



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:28 PM GMT

PDB ID : 1JJ2
Title : Fully Refined Crystal Structure of the Haloarcula marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-07-03
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

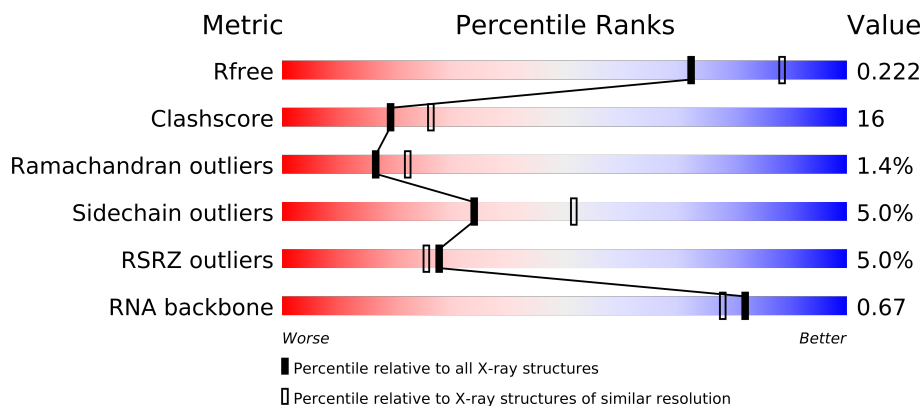
The following versions of software and data (see [references](#)) were used in the production of this report:

| | | |
|--------------------------------|---|--------------------------|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.15 2013 |
| Xtriage (Phenix) | : | dev-1323 |
| EDS | : | stable22639 |
| Percentile statistics | : | 21963 |
| Refmac | : | 5.8.0049 |
| CCP4 | : | 6.3.0 (Settle) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | stable22683 |

1 Overall quality at a glance

The reported resolution of this entry is 2.40 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 2207 (2.40-2.40) |
| Clashscore | 79885 | 2789 (2.40-2.40) |
| Ramachandran outliers | 78287 | 2736 (2.40-2.40) |
| Sidechain outliers | 78261 | 2737 (2.40-2.40) |
| RSRZ outliers | 66119 | 2210 (2.40-2.40) |
| RNA backbone | 1838 | 1029 (3.00-1.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 0 | 2922 | |
| 2 | 9 | 122 | |
| 3 | A | 239 | |
| 4 | B | 337 | |
| 5 | C | 246 | |
| 6 | D | 176 | |
| 7 | E | 177 | |
| 8 | F | 119 | |
| 9 | G | 348 | |
| 10 | H | 167 | |
| 11 | I | 145 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 12 | J | 132 | |
| 13 | K | 164 | |
| 14 | L | 194 | |
| 15 | M | 186 | |
| 16 | N | 115 | |
| 17 | O | 148 | |
| 18 | P | 95 | |
| 19 | Q | 154 | |
| 20 | R | 84 | |
| 21 | S | 119 | |
| 22 | T | 66 | |
| 23 | U | 70 | |
| 24 | V | 154 | |
| 25 | W | 91 | |
| 26 | X | 240 | |
| 27 | Y | 73 | |
| 28 | Z | 56 | |
| 29 | 1 | 48 | |
| 30 | 2 | 92 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 31 | MG | 0 | 8007 | - | X |
| 31 | MG | 0 | 8012 | - | X |
| 31 | MG | 0 | 8042 | - | X |
| 31 | MG | 0 | 8060 | - | X |
| 31 | MG | 0 | 8066 | - | X |
| 31 | MG | 0 | 8082 | - | X |
| 31 | MG | 0 | 8087 | - | X |
| 31 | MG | 0 | 8090 | - | X |
| 31 | MG | 0 | 8099 | - | X |
| 31 | MG | 0 | 8101 | - | X |
| 31 | MG | 0 | 8103 | - | X |
| 31 | MG | 0 | 8117 | - | X |
| 33 | NA | 0 | 8302 | - | X |
| 33 | NA | 0 | 8307 | - | X |
| 33 | NA | 0 | 8314 | - | X |
| 33 | NA | 0 | 8318 | - | X |
| 33 | NA | 0 | 8320 | - | X |
| 33 | NA | 0 | 8325 | - | X |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 33 | NA | 0 | 8326 | - | X |
| 33 | NA | 0 | 8327 | - | X |
| 33 | NA | 0 | 8329 | - | X |
| 33 | NA | 0 | 8331 | - | X |
| 33 | NA | 0 | 8340 | - | X |
| 33 | NA | 0 | 8350 | - | X |
| 33 | NA | 0 | 8355 | - | X |
| 33 | NA | 0 | 8358 | - | X |
| 33 | NA | 0 | 8359 | - | X |
| 33 | NA | 0 | 8360 | - | X |
| 33 | NA | 0 | 8361 | - | X |
| 33 | NA | 0 | 8362 | - | X |
| 33 | NA | 0 | 8363 | - | X |
| 33 | NA | 0 | 8364 | - | X |
| 33 | NA | 0 | 8366 | - | X |
| 33 | NA | 0 | 8367 | - | X |
| 33 | NA | 0 | 8369 | - | X |
| 33 | NA | 0 | 8370 | - | X |
| 33 | NA | 0 | 8371 | - | X |
| 33 | NA | 0 | 8372 | - | X |
| 33 | NA | 0 | 8373 | - | X |
| 33 | NA | 0 | 8374 | - | X |
| 33 | NA | 0 | 8376 | - | X |
| 33 | NA | 0 | 8377 | - | X |
| 33 | NA | 0 | 8379 | - | X |
| 33 | NA | 0 | 8384 | - | X |
| 33 | NA | 0 | 8385 | - | X |
| 33 | NA | 9 | 8383 | - | X |
| 33 | NA | K | 8380 | - | X |
| 33 | NA | Q | 8386 | - | X |
| 34 | CL | 0 | 8522 | - | X |

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 98543 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | 0 | 2754 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59017 | 26346 | 10878 | 19048 | 2745 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 0 | 560 | C | U | CONFLICT | GB 3377779 |

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1754 | 1072 | 352 | 325 | 5 | | | |

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | B | 337 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2624 | 1616 | 493 | 510 | 5 | | | |

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 5 is a protein called RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | C | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1858 | 1131 | 344 | 382 | 1 | | | |

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

| 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 RIBOSOMAL PROTEIN L6.

| 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 RIBOSOMAL PROTEIN L7AE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | F | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 552 | 141 | 191 | 1 | | | |

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | H | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1215 | 766 | 233 | 212 | 4 | | | |

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | I | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1119 | 696 | 199 | 221 | 3 | | | |

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | J | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 993 | 609 | 189 | 191 | 4 | | | |

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 13 | K | 145 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1114 | 668 | 222 | 224 | | | | |

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | L | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 988 | 346 | 266 | 5 | | | |

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | M | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1444 | 895 | 262 | 285 | 2 | | | |

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 16 | N | 115 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 864 | 529 | 161 | 174 | | | | |

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17 | 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 18 is a protein called RIBOSOMAL PROTEIN L21E.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18 | P | 95 | Total | C | N | O | 0 | 0 | 0 |
| | | | 734 | 450 | 141 | 143 | | | |

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 21 | S | 119 | Total | C | N | O | 0 | 0 | 0 |
| | | | 949 | 568 | 180 | 201 | | | |

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | V | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 737 | 209 | 243 | 6 | | | |

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 27 | Y | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 563 | 359 | 111 | 86 | 7 | | | |

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | Z | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 258 | 86 | 82 | 4 | | | |

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 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 30 is a protein called RIBOSOMAL PROTEIN L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | 2 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 31 | 0 | 109 | Total Mg 109 109 | 0 | 0 |
| 31 | J | 1 | Total Mg 1 1 | 0 | 0 |
| 31 | B | 1 | Total Mg 1 1 | 0 | 0 |
| 31 | A | 2 | Total Mg 2 2 | 0 | 0 |
| 31 | X | 1 | Total Mg 1 1 | 0 | 0 |
| 31 | 2 | 1 | Total Mg 1 1 | 0 | 0 |
| 31 | 9 | 1 | Total Mg 1 1 | 0 | 0 |
| 31 | S | 1 | Total Mg 1 1 | 0 | 0 |

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 32 | 0 | 2 | Total K 2 2 | 0 | 0 |

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 33 | 0 | 72 | Total Na 72 72 | 0 | 0 |
| 33 | P | 1 | Total Na 1 1 | 0 | 0 |
| 33 | Q | 2 | Total Na 2 2 | 0 | 0 |
| 33 | K | 1 | Total Na 1 1 | 0 | 0 |
| 33 | H | 2 | Total Na 2 2 | 0 | 0 |
| 33 | I | 1 | Total Na 1 1 | 0 | 0 |
| 33 | C | 1 | Total Na 1 1 | 0 | 0 |
| 33 | A | 1 | Total Na 1 1 | 0 | 0 |
| 33 | R | 1 | Total Na 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 33 | 9 | 2 | Total 2 | Na 2 | 0 | 0 |
| 33 | L | 1 | Total 1 | Na 1 | 0 | 0 |
| 33 | S | 1 | Total 1 | Na 1 | 0 | 0 |

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 34 | 0 | 10 | Total 10 | Cl 10 | 0 | 0 |
| 34 | Q | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | K | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | B | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | I | 3 | Total 3 | Cl 3 | 0 | 0 |
| 34 | A | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | N | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | X | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | 2 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | L | 1 | Total 1 | Cl 1 | 0 | 0 |
| 34 | M | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 35 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35 | Z | 1 | Total 1 | Cd 1 | 0 | 0 |
| 35 | Y | 1 | Total 1 | Cd 1 | 0 | 0 |
| 35 | T | 1 | Total 1 | Cd 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 35 | 2 | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | N | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 36 is water.

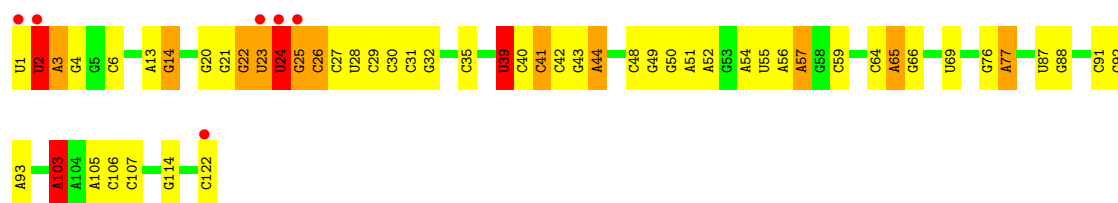
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 36 | 0 | 5938 | Total | O | 0 | 0 |
| | | | 5938 | 5938 | | |
| 36 | 9 | 135 | Total | O | 0 | 0 |
| | | | 135 | 135 | | |
| 36 | A | 126 | Total | O | 0 | 0 |
| | | | 126 | 126 | | |
| 36 | B | 150 | Total | O | 0 | 0 |
| | | | 150 | 150 | | |
| 36 | C | 172 | Total | O | 0 | 0 |
| | | | 172 | 172 | | |
| 36 | D | 53 | Total | O | 0 | 0 |
| | | | 53 | 53 | | |
| 36 | E | 46 | Total | O | 0 | 0 |
| | | | 46 | 46 | | |
| 36 | F | 28 | Total | O | 0 | 0 |
| | | | 28 | 28 | | |
| 36 | G | 21 | Total | O | 0 | 0 |
| | | | 21 | 21 | | |
| 36 | H | 74 | Total | O | 0 | 0 |
| | | | 74 | 74 | | |
| 36 | I | 56 | Total | O | 0 | 0 |
| | | | 56 | 56 | | |
| 36 | J | 62 | Total | O | 0 | 0 |
| | | | 62 | 62 | | |
| 36 | K | 80 | Total | O | 0 | 0 |
| | | | 80 | 80 | | |
| 36 | L | 127 | Total | O | 0 | 0 |
| | | | 127 | 127 | | |
| 36 | M | 70 | Total | O | 0 | 0 |
| | | | 70 | 70 | | |
| 36 | N | 43 | Total | O | 0 | 0 |
| | | | 43 | 43 | | |
| 36 | O | 68 | Total | O | 0 | 0 |
| | | | 68 | 68 | | |

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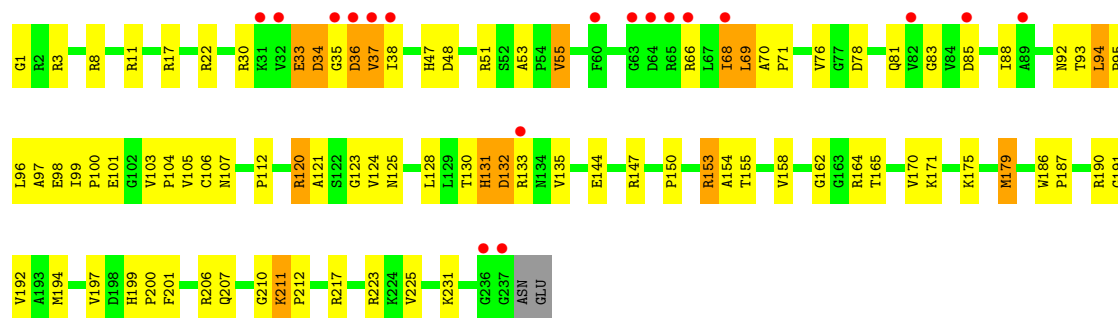
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 36 | P | 53 | Total 53 | O 53 | 0 | 0 |
| 36 | Q | 81 | Total 81 | O 81 | 0 | 0 |
| 36 | R | 32 | Total 32 | O 32 | 0 | 0 |
| 36 | S | 39 | Total 39 | O 39 | 0 | 0 |
| 36 | T | 25 | Total 25 | O 25 | 0 | 0 |
| 36 | U | 15 | Total 15 | O 15 | 0 | 0 |
| 36 | V | 67 | Total 67 | O 67 | 0 | 0 |
| 36 | W | 29 | Total 29 | O 29 | 0 | 0 |
| 36 | X | 99 | Total 99 | O 99 | 0 | 0 |
| 36 | Y | 39 | Total 39 | O 39 | 0 | 0 |
| 36 | Z | 53 | Total 53 | O 53 | 0 | 0 |
| 36 | 1 | 40 | Total 40 | O 40 | 0 | 0 |
| 36 | 2 | 72 | Total 72 | O 72 | 0 | 0 |





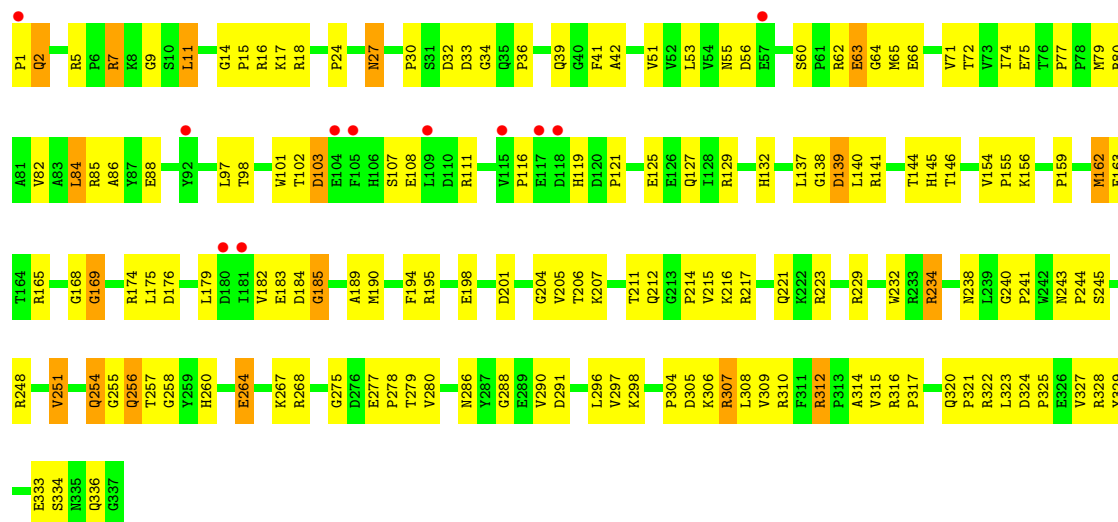
• Molecule 3: RIBOSOMAL PROTEIN L2

Chain A:



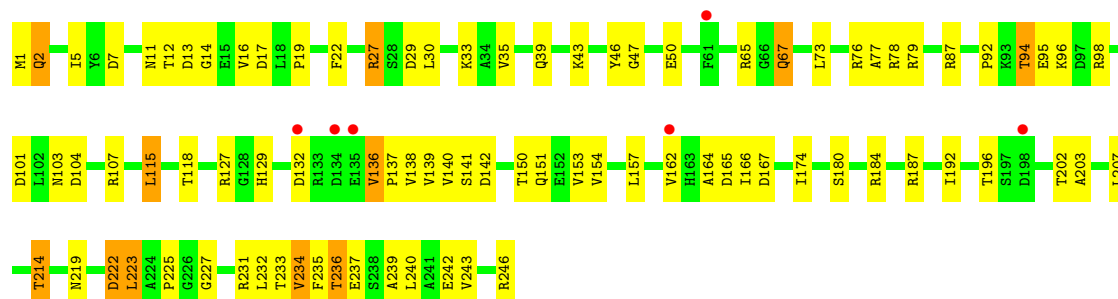
• Molecule 4: RIBOSOMAL PROTEIN L3

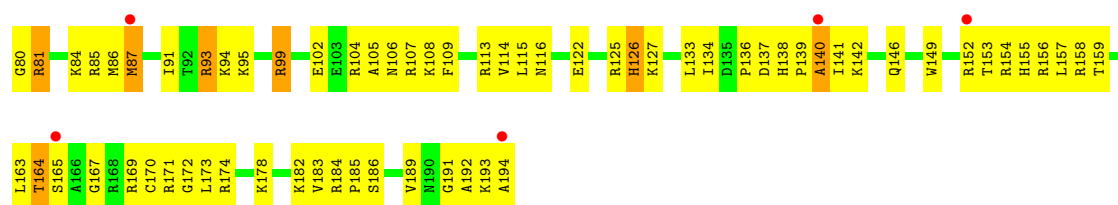
Chain B:



• Molecule 5: RIBOSOMAL PROTEIN L4

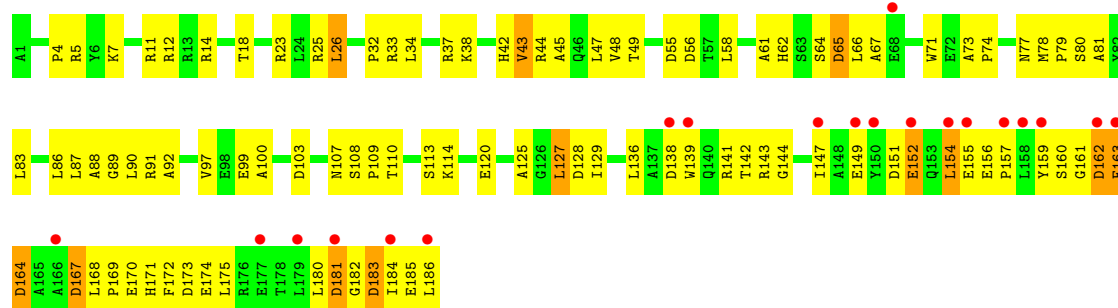
Chain C:





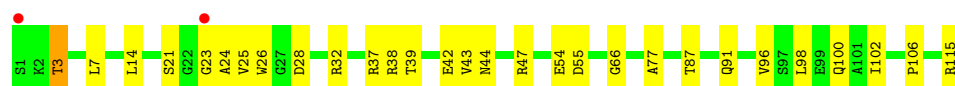
• Molecule 15: RIBOSOMAL PROTEIN L18

Chain M:



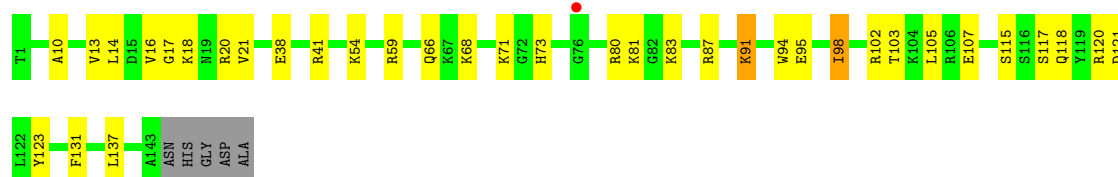
• Molecule 16: RIBOSOMAL PROTEIN L18E

Chain N:



• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain O:



• Molecule 18: RIBOSOMAL PROTEIN L21E

Chain P:



• Molecule 19: RIBOSOMAL PROTEIN L22

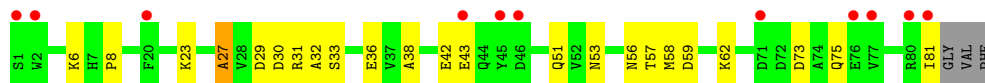
Chain Q:





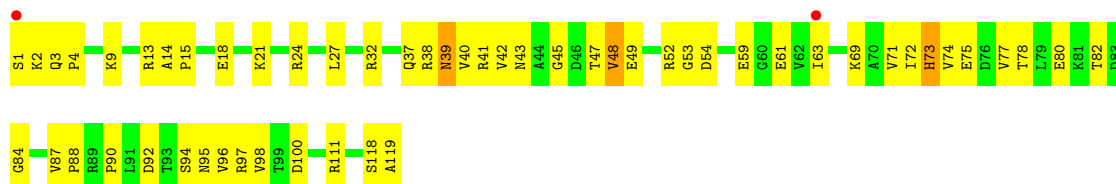
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain R:



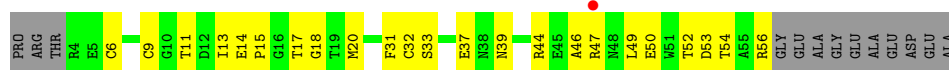
• Molecule 21: RIBOSOMAL PROTEIN L24

Chain S:



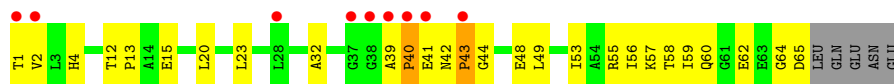
• Molecule 22: RIBOSOMAL PROTEIN L24E

Chain T:



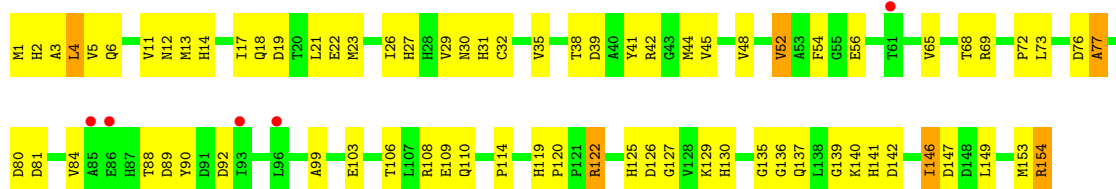
• Molecule 23: RIBOSOMAL PROTEIN L29

Chain U:



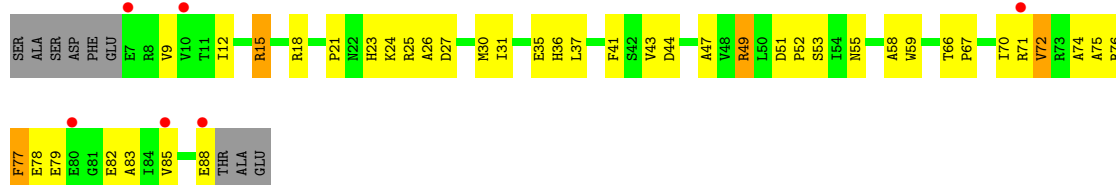
• Molecule 24: RIBOSOMAL PROTEIN L30

Chain V:



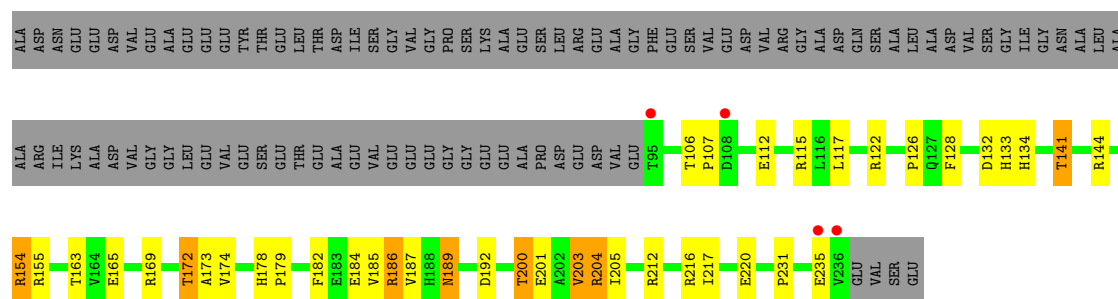
• Molecule 25: RIBOSOMAL PROTEIN L31E

Chain W:



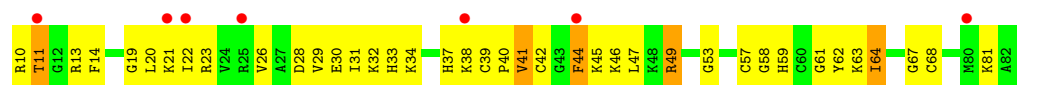
- Molecule 26: RIBOSOMAL PROTEIN L32E

Chain X:



- Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain Y:



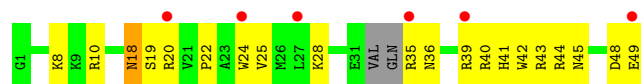
- Molecule 28: RIBOSOMAL PROTEIN L37E

Chain Z:



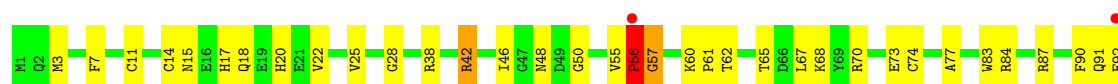
- Molecule 29: RIBOSOMAL PROTEIN L39E

Chain 1:



- Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 2:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 2.40 85.48 – 2.40 | Depositor EDS |
| % Data completeness (in resolution range) | 90.2 (15.00-2.40) 90.7 (85.48-2.40) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.37 (at 2.40Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.189 , 0.222 0.191 , 0.222 | Depositor DCC |
| R_{free} test set | 6222 reflections (0.99%) | DCC |
| Wilson B-factor (Å ²) | 38.9 | Xtriage |
| Anisotropy | 0.263 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 32.1 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 0 of 666819 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 98543 | wwPDB-VP |
| Average B, all atoms (Å ²) | 43.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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 | 0.38 | 3/66076 (0.0%) | 0.71 | 32/103052 (0.0%) |
| 2 | 9 | 0.44 | 3/2905 (0.1%) | 0.85 | 11/4528 (0.2%) |
| 3 | A | 0.34 | 0/1787 | 0.66 | 0/2409 |
| 4 | B | 0.34 | 0/2689 | 0.64 | 0/3652 |
| 5 | C | 0.39 | 0/1883 | 0.67 | 0/2551 |
| 6 | D | 0.31 | 0/1111 | 0.59 | 0/1498 |
| 7 | E | 0.31 | 0/1382 | 0.57 | 0/1880 |
| 8 | F | 0.33 | 0/896 | 0.56 | 0/1219 |
| 9 | G | 0.25 | 0/241 | 0.47 | 0/324 |
| 10 | H | 0.38 | 0/1246 | 0.74 | 1/1686 (0.1%) |
| 11 | I | 0.33 | 0/1135 | 0.61 | 0/1530 |
| 12 | J | 0.33 | 0/1003 | 0.65 | 0/1351 |
| 13 | K | 0.34 | 0/1126 | 0.68 | 0/1504 |
| 14 | L | 0.41 | 0/1633 | 0.71 | 1/2180 (0.0%) |
| 15 | M | 0.29 | 0/1473 | 0.64 | 0/1999 |
| 16 | N | 0.32 | 0/873 | 0.61 | 1/1181 (0.1%) |
| 17 | O | 0.33 | 0/1143 | 0.54 | 0/1521 |
| 18 | P | 0.35 | 0/748 | 0.68 | 0/1005 |
| 19 | Q | 0.35 | 0/1172 | 0.67 | 0/1578 |
| 20 | R | 0.32 | 0/648 | 0.59 | 1/875 (0.1%) |
| 21 | S | 0.31 | 0/957 | 0.63 | 0/1289 |
| 22 | T | 0.32 | 0/417 | 0.58 | 0/562 |
| 23 | U | 0.29 | 0/502 | 0.54 | 0/675 |
| 24 | V | 0.33 | 0/1218 | 0.62 | 0/1655 |
| 25 | W | 0.32 | 0/664 | 0.60 | 0/895 |
| 26 | X | 0.34 | 0/1146 | 0.63 | 0/1536 |
| 27 | Y | 0.37 | 0/575 | 0.69 | 0/763 |
| 28 | Z | 0.42 | 0/437 | 0.67 | 0/578 |
| 29 | 1 | 0.34 | 0/398 | 0.54 | 0/527 |
| 30 | 2 | 0.38 | 0/771 | 0.62 | 0/1024 |
| All | All | 0.37 | 6/98255 (0.0%) | 0.70 | 47/147027 (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 | 62 |
| 2 | 9 | 0 | 2 |
| All | All | 1 | 64 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | 9 | 3 | A | C2'-O2' | -7.92 | 1.31 | 1.41 |
| 1 | 0 | 1206 | U | P-OP2 | 6.22 | 1.59 | 1.49 |
| 2 | 9 | 3 | A | O5'-C5' | 6.21 | 1.54 | 1.44 |
| 1 | 0 | 1206 | U | C3'-O3' | -5.28 | 1.34 | 1.42 |
| 1 | 0 | 1205 | U | C3'-O3' | -5.23 | 1.34 | 1.42 |

The worst 5 of 47 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | 0 | 1165 | G | O5'-P-OP1 | -22.95 | 83.17 | 110.70 |
| 1 | 0 | 1164 | U | OP1-P-O3' | -20.79 | 59.47 | 105.20 |
| 1 | 0 | 1165 | G | O5'-P-OP2 | -15.10 | 92.11 | 105.70 |
| 2 | 9 | 3 | A | OP1-P-O3' | -13.36 | 75.82 | 105.20 |
| 1 | 0 | 1164 | U | OP2-P-O3' | -13.28 | 75.98 | 105.20 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | 0 | 1563 | G | C3' |

5 of 64 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | 0 | 182 | G | Sidechain |
| 1 | 0 | 191 | A | Sidechain |
| 1 | 0 | 22 | U | Sidechain |
| 1 | 0 | 221 | G | Sidechain |
| 1 | 0 | 246 | G | Sidechain |

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 0 | 59017 | 0 | 29807 | 760 | 0 |
| 2 | 9 | 2600 | 0 | 1326 | 78 | 0 |
| 3 | A | 1754 | 0 | 1763 | 109 | 0 |
| 4 | B | 2624 | 0 | 2533 | 176 | 0 |
| 5 | C | 1858 | 0 | 1816 | 105 | 0 |
| 6 | D | 1094 | 0 | 1085 | 130 | 0 |
| 7 | E | 1357 | 0 | 1266 | 79 | 0 |
| 8 | F | 885 | 0 | 854 | 59 | 0 |
| 9 | G | 240 | 0 | 231 | 18 | 0 |
| 10 | H | 1215 | 0 | 1215 | 150 | 0 |
| 11 | I | 1119 | 0 | 1098 | 62 | 0 |
| 12 | J | 993 | 0 | 1027 | 56 | 0 |
| 13 | K | 1114 | 0 | 1072 | 55 | 0 |
| 14 | L | 1605 | 0 | 1676 | 141 | 0 |
| 15 | M | 1444 | 0 | 1401 | 119 | 0 |
| 16 | N | 864 | 0 | 873 | 31 | 0 |
| 17 | O | 1133 | 0 | 1127 | 38 | 0 |
| 18 | P | 734 | 0 | 728 | 18 | 0 |
| 19 | Q | 1149 | 0 | 1122 | 49 | 0 |
| 20 | R | 641 | 0 | 605 | 21 | 0 |
| 21 | S | 949 | 0 | 923 | 52 | 0 |
| 22 | T | 410 | 0 | 364 | 31 | 0 |
| 23 | U | 499 | 0 | 511 | 28 | 0 |
| 24 | V | 1195 | 0 | 1137 | 91 | 0 |
| 25 | W | 654 | 0 | 653 | 44 | 0 |
| 26 | X | 1130 | 0 | 1133 | 52 | 0 |
| 27 | Y | 563 | 0 | 597 | 53 | 0 |
| 28 | Z | 430 | 0 | 426 | 22 | 0 |
| 29 | 1 | 393 | 0 | 406 | 32 | 0 |
| 30 | 2 | 755 | 0 | 728 | 36 | 0 |
| 31 | 0 | 109 | 0 | 0 | 0 | 0 |
| 31 | 2 | 1 | 0 | 0 | 0 | 0 |
| 31 | 9 | 1 | 0 | 0 | 0 | 0 |
| 31 | A | 2 | 0 | 0 | 0 | 0 |
| 31 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31 | J | 1 | 0 | 0 | 0 | 0 |
| 31 | S | 1 | 0 | 0 | 0 | 0 |
| 31 | X | 1 | 0 | 0 | 0 | 0 |
| 32 | 0 | 2 | 0 | 0 | 0 | 0 |
| 33 | 0 | 72 | 0 | 0 | 0 | 0 |
| 33 | 9 | 2 | 0 | 0 | 0 | 0 |
| 33 | A | 1 | 0 | 0 | 0 | 0 |
| 33 | C | 1 | 0 | 0 | 0 | 0 |
| 33 | H | 2 | 0 | 0 | 0 | 0 |
| 33 | I | 1 | 0 | 0 | 0 | 0 |
| 33 | K | 1 | 0 | 0 | 0 | 0 |
| 33 | L | 1 | 0 | 0 | 0 | 0 |
| 33 | P | 1 | 0 | 0 | 0 | 0 |
| 33 | Q | 2 | 0 | 0 | 0 | 0 |
| 33 | R | 1 | 0 | 0 | 0 | 0 |
| 33 | S | 1 | 0 | 0 | 0 | 0 |
| 34 | 0 | 10 | 0 | 0 | 0 | 0 |
| 34 | 2 | 1 | 0 | 0 | 0 | 0 |
| 34 | A | 1 | 0 | 0 | 0 | 0 |
| 34 | B | 1 | 0 | 0 | 0 | 0 |
| 34 | I | 3 | 0 | 0 | 1 | 0 |
| 34 | K | 1 | 0 | 0 | 0 | 0 |
| 34 | L | 1 | 0 | 0 | 1 | 0 |
| 34 | M | 1 | 0 | 0 | 0 | 0 |
| 34 | N | 1 | 0 | 0 | 0 | 0 |
| 34 | Q | 1 | 0 | 0 | 0 | 0 |
| 34 | X | 1 | 0 | 0 | 0 | 0 |
| 35 | 2 | 1 | 0 | 0 | 0 | 0 |
| 35 | N | 1 | 0 | 0 | 0 | 0 |
| 35 | T | 1 | 0 | 0 | 0 | 0 |
| 35 | Y | 1 | 0 | 0 | 0 | 0 |
| 35 | Z | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 5938 | 0 | 0 | 173 | 0 |
| 36 | 1 | 40 | 0 | 0 | 6 | 0 |
| 36 | 2 | 72 | 0 | 0 | 10 | 0 |
| 36 | 9 | 135 | 0 | 0 | 14 | 0 |
| 36 | A | 126 | 0 | 0 | 20 | 0 |
| 36 | B | 150 | 0 | 0 | 30 | 0 |
| 36 | C | 172 | 0 | 0 | 30 | 0 |
| 36 | D | 53 | 0 | 0 | 18 | 0 |
| 36 | E | 46 | 0 | 0 | 12 | 0 |
| 36 | F | 28 | 0 | 0 | 7 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36 | G | 21 | 0 | 0 | 4 | 0 |
| 36 | H | 74 | 0 | 0 | 21 | 0 |
| 36 | I | 56 | 0 | 0 | 5 | 0 |
| 36 | J | 62 | 0 | 0 | 13 | 0 |
| 36 | K | 80 | 0 | 0 | 17 | 0 |
| 36 | L | 127 | 0 | 0 | 19 | 0 |
| 36 | M | 70 | 0 | 0 | 16 | 0 |
| 36 | N | 43 | 0 | 0 | 6 | 0 |
| 36 | O | 68 | 0 | 0 | 1 | 0 |
| 36 | P | 53 | 0 | 0 | 1 | 0 |
| 36 | Q | 81 | 0 | 0 | 9 | 0 |
| 36 | R | 32 | 0 | 0 | 5 | 0 |
| 36 | S | 39 | 0 | 0 | 5 | 0 |
| 36 | T | 25 | 0 | 0 | 6 | 0 |
| 36 | U | 15 | 0 | 0 | 4 | 0 |
| 36 | V | 67 | 0 | 0 | 10 | 0 |
| 36 | W | 29 | 0 | 0 | 3 | 0 |
| 36 | X | 99 | 0 | 0 | 15 | 0 |
| 36 | Y | 39 | 0 | 0 | 12 | 0 |
| 36 | Z | 53 | 0 | 0 | 1 | 0 |
| All | All | 98543 | 0 | 59503 | 2453 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 2453 close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:0:1160:G:H5' | 1:0:1161:A:H5' | 1.26 | 1.14 |
| 10:H:86:ARG:NH1 | 10:H:133:ILE:HG13 | 1.62 | 1.12 |
| 5:C:5:ILE:HD11 | 5:C:16:VAL:HG23 | 1.35 | 1.07 |
| 25:W:37:LEU:HD13 | 25:W:85:VAL:HG21 | 1.29 | 1.06 |
| 1:0:960:G:H4' | 36:0:6956:HOH:O | 1.54 | 1.06 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3 | A | 235/239 (98%) | 216 (92%) | 14 (6%) | 5 (2%) | 11 | 12 |
| 4 | B | 335/337 (99%) | 314 (94%) | 14 (4%) | 7 (2%) | 11 | 12 |
| 5 | C | 244/246 (99%) | 226 (93%) | 18 (7%) | 0 | 100 | 100 |
| 6 | D | 134/176 (76%) | 97 (72%) | 28 (21%) | 9 (7%) | 2 | 1 |
| 7 | E | 170/177 (96%) | 161 (95%) | 8 (5%) | 1 (1%) | 33 | 47 |
| 8 | F | 117/119 (98%) | 106 (91%) | 9 (8%) | 2 (2%) | 14 | 17 |
| 9 | G | 25/348 (7%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 10 | H | 152/167 (91%) | 135 (89%) | 12 (8%) | 5 (3%) | 6 | 5 |
| 11 | I | 140/145 (97%) | 130 (93%) | 7 (5%) | 3 (2%) | 11 | 12 |
| 12 | J | 130/132 (98%) | 121 (93%) | 8 (6%) | 1 (1%) | 27 | 39 |
| 13 | K | 141/164 (86%) | 121 (86%) | 19 (14%) | 1 (1%) | 30 | 43 |
| 14 | L | 192/194 (99%) | 181 (94%) | 10 (5%) | 1 (0%) | 38 | 53 |
| 15 | M | 184/186 (99%) | 167 (91%) | 10 (5%) | 7 (4%) | 5 | 4 |
| 16 | N | 113/115 (98%) | 109 (96%) | 4 (4%) | 0 | 100 | 100 |
| 17 | O | 141/148 (95%) | 138 (98%) | 3 (2%) | 0 | 100 | 100 |
| 18 | P | 93/95 (98%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 19 | Q | 148/154 (96%) | 143 (97%) | 4 (3%) | 1 (1%) | 30 | 43 |
| 20 | R | 79/84 (94%) | 75 (95%) | 4 (5%) | 0 | 100 | 100 |
| 21 | S | 117/119 (98%) | 112 (96%) | 5 (4%) | 0 | 100 | 100 |
| 22 | T | 51/66 (77%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 23 | U | 63/70 (90%) | 58 (92%) | 3 (5%) | 2 (3%) | 6 | 5 |
| 24 | V | 152/154 (99%) | 147 (97%) | 4 (3%) | 1 (1%) | 30 | 43 |
| 25 | W | 80/91 (88%) | 70 (88%) | 8 (10%) | 2 (2%) | 9 | 8 |
| 26 | X | 140/240 (58%) | 140 (100%) | 0 | 0 | 100 | 100 |
| 27 | Y | 71/73 (97%) | 64 (90%) | 5 (7%) | 2 (3%) | 8 | 6 |
| 28 | Z | 54/56 (96%) | 52 (96%) | 2 (4%) | 0 | 100 | 100 |
| 29 | 1 | 42/48 (88%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 30 | 2 | 90/92 (98%) | 86 (96%) | 2 (2%) | 2 (2%) | 10 | 11 |
| All | All | 3633/4235 (86%) | 3372 (93%) | 209 (6%) | 52 (1%) | 16 | 22 |

5 of 52 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 139 | ASP |
| 6 | D | 93 | LEU |
| 6 | D | 95 | THR |
| 6 | D | 137 | PRO |
| 6 | D | 173 | GLU |

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 | 179/181 (99%) | 166 (93%) | 13 (7%) | 20 | 30 |
| 4 | B | 282/282 (100%) | 264 (94%) | 18 (6%) | 25 | 37 |
| 5 | C | 193/193 (100%) | 179 (93%) | 14 (7%) | 20 | 30 |
| 6 | D | 117/147 (80%) | 106 (91%) | 11 (9%) | 13 | 18 |
| 7 | E | 152/155 (98%) | 148 (97%) | 4 (3%) | 59 | 79 |
| 8 | F | 92/92 (100%) | 91 (99%) | 1 (1%) | 84 | 94 |
| 9 | G | 27/283 (10%) | 27 (100%) | 0 | 100 | 100 |
| 10 | H | 122/122 (100%) | 109 (89%) | 13 (11%) | 10 | 13 |
| 11 | I | 118/121 (98%) | 109 (92%) | 9 (8%) | 19 | 28 |
| 12 | J | 106/106 (100%) | 103 (97%) | 3 (3%) | 56 | 77 |
| 13 | K | 112/126 (89%) | 108 (96%) | 4 (4%) | 47 | 68 |
| 14 | L | 166/166 (100%) | 157 (95%) | 9 (5%) | 31 | 47 |
| 15 | M | 149/149 (100%) | 143 (96%) | 6 (4%) | 42 | 63 |
| 16 | N | 93/93 (100%) | 91 (98%) | 2 (2%) | 64 | 83 |
| 17 | O | 113/116 (97%) | 111 (98%) | 2 (2%) | 71 | 88 |
| 18 | P | 79/79 (100%) | 75 (95%) | 4 (5%) | 33 | 50 |
| 19 | Q | 117/121 (97%) | 114 (97%) | 3 (3%) | 59 | 79 |
| 20 | R | 71/73 (97%) | 71 (100%) | 0 | 100 | 100 |
| 21 | S | 105/105 (100%) | 101 (96%) | 4 (4%) | 44 | 65 |
| 22 | T | 44/52 (85%) | 44 (100%) | 0 | 100 | 100 |
| 23 | U | 51/56 (91%) | 50 (98%) | 1 (2%) | 68 | 86 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 24 | V | 130/130 (100%) | 122 (94%) | 8 (6%) | 26 | 39 |
| 25 | W | 66/73 (90%) | 62 (94%) | 4 (6%) | 26 | 40 |
| 26 | X | 120/195 (62%) | 110 (92%) | 10 (8%) | 16 | 24 |
| 27 | Y | 56/56 (100%) | 52 (93%) | 4 (7%) | 21 | 32 |
| 28 | Z | 46/46 (100%) | 46 (100%) | 0 | 100 | 100 |
| 29 | 1 | 42/44 (96%) | 41 (98%) | 1 (2%) | 61 | 81 |
| 30 | 2 | 79/79 (100%) | 76 (96%) | 3 (4%) | 44 | 65 |
| All | All | 3027/3441 (88%) | 2876 (95%) | 151 (5%) | 34 | 51 |

5 of 151 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | H | 86 | ARG |
| 12 | J | 10 | GLN |
| 26 | X | 200 | THR |
| 10 | H | 129 | ASN |
| 11 | I | 74 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | K | 116 | HIS |
| 17 | O | 50 | GLN |
| 28 | Z | 28 | HIS |
| 14 | L | 26 | HIS |
| 15 | M | 21 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 0 | 2747/2922 (94%) | 239 (8%) | 35 (1%) |
| 2 | 9 | 121/122 (99%) | 16 (13%) | 5 (4%) |
| All | All | 2868/3044 (94%) | 255 (8%) | 40 (1%) |

5 of 255 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 40 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1377 | C |
| 1 | 0 | 1856 | C |
| 2 | 9 | 23 | U |
| 1 | 0 | 1563 | G |
| 1 | 0 | 1942 | A |

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 232 ligands modelled in this entry, 232 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | 0 | 2754/2922 (94%) | -0.14 | 58 (2%) 60 58 | 17, 36, 79, 127 | 0 |
| 2 | 9 | 122/122 (100%) | -0.07 | 6 (4%) 28 26 | 31, 54, 78, 136 | 0 |
| 3 | A | 237/239 (99%) | 0.24 | 18 (7%) 14 12 | 19, 38, 71, 92 | 0 |
| 4 | B | 337/337 (100%) | 0.28 | 11 (3%) 44 42 | 21, 45, 71, 82 | 0 |
| 5 | C | 246/246 (100%) | 0.14 | 6 (2%) 56 54 | 15, 35, 58, 70 | 0 |
| 6 | D | 140/176 (79%) | 2.20 | 73 (52%) 0 0 | 43, 86, 105, 108 | 0 |
| 7 | E | 172/177 (97%) | 0.58 | 8 (4%) 30 28 | 37, 59, 77, 81 | 0 |
| 8 | F | 119/119 (100%) | 0.71 | 15 (12%) 4 4 | 37, 58, 83, 88 | 0 |
| 9 | G | 29/348 (8%) | 2.33 | 18 (62%) 0 0 | 64, 79, 86, 91 | 0 |
| 10 | H | 156/167 (93%) | 0.63 | 18 (11%) 5 5 | 30, 47, 75, 79 | 0 |
| 11 | I | 142/145 (97%) | 0.29 | 5 (3%) 42 40 | 29, 42, 63, 84 | 0 |
| 12 | J | 132/132 (100%) | 0.09 | 3 (2%) 57 55 | 27, 42, 61, 71 | 0 |
| 13 | K | 145/164 (88%) | 0.58 | 14 (9%) 8 7 | 18, 54, 90, 102 | 0 |
| 14 | L | 194/194 (100%) | -0.03 | 6 (3%) 47 44 | 19, 32, 50, 62 | 0 |
| 15 | M | 186/186 (100%) | 0.54 | 20 (10%) 6 6 | 31, 50, 91, 103 | 0 |
| 16 | N | 115/115 (100%) | 0.02 | 2 (1%) 67 65 | 27, 44, 60, 69 | 0 |
| 17 | O | 143/148 (96%) | 0.15 | 1 (0%) 84 84 | 30, 44, 57, 64 | 0 |
| 18 | P | 95/95 (100%) | 0.07 | 2 (2%) 60 58 | 25, 34, 50, 61 | 0 |
| 19 | Q | 150/154 (97%) | -0.13 | 0 100 100 | 23, 36, 54, 63 | 0 |
| 20 | R | 81/84 (96%) | 0.51 | 11 (13%) 4 3 | 31, 47, 68, 72 | 0 |
| 21 | S | 119/119 (100%) | 0.40 | 2 (1%) 67 65 | 28, 45, 69, 81 | 0 |
| 22 | T | 53/66 (80%) | 0.08 | 1 (1%) 64 61 | 33, 47, 63, 71 | 0 |
| 23 | U | 65/70 (92%) | 1.42 | 9 (13%) 4 3 | 39, 59, 97, 101 | 0 |
| 24 | V | 154/154 (100%) | 0.26 | 5 (3%) 45 43 | 27, 40, 57, 65 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | W | 82/91 (90%) | 0.46 | 6 (7%) 15 13 | 35, 48, 73, 91 | 0 |
| 26 | X | 142/240 (59%) | -0.05 | 4 (2%) 50 48 | 22, 35, 59, 74 | 0 |
| 27 | Y | 73/73 (100%) | 0.47 | 7 (9%) 8 8 | 36, 49, 63, 77 | 0 |
| 28 | Z | 56/56 (100%) | -0.13 | 0 100 100 | 17, 24, 32, 35 | 0 |
| 29 | 1 | 46/48 (95%) | 0.48 | 6 (13%) 4 4 | 27, 49, 77, 86 | 0 |
| 30 | 2 | 92/92 (100%) | 0.09 | 2 (2%) 59 57 | 23, 44, 59, 72 | 0 |
| All | All | 6577/7279 (90%) | 0.15 | 337 (5%) 28 25 | 15, 41, 80, 136 | 0 |

The worst 5 of 337 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 23 | U | 1 | THR | 12.5 |
| 23 | U | 39 | ALA | 9.7 |
| 6 | D | 63 | ILE | 9.2 |
| 6 | D | 57 | THR | 7.5 |
| 23 | U | 40 | PRO | 7.4 |

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

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

6.3 Carbohydrates ⓘ

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 | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 33 | NA | 0 | 8370 | 1/1 | 0.40 | 74.46 | 61,61,61,61 | 0 |
| 31 | MG | 0 | 8087 | 1/1 | 0.26 | 34.54 | 72,72,72,72 | 0 |
| 31 | MG | 0 | 8101 | 1/1 | 0.27 | 30.69 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 33 | NA | 0 | 8358 | 1/1 | 0.31 | 22.79 | 74,74,74,74 | 0 |
| 33 | NA | 0 | 8379 | 1/1 | 0.32 | 20.33 | 48,48,48,48 | 0 |
| 33 | NA | 0 | 8366 | 1/1 | 0.26 | 19.42 | 54,54,54,54 | 0 |
| 33 | NA | 0 | 8350 | 1/1 | 0.28 | 18.59 | 36,36,36,36 | 0 |
| 33 | NA | 0 | 8371 | 1/1 | 0.26 | 17.92 | 49,49,49,49 | 0 |
| 33 | NA | 0 | 8320 | 1/1 | 0.21 | 17.75 | 38,38,38,38 | 0 |
| 33 | NA | 0 | 8363 | 1/1 | 0.24 | 17.44 | 52,52,52,52 | 0 |
| 31 | MG | 0 | 8103 | 1/1 | 0.23 | 15.15 | 54,54,54,54 | 0 |
| 33 | NA | 0 | 8372 | 1/1 | 0.29 | 13.11 | 54,54,54,54 | 0 |
| 31 | MG | 0 | 8082 | 1/1 | 0.18 | 12.67 | 56,56,56,56 | 0 |
| 33 | NA | 0 | 8385 | 1/1 | 0.32 | 12.36 | 48,48,48,48 | 0 |
| 33 | NA | 0 | 8327 | 1/1 | 0.22 | 12.32 | 38,38,38,38 | 0 |
| 33 | NA | 0 | 8340 | 1/1 | 0.19 | 10.84 | 47,47,47,47 | 0 |
| 33 | NA | 0 | 8367 | 1/1 | 0.22 | 10.16 | 45,45,45,45 | 0 |
| 33 | NA | Q | 8386 | 1/1 | 0.36 | 9.60 | 74,74,74,74 | 0 |
| 33 | NA | 0 | 8326 | 1/1 | 0.19 | 8.43 | 37,37,37,37 | 0 |
| 33 | NA | K | 8380 | 1/1 | 0.27 | 7.73 | 42,42,42,42 | 0 |
| 33 | NA | 0 | 8373 | 1/1 | 0.15 | 7.34 | 43,43,43,43 | 0 |
| 34 | CL | 0 | 8522 | 1/1 | 0.17 | 7.16 | 44,44,44,44 | 0 |
| 33 | NA | 0 | 8364 | 1/1 | 0.20 | 6.98 | 38,38,38,38 | 0 |
| 33 | NA | 0 | 8314 | 1/1 | 0.25 | 6.97 | 40,40,40,40 | 0 |
| 31 | MG | 0 | 8042 | 1/1 | 0.13 | 6.17 | 29,29,29,29 | 0 |
| 33 | NA | 0 | 8376 | 1/1 | 0.21 | 6.08 | 39,39,39,39 | 0 |
| 33 | NA | 0 | 8362 | 1/1 | 0.23 | 6.06 | 51,51,51,51 | 0 |
| 33 | NA | 0 | 8302 | 1/1 | 0.18 | 5.40 | 44,44,44,44 | 0 |
| 31 | MG | 0 | 8066 | 1/1 | 0.39 | 5.20 | 85,85,85,85 | 0 |
| 33 | NA | 0 | 8318 | 1/1 | 0.18 | 5.11 | 49,49,49,49 | 0 |
| 33 | NA | 0 | 8359 | 1/1 | 0.22 | 4.57 | 39,39,39,39 | 0 |
| 33 | NA | 0 | 8329 | 1/1 | 0.14 | 4.20 | 48,48,48,48 | 0 |
| 33 | NA | 0 | 8331 | 1/1 | 0.20 | 4.11 | 39,39,39,39 | 0 |
| 31 | MG | 0 | 8090 | 1/1 | 0.23 | 3.95 | 53,53,53,53 | 0 |
| 33 | NA | 0 | 8384 | 1/1 | 0.14 | 3.61 | 52,52,52,52 | 0 |
| 33 | NA | 0 | 8374 | 1/1 | 0.14 | 3.22 | 44,44,44,44 | 0 |
| 33 | NA | 0 | 8369 | 1/1 | 0.19 | 3.05 | 40,40,40,40 | 0 |
| 33 | NA | 0 | 8377 | 1/1 | 0.16 | 3.03 | 50,50,50,50 | 0 |
| 33 | NA | 9 | 8383 | 1/1 | 0.21 | 2.91 | 43,43,43,43 | 0 |
| 33 | NA | 0 | 8307 | 1/1 | 0.15 | 2.83 | 42,42,42,42 | 0 |
| 31 | MG | 0 | 8099 | 1/1 | 0.20 | 2.67 | 44,44,44,44 | 0 |
| 31 | MG | 0 | 8012 | 1/1 | 0.14 | 2.67 | 32,32,32,32 | 0 |
| 33 | NA | 0 | 8360 | 1/1 | 0.17 | 2.59 | 41,41,41,41 | 0 |
| 31 | MG | 0 | 8060 | 1/1 | 0.19 | 2.54 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 33 | NA | 0 | 8361 | 1/1 | 0.18 | 2.53 | 38,38,38,38 | 0 |
| 31 | MG | 0 | 8007 | 1/1 | 0.19 | 2.48 | 21,21,21,21 | 0 |
| 33 | NA | 0 | 8355 | 1/1 | 0.33 | 2.42 | 47,47,47,47 | 0 |
| 31 | MG | 0 | 8117 | 1/1 | 0.17 | 2.41 | 36,36,36,36 | 0 |
| 33 | NA | 0 | 8325 | 1/1 | 0.18 | 2.03 | 47,47,47,47 | 0 |
| 33 | NA | 0 | 8382 | 1/1 | 0.14 | 1.93 | 64,64,64,64 | 0 |
| 33 | NA | 0 | 8365 | 1/1 | 0.28 | 1.84 | 28,28,28,28 | 0 |
| 33 | NA | 0 | 8308 | 1/1 | 0.15 | 1.72 | 42,42,42,42 | 0 |
| 33 | NA | 0 | 8321 | 1/1 | 0.19 | 1.02 | 40,40,40,40 | 0 |
| 33 | NA | 0 | 8328 | 1/1 | 0.13 | 0.89 | 28,28,28,28 | 0 |
| 33 | NA | H | 8322 | 1/1 | 0.17 | 0.58 | 52,52,52,52 | 0 |
| 31 | MG | 0 | 8015 | 1/1 | 0.17 | 0.50 | 26,26,26,26 | 0 |
| 31 | MG | 0 | 8041 | 1/1 | 0.12 | 0.32 | 33,33,33,33 | 0 |
| 34 | CL | 0 | 8514 | 1/1 | 0.15 | 0.28 | 36,36,36,36 | 0 |
| 34 | CL | 0 | 8516 | 1/1 | 0.13 | 0.20 | 42,42,42,42 | 0 |
| 34 | CL | 0 | 8503 | 1/1 | 0.13 | 0.07 | 40,40,40,40 | 0 |
| 33 | NA | 0 | 8356 | 1/1 | 0.15 | 0.02 | 37,37,37,37 | 0 |
| 33 | NA | 0 | 8315 | 1/1 | 0.17 | -0.18 | 30,30,30,30 | 0 |
| 33 | NA | 0 | 8324 | 1/1 | 0.12 | -0.22 | 48,48,48,48 | 0 |
| 31 | MG | 0 | 8010 | 1/1 | 0.14 | -0.35 | 24,24,24,24 | 0 |
| 31 | MG | 0 | 8026 | 1/1 | 0.15 | -0.36 | 26,26,26,26 | 0 |
| 33 | NA | 0 | 8375 | 1/1 | 0.17 | -0.50 | 39,39,39,39 | 0 |
| 31 | MG | 0 | 8067 | 1/1 | 0.12 | -0.56 | 34,34,34,34 | 0 |
| 31 | MG | 9 | 8095 | 1/1 | 0.14 | -0.57 | 69,69,69,69 | 0 |
| 31 | MG | J | 8069 | 1/1 | 0.12 | -0.59 | 46,46,46,46 | 0 |
| 35 | CD | Y | 8403 | 1/1 | 0.13 | -0.65 | 49,49,49,49 | 0 |
| 33 | NA | C | 8304 | 1/1 | 0.12 | -0.66 | 30,30,30,30 | 0 |
| 31 | MG | 0 | 8013 | 1/1 | 0.13 | -0.77 | 22,22,22,22 | 0 |
| 31 | MG | 0 | 8049 | 1/1 | 0.11 | -0.92 | 56,56,56,56 | 0 |
| 35 | CD | T | 8401 | 1/1 | 0.10 | -0.92 | 49,49,49,49 | 0 |
| 31 | MG | 0 | 8086 | 1/1 | 0.07 | -0.94 | 33,33,33,33 | 0 |
| 34 | CL | L | 8518 | 1/1 | 0.12 | -1.05 | 32,32,32,32 | 0 |
| 34 | CL | A | 8509 | 1/1 | 0.11 | -1.11 | 50,50,50,50 | 0 |
| 31 | MG | 0 | 8061 | 1/1 | 0.13 | -1.17 | 32,32,32,32 | 0 |
| 33 | NA | 0 | 8378 | 1/1 | 0.14 | -1.18 | 39,39,39,39 | 0 |
| 33 | NA | L | 8347 | 1/1 | 0.11 | -1.20 | 18,18,18,18 | 0 |
| 31 | MG | A | 8105 | 1/1 | 0.12 | -1.22 | 27,27,27,27 | 0 |
| 33 | NA | 0 | 8368 | 1/1 | 0.10 | -1.24 | 48,48,48,48 | 0 |
| 33 | NA | 0 | 8342 | 1/1 | 0.15 | -1.26 | 33,33,33,33 | 0 |
| 34 | CL | X | 8520 | 1/1 | 0.10 | -1.26 | 38,38,38,38 | 0 |
| 34 | CL | I | 8521 | 1/1 | 0.12 | -1.31 | 47,47,47,47 | 0 |
| 31 | MG | 0 | 8079 | 1/1 | 0.15 | -1.44 | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 31 | MG | 0 | 8106 | 1/1 | 0.11 | -1.63 | 42,42,42,42 | 0 |
| 35 | CD | 2 | 8404 | 1/1 | 0.08 | -1.66 | 47,47,47,47 | 0 |
| 31 | MG | 0 | 8038 | 1/1 | 0.11 | -1.69 | 22,22,22,22 | 0 |
| 33 | NA | 0 | 8311 | 1/1 | 0.11 | -1.70 | 48,48,48,48 | 0 |
| 31 | MG | 0 | 8102 | 1/1 | 0.10 | -1.73 | 51,51,51,51 | 0 |
| 31 | MG | 0 | 8054 | 1/1 | 0.14 | -1.87 | 18,18,18,18 | 0 |
| 33 | NA | H | 8309 | 1/1 | 0.06 | -1.89 | 28,28,28,28 | 0 |
| 33 | NA | 9 | 8351 | 1/1 | 0.11 | -1.90 | 42,42,42,42 | 0 |
| 34 | CL | I | 8502 | 1/1 | 0.07 | -1.92 | 53,53,53,53 | 0 |
| 31 | MG | 0 | 8104 | 1/1 | 0.12 | -2.02 | 45,45,45,45 | 0 |
| 34 | CL | 0 | 8511 | 1/1 | 0.08 | -2.05 | 37,37,37,37 | 0 |
| 31 | MG | 0 | 8064 | 1/1 | 0.11 | -2.08 | 26,26,26,26 | 0 |
| 33 | NA | I | 8346 | 1/1 | 0.07 | -2.15 | 34,34,34,34 | 0 |
| 33 | NA | 0 | 8319 | 1/1 | 0.10 | -2.17 | 29,29,29,29 | 0 |
| 31 | MG | 0 | 8023 | 1/1 | 0.13 | -2.21 | 30,30,30,30 | 0 |
| 31 | MG | 0 | 8077 | 1/1 | 0.14 | -2.21 | 23,23,23,23 | 0 |
| 31 | MG | 0 | 8093 | 1/1 | 0.12 | -2.22 | 35,35,35,35 | 0 |
| 33 | NA | 0 | 8305 | 1/1 | 0.12 | -2.23 | 32,32,32,32 | 0 |
| 33 | NA | 0 | 8344 | 1/1 | 0.08 | -2.28 | 24,24,24,24 | 0 |
| 34 | CL | I | 8501 | 1/1 | 0.07 | -2.36 | 44,44,44,44 | 0 |
| 35 | CD | N | 8405 | 1/1 | 0.07 | -2.38 | 71,71,71,71 | 0 |
| 34 | CL | K | 8510 | 1/1 | 0.06 | -2.39 | 36,36,36,36 | 0 |
| 33 | NA | 0 | 8317 | 1/1 | 0.09 | -2.40 | 27,27,27,27 | 0 |
| 31 | MG | 0 | 8003 | 1/1 | 0.10 | -2.52 | 21,21,21,21 | 0 |
| 31 | MG | 0 | 8091 | 1/1 | 0.09 | -2.53 | 41,41,41,41 | 0 |
| 33 | NA | 0 | 8316 | 1/1 | 0.15 | -2.57 | 35,35,35,35 | 0 |
| 33 | NA | P | 8348 | 1/1 | 0.06 | -2.57 | 32,32,32,32 | 0 |
| 34 | CL | N | 8508 | 1/1 | 0.06 | -2.61 | 52,52,52,52 | 0 |
| 31 | MG | S | 8073 | 1/1 | 0.04 | -2.62 | 39,39,39,39 | 0 |
| 33 | NA | 0 | 8339 | 1/1 | 0.11 | -2.63 | 20,20,20,20 | 0 |
| 31 | MG | 0 | 8074 | 1/1 | 0.05 | -2.63 | 36,36,36,36 | 0 |
| 33 | NA | 0 | 8349 | 1/1 | 0.13 | -2.68 | 37,37,37,37 | 0 |
| 31 | MG | 0 | 8027 | 1/1 | 0.04 | -2.68 | 37,37,37,37 | 0 |
| 31 | MG | 0 | 8108 | 1/1 | 0.09 | -2.76 | 62,62,62,62 | 0 |
| 34 | CL | B | 8519 | 1/1 | 0.10 | -2.81 | 33,33,33,33 | 0 |
| 34 | CL | M | 8507 | 1/1 | 0.06 | -2.82 | 45,45,45,45 | 0 |
| 33 | NA | S | 8343 | 1/1 | 0.05 | -2.85 | 29,29,29,29 | 0 |
| 31 | MG | 0 | 8001 | 1/1 | 0.12 | -2.92 | 25,25,25,25 | 0 |
| 33 | NA | 0 | 8334 | 1/1 | 0.06 | -2.96 | 33,33,33,33 | 0 |
| 34 | CL | 0 | 8515 | 1/1 | 0.09 | -2.98 | 48,48,48,48 | 0 |
| 34 | CL | 0 | 8512 | 1/1 | 0.07 | -3.04 | 34,34,34,34 | 0 |
| 34 | CL | Q | 8506 | 1/1 | 0.09 | -3.04 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 33 | NA | A | 8345 | 1/1 | 0.08 | -3.05 | 46,46,46,46 | 0 |
| 31 | MG | 0 | 8070 | 1/1 | 0.14 | -3.08 | 40,40,40,40 | 0 |
| 33 | NA | 0 | 8306 | 1/1 | 0.11 | -3.10 | 28,28,28,28 | 0 |
| 31 | MG | B | 8055 | 1/1 | 0.08 | -3.11 | 40,40,40,40 | 0 |
| 31 | MG | 0 | 8004 | 1/1 | 0.12 | -3.12 | 21,21,21,21 | 0 |
| 31 | MG | 0 | 8081 | 1/1 | 0.09 | -3.20 | 39,39,39,39 | 0 |
| 31 | MG | 0 | 8047 | 1/1 | 0.09 | -3.21 | 54,54,54,54 | 0 |
| 33 | NA | 0 | 8332 | 1/1 | 0.09 | -3.21 | 33,33,33,33 | 0 |
| 31 | MG | 0 | 8024 | 1/1 | 0.08 | -3.25 | 22,22,22,22 | 0 |
| 31 | MG | 0 | 8020 | 1/1 | 0.10 | -3.26 | 24,24,24,24 | 0 |
| 33 | NA | 0 | 8335 | 1/1 | 0.10 | -3.30 | 31,31,31,31 | 0 |
| 31 | MG | 0 | 8009 | 1/1 | 0.13 | -3.34 | 24,24,24,24 | 0 |
| 31 | MG | 0 | 8107 | 1/1 | 0.03 | -3.49 | 30,30,30,30 | 0 |
| 33 | NA | 0 | 8310 | 1/1 | 0.07 | -3.56 | 27,27,27,27 | 0 |
| 34 | CL | 0 | 8505 | 1/1 | 0.08 | -3.57 | 41,41,41,41 | 0 |
| 31 | MG | 0 | 8046 | 1/1 | 0.05 | -3.60 | 38,38,38,38 | 0 |
| 31 | MG | 0 | 8005 | 1/1 | 0.14 | -3.60 | 24,24,24,24 | 0 |
| 31 | MG | 0 | 8080 | 1/1 | 0.07 | -3.61 | 41,41,41,41 | 0 |
| 33 | NA | 0 | 8333 | 1/1 | 0.06 | -3.61 | 23,23,23,23 | 0 |
| 31 | MG | 0 | 8016 | 1/1 | 0.09 | -3.64 | 32,32,32,32 | 0 |
| 31 | MG | 0 | 8096 | 1/1 | 0.08 | -3.64 | 37,37,37,37 | 0 |
| 33 | NA | 0 | 8341 | 1/1 | 0.09 | -3.68 | 37,37,37,37 | 0 |
| 31 | MG | 2 | 8078 | 1/1 | 0.08 | -3.85 | 39,39,39,39 | 0 |
| 31 | MG | 0 | 8033 | 1/1 | 0.08 | -3.93 | 20,20,20,20 | 0 |
| 31 | MG | 0 | 8050 | 1/1 | 0.13 | -3.94 | 56,56,56,56 | 0 |
| 31 | MG | 0 | 8053 | 1/1 | 0.09 | -3.95 | 28,28,28,28 | 0 |
| 31 | MG | 0 | 8008 | 1/1 | 0.08 | -3.98 | 22,22,22,22 | 0 |
| 31 | MG | X | 8109 | 1/1 | 0.07 | -3.99 | 25,25,25,25 | 0 |
| 31 | MG | 0 | 8045 | 1/1 | 0.05 | -4.09 | 51,51,51,51 | 0 |
| 31 | MG | 0 | 8030 | 1/1 | 0.07 | -4.10 | 22,22,22,22 | 0 |
| 33 | NA | Q | 8337 | 1/1 | 0.06 | -4.17 | 33,33,33,33 | 0 |
| 35 | CD | Z | 8402 | 1/1 | 0.03 | -4.19 | 37,37,37,37 | 0 |
| 31 | MG | 0 | 8051 | 1/1 | 0.07 | -4.32 | 56,56,56,56 | 0 |
| 31 | MG | 0 | 8116 | 1/1 | 0.08 | -4.34 | 42,42,42,42 | 0 |
| 31 | MG | 0 | 8025 | 1/1 | 0.07 | -4.36 | 36,36,36,36 | 0 |
| 31 | MG | 0 | 8068 | 1/1 | 0.04 | -4.37 | 44,44,44,44 | 0 |
| 31 | MG | 0 | 8011 | 1/1 | 0.10 | -4.51 | 23,23,23,23 | 0 |
| 31 | MG | 0 | 8058 | 1/1 | 0.07 | -4.60 | 27,27,27,27 | 0 |
| 34 | CL | 2 | 8504 | 1/1 | 0.05 | -4.66 | 45,45,45,45 | 0 |
| 31 | MG | 0 | 8075 | 1/1 | 0.07 | -4.68 | 28,28,28,28 | 0 |
| 31 | MG | 0 | 8034 | 1/1 | 0.10 | -4.69 | 31,31,31,31 | 0 |
| 34 | CL | 0 | 8517 | 1/1 | 0.08 | -4.71 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 31 | MG | 0 | 8056 | 1/1 | 0.06 | -4.72 | 31,31,31,31 | 0 |
| 31 | MG | 0 | 8022 | 1/1 | 0.13 | -4.89 | 32,32,32,32 | 0 |
| 31 | MG | 0 | 8037 | 1/1 | 0.06 | -4.91 | 35,35,35,35 | 0 |
| 31 | MG | 0 | 8114 | 1/1 | 0.06 | -4.92 | 35,35,35,35 | 0 |
| 31 | MG | A | 8065 | 1/1 | 0.06 | -4.92 | 24,24,24,24 | 0 |
| 34 | CL | 0 | 8513 | 1/1 | 0.07 | -4.97 | 44,44,44,44 | 0 |
| 31 | MG | 0 | 8040 | 1/1 | 0.10 | -5.18 | 38,38,38,38 | 0 |
| 31 | MG | 0 | 8084 | 1/1 | 0.05 | -5.28 | 39,39,39,39 | 0 |
| 33 | NA | 0 | 8338 | 1/1 | 0.05 | -5.36 | 36,36,36,36 | 0 |
| 31 | MG | 0 | 8035 | 1/1 | 0.07 | -5.37 | 36,36,36,36 | 0 |
| 31 | MG | 0 | 8088 | 1/1 | 0.06 | -5.50 | 20,20,20,20 | 0 |
| 31 | MG | 0 | 8112 | 1/1 | 0.06 | -5.52 | 23,23,23,23 | 0 |
| 31 | MG | 0 | 8057 | 1/1 | 0.10 | -5.53 | 35,35,35,35 | 0 |
| 31 | MG | 0 | 8094 | 1/1 | 0.08 | -5.59 | 59,59,59,59 | 0 |
| 31 | MG | 0 | 8072 | 1/1 | 0.09 | -5.60 | 47,47,47,47 | 0 |
| 31 | MG | 0 | 8036 | 1/1 | 0.08 | -5.65 | 35,35,35,35 | 0 |
| 31 | MG | 0 | 8098 | 1/1 | 0.08 | -5.66 | 27,27,27,27 | 0 |
| 33 | NA | 0 | 8353 | 1/1 | 0.08 | -5.68 | 18,18,18,18 | 0 |
| 31 | MG | 0 | 8017 | 1/1 | 0.12 | -6.20 | 12,12,12,12 | 0 |
| 33 | NA | 0 | 8357 | 1/1 | 0.06 | -6.23 | 39,39,39,39 | 0 |
| 33 | NA | 0 | 8330 | 1/1 | 0.05 | -6.46 | 39,39,39,39 | 0 |
| 33 | NA | 0 | 8354 | 1/1 | 0.13 | -6.56 | 25,25,25,25 | 0 |
| 31 | MG | 0 | 8031 | 1/1 | 0.10 | -6.68 | 24,24,24,24 | 0 |
| 31 | MG | 0 | 8021 | 1/1 | 0.08 | -6.68 | 24,24,24,24 | 0 |
| 31 | MG | 0 | 8044 | 1/1 | 0.07 | -6.69 | 32,32,32,32 | 0 |
| 31 | MG | 0 | 8110 | 1/1 | 0.07 | -6.77 | 24,24,24,24 | 0 |
| 33 | NA | R | 8312 | 1/1 | 0.07 | -6.91 | 26,26,26,26 | 0 |
| 31 | MG | 0 | 8063 | 1/1 | 0.07 | -7.17 | 62,62,62,62 | 0 |
| 31 | MG | 0 | 8085 | 1/1 | 0.07 | -7.25 | 35,35,35,35 | 0 |
| 33 | NA | 0 | 8323 | 1/1 | 0.07 | -7.48 | 31,31,31,31 | 0 |
| 33 | NA | 0 | 8313 | 1/1 | 0.06 | -7.68 | 48,48,48,48 | 0 |
| 31 | MG | 0 | 8113 | 1/1 | 0.10 | -7.71 | 36,36,36,36 | 0 |
| 31 | MG | 0 | 8029 | 1/1 | 0.09 | -7.78 | 35,35,35,35 | 0 |
| 31 | MG | 0 | 8059 | 1/1 | 0.06 | -7.99 | 25,25,25,25 | 0 |
| 33 | NA | 0 | 8381 | 1/1 | 0.05 | -8.03 | 41,41,41,41 | 0 |
| 31 | MG | 0 | 8062 | 1/1 | 0.07 | -8.07 | 41,41,41,41 | 0 |
| 32 | K | 0 | 8201 | 1/1 | 0.08 | -8.08 | 62,62,62,62 | 0 |
| 31 | MG | 0 | 8039 | 1/1 | 0.07 | -8.12 | 32,32,32,32 | 0 |
| 31 | MG | 0 | 8019 | 1/1 | 0.04 | -8.31 | 23,23,23,23 | 0 |
| 31 | MG | 0 | 8071 | 1/1 | 0.05 | -8.45 | 62,62,62,62 | 0 |
| 33 | NA | 0 | 8301 | 1/1 | 0.07 | -8.58 | 33,33,33,33 | 0 |
| 33 | NA | 0 | 8303 | 1/1 | 0.10 | -8.64 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|-----------------------------|-------|
| 31 | MG | 0 | 8032 | 1/1 | 0.04 | -8.76 | 23,23,23,23 | 0 |
| 31 | MG | 0 | 8018 | 1/1 | 0.05 | -8.97 | 27,27,27,27 | 0 |
| 31 | MG | 0 | 8006 | 1/1 | 0.07 | -9.10 | 27,27,27,27 | 0 |
| 31 | MG | 0 | 8076 | 1/1 | 0.04 | -9.11 | 46,46,46,46 | 0 |
| 31 | MG | 0 | 8052 | 1/1 | 0.06 | -9.76 | 45,45,45,45 | 0 |
| 31 | MG | 0 | 8083 | 1/1 | 0.06 | -10.16 | 30,30,30,30 | 0 |
| 33 | NA | 0 | 8352 | 1/1 | 0.07 | -10.16 | 40,40,40,40 | 0 |
| 32 | K | 0 | 8202 | 1/1 | 0.06 | -10.17 | 37,37,37,37 | 0 |
| 31 | MG | 0 | 8100 | 1/1 | 0.07 | -10.35 | 64,64,64,64 | 0 |
| 31 | MG | 0 | 8111 | 1/1 | 0.06 | -10.79 | 32,32,32,32 | 0 |
| 31 | MG | 0 | 8092 | 1/1 | 0.07 | -11.28 | 66,66,66,66 | 0 |
| 31 | MG | 0 | 8028 | 1/1 | 0.04 | -11.71 | 25,25,25,25 | 0 |
| 31 | MG | 0 | 8002 | 1/1 | 0.06 | -12.28 | 26,26,26,26 | 0 |
| 31 | MG | 0 | 8014 | 1/1 | 0.07 | -12.39 | 25,25,25,25 | 0 |
| 31 | MG | 0 | 8043 | 1/1 | 0.05 | -12.84 | 33,33,33,33 | 0 |
| 31 | MG | 0 | 8048 | 1/1 | 0.05 | -13.00 | 39,39,39,39 | 0 |
| 31 | MG | 0 | 8089 | 1/1 | 0.06 | -17.58 | 51,51,51,51 | 0 |
| 33 | NA | 0 | 8336 | 1/1 | 0.04 | -17.64 | 37,37,37,37 | 0 |
| 31 | MG | 0 | 8115 | 1/1 | 0.07 | -23.50 | 36,36,36,36 | 0 |
| 31 | MG | 0 | 8097 | 1/1 | 0.06 | -26.68 | 30,30,30,30 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.