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 993 | 609 | 189 | 191 | 4 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | K | 145 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1114 | 668 | 222 | 224 | | | |

- Molecule 15 is a protein called L15 Ribosomal Protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | L | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 988 | 346 | 266 | 5 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | M | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1444 | 895 | 262 | 285 | 2 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | N | 115 | Total | C | N | O | 0 | 0 | 0 |
| | | | 864 | 529 | 161 | 174 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L19E.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | O | 143 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1133 | 680 | 230 | 223 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| O | 71 | LYS | TYR | CONFLICT | UNP P14119 |

- Molecule 19 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | P | 95 | Total | C | N | O | 0 | 0 | 0 |
| | | | 734 | 450 | 141 | 143 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | Q | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1149 | 713 | 209 | 223 | 4 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | R | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 641 | 389 | 111 | 138 | 3 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L24P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | S | 119 | Total | C | N | O | 0 | 0 | 0 |
| | | | 949 | 568 | 180 | 201 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L24E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | T | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 410 | 244 | 75 | 86 | 5 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | U | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 499 | 304 | 94 | 100 | 1 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | V | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 737 | 209 | 243 | 6 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | W | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 654 | 402 | 129 | 122 | 1 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L32E.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | X | 142 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1130 | 686 | 228 | 216 | | | |

- Molecule 28 is a protein called L37Ae 50S ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | Y | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 563 | 359 | 111 | 86 | 7 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | Z | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 258 | 86 | 82 | 4 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | 1 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 393 | 238 | 86 | 68 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 1 | ? | - | ARG | DELETION | UNP P22452 |

- Molecule 31 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | 2 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 32 | 0 | 107 | Total | Mg | 0 | 0 |
| | | | 107 | 107 | | |
| 32 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 32 | X | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 2 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | S | 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 | 73 | Total | Na | 0 | 0 |
| | | | 73 | 73 | | |
| 34 | P | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | Q | 3 | Total | Na | 0 | 0 |
| | | | 3 | 3 | | |
| 34 | K | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | H | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 34 | I | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | C | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | A | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | R | 1 | Total Na<br>1 1 | 0 | 0 |
| 34 | 9 | 2 | Total Na<br>2 2 | 0 | 0 |
| 34 | L | 1 | Total Na<br>1 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 35 | 0 | 9 | Total Cl<br>9 9 | 0 | 0 |
| 35 | J | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | Q | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | K | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | B | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | I | 3 | Total Cl<br>3 3 | 0 | 0 |
| 35 | A | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | N | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | X | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | 2 | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | L | 1 | Total Cl<br>1 1 | 0 | 0 |
| 35 | M | 1 | Total Cl<br>1 1 | 0 | 0 |

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 36 | Z | 1 | Total Cd<br>1 1 | 0 | 0 |
| 36 | Y | 1 | Total Cd<br>1 1 | 0 | 0 |
| 36 | T | 1 | Total Cd<br>1 1 | 0 | 0 |
| 36 | 2 | 1 | Total Cd<br>1 1 | 0 | 0 |
| 36 | N | 1 | Total Cd<br>1 1 | 0 | 0 |

- Molecule 37 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 37 | 0 | 5766 | Total O<br>5766 5766 | 0 | 0 |
| 37 | 9 | 148 | Total O<br>148 148 | 0 | 0 |
| 37 | 4 | 1 | Total O<br>1 1 | 0 | 0 |
| 37 | 5 | 2 | Total O<br>2 2 | 0 | 0 |
| 37 | A | 115 | Total O<br>115 115 | 0 | 0 |
| 37 | B | 146 | Total O<br>146 146 | 0 | 0 |
| 37 | C | 166 | Total O<br>166 166 | 0 | 0 |
| 37 | D | 48 | Total O<br>48 48 | 0 | 0 |
| 37 | E | 43 | Total O<br>43 43 | 0 | 0 |
| 37 | F | 25 | Total O<br>25 25 | 0 | 0 |
| 37 | G | 20 | Total O<br>20 20 | 0 | 0 |
| 37 | H | 77 | Total O<br>77 77 | 0 | 0 |
| 37 | I | 56 | Total O<br>56 56 | 0 | 0 |
| 37 | J | 56 | Total O<br>56 56 | 0 | 0 |
| 37 | K | 80 | Total O<br>80 80 | 0 | 0 |

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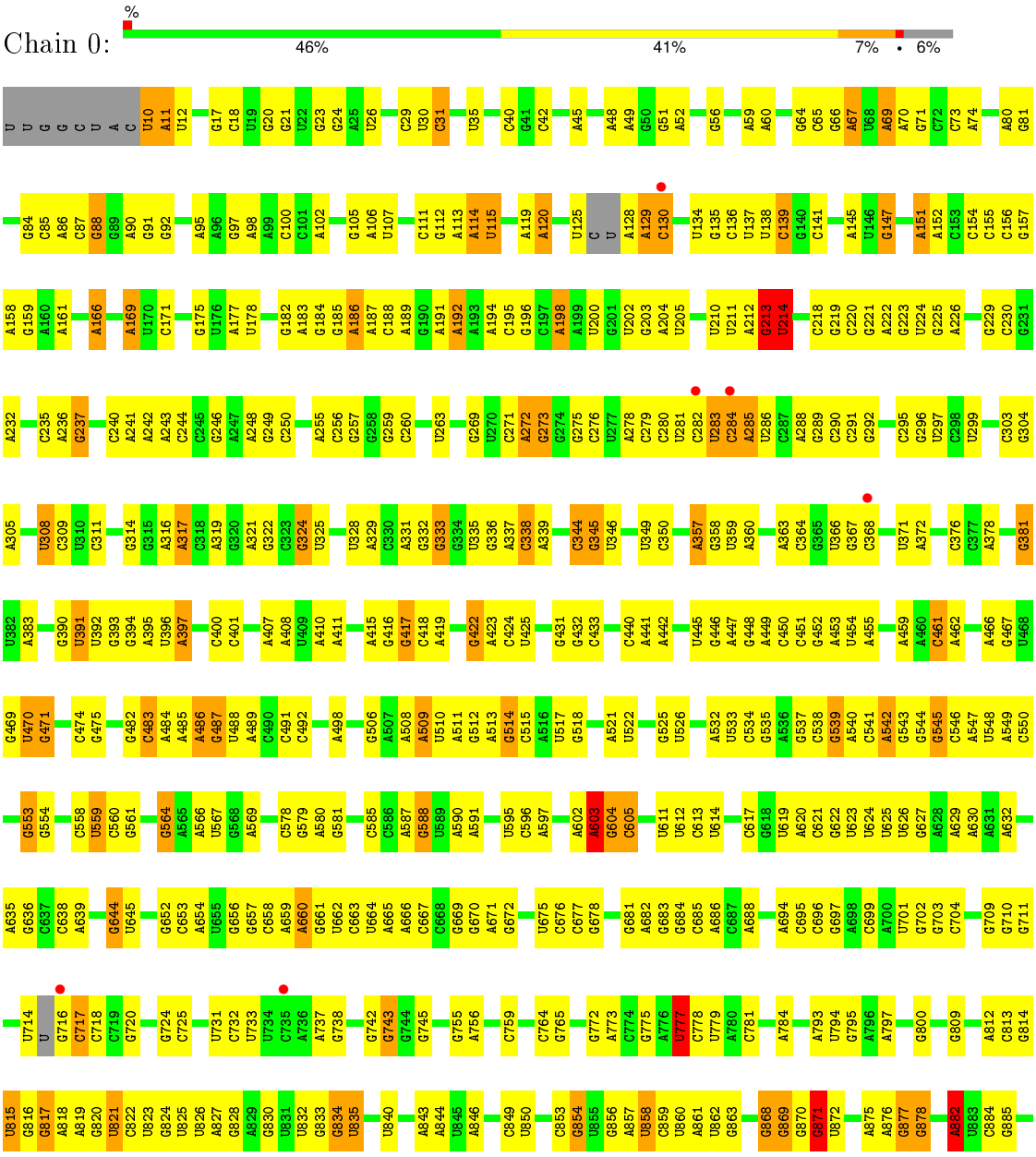
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 37 | L | 129 | Total O<br>129 129 | 0 | 0 |
| 37 | M | 56 | Total O<br>56 56 | 0 | 0 |
| 37 | N | 43 | Total O<br>43 43 | 0 | 0 |
| 37 | O | 58 | Total O<br>58 58 | 0 | 0 |
| 37 | P | 57 | Total O<br>57 57 | 0 | 0 |
| 37 | Q | 85 | Total O<br>85 85 | 0 | 0 |
| 37 | R | 31 | Total O<br>31 31 | 0 | 0 |
| 37 | S | 38 | Total O<br>38 38 | 0 | 0 |
| 37 | T | 30 | Total O<br>30 30 | 0 | 0 |
| 37 | U | 12 | Total O<br>12 12 | 0 | 0 |
| 37 | V | 69 | Total O<br>69 69 | 0 | 0 |
| 37 | W | 27 | Total O<br>27 27 | 0 | 0 |
| 37 | X | 97 | Total O<br>97 97 | 0 | 0 |
| 37 | Y | 35 | Total O<br>35 35 | 0 | 0 |
| 37 | Z | 54 | Total O<br>54 54 | 0 | 0 |
| 37 | 1 | 42 | Total O<br>42 42 | 0 | 0 |
| 37 | 2 | 56 | Total O<br>56 56 | 0 | 0 |

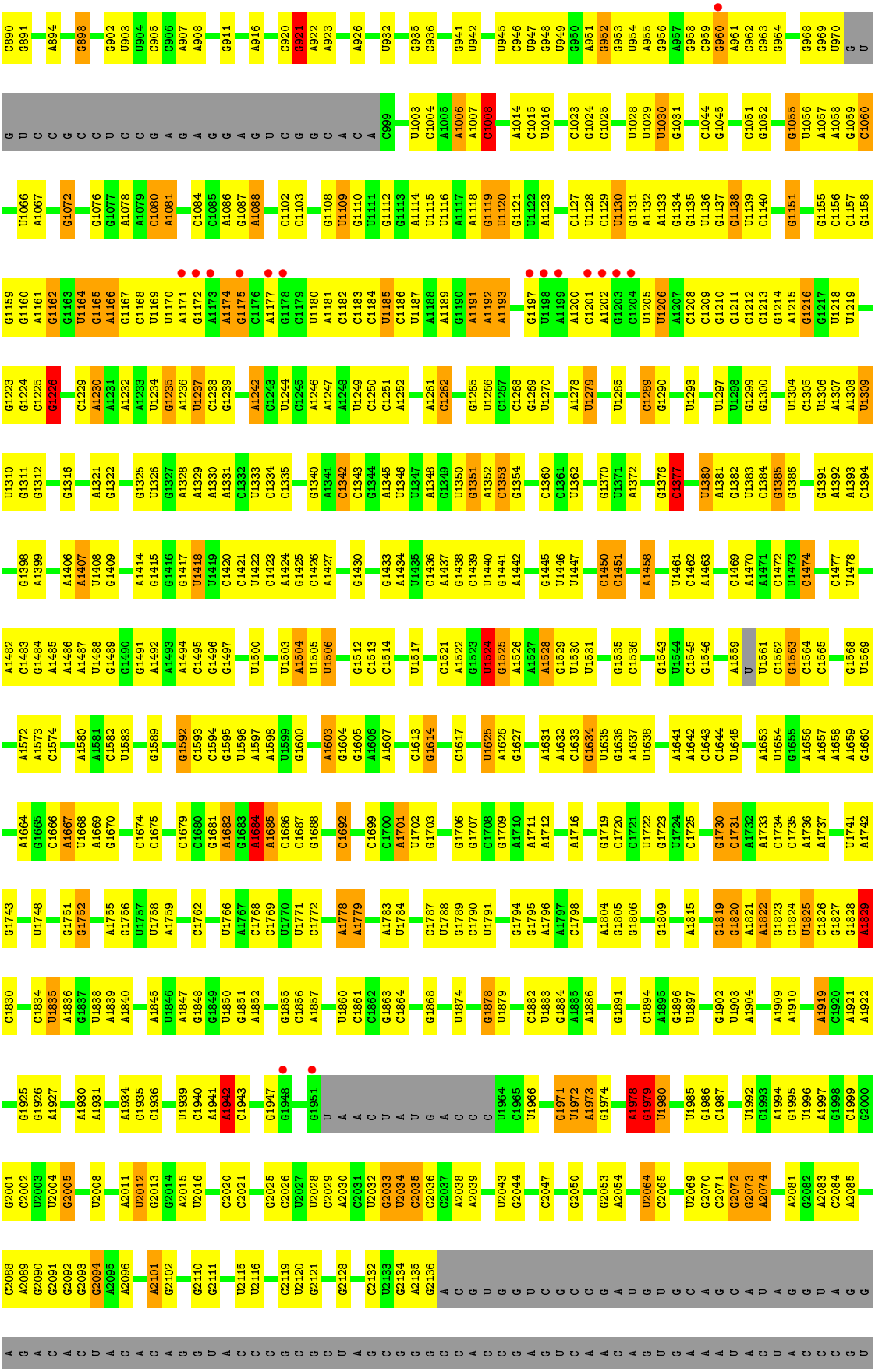
# 3 Residue-property plots (i)

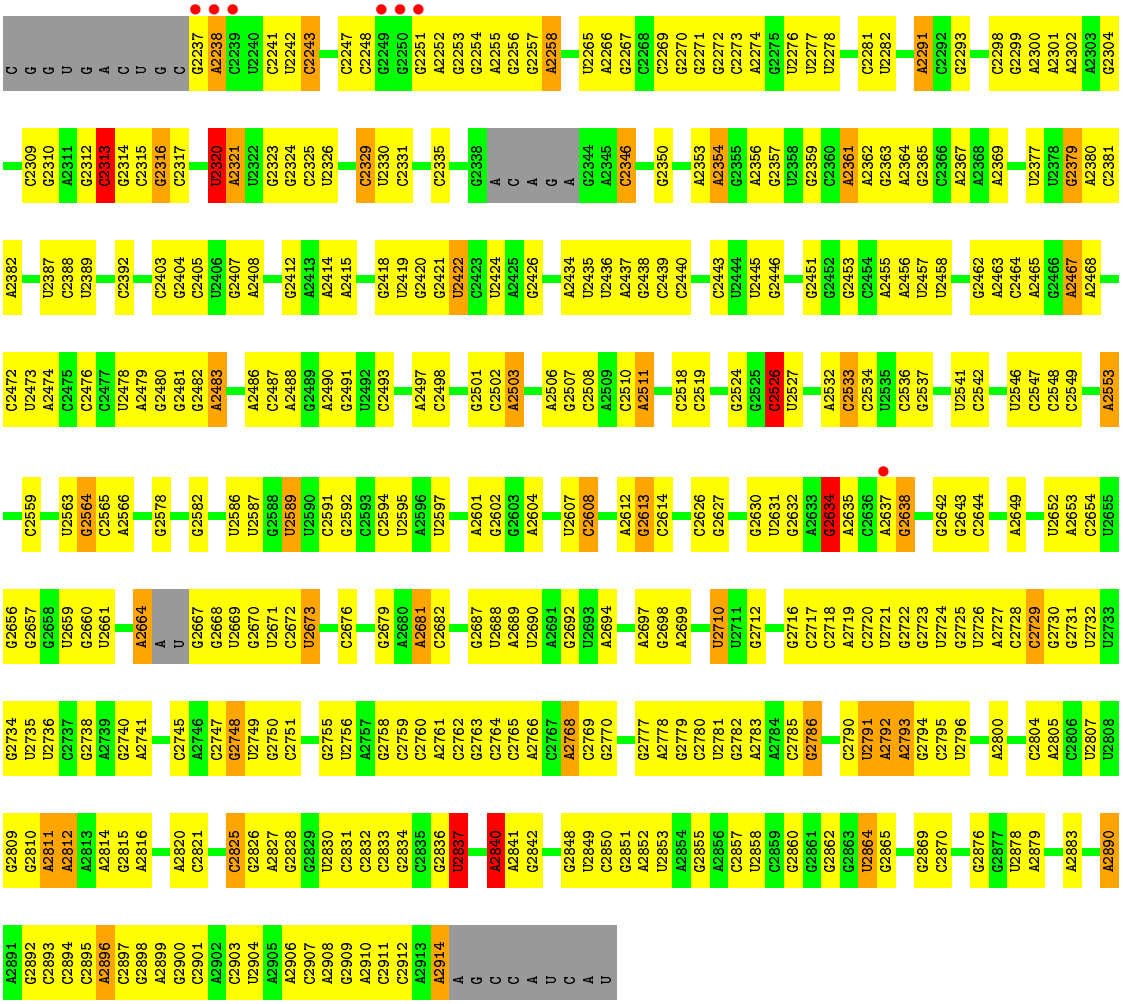
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

Chain 0:

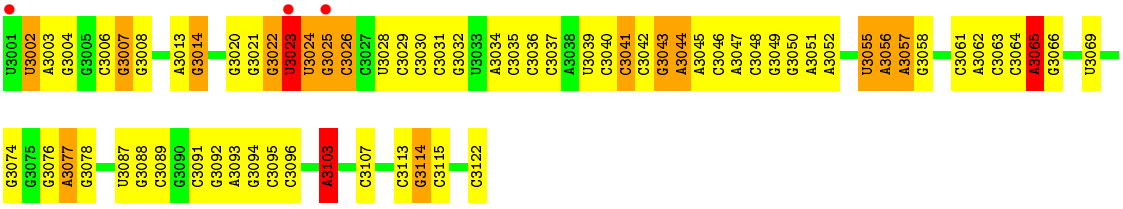






• Molecule 2: 5S ribosomal RNA

Chain 9:

• Molecule 3: Oligonucleotide CCA

Chain 3:


• Molecule 3: Oligonucleotide CCA

Chain 4:

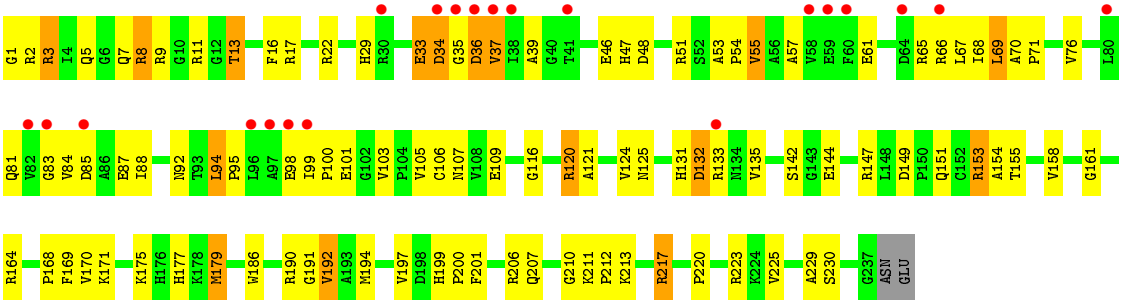

• Molecule 3: Oligonucleotide CCA

Chain 5:



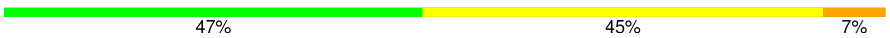
• Molecule 4: 50S ribosomal protein L2P

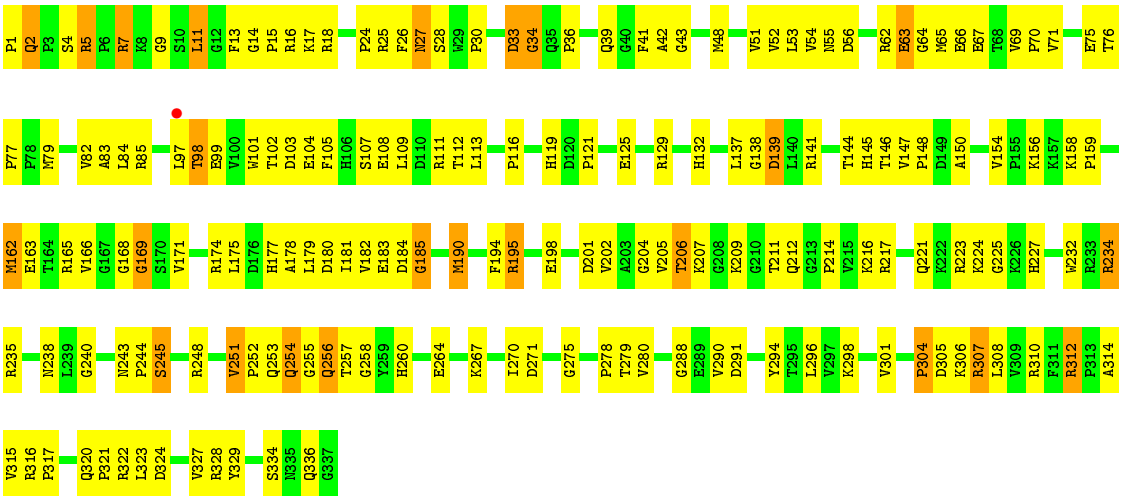
Chain A:


• Molecule 5: 50S ribosomal protein L3P

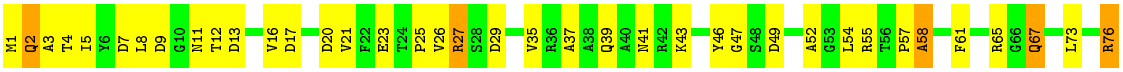
Chain B:

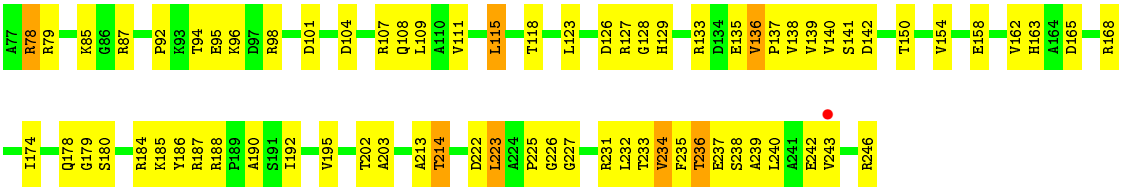



• Molecule 6: 50S ribosomal protein L4E

Chain C:

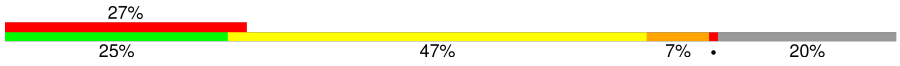



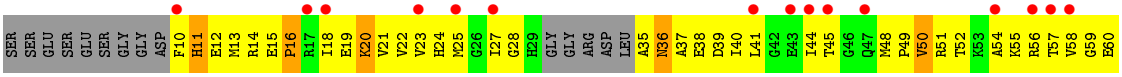


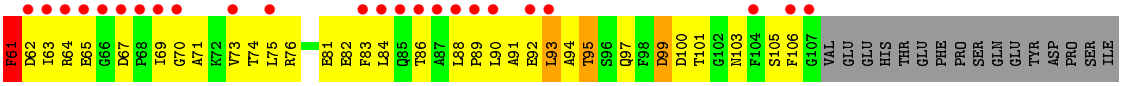


• Molecule 7: 50S ribosomal protein L5P

Chain D:

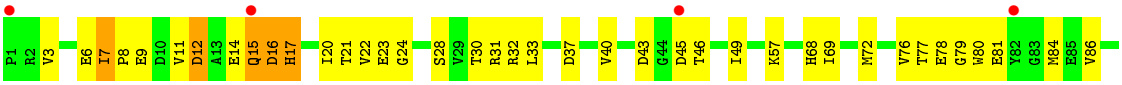


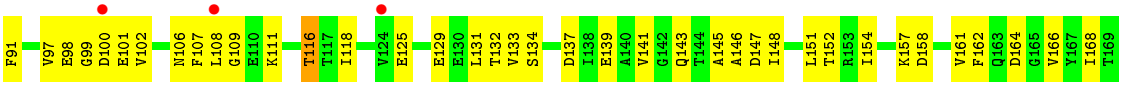





• Molecule 8: 50S ribosomal protein L6P

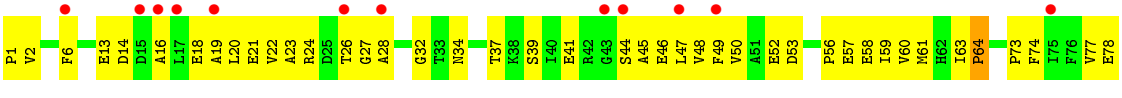
Chain E:

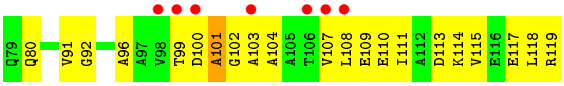





• Molecule 9: 50S ribosomal protein L7Ae

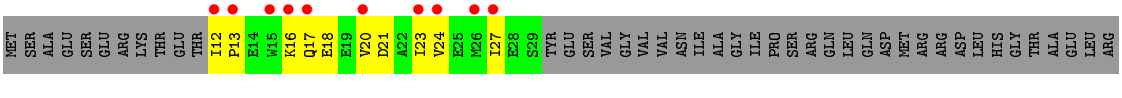
Chain F:

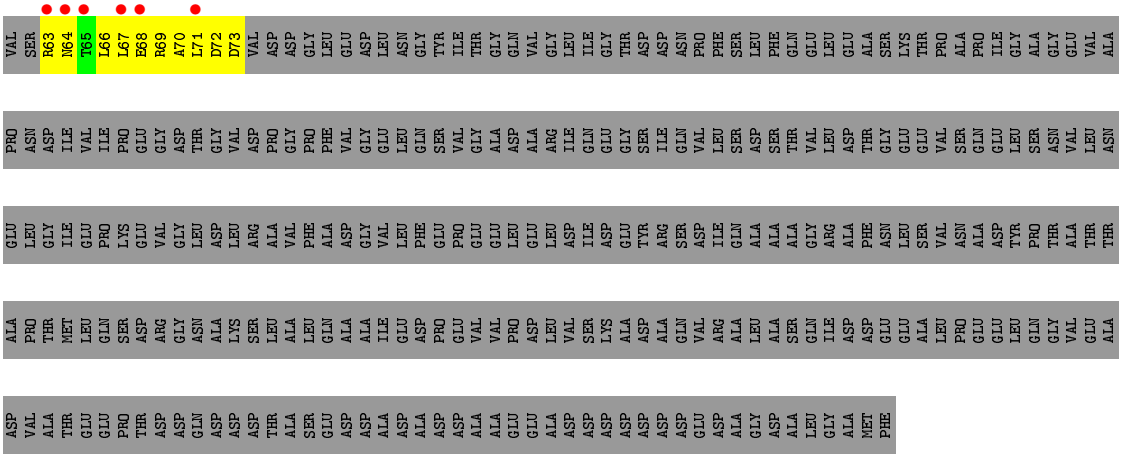





• Molecule 10: 50S RIBOSOMAL PROTEIN L10E

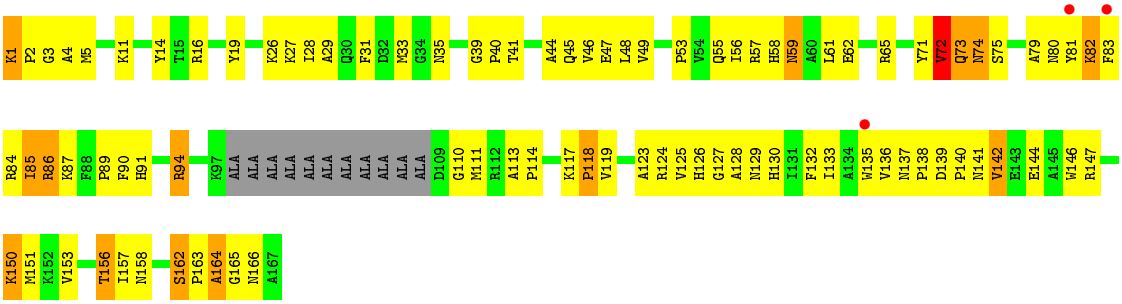
Chain G:



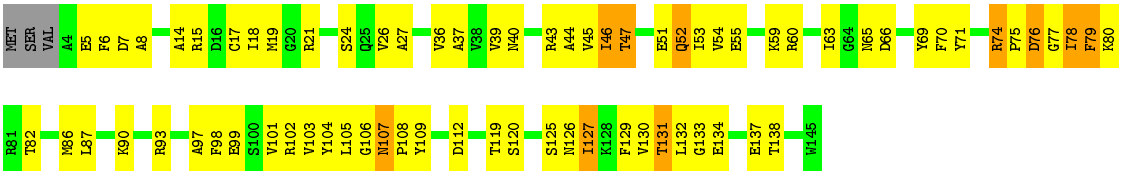
- Molecule 11: L10 Ribosomal Protein

Chain H:

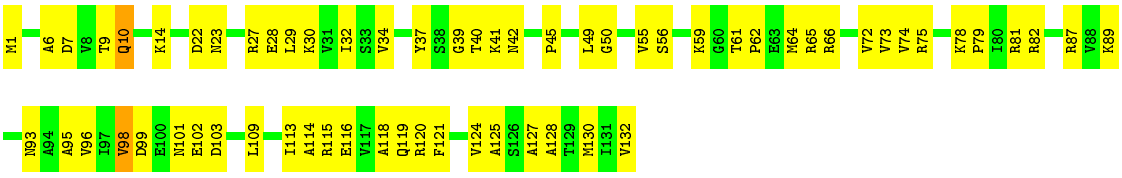
- Molecule 12: 50S ribosomal protein L13P

Chain I:

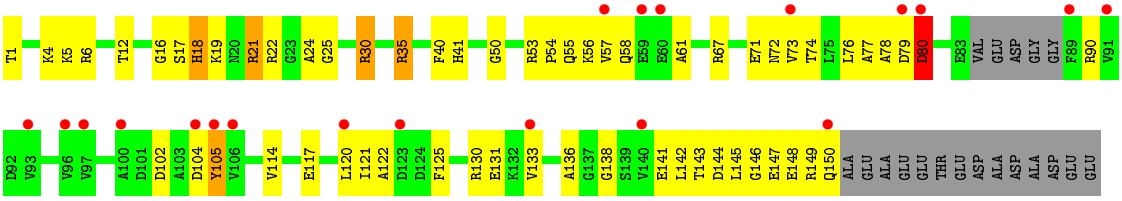
- Molecule 13: 50S ribosomal protein L14P

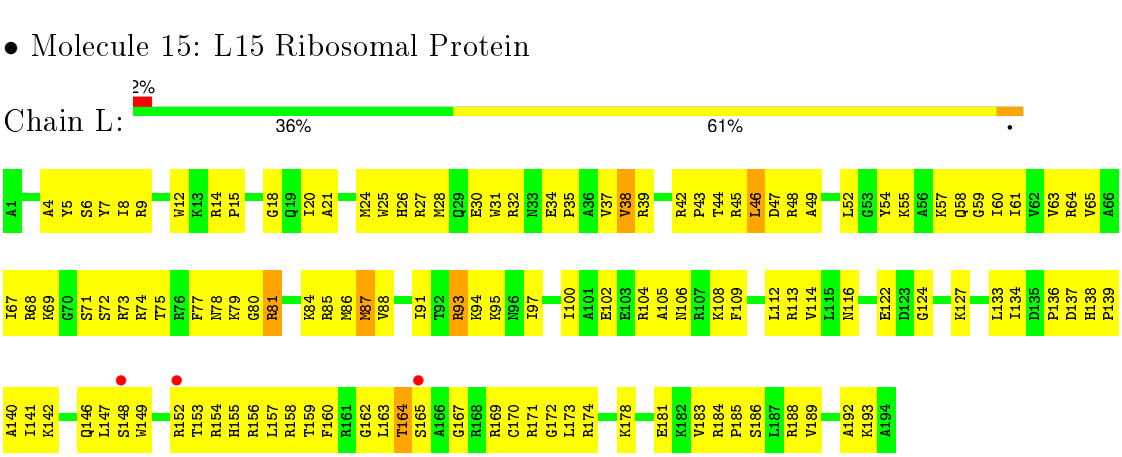
Chain J:

- Molecule 14: 50S ribosomal protein L15P

Chain K:





• Molecule 15: L15 Ribosomal Protein

Chain L:



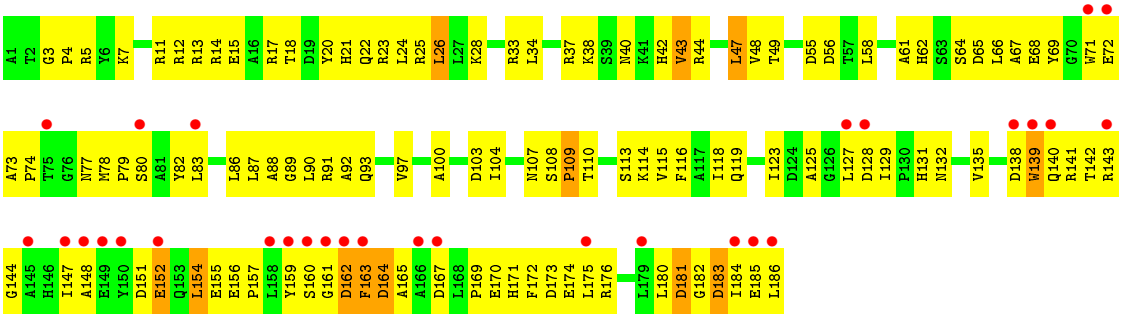







• Molecule 16: 50S ribosomal protein L18P

Chain M:

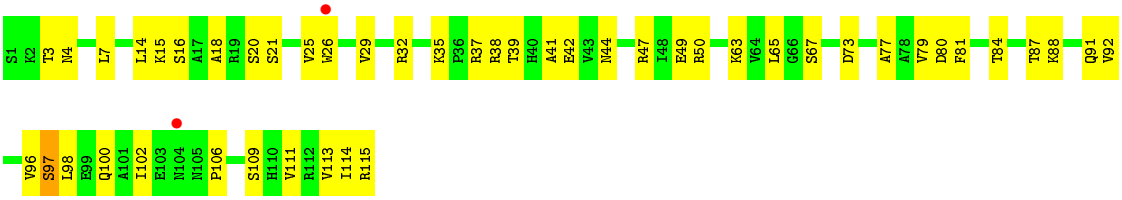







• Molecule 17: 50S ribosomal protein L18e

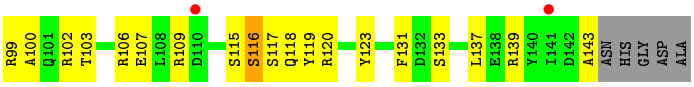
Chain N:

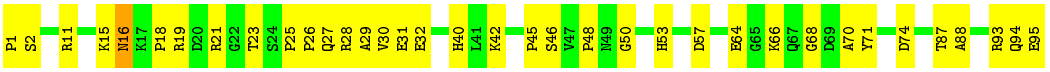


• Molecule 18: 50S ribosomal protein L19E

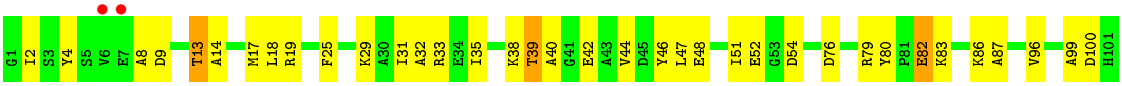
Chain O:

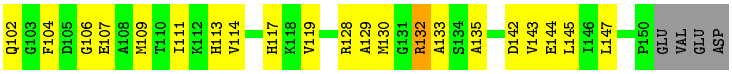




• Molecule 19: 50S ribosomal protein L21e

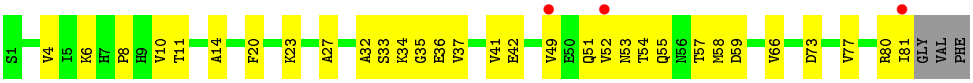




• Molecule 20: 50S ribosomal protein L22P

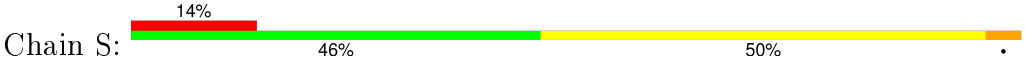



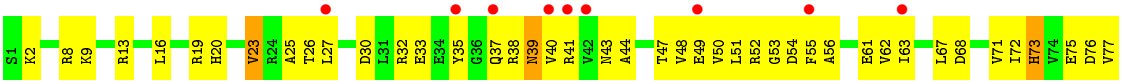



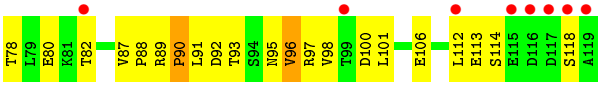

• Molecule 21: 50S ribosomal protein L23P

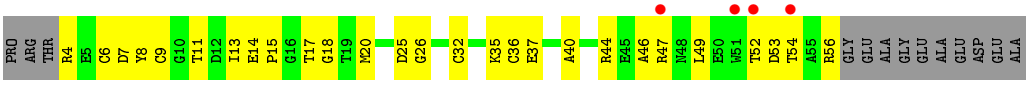

• Molecule 22: 50S ribosomal protein L24P



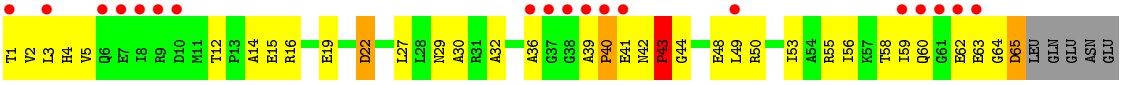




• Molecule 23: 50S ribosomal protein L24E

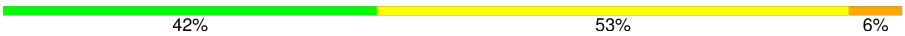



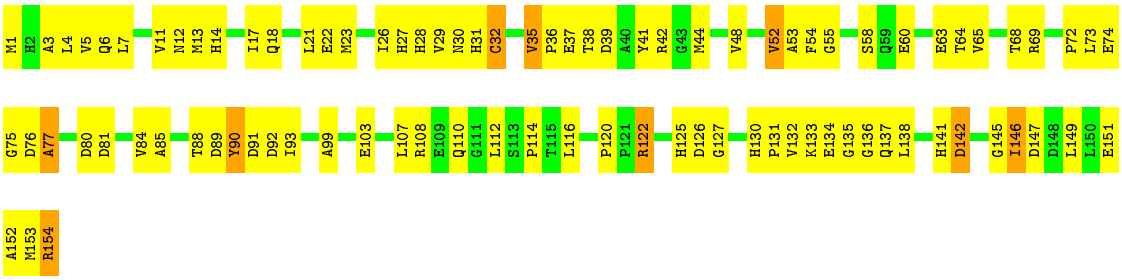

• Molecule 24: 50S ribosomal protein L29P



- Molecule 25: 50S ribosomal protein L30P

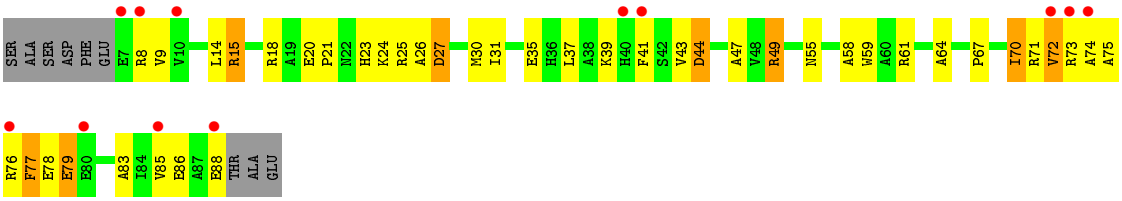
Chain V:



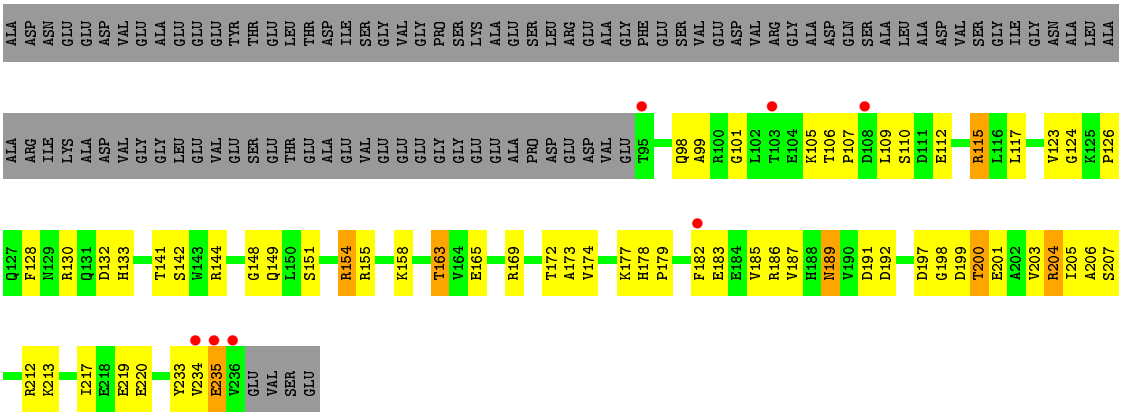
- Molecule 26: 50S ribosomal protein L31e

Chain W:

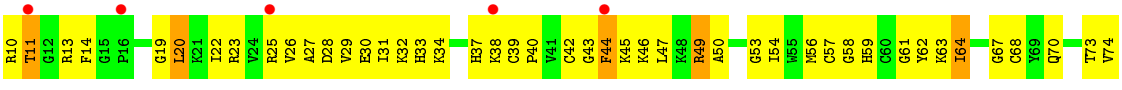
- Molecule 27: 50S ribosomal protein L32E

Chain X:

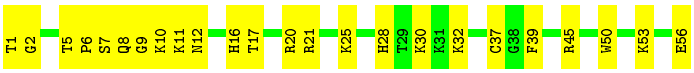
- Molecule 28: L37Ae 50S ribosomal protein

Chain Y:

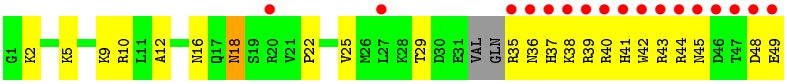

• Molecule 29: 50S ribosomal protein L37e

Chain Z:

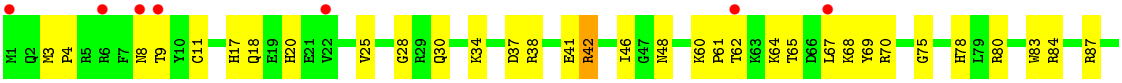

• Molecule 30: 50S ribosomal protein L39e

Chain 1:


• Molecule 31: 50S ribosomal protein L44E

Chain 2:


# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 213.52Å 300.61Å 573.93Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 2.90<br>47.91 – 2.80 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | (Not available) (50.00-2.90)<br>87.2 (47.91-2.80) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.62 (at 2.81Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.201 , 0.258<br>0.201 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | DCC |
| Wilson B-factor (Å$^2$) | 51.8 | Xtriage |
| Anisotropy | 0.440 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 68.8 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Outliers | 0 of 443536 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 98494 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 60.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, MG, CD, K, CL

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 | 0.75 | 2/66076 (0.0%) | 0.75 | 24/103052 (0.0%) |
| 2 | 9 | 0.67 | 0/2905 | 0.78 | 2/4528 (0.0%) |
| 3 | 3 | 0.70 | 0/65 | 0.61 | 0/99 |
| 3 | 4 | 0.79 | 0/65 | 0.79 | 0/99 |
| 3 | 5 | 0.72 | 0/65 | 0.66 | 0/99 |
| 4 | A | 0.51 | 0/1787 | 0.72 | 0/2409 |
| 5 | B | 0.57 | 0/2689 | 0.74 | 0/3652 |
| 6 | C | 0.61 | 0/1883 | 0.77 | 0/2551 |
| 7 | D | 0.46 | 0/1111 | 0.66 | 0/1498 |
| 8 | E | 0.57 | 0/1382 | 0.68 | 0/1880 |
| 9 | F | 0.47 | 0/896 | 0.63 | 0/1219 |
| 10 | G | 0.47 | 0/241 | 0.57 | 0/324 |
| 11 | H | 0.62 | 0/1246 | 0.86 | 2/1686 (0.1%) |
| 12 | I | 0.66 | 0/1135 | 0.73 | 0/1530 |
| 13 | J | 0.58 | 0/1003 | 0.77 | 0/1351 |
| 14 | K | 0.53 | 0/1126 | 0.74 | 0/1504 |
| 15 | L | 0.60 | 0/1633 | 0.76 | 0/2180 |
| 16 | M | 0.46 | 0/1473 | 0.72 | 0/1999 |
| 17 | N | 0.58 | 0/873 | 0.70 | 0/1181 |
| 18 | O | 0.52 | 0/1143 | 0.65 | 0/1521 |
| 19 | P | 0.61 | 0/748 | 0.80 | 1/1005 (0.1%) |
| 20 | Q | 0.60 | 0/1172 | 0.75 | 0/1578 |
| 21 | R | 0.48 | 0/648 | 0.64 | 0/875 |
| 22 | S | 0.49 | 0/957 | 0.70 | 0/1289 |
| 23 | T | 0.53 | 0/417 | 0.68 | 0/562 |
| 24 | U | 0.40 | 0/502 | 0.60 | 0/675 |
| 25 | V | 0.61 | 0/1218 | 0.75 | 0/1655 |
| 26 | W | 0.61 | 0/664 | 0.72 | 0/895 |
| 27 | X | 0.59 | 0/1146 | 0.74 | 0/1536 |
| 28 | Y | 0.55 | 0/575 | 0.77 | 0/763 |
| 29 | Z | 0.59 | 0/437 | 0.71 | 0/578 |
| 30 | 1 | 0.49 | 0/398 | 0.60 | 0/527 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 31 | 2 | 0.64 | 1/771 (0.1%) | 0.71 | 0/1024 |
| All | All | 0.70 | 3/98450 (0.0%) | 0.74 | 29/147324 (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 | 0 | 105 |
| 2 | 9 | 0 | 4 |
| 25 | V | 0 | 1 |
| All | All | 0 | 110 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 854 | G | N9-C8 | 5.34 | 1.41 | 1.37 |
| 31 | 2 | 41 | GLU | CG-CD | 5.17 | 1.59 | 1.51 |
| 1 | 0 | 871 | G | C5-C6 | -5.03 | 1.37 | 1.42 |

The worst 5 of 29 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1563 | G | C2'-C3'-O3' | 9.85 | 131.17 | 109.50 |
| 1 | 0 | 1979 | G | C2'-C3'-O3' | 7.29 | 125.53 | 109.50 |
| 11 | H | 74 | ASN | N-CA-C | -7.20 | 91.57 | 111.00 |
| 1 | 0 | 1030 | U | C5'-C4'-O4' | 7.16 | 117.69 | 109.10 |
| 1 | 0 | 2467 | A | C1'-O4'-C4' | -6.58 | 104.64 | 109.90 |

There are no chirality outliers.

5 of 110 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | 0 | 147 | G | Sidechain |
| 1 | 0 | 171 | C | Sidechain |
| 1 | 0 | 26 | U | Sidechain |
| 1 | 0 | 48 | A | Sidechain |
| 1 | 0 | 49 | A | 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 | 59017 | 0 | 29802 | 1339 | 0 |
| 2 | 9 | 2600 | 0 | 1326 | 87 | 0 |
| 3 | 3 | 59 | 0 | 35 | 1 | 0 |
| 3 | 4 | 59 | 0 | 35 | 3 | 0 |
| 3 | 5 | 59 | 0 | 35 | 0 | 0 |
| 4 | A | 1754 | 0 | 1763 | 120 | 0 |
| 5 | B | 2624 | 0 | 2533 | 208 | 0 |
| 6 | C | 1858 | 0 | 1816 | 132 | 0 |
| 7 | D | 1094 | 0 | 1085 | 140 | 0 |
| 8 | E | 1357 | 0 | 1266 | 86 | 0 |
| 9 | F | 885 | 0 | 854 | 65 | 0 |
| 10 | G | 240 | 0 | 231 | 28 | 0 |
| 11 | H | 1215 | 0 | 1215 | 172 | 0 |
| 12 | I | 1119 | 0 | 1098 | 83 | 0 |
| 13 | J | 993 | 0 | 1027 | 78 | 0 |
| 14 | K | 1114 | 0 | 1072 | 66 | 0 |
| 15 | L | 1605 | 0 | 1676 | 167 | 0 |
| 16 | M | 1444 | 0 | 1401 | 161 | 0 |
| 17 | N | 864 | 0 | 873 | 45 | 0 |
| 18 | O | 1133 | 0 | 1127 | 61 | 0 |
| 19 | P | 734 | 0 | 728 | 35 | 0 |
| 20 | Q | 1149 | 0 | 1122 | 75 | 0 |
| 21 | R | 641 | 0 | 605 | 33 | 0 |
| 22 | S | 949 | 0 | 923 | 75 | 0 |
| 23 | T | 410 | 0 | 364 | 40 | 0 |
| 24 | U | 499 | 0 | 511 | 36 | 0 |
| 25 | V | 1195 | 0 | 1137 | 112 | 0 |
| 26 | W | 654 | 0 | 653 | 54 | 0 |
| 27 | X | 1130 | 0 | 1133 | 78 | 0 |
| 28 | Y | 563 | 0 | 597 | 56 | 0 |
| 29 | Z | 430 | 0 | 426 | 33 | 0 |
| 30 | 1 | 393 | 0 | 406 | 43 | 0 |
| 31 | 2 | 755 | 0 | 728 | 34 | 0 |
| 32 | 0 | 107 | 0 | 0 | 0 | 0 |
| 32 | 2 | 1 | 0 | 0 | 0 | 0 |
| 32 | 9 | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 32 | B | 1 | 0 | 0 | 0 | 0 |
| 32 | J | 1 | 0 | 0 | 0 | 0 |
| 32 | S | 1 | 0 | 0 | 0 | 0 |
| 32 | X | 1 | 0 | 0 | 0 | 0 |
| 33 | 0 | 2 | 0 | 0 | 0 | 0 |
| 34 | 0 | 73 | 0 | 0 | 0 | 0 |
| 34 | 9 | 2 | 0 | 0 | 0 | 0 |
| 34 | A | 1 | 0 | 0 | 0 | 0 |
| 34 | C | 1 | 0 | 0 | 0 | 0 |
| 34 | H | 1 | 0 | 0 | 0 | 0 |
| 34 | I | 1 | 0 | 0 | 0 | 0 |
| 34 | K | 1 | 0 | 0 | 0 | 0 |
| 34 | L | 1 | 0 | 0 | 0 | 0 |
| 34 | P | 1 | 0 | 0 | 0 | 0 |
| 34 | Q | 3 | 0 | 0 | 0 | 0 |
| 34 | R | 1 | 0 | 0 | 0 | 0 |
| 35 | 0 | 9 | 0 | 0 | 1 | 0 |
| 35 | 2 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 1 | 0 | 0 | 0 | 0 |
| 35 | B | 1 | 0 | 0 | 0 | 0 |
| 35 | I | 3 | 0 | 0 | 2 | 0 |
| 35 | J | 1 | 0 | 0 | 1 | 0 |
| 35 | K | 1 | 0 | 0 | 0 | 0 |
| 35 | L | 1 | 0 | 0 | 1 | 0 |
| 35 | M | 1 | 0 | 0 | 1 | 0 |
| 35 | N | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 1 | 0 | 0 | 0 | 0 |
| 35 | X | 1 | 0 | 0 | 0 | 0 |
| 36 | 2 | 1 | 0 | 0 | 0 | 0 |
| 36 | N | 1 | 0 | 0 | 0 | 0 |
| 36 | T | 1 | 0 | 0 | 0 | 0 |
| 36 | Y | 1 | 0 | 0 | 0 | 0 |
| 36 | Z | 1 | 0 | 0 | 0 | 0 |
| 37 | 0 | 5766 | 0 | 0 | 298 | 0 |
| 37 | 1 | 42 | 0 | 0 | 4 | 0 |
| 37 | 2 | 56 | 0 | 0 | 10 | 0 |
| 37 | 4 | 1 | 0 | 0 | 0 | 0 |
| 37 | 5 | 2 | 0 | 0 | 0 | 0 |
| 37 | 9 | 148 | 0 | 0 | 15 | 0 |
| 37 | A | 115 | 0 | 0 | 22 | 0 |
| 37 | B | 146 | 0 | 0 | 25 | 0 |
| 37 | C | 166 | 0 | 0 | 38 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 37 | D | 48 | 0 | 0 | 22 | 0 |
| 37 | E | 43 | 0 | 0 | 14 | 0 |
| 37 | F | 25 | 0 | 0 | 10 | 0 |
| 37 | G | 20 | 0 | 0 | 6 | 0 |
| 37 | H | 77 | 0 | 0 | 27 | 0 |
| 37 | I | 56 | 0 | 0 | 10 | 0 |
| 37 | J | 56 | 0 | 0 | 12 | 0 |
| 37 | K | 80 | 0 | 0 | 17 | 0 |
| 37 | L | 129 | 0 | 0 | 21 | 0 |
| 37 | M | 56 | 0 | 0 | 27 | 0 |
| 37 | N | 43 | 0 | 0 | 13 | 0 |
| 37 | O | 58 | 0 | 0 | 5 | 0 |
| 37 | P | 57 | 0 | 0 | 7 | 0 |
| 37 | Q | 85 | 0 | 0 | 11 | 0 |
| 37 | R | 31 | 0 | 0 | 9 | 0 |
| 37 | S | 38 | 0 | 0 | 6 | 0 |
| 37 | T | 30 | 0 | 0 | 10 | 0 |
| 37 | U | 12 | 0 | 0 | 2 | 0 |
| 37 | V | 69 | 0 | 0 | 12 | 0 |
| 37 | W | 27 | 0 | 0 | 7 | 0 |
| 37 | X | 97 | 0 | 0 | 21 | 0 |
| 37 | Y | 35 | 0 | 0 | 8 | 0 |
| 37 | Z | 54 | 0 | 0 | 5 | 0 |
| All | All | 98494 | 0 | 59603 | 3417 | 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 23.

The worst 5 of 3417 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) |
|---|---|---|---|
| 11:H:86:ARG:NH1 | 11:H:133:ILE:HG13 | 1.55 | 1.20 |
| 24:U:12:THR:HG22 | 24:U:15:GLU:HG3 | 1.32 | 1.11 |
| 6:C:236:THR:HG22 | 6:C:239:ALA:H | 1.00 | 1.07 |
| 6:C:127:ARG:NH2 | 6:C:225:PRO:HG2 | 1.70 | 1.06 |
| 11:H:86:ARG:HH11 | 11:H:133:ILE:CG1 | 1.68 | 1.06 |

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 |
|---|---|---|---|---|---|---|
| 4 | A | 235/239 (98%) | 204 (87%) | 27 (12%) | 4 (2%) | 11 38 |
| 5 | B | 335/337 (99%) | 295 (88%) | 31 (9%) | 9 (3%) | 6 25 |
| 6 | C | 244/246 (99%) | 221 (91%) | 21 (9%) | 2 (1%) | 24 60 |
| 7 | D | 134/176 (76%) | 93 (69%) | 29 (22%) | 12 (9%) | 1 2 |
| 8 | E | 170/177 (96%) | 157 (92%) | 12 (7%) | 1 (1%) | 30 67 |
| 9 | F | 117/119 (98%) | 103 (88%) | 11 (9%) | 3 (3%) | 7 26 |
| 10 | G | 25/348 (7%) | 21 (84%) | 3 (12%) | 1 (4%) | 4 15 |
| 11 | H | 152/167 (91%) | 131 (86%) | 16 (10%) | 5 (3%) | 5 20 |
| 12 | I | 140/145 (97%) | 128 (91%) | 8 (6%) | 4 (3%) | 6 23 |
| 13 | J | 130/132 (98%) | 111 (85%) | 18 (14%) | 1 (1%) | 24 60 |
| 14 | K | 141/164 (86%) | 118 (84%) | 20 (14%) | 3 (2%) | 9 32 |
| 15 | L | 192/194 (99%) | 165 (86%) | 24 (12%) | 3 (2%) | 12 40 |
| 16 | M | 184/186 (99%) | 161 (88%) | 15 (8%) | 8 (4%) | 3 13 |
| 17 | N | 113/115 (98%) | 104 (92%) | 7 (6%) | 2 (2%) | 11 37 |
| 18 | O | 141/148 (95%) | 132 (94%) | 8 (6%) | 1 (1%) | 26 63 |
| 19 | P | 93/95 (98%) | 88 (95%) | 4 (4%) | 1 (1%) | 17 51 |
| 20 | Q | 148/154 (96%) | 136 (92%) | 12 (8%) | 0 | 100 100 |
| 21 | R | 79/84 (94%) | 75 (95%) | 3 (4%) | 1 (1%) | 15 46 |
| 22 | S | 117/119 (98%) | 99 (85%) | 17 (14%) | 1 (1%) | 21 57 |
| 23 | T | 51/66 (77%) | 45 (88%) | 5 (10%) | 1 (2%) | 9 33 |
| 24 | U | 63/70 (90%) | 56 (89%) | 5 (8%) | 2 (3%) | 5 20 |
| 25 | V | 152/154 (99%) | 139 (91%) | 12 (8%) | 1 (1%) | 26 63 |
| 26 | W | 80/91 (88%) | 72 (90%) | 6 (8%) | 2 (2%) | 7 27 |
| 27 | X | 140/240 (58%) | 134 (96%) | 6 (4%) | 0 | 100 100 |
| 28 | Y | 71/73 (97%) | 57 (80%) | 13 (18%) | 1 (1%) | 14 44 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 29 | Z | 54/56 (96%) | 51 (94%) | 3 (6%) | 0 | 100 100 |
| 30 | 1 | 42/48 (88%) | 40 (95%) | 2 (5%) | 0 | 100 100 |
| 31 | 2 | 90/92 (98%) | 84 (93%) | 6 (7%) | 0 | 100 100 |
| All | All | 3633/4235 (86%) | 3220 (89%) | 344 (10%) | 69 (2%) | 10 35 |

5 of 69 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | B | 139 | ASP |
| 7 | D | 16 | PRO |
| 7 | D | 93 | LEU |
| 7 | D | 95 | THR |
| 7 | D | 137 | PRO |

### 5.3.2 Protein sidechains (i)

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 |
|---|---|---|---|---|---|
| 4 | A | 179/181 (99%) | 166 (93%) | 13 (7%) | 17 45 |
| 5 | B | 282/282 (100%) | 263 (93%) | 19 (7%) | 20 50 |
| 6 | C | 193/193 (100%) | 177 (92%) | 16 (8%) | 14 38 |
| 7 | D | 117/147 (80%) | 107 (92%) | 10 (8%) | 13 37 |
| 8 | E | 152/155 (98%) | 146 (96%) | 6 (4%) | 39 75 |
| 9 | F | 92/92 (100%) | 92 (100%) | 0 | 100 100 |
| 10 | G | 27/283 (10%) | 27 (100%) | 0 | 100 100 |
| 11 | H | 122/122 (100%) | 111 (91%) | 11 (9%) | 12 34 |
| 12 | I | 118/121 (98%) | 107 (91%) | 11 (9%) | 11 32 |
| 13 | J | 106/106 (100%) | 103 (97%) | 3 (3%) | 51 84 |
| 14 | K | 112/126 (89%) | 107 (96%) | 5 (4%) | 34 70 |
| 15 | L | 166/166 (100%) | 158 (95%) | 8 (5%) | 31 67 |
| 16 | M | 149/149 (100%) | 143 (96%) | 6 (4%) | 38 74 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 17 | N | 93/93 (100%) | 89 (96%) | 4 (4%) | 35 71 |
| 18 | O | 113/116 (97%) | 109 (96%) | 4 (4%) | 43 78 |
| 19 | P | 79/79 (100%) | 76 (96%) | 3 (4%) | 40 76 |
| 20 | Q | 117/121 (97%) | 113 (97%) | 4 (3%) | 44 79 |
| 21 | R | 71/73 (97%) | 71 (100%) | 0 | 100 100 |
| 22 | S | 105/105 (100%) | 101 (96%) | 4 (4%) | 40 76 |
| 23 | T | 44/52 (85%) | 44 (100%) | 0 | 100 100 |
| 24 | U | 51/56 (91%) | 48 (94%) | 3 (6%) | 24 58 |
| 25 | V | 130/130 (100%) | 122 (94%) | 8 (6%) | 23 55 |
| 26 | W | 66/73 (90%) | 60 (91%) | 6 (9%) | 12 34 |
| 27 | X | 120/195 (62%) | 112 (93%) | 8 (7%) | 20 50 |
| 28 | Y | 56/56 (100%) | 52 (93%) | 4 (7%) | 18 47 |
| 29 | Z | 46/46 (100%) | 46 (100%) | 0 | 100 100 |
| 30 | 1 | 42/44 (96%) | 41 (98%) | 1 (2%) | 57 86 |
| 31 | 2 | 79/79 (100%) | 78 (99%) | 1 (1%) | 76 94 |
| All | All | 3027/3441 (88%) | 2869 (95%) | 158 (5%) | 29 64 |

5 of 158 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | H | 94 | ARG |
| 13 | J | 98 | VAL |
| 27 | X | 163 | THR |
| 11 | H | 142 | VAL |
| 12 | I | 79 | PHE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | L | 26 | HIS |
| 18 | O | 73 | HIS |
| 30 | 1 | 16 | ASN |
| 15 | L | 176 | GLN |
| 17 | N | 53 | GLN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 0 | 2746/2922 (93%) | 264 (9%) | 55 (2%) |
| 2 | 9 | 121/122 (99%) | 18 (14%) | 7 (5%) |
| 3 | 3 | 2/3 (66%) | 1 (50%) | 0 |
| 3 | 4 | 2/3 (66%) | 0 | 0 |
| 3 | 5 | 2/3 (66%) | 1 (50%) | 0 |
| All | All | 2873/3053 (94%) | 284 (9%) | 62 (2%) |

5 of 284 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 11 | A |
| 1 | 0 | 31 | C |
| 1 | 0 | 60 | A |
| 1 | 0 | 67 | A |
| 1 | 0 | 69 | A |

5 of 62 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 1380 | U |
| 1 | 0 | 1730 | G |
| 2 | 9 | 3024 | U |
| 1 | 0 | 1563 | G |
| 1 | 0 | 1856 | C |

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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, $95^{th}$ 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 | 2754/2922 (94%) | -0.14 | 29 (1%) 82 80 | 23, 53, 103, 166 | 0 |
| 2 | 9 | 122/122 (100%) | -0.01 | 3 (2%) 61 55 | 36, 67, 104, 164 | 0 |
| 3 | 3 | 3/3 (100%) | 1.53 | 1 (33%) 0 0 | 68, 68, 83, 120 | 0 |
| 3 | 4 | 3/3 (100%) | 1.40 | 1 (33%) 0 0 | 88, 88, 89, 103 | 0 |
| 3 | 5 | 3/3 (100%) | -0.04 | 0 100 100 | 57, 57, 58, 64 | 0 |
| 4 | A | 237/239 (99%) | 0.31 | 21 (8%) 12 7 | 33, 66, 100, 126 | 0 |
| 5 | B | 337/337 (100%) | -0.04 | 1 (0%) 94 94 | 27, 60, 86, 95 | 0 |
| 6 | C | 246/246 (100%) | -0.06 | 1 (0%) 93 92 | 27, 57, 81, 88 | 0 |
| 7 | D | 140/176 (79%) | 1.79 | 47 (33%) 0 0 | 65, 111, 129, 137 | 0 |
| 8 | E | 172/177 (97%) | 0.47 | 7 (4%) 41 34 | 43, 69, 95, 101 | 0 |
| 9 | F | 119/119 (100%) | 0.79 | 19 (15%) 3 1 | 65, 88, 112, 117 | 0 |
| 10 | G | 29/348 (8%) | 2.14 | 16 (55%) 0 0 | 72, 95, 107, 111 | 0 |
| 11 | H | 156/167 (93%) | 0.09 | 3 (1%) 70 66 | 31, 56, 83, 92 | 0 |
| 12 | I | 142/145 (97%) | -0.16 | 0 100 100 | 37, 50, 75, 87 | 0 |
| 13 | J | 132/132 (100%) | 0.01 | 0 100 100 | 41, 60, 83, 90 | 0 |
| 14 | K | 145/164 (88%) | 0.54 | 20 (13%) 4 2 | 31, 77, 121, 127 | 0 |
| 15 | L | 194/194 (100%) | -0.00 | 3 (1%) 76 74 | 37, 56, 80, 88 | 0 |
| 16 | M | 186/186 (100%) | 0.74 | 30 (16%) 3 1 | 43, 78, 123, 135 | 0 |
| 17 | N | 115/115 (100%) | 0.10 | 2 (1%) 73 70 | 47, 65, 83, 86 | 0 |
| 18 | O | 143/148 (96%) | 0.43 | 4 (2%) 56 50 | 39, 65, 85, 94 | 0 |
| 19 | P | 95/95 (100%) | 0.02 | 0 100 100 | 35, 49, 67, 86 | 0 |
| 20 | Q | 150/154 (97%) | -0.14 | 2 (1%) 79 78 | 35, 47, 69, 80 | 0 |
| 21 | R | 81/84 (96%) | 0.34 | 3 (3%) 45 38 | 56, 80, 96, 103 | 0 |
| 22 | S | 119/119 (100%) | 0.87 | 17 (14%) 4 2 | 52, 71, 101, 120 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 23 | T | 53/66 (80%) | 0.39 | 4 (7%) 17 11 | 48, 62, 79, 91 | 0 |
| 24 | U | 65/70 (92%) | 1.47 | 19 (29%) 1 0 | 67, 93, 127, 133 | 0 |
| 25 | V | 154/154 (100%) | -0.21 | 0 100 100 | 32, 49, 70, 80 | 0 |
| 26 | W | 82/91 (90%) | 0.69 | 12 (14%) 3 2 | 46, 63, 84, 101 | 0 |
| 27 | X | 142/240 (59%) | 0.02 | 7 (4%) 33 27 | 28, 52, 77, 93 | 0 |
| 28 | Y | 73/73 (100%) | 0.39 | 5 (6%) 20 14 | 55, 72, 90, 96 | 0 |
| 29 | Z | 56/56 (100%) | -0.34 | 0 100 100 | 29, 42, 50, 53 | 0 |
| 30 | 1 | 46/48 (95%) | 2.14 | 17 (36%) 0 0 | 42, 77, 136, 138 | 0 |
| 31 | 2 | 92/92 (100%) | 0.53 | 8 (8%) 13 8 | 44, 67, 80, 91 | 0 |
| All | All | 6586/7288 (90%) | 0.13 | 302 (4%) 36 30 | 23, 60, 108, 166 | 0 |

The worst 5 of 302 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 24 | U | 1 | THR | 10.0 |
| 30 | 1 | 48 | ASP | 8.9 |
| 30 | 1 | 36 | ASN | 8.9 |
| 30 | 1 | 42 | TRP | 8.6 |
| 30 | 1 | 45 | ASN | 7.8 |

## 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, 95$^{th}$ 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 |
|---|---|---|---|---|---|---|---|---|---|
| 35 | CL | 0 | 8515 | 1/1 | 0.92 | 0.41 | 45.14 | 96,96,96,96 | 0 |
| 34 | NA | 0 | 8371 | 1/1 | 0.71 | 0.42 | 41.11 | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8374 | 1/1 | 0.77 | 0.98 | 37.63 | 74,74,74,74 | 0 |
| 34 | NA | 0 | 8378 | 1/1 | 0.96 | 0.59 | 36.30 | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8359 | 1/1 | 0.90 | 0.43 | 32.55 | 66,66,66,66 | 0 |
| 34 | NA | 0 | 8356 | 1/1 | 0.92 | 0.47 | 32.18 | 77,77,77,77 | 0 |
| 34 | NA | 0 | 8350 | 1/1 | 0.95 | 0.27 | 25.69 | 61,61,61,61 | 0 |
| 34 | NA | Q | 8386 | 1/1 | 0.89 | 0.73 | 23.15 | 84,84,84,84 | 0 |
| 34 | NA | 0 | 8372 | 1/1 | 0.56 | 0.47 | 20.41 | 71,71,71,71 | 0 |
| 34 | NA | K | 8380 | 1/1 | 0.86 | 0.49 | 19.85 | 77,77,77,77 | 0 |
| 34 | NA | 0 | 8361 | 1/1 | 0.96 | 0.58 | 18.58 | 47,47,47,47 | 0 |
| 34 | NA | 9 | 8383 | 1/1 | 0.83 | 0.38 | 18.52 | 62,62,62,62 | 0 |
| 35 | CL | 0 | 8505 | 1/1 | 0.54 | 0.44 | 16.91 | 87,87,87,87 | 0 |
| 34 | NA | 0 | 8376 | 1/1 | 0.98 | 0.27 | 15.39 | 33,33,33,33 | 0 |
| 34 | NA | 0 | 8335 | 1/1 | 0.92 | 0.35 | 15.24 | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8320 | 1/1 | 0.95 | 0.21 | 9.69 | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8054 | 1/1 | 0.97 | 0.23 | 9.41 | 17,17,17,17 | 0 |
| 34 | NA | 0 | 8310 | 1/1 | 0.96 | 0.30 | 8.79 | 20,20,20,20 | 0 |
| 34 | NA | 0 | 8373 | 1/1 | 0.94 | 0.33 | 7.40 | 53,53,53,53 | 0 |
| 34 | NA | 0 | 8362 | 1/1 | 0.91 | 0.25 | 7.39 | 73,73,73,73 | 0 |
| 34 | NA | 0 | 8355 | 1/1 | 0.95 | 0.42 | 7.11 | 59,59,59,59 | 0 |
| 34 | NA | 0 | 8328 | 1/1 | 0.95 | 0.27 | 6.93 | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8365 | 1/1 | 0.91 | 0.43 | 6.92 | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8326 | 1/1 | 0.85 | 0.40 | 6.69 | 52,52,52,52 | 0 |
| 34 | NA | 0 | 8367 | 1/1 | 0.90 | 0.22 | 6.29 | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8049 | 1/1 | 0.90 | 0.30 | 5.67 | 64,64,64,64 | 0 |
| 34 | NA | 0 | 8325 | 1/1 | 0.96 | 0.19 | 4.33 | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8382 | 1/1 | 0.90 | 0.20 | 4.19 | 64,64,64,64 | 0 |
| 35 | CL | N | 8508 | 1/1 | 0.78 | 0.37 | 3.89 | 101,101,101,101 | 0 |
| 35 | CL | B | 8519 | 1/1 | 0.95 | 0.26 | 3.81 | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8321 | 1/1 | 0.97 | 0.25 | 3.74 | 45,45,45,45 | 0 |
| 34 | NA | 0 | 8379 | 1/1 | 0.88 | 0.17 | 2.86 | 34,34,34,34 | 0 |
| 34 | NA | Q | 8337 | 1/1 | 0.91 | 0.26 | 2.59 | 43,43,43,43 | 0 |
| 34 | NA | C | 8304 | 1/1 | 0.89 | 0.30 | 2.21 | 59,59,59,59 | 0 |
| 32 | MG | 0 | 8044 | 1/1 | 0.95 | 0.18 | 1.93 | 54,54,54,54 | 0 |
| 35 | CL | 0 | 8516 | 1/1 | 0.96 | 0.18 | 0.91 | 65,65,65,65 | 0 |
| 32 | MG | 0 | 8013 | 1/1 | 0.96 | 0.16 | 0.87 | 64,64,64,64 | 0 |
| 32 | MG | 0 | 8070 | 1/1 | 0.99 | 0.17 | 0.80 | 41,41,41,41 | 0 |
| 34 | NA | A | 8345 | 1/1 | 0.95 | 0.19 | 0.73 | 58,58,58,58 | 0 |
| 33 | K | 0 | 8201 | 1/1 | 0.98 | 0.16 | 0.26 | 74,74,74,74 | 0 |
| 34 | NA | 0 | 8366 | 1/1 | 0.92 | 0.15 | 0.08 | 48,48,48,48 | 0 |
| 34 | NA | 0 | 8323 | 1/1 | 0.97 | 0.17 | -0.03 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 34 | NA | 0 | 8308 | 1/1 | 0.82 | 0.13 | -0.13 | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8112 | 1/1 | 0.89 | 0.15 | -0.14 | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8064 | 1/1 | 0.98 | 0.13 | -0.26 | 22,22,22,22 | 0 |
| 34 | NA | 0 | 8317 | 1/1 | 0.84 | 0.37 | -0.33 | 75,75,75,75 | 0 |
| 34 | NA | 0 | 8332 | 1/1 | 0.84 | 0.13 | -0.49 | 30,30,30,30 | 0 |
| 34 | NA | 0 | 8305 | 1/1 | 0.94 | 0.14 | -0.50 | 39,39,39,39 | 0 |
| 34 | NA | Q | 8338 | 1/1 | 0.94 | 0.13 | -0.68 | 96,96,96,96 | 0 |
| 32 | MG | 0 | 8027 | 1/1 | 0.96 | 0.12 | -1.00 | 69,69,69,69 | 0 |
| 32 | MG | 0 | 8108 | 1/1 | 0.94 | 0.12 | -1.07 | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8333 | 1/1 | 0.94 | 0.11 | -1.07 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8057 | 1/1 | 0.94 | 0.15 | -1.11 | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8010 | 1/1 | 0.97 | 0.12 | -1.13 | 19,19,19,19 | 0 |
| 32 | MG | B | 8056 | 1/1 | 0.99 | 0.18 | -1.22 | 65,65,65,65 | 0 |
| 35 | CL | I | 8521 | 1/1 | 0.93 | 0.14 | -1.22 | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8353 | 1/1 | 0.94 | 0.13 | -1.35 | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8303 | 1/1 | 0.94 | 0.13 | -1.37 | 54,54,54,54 | 0 |
| 36 | CD | 2 | 8404 | 1/1 | 0.97 | 0.09 | -1.38 | 76,76,76,76 | 0 |
| 34 | NA | 0 | 8331 | 1/1 | 0.97 | 0.12 | -1.41 | 50,50,50,50 | 0 |
| 36 | CD | Z | 8402 | 1/1 | 0.99 | 0.08 | -1.48 | 75,75,75,75 | 0 |
| 36 | CD | Y | 8403 | 1/1 | 0.99 | 0.08 | -1.54 | 82,82,82,82 | 0 |
| 32 | MG | 0 | 8018 | 1/1 | 0.95 | 0.11 | -1.59 | 75,75,75,75 | 0 |
| 34 | NA | P | 8348 | 1/1 | 0.90 | 0.12 | -1.61 | 47,47,47,47 | 0 |
| 34 | NA | H | 8309 | 1/1 | 0.96 | 0.11 | -1.74 | 29,29,29,29 | 0 |
| 35 | CL | 2 | 8504 | 1/1 | 0.93 | 0.14 | -1.78 | 77,77,77,77 | 0 |
| 32 | MG | 2 | 8078 | 1/1 | 0.98 | 0.06 | -1.87 | 31,31,31,31 | 0 |
| 34 | NA | 0 | 8339 | 1/1 | 0.91 | 0.13 | -1.90 | 34,34,34,34 | 0 |
| 36 | CD | T | 8401 | 1/1 | 0.99 | 0.07 | -1.95 | 78,78,78,78 | 0 |
| 32 | MG | S | 8073 | 1/1 | 0.98 | 0.14 | -2.00 | 64,64,64,64 | 0 |
| 32 | MG | 0 | 8055 | 1/1 | 0.84 | 0.10 | -2.11 | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8048 | 1/1 | 0.99 | 0.10 | -2.16 | 35,35,35,35 | 0 |
| 34 | NA | 0 | 8343 | 1/1 | 0.95 | 0.08 | -2.41 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8060 | 1/1 | 0.98 | 0.11 | -2.47 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8032 | 1/1 | 0.94 | 0.07 | -2.63 | 26,26,26,26 | 0 |
| 34 | NA | 0 | 8368 | 1/1 | 0.88 | 0.10 | -2.78 | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8004 | 1/1 | 0.95 | 0.06 | -3.11 | 44,44,44,44 | 0 |
| 32 | MG | A | 8065 | 1/1 | 0.99 | 0.10 | -3.11 | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8096 | 1/1 | 0.98 | 0.07 | -3.14 | 39,39,39,39 | 0 |
| 35 | CL | J | 8512 | 1/1 | 0.97 | 0.08 | -3.20 | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8003 | 1/1 | 0.97 | 0.11 | -3.27 | 26,26,26,26 | 0 |
| 32 | MG | 0 | 8012 | 1/1 | 0.99 | 0.09 | -3.31 | 18,18,18,18 | 0 |
| 32 | MG | 0 | 8077 | 1/1 | 0.96 | 0.06 | -3.34 | 31,31,31,31 | 0 |
| 32 | MG | 0 | 8038 | 1/1 | 0.98 | 0.09 | -3.39 | 23,23,23,23 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8033 | 1/1 | 0.99 | 0.12 | -3.39 | 15,15,15,15 | 0 |
| 32 | MG | 0 | 8017 | 1/1 | 0.99 | 0.04 | -3.57 | 33,33,33,33 | 0 |
| 32 | MG | X | 8109 | 1/1 | 0.94 | 0.07 | -3.66 | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8088 | 1/1 | 0.93 | 0.12 | -3.77 | 34,34,34,34 | 0 |
| 35 | CL | 0 | 8513 | 1/1 | 0.98 | 0.08 | -3.82 | 62,62,62,62 | 0 |
| 32 | MG | 0 | 8020 | 1/1 | 0.99 | 0.08 | -3.87 | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8071 | 1/1 | 0.88 | 0.10 | -3.88 | 104,104,104,104 | 0 |
| 32 | MG | 0 | 8067 | 1/1 | 0.98 | 0.14 | -3.96 | 78,78,78,78 | 0 |
| 34 | NA | I | 8346 | 1/1 | 0.97 | 0.05 | -3.98 | 39,39,39,39 | 0 |
| 34 | NA | 0 | 8344 | 1/1 | 0.97 | 0.04 | -4.07 | 21,21,21,21 | 0 |
| 35 | CL | L | 8518 | 1/1 | 0.99 | 0.10 | -4.19 | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8001 | 1/1 | 0.99 | 0.11 | -4.36 | 40,40,40,40 | 0 |
| 34 | NA | 0 | 8327 | 1/1 | 0.98 | 0.09 | -4.36 | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8107 | 1/1 | 0.98 | 0.05 | -4.82 | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8074 | 1/1 | 0.96 | 0.04 | -5.08 | 29,29,29,29 | 0 |
| 32 | MG | 0 | 8053 | 1/1 | 0.99 | 0.07 | -5.10 | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8091 | 1/1 | 0.82 | 0.09 | -5.19 | 73,73,73,73 | 0 |
| 33 | K | 0 | 8202 | 1/1 | 0.94 | 0.11 | -5.52 | 79,79,79,79 | 0 |
| 32 | MG | 0 | 8052 | 1/1 | 0.92 | 0.08 | -5.64 | 42,42,42,42 | 0 |
| 32 | MG | 0 | 8015 | 1/1 | 0.95 | 0.06 | -5.75 | 61,61,61,61 | 0 |
| 34 | NA | L | 8347 | 1/1 | 0.96 | 0.09 | -5.77 | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8062 | 1/1 | 0.93 | 0.05 | -6.44 | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8019 | 1/1 | 0.99 | 0.04 | -6.73 | 24,24,24,24 | 0 |
| 32 | MG | 0 | 8006 | 1/1 | 0.98 | 0.06 | -6.87 | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8014 | 1/1 | 0.98 | 0.07 | -7.07 | 16,16,16,16 | 0 |
| 32 | MG | 0 | 8080 | 1/1 | 0.98 | 0.07 | -7.37 | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8008 | 1/1 | 0.94 | 0.08 | -7.56 | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8007 | 1/1 | 0.99 | 0.06 | -8.06 | 14,14,14,14 | 0 |
| 32 | MG | 0 | 8002 | 1/1 | 0.98 | 0.05 | -9.68 | 23,23,23,23 | 0 |
| 32 | MG | 0 | 8022 | 1/1 | 0.98 | 0.04 | -9.97 | 27,27,27,27 | 0 |
| 32 | MG | 0 | 8035 | 1/1 | 0.98 | 0.05 | -12.35 | 50,50,50,50 | 0 |
| 32 | MG | 0 | 8084 | 1/1 | 0.99 | 0.07 | -13.39 | 101,101,101,101 | 0 |
| 32 | MG | 0 | 8058 | 1/1 | 0.98 | 0.06 | -14.14 | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8110 | 1/1 | 0.93 | 0.09 | - | 34,34,34,34 | 0 |
| 32 | MG | 0 | 8046 | 1/1 | 0.82 | 0.10 | - | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8318 | 1/1 | 0.98 | 0.13 | - | 20,20,20,20 | 0 |
| 32 | MG | 0 | 8040 | 1/1 | 0.97 | 0.10 | - | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8099 | 1/1 | 0.79 | 0.14 | - | 73,73,73,73 | 0 |
| 35 | CL | I | 8502 | 1/1 | 0.90 | 0.11 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8102 | 1/1 | 0.97 | 0.12 | - | 61,61,61,61 | 0 |
| 32 | MG | 0 | 8085 | 1/1 | 0.90 | 0.14 | - | 82,82,82,82 | 0 |
| 34 | NA | 0 | 8342 | 1/1 | 0.93 | 0.21 | - | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8093 | 1/1 | 0.91 | 0.08 | - | 37,37,37,37 | 0 |
| 34 | NA | 0 | 8324 | 1/1 | 0.90 | 0.19 | - | 62,62,62,62 | 0 |
| 32 | MG | 0 | 8116 | 1/1 | 0.93 | 0.11 | - | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8047 | 1/1 | 0.99 | 0.10 | - | 48,48,48,48 | 0 |
| 32 | MG | 0 | 8092 | 1/1 | 0.62 | 0.53 | - | 109,109,109,109 | 0 |
| 32 | MG | 0 | 8041 | 1/1 | 0.96 | 0.12 | - | 53,53,53,53 | 0 |
| 34 | NA | 0 | 8306 | 1/1 | 0.87 | 0.69 | - | 57,57,57,57 | 0 |
| 34 | NA | 0 | 8352 | 1/1 | 0.81 | 0.71 | - | 61,61,61,61 | 0 |
| 32 | MG | 0 | 8042 | 1/1 | 0.97 | 0.06 | - | 32,32,32,32 | 0 |
| 34 | NA | 0 | 8341 | 1/1 | 0.75 | 0.15 | - | 42,42,42,42 | 0 |
| 34 | NA | R | 8312 | 1/1 | 0.60 | 0.25 | - | 60,60,60,60 | 0 |
| 32 | MG | 0 | 8094 | 1/1 | 0.97 | 0.14 | - | 56,56,56,56 | 0 |
| 35 | CL | X | 8520 | 1/1 | 0.96 | 0.14 | - | 43,43,43,43 | 0 |
| 32 | MG | 0 | 8023 | 1/1 | 0.98 | 0.12 | - | 20,20,20,20 | 0 |
| 35 | CL | 0 | 8522 | 1/1 | 0.97 | 0.37 | - | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8076 | 1/1 | 0.88 | 0.18 | - | 83,83,83,83 | 0 |
| 32 | MG | 0 | 8106 | 1/1 | 0.99 | 0.08 | - | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8079 | 1/1 | 0.97 | 0.10 | - | 50,50,50,50 | 0 |
| 34 | NA | 0 | 8381 | 1/1 | 0.91 | 0.13 | - | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8031 | 1/1 | 0.97 | 0.04 | - | 19,19,19,19 | 0 |
| 32 | MG | 0 | 8039 | 1/1 | 0.98 | 0.06 | - | 39,39,39,39 | 0 |
| 32 | MG | 0 | 8011 | 1/1 | 0.99 | 0.39 | - | 1,1,1,1 | 0 |
| 34 | NA | 0 | 8385 | 1/1 | 0.91 | 0.34 | - | 44,44,44,44 | 0 |
| 34 | NA | 0 | 8314 | 1/1 | 0.95 | 0.12 | - | 26,26,26,26 | 0 |
| 32 | MG | 0 | 8103 | 1/1 | 0.89 | 0.27 | - | 88,88,88,88 | 0 |
| 34 | NA | 0 | 8313 | 1/1 | 0.97 | 0.17 | - | 77,77,77,77 | 0 |
| 32 | MG | 9 | 8095 | 1/1 | 0.92 | 0.15 | - | 73,73,73,73 | 0 |
| 34 | NA | 0 | 8369 | 1/1 | 0.75 | 0.55 | - | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8026 | 1/1 | 0.97 | 0.11 | - | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8036 | 1/1 | 0.98 | 0.10 | - | 36,36,36,36 | 0 |
| 35 | CL | A | 8509 | 1/1 | 0.79 | 0.31 | - | 78,78,78,78 | 0 |
| 32 | MG | 0 | 8061 | 1/1 | 0.99 | 0.08 | - | 23,23,23,23 | 0 |
| 34 | NA | 0 | 8354 | 1/1 | 0.94 | 0.20 | - | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8063 | 1/1 | 0.90 | 0.11 | - | 143,143,143,143 | 0 |
| 34 | NA | 9 | 8351 | 1/1 | 0.70 | 0.23 | - | 89,89,89,89 | 0 |
| 32 | MG | 0 | 8115 | 1/1 | 0.99 | 0.04 | - | 27,27,27,27 | 0 |
| 32 | MG | 0 | 8051 | 1/1 | 0.94 | 0.10 | - | 86,86,86,86 | 0 |
| 34 | NA | 0 | 8329 | 1/1 | 0.78 | 0.23 | - | 135,135,135,135 | 0 |
| 35 | CL | I | 8501 | 1/1 | 0.92 | 0.16 | - | 64,64,64,64 | 0 |
| 32 | MG | 0 | 8025 | 1/1 | 0.99 | 0.11 | - | 24,24,24,24 | 0 |
| 32 | MG | 0 | 8098 | 1/1 | 0.98 | 0.12 | - | 18,18,18,18 | 0 |
| 34 | NA | 0 | 8384 | 1/1 | 0.16 | 0.76 | - | 132,132,132,132 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8024 | 1/1 | 0.21 | 0.46 | - | 146,146,146,146 | 0 |
| 32 | MG | 0 | 8100 | 1/1 | 0.86 | 0.32 | - | 74,74,74,74 | 0 |
| 32 | MG | 0 | 8075 | 1/1 | 0.92 | 0.09 | - | 54,54,54,54 | 0 |
| 34 | NA | 0 | 8375 | 1/1 | 0.91 | 0.48 | - | 55,55,55,55 | 0 |
| 34 | NA | 0 | 8340 | 1/1 | 0.97 | 0.17 | - | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8068 | 1/1 | 0.97 | 0.06 | - | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8089 | 1/1 | 0.97 | 0.08 | - | 60,60,60,60 | 0 |
| 32 | MG | 0 | 8059 | 1/1 | 0.82 | 0.18 | - | 84,84,84,84 | 0 |
| 35 | CL | 0 | 8503 | 1/1 | 0.85 | 0.24 | - | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8364 | 1/1 | 0.85 | 0.20 | - | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8021 | 1/1 | 0.99 | 0.08 | - | 19,19,19,19 | 0 |
| 34 | NA | 0 | 8377 | 1/1 | 0.96 | 0.13 | - | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8043 | 1/1 | 0.94 | 0.09 | - | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8316 | 1/1 | 0.93 | 0.21 | - | 39,39,39,39 | 0 |
| 35 | CL | 0 | 8514 | 1/1 | 0.95 | 0.11 | - | 80,80,80,80 | 0 |
| 32 | MG | 0 | 8005 | 1/1 | 0.97 | 0.13 | - | 55,55,55,55 | 0 |
| 32 | MG | 0 | 8072 | 1/1 | 0.99 | 0.08 | - | 38,38,38,38 | 0 |
| 35 | CL | Q | 8506 | 1/1 | 0.97 | 0.17 | - | 52,52,52,52 | 0 |
| 34 | NA | 0 | 8358 | 1/1 | 0.98 | 0.31 | - | 102,102,102,102 | 0 |
| 32 | MG | 0 | 8104 | 1/1 | 0.88 | 0.24 | - | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8029 | 1/1 | 0.97 | 0.12 | - | 38,38,38,38 | 0 |
| 32 | MG | 0 | 8097 | 1/1 | 0.93 | 0.20 | - | 37,37,37,37 | 0 |
| 34 | NA | 0 | 8360 | 1/1 | 0.92 | 0.59 | - | 47,47,47,47 | 0 |
| 36 | CD | N | 8405 | 1/1 | 0.96 | 0.10 | - | 90,90,90,90 | 0 |
| 34 | NA | 0 | 8363 | 1/1 | 0.84 | 0.38 | - | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8101 | 1/1 | 0.92 | 0.14 | - | 68,68,68,68 | 0 |
| 34 | NA | 0 | 8311 | 1/1 | 0.93 | 0.14 | - | 44,44,44,44 | 0 |
| 34 | NA | 0 | 8370 | 1/1 | 0.96 | 0.19 | - | 60,60,60,60 | 0 |
| 34 | NA | 0 | 8322 | 1/1 | 0.93 | 0.27 | - | 65,65,65,65 | 0 |
| 35 | CL | 0 | 8517 | 1/1 | 0.96 | 0.07 | - | 64,64,64,64 | 0 |
| 35 | CL | 0 | 8511 | 1/1 | 0.90 | 0.31 | - | 90,90,90,90 | 0 |
| 34 | NA | 0 | 8315 | 1/1 | 0.95 | 0.12 | - | 41,41,41,41 | 0 |
| 32 | MG | 0 | 8086 | 1/1 | 0.98 | 0.10 | - | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8330 | 1/1 | 0.94 | 0.17 | - | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8030 | 1/1 | 0.98 | 0.15 | - | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8082 | 1/1 | 0.90 | 0.13 | - | 77,77,77,77 | 0 |
| 35 | CL | K | 8510 | 1/1 | 0.83 | 0.20 | - | 71,71,71,71 | 0 |
| 34 | NA | 0 | 8301 | 1/1 | 0.94 | 0.09 | - | 30,30,30,30 | 0 |
| 34 | NA | 0 | 8336 | 1/1 | 0.86 | 0.07 | - | 50,50,50,50 | 0 |
| 32 | MG | J | 8069 | 1/1 | 0.98 | 0.24 | - | 114,114,114,114 | 0 |
| 32 | MG | 0 | 8111 | 1/1 | 0.94 | 0.07 | - | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8090 | 1/1 | 0.93 | 0.26 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 32 | MG | 0 | 8009 | 1/1 | 0.96 | 0.07 | - | 53,53,53,53 | 0 |
| 35 | CL | M | 8507 | 1/1 | 0.81 | 0.30 | - | 66,66,66,66 | 0 |
| 34 | NA | 0 | 8302 | 1/1 | 0.83 | 0.11 | - | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8050 | 1/1 | 0.93 | 0.10 | - | 50,50,50,50 | 0 |
| 32 | MG | 0 | 8037 | 1/1 | 0.99 | 0.10 | - | 32,32,32,32 | 0 |
| 32 | MG | 0 | 8113 | 1/1 | 0.76 | 0.15 | - | 39,39,39,39 | 0 |
| 34 | NA | 0 | 8319 | 1/1 | 0.93 | 0.10 | - | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8081 | 1/1 | 0.95 | 0.10 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 8105 | 1/1 | 0.98 | 0.19 | - | 29,29,29,29 | 0 |
| 32 | MG | 0 | 8034 | 1/1 | 0.99 | 0.07 | - | 16,16,16,16 | 0 |
| 32 | MG | 0 | 8087 | 1/1 | 0.90 | 0.08 | - | 83,83,83,83 | 0 |
| 32 | MG | 0 | 8117 | 1/1 | 0.97 | 0.08 | - | 28,28,28,28 | 0 |
| 34 | NA | 0 | 8357 | 1/1 | 0.89 | 0.12 | - | 63,63,63,63 | 0 |
| 32 | MG | 0 | 8028 | 1/1 | 0.89 | 0.06 | - | 93,93,93,93 | 0 |
| 32 | MG | 0 | 8016 | 1/1 | 0.88 | 0.14 | - | 50,50,50,50 | 0 |
| 34 | NA | 0 | 8334 | 1/1 | 0.98 | 0.04 | - | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8349 | 1/1 | 0.98 | 0.15 | - | 51,51,51,51 | 0 |
| 32 | MG | 0 | 8083 | 1/1 | 0.97 | 0.06 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 8066 | 1/1 | 0.92 | 0.06 | - | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8045 | 1/1 | 0.97 | 0.08 | - | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8307 | 1/1 | 0.88 | 0.30 | - | 40,40,40,40 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.