



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:56 PM GMT

PDB ID : 1M90
Title : Co-crystal structure of CCA-Phe-caproic acid-biotin and sparsomycin bound to the 50S ribosomal subunit
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-07-26
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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

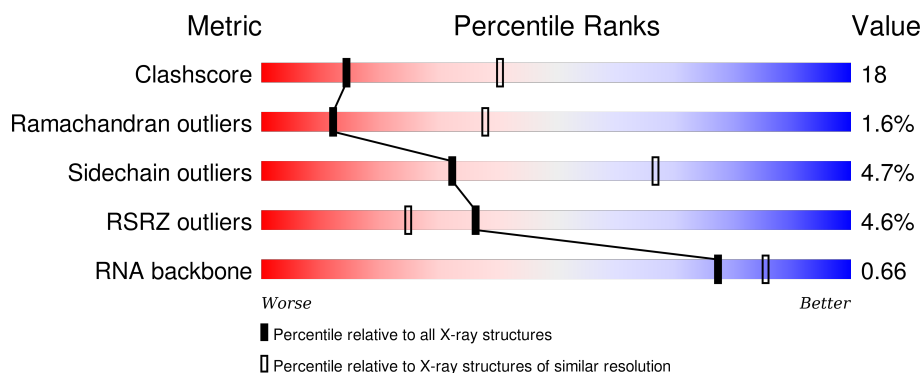
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.




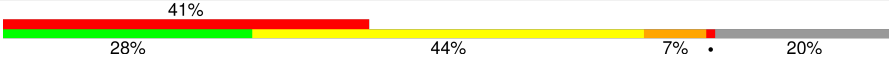
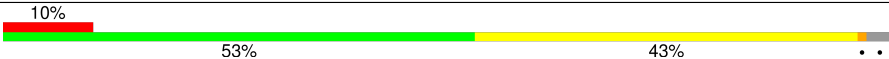
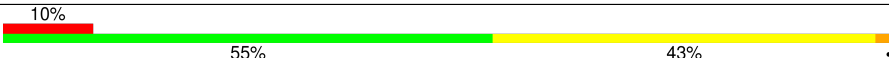
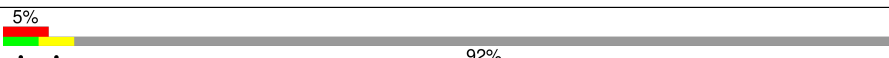
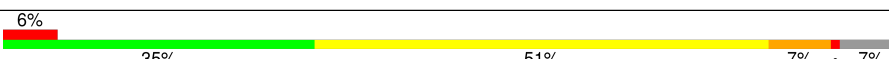
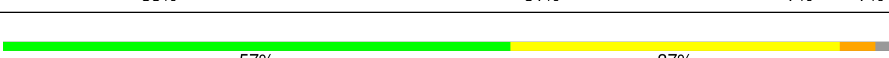
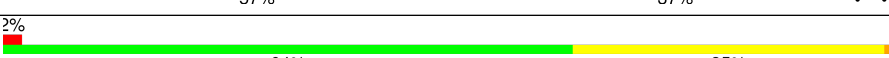
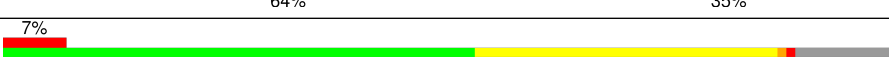
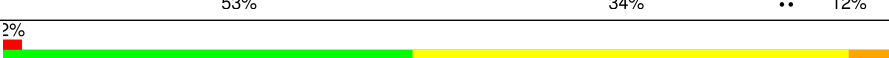








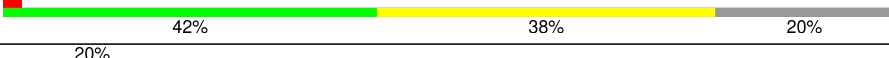
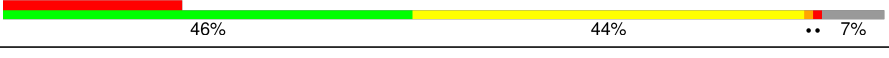

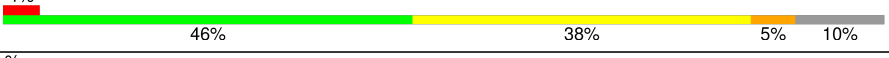
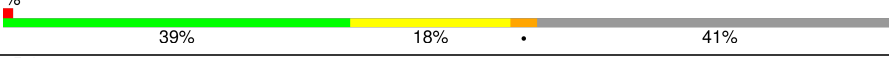


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 2827 (2.80-2.80) |
| Ramachandran outliers | 100387 | 2782 (2.80-2.80) |
| Sidechain outliers | 100360 | 2784 (2.80-2.80) |
| RSRZ outliers | 91569 | 2404 (2.80-2.80) |
| RNA backbone | 2183 | 1091 (3.20-2.40) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 2922 | <div> <div>2%</div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div> |
| 2 | B | 122 | <div> <div>3%</div> <div>49%</div> <div>38%</div> <div>11%</div> <div>•</div> </div> |
| 3 | 5 | 3 | <div> <div>67%</div> <div>33%</div> </div> |
| 4 | C | 239 | <div> <div>5%</div> <div>60%</div> <div>32%</div> <div>7%</div> <div>•</div> </div> |
| 5 | D | 337 | <div> <div>%</div> <div>50%</div> <div>44%</div> <div>6%</div> </div> |


Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 6 | E | 246 |  |
| 7 | F | 176 |  |
| 8 | G | 177 |  |
| 9 | H | 119 |  |
| 10 | I | 348 |  |
| 11 | J | 167 |  |
| 12 | K | 145 |  |
| 13 | L | 132 |  |
| 14 | M | 164 |  |
| 15 | N | 194 |  |
| 16 | O | 186 |  |
| 17 | P | 115 |  |
| 18 | Q | 148 |  |
| 19 | R | 95 |  |
| 20 | S | 154 |  |
| 21 | T | 84 |  |
| 22 | U | 119 |  |
| 23 | V | 66 |  |
| 24 | W | 70 |  |
| 25 | X | 154 |  |
| 26 | Y | 91 |  |
| 27 | Z | 240 |  |
| 28 | 1 | 73 |  |
| 29 | 2 | 56 |  |
| 30 | 3 | 48 |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 31 | 4 | 92 |  % 61% 35% |

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 | A | 8060 | - | - | - | X |
| 33 | NA | A | 8303 | - | - | - | X |
| 33 | NA | A | 8310 | - | - | - | X |
| 33 | NA | A | 8321 | - | - | - | X |
| 33 | NA | A | 8325 | - | - | - | X |
| 33 | NA | A | 8331 | - | - | - | X |
| 33 | NA | A | 8335 | - | - | - | X |
| 33 | NA | A | 8340 | - | - | - | X |
| 33 | NA | A | 8350 | - | - | - | X |
| 33 | NA | A | 8356 | - | - | - | X |
| 33 | NA | A | 8359 | - | - | - | X |
| 33 | NA | A | 8361 | - | - | - | X |
| 33 | NA | A | 8362 | - | - | - | X |
| 33 | NA | A | 8364 | - | - | - | X |
| 33 | NA | A | 8366 | - | - | - | X |
| 33 | NA | A | 8368 | - | - | - | X |
| 33 | NA | A | 8371 | - | - | - | X |
| 33 | NA | A | 8372 | - | - | - | X |
| 33 | NA | A | 8373 | - | - | - | X |
| 33 | NA | A | 8374 | - | - | - | X |
| 33 | NA | A | 8378 | - | - | - | X |
| 33 | NA | B | 8383 | - | - | - | X |
| 33 | NA | M | 8380 | - | - | - | X |
| 33 | NA | S | 8386 | - | - | - | X |
| 34 | K | A | 8390 | - | - | - | X |
| 34 | K | A | 8391 | - | - | - | X |
| 35 | CL | A | 8515 | - | - | - | X |
| 36 | SPS | 5 | 9080 | - | - | - | X |
| 37 | PHA | 5 | 9077 | - | - | - | X |
| 38 | ACA | 5 | 9078 | - | - | - | X |

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98611 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 RRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | A | 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 |
|-------|---------|----------|--------|----------|------------|
| A | 560 | C | U | CONFLICT | GB 3377779 |

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

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

- Molecule 3 is a RNA chain called CCA.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | D | 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 |
|-------|---------|----------|--------|----------|------------|
| D | ? | - | PRO | DELETION | UNP P20279 |
| D | 310 | ARG | PHE | CONFLICT | UNP P20279 |

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 28 | 1 | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 563 | 359 | 111 | 86 | 7 | | | |

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 2 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 258 | 86 | 82 | 4 | | | |

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | 3 | 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 |
|-------|---------|----------|--------|----------|------------|
| 3 | ? | - | ARG | DELETION | UNP P22452 |

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | 4 | 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 | 1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | C | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | Z | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 111 | Total | Mg | 0 | 0 |
| | | | 111 | 111 | | |
| 32 | 4 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | U | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | L | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 33 | J | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | K | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | E | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | B | 2 | Total | Na | 0 | 0 |
| | | | 2 | 2 | | |
| 33 | C | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | A | 73 | Total | Na | 0 | 0 |
| | | | 73 | 73 | | |
| 33 | T | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | N | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 33 | U | 1 | Total 1 | Na 1 | 0 | 0 |
| 33 | R | 1 | Total 1 | Na 1 | 0 | 0 |
| 33 | S | 2 | Total 2 | Na 2 | 0 | 0 |
| 33 | M | 1 | Total 1 | Na 1 | 0 | 0 |

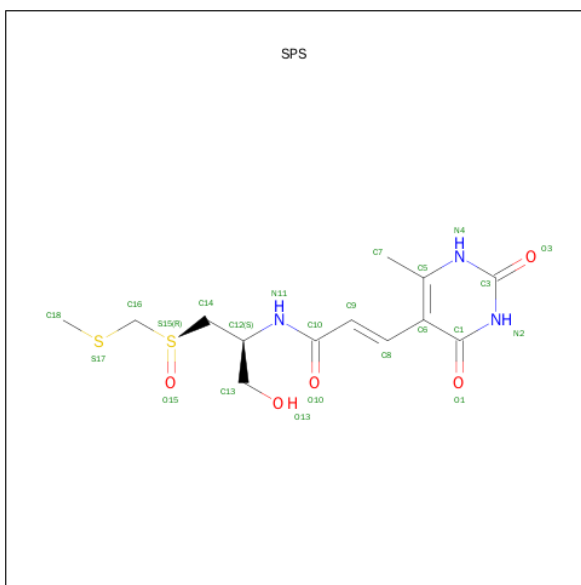
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 34 | A | 2 | Total 2 | K 2 | 0 | 0 |

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

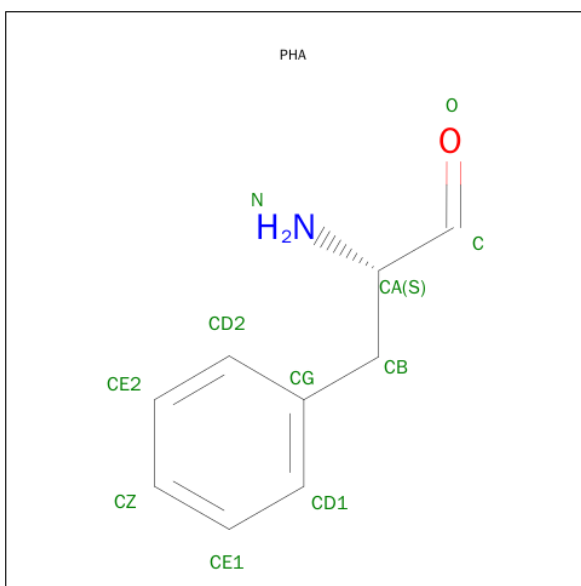
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 35 | P | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | D | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | K | 3 | Total 3 | Cl 3 | 0 | 0 |
| 35 | C | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | Z | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | A | 10 | Total 10 | Cl 10 | 0 | 0 |
| 35 | 4 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | N | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | O | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | S | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | M | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 36 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



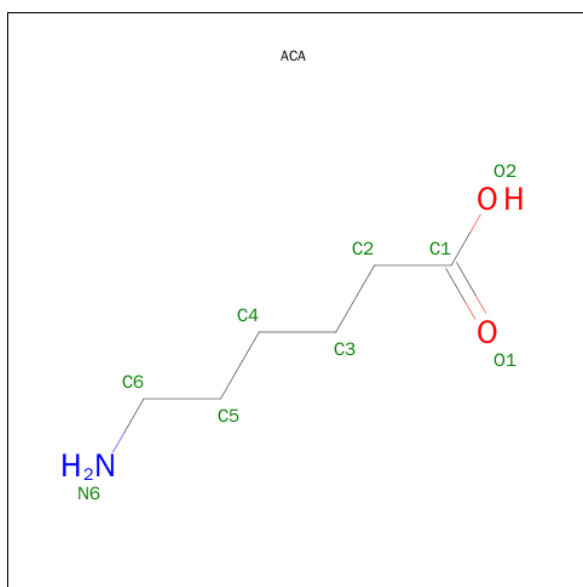
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 36 | 5 | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 23 | 13 | 3 | 5 | 2 | | |

- Molecule 37 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 37 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 11 | 9 | 1 | 1 | | |

- Molecule 38 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula: $C_6H_{13}NO_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 38 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 8 | 6 | 1 | 1 | | |

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 39 | P | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |
| 39 | 2 | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |
| 39 | 1 | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |
| 39 | 4 | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |
| 39 | V | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 40 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 40 | A | 5920 | Total | O | 0 | 0 |
| | | | 5920 | 5920 | | |
| 40 | B | 136 | Total | O | 0 | 0 |
| | | | 136 | 136 | | |
| 40 | 5 | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 40 | C | 119 | Total 119 | O 119 | 0 | 0 |
| 40 | D | 142 | Total 142 | O 142 | 0 | 0 |
| 40 | E | 172 | Total 172 | O 172 | 0 | 0 |
| 40 | F | 51 | Total 51 | O 51 | 0 | 0 |
| 40 | G | 44 | Total 44 | O 44 | 0 | 0 |
| 40 | H | 28 | Total 28 | O 28 | 0 | 0 |
| 40 | I | 21 | Total 21 | O 21 | 0 | 0 |
| 40 | J | 75 | Total 75 | O 75 | 0 | 0 |
| 40 | K | 56 | Total 56 | O 56 | 0 | 0 |
| 40 | L | 61 | Total 61 | O 61 | 0 | 0 |
| 40 | M | 86 | Total 86 | O 86 | 0 | 0 |
| 40 | N | 125 | Total 125 | O 125 | 0 | 0 |
| 40 | O | 69 | Total 69 | O 69 | 0 | 0 |
| 40 | P | 43 | Total 43 | O 43 | 0 | 0 |
| 40 | Q | 67 | Total 67 | O 67 | 0 | 0 |
| 40 | R | 49 | Total 49 | O 49 | 0 | 0 |
| 40 | S | 83 | Total 83 | O 83 | 0 | 0 |
| 40 | T | 35 | Total 35 | O 35 | 0 | 0 |
| 40 | U | 37 | Total 37 | O 37 | 0 | 0 |
| 40 | V | 24 | Total 24 | O 24 | 0 | 0 |
| 40 | W | 16 | Total 16 | O 16 | 0 | 0 |

Continued on next page...

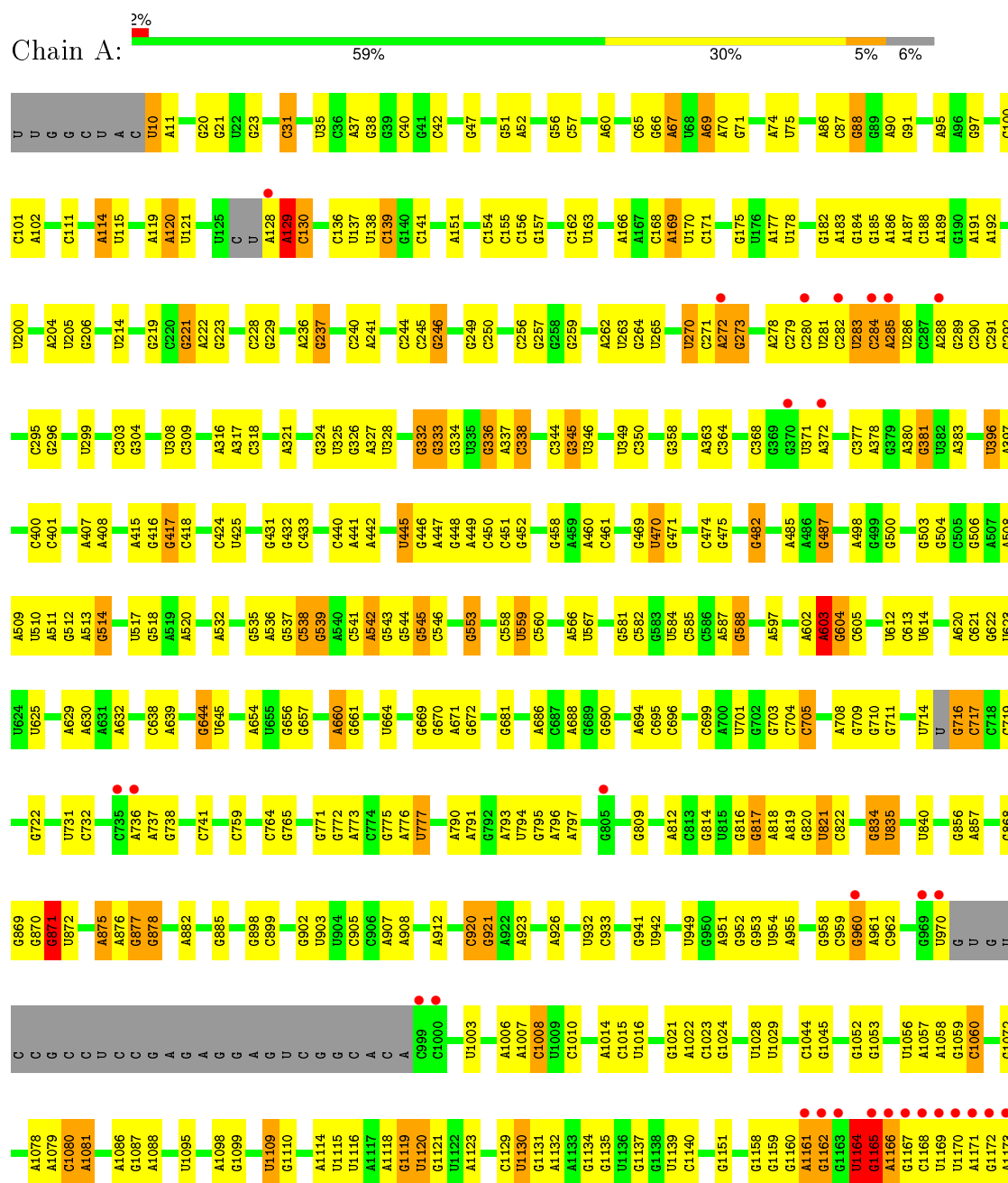
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 40 | X | 71 | Total 71 | O 71 | 0 | 0 |
| 40 | Y | 31 | Total 31 | O 31 | 0 | 0 |
| 40 | Z | 92 | Total 92 | O 92 | 0 | 0 |
| 40 | 1 | 36 | Total 36 | O 36 | 0 | 0 |
| 40 | 2 | 55 | Total 55 | O 55 | 0 | 0 |
| 40 | 3 | 40 | Total 40 | O 40 | 0 | 0 |
| 40 | 4 | 73 | Total 73 | O 73 | 0 | 0 |

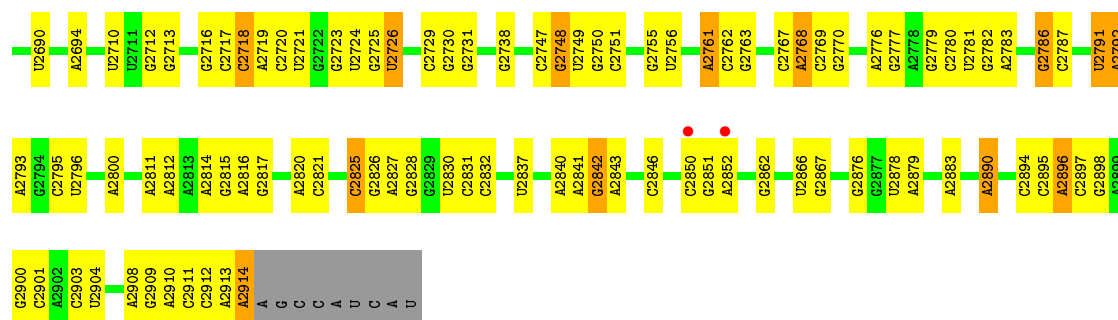
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

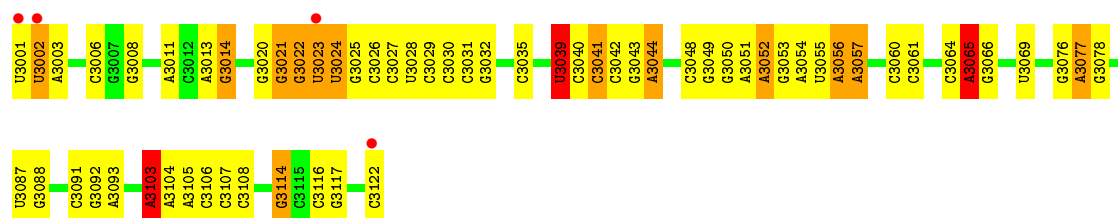
• Molecule 1: 23S rRNA



| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|---|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C2582 | A2479 | G2379 | G2275 | U | G | U2034 | A1941 | G1819 | U1702 | U1596 | C1472 | G1351 | A1242 | A1174 |
| G2480 | G2480 | G2383 | C2281 | C | C | G2044 | A1942 | G1820 | A1717 | A1597 | U1473 | G1352 | C1243 | G1175 |
| A2483 | A2483 | U2384 | U2282 | A | C | G | C1943 | G1827 | G | A1598 | C1474 | A1352 | U1244 | C1176 |
| A2485 | A2485 | G2385 | U2282 | A | C | A2054 | G1946 | G1828 | U1723 | A1503 | G1477 | C1353 | A1246 | A1177 |
| A2490 | A2490 | U2387 | A2291 | A | U | A2055 | G1947 | A1829 | G1723 | G1604 | U1478 | U1359 | U1249 | G1178 |
| C2591 | C2588 | C2388 | A2300 | C | U | C2061 | G1948 | C1830 | U1724 | G1605 | U1482 | C1360 | C1250 | U1180 |
| C2494 | A2401 | U2387 | A2301 | U | G | A2062 | G1949 | C1834 | G1730 | C1609 | A1483 | C1251 | C1250 | A1181 |
| C2494 | A2402 | U2387 | A2302 | U | C | U2063 | G1950 | U1835 | C1731 | G1610 | C1483 | C1252 | C1251 | C1182 |
| C2502 | C2403 | C2403 | U2308 | A | C | U2064 | U | U1835 | G1731 | G1613 | A1485 | C1253 | C1253 | C1183 |
| A2503 | A2408 | A | U2309 | A | G | G2068 | A | A1840 | A1732 | C1614 | U1488 | U1266 | U1266 | U1185 |
| A2504 | A2408 | A | G2310 | U | C | G2069 | A | A1845 | A1733 | G1614 | U1488 | U1267 | U1267 | U1186 |
| A2506 | G2412 | C | G2311 | A | A | U2069 | C | U1846 | G1734 | A1615 | A1494 | C1268 | C1268 | A1188 |
| G2507 | A2413 | U | C2313 | U | U | G2070 | U | U1847 | C1735 | U1625 | G1497 | C1269 | C1269 | A1189 |
| A2508 | A2414 | A | G2314 | C | G | G2071 | A | G1848 | A1736 | A1626 | U1497 | U1270 | U1270 | G1190 |
| A2509 | A2415 | C | G2315 | C | G | G2072 | G | G1856 | U1741 | G1627 | U1500 | C1275 | C1275 | A1191 |
| A2510 | G2416 | U | G2316 | C | U | A2074 | A | A1857 | A1742 | A1630 | U1500 | U1276 | U1276 | A1192 |
| A2511 | U2419 | C | C2317 | C | G | U2078 | C | G1867 | G1743 | A1637 | U1500 | U1277 | U1277 | A1193 |
| A2515 | G2420 | U | U2320 | G | A | G2079 | C | G1868 | G1744 | C1633 | U1503 | U1279 | U1279 | G1197 |
| A2516 | G2421 | C | A2321 | U | A | G2080 | U1964 | G1877 | G1745 | U1634 | A1504 | U1287 | U1287 | U1198 |
| G2526 | U2422 | G | G2324 | G | G | A2081 | C1965 | U1874 | U1751 | U1635 | A1505 | U1288 | U1288 | A1199 |
| G2527 | C2423 | U | C2325 | U | C | C2088 | U1967 | G1877 | G1752 | A1636 | U1506 | C1289 | C1289 | A1200 |
| G2533 | U2424 | C | U2326 | C | A | A2089 | C | G1878 | G1753 | A1637 | A1515 | U1290 | U1290 | C1201 |
| C2536 | U2425 | G | U2327 | G | C | G2090 | U1967 | G1878 | A1754 | A1641 | C1516 | G1290 | G1290 | G1202 |
| C2537 | U2426 | U | U2328 | U | C | G2091 | G1975 | U1879 | G1756 | A1642 | U1523 | A1294 | A1294 | U1205 |
| U2541 | G2427 | C | U2329 | C | U | G2092 | G1976 | U1880 | U1766 | U1654 | U1524 | U1298 | U1298 | U1206 |
| G2542 | G2428 | G | U2330 | C | A | G2093 | A1978 | U1881 | U1767 | G1855 | G1525 | G1299 | G1299 | A1207 |
| G2543 | U2434 | C | G2338 | C | C | G2094 | G1979 | U1882 | U1771 | U1667 | A1526 | U1304 | U1304 | C1208 |
| G2547 | U2435 | U | C2339 | C | C | A2095 | U1979 | U1883 | C1772 | A1656 | A1527 | U1305 | U1305 | G1210 |
| C2548 | G2436 | C | U2340 | C | G | G2096 | G1977 | U1884 | G1773 | A1657 | G1528 | A1309 | U1310 | G1211 |
| C2551 | A2438 | C | U2341 | C | A | A2101 | U1978 | G1887 | U1774 | U1666 | G1535 | U1309 | U1309 | C1212 |
| C2552 | U2439 | C | U2342 | C | U | G2102 | G1979 | U1887 | C1772 | U1667 | C1536 | U1310 | U1310 | G1213 |
| A2553 | U2440 | C | U2343 | C | C | A2103 | U1980 | U1887 | G1773 | U1668 | G1543 | G1433 | G1311 | G1214 |
| U2557 | G2441 | C | U2344 | C | C | G2104 | A1981 | U1887 | U1778 | A1669 | U1543 | G1434 | G1312 | G1215 |
| G2558 | U2442 | C | U2345 | C | C | U2107 | G1982 | U1887 | U1779 | C1675 | G1555 | U1435 | A1313 | G1216 |
| G2559 | U2443 | C | U2346 | C | C | U2108 | C1993 | G1891 | A1778 | G1676 | G1555 | U1436 | U1314 | U1218 |
| U2563 | A2456 | C | A2353 | C | C | U2109 | U1996 | G1902 | A1783 | A1677 | A1559 | A1441 | G1315 | U1219 |
| G2564 | U2457 | C | A2354 | C | C | G2110 | A1997 | U1903 | U1784 | A1678 | U | A1442 | G1316 | |
| G2565 | G2462 | C | G2355 | C | C | G2111 | U2004 | A1904 | C1787 | C1679 | U1561 | A1328 | A1328 | G1224 |
| G2567 | U2463 | C | A2356 | C | U | U2115 | G2005 | A1909 | U1788 | G1680 | C1562 | A1329 | G1225 | |
| G2568 | U2464 | C | A2357 | C | A | U2116 | G2006 | A1913 | G1789 | G1681 | C1563 | A1330 | C1225 | |
| G2569 | U2465 | C | A2358 | C | C | G2128 | U2008 | G1913 | C1798 | A1682 | C1564 | A1331 | C1229 | |
| G2570 | U2466 | C | U2285 | C | G | G2136 | G2009 | A1919 | C1798 | A1684 | C1565 | C1332 | A1230 | |
| G2571 | U2467 | C | A2286 | C | G | A | A2010 | C1920 | A1804 | A1685 | A1580 | U1333 | A1231 | |
| G2572 | U2468 | C | G2287 | C | C | C | U2011 | C1921 | C1686 | U1457 | C1450 | C1334 | A1232 | |
| G2573 | U2469 | C | C2288 | C | C | G | U2012 | A1921 | G1588 | A1458 | C1451 | C1335 | U1234 | |
| G2574 | G2472 | C | G2289 | C | A | U | G2013 | A1922 | G1589 | C1462 | G1452 | U1336 | G1235 | |
| G2575 | U2474 | C | G2290 | C | C | G | G2014 | G1926 | C1809 | A1463 | G1453 | G1339 | G1236 | |
| G2576 | U2475 | C | G2291 | C | C | U | A2015 | A1927 | C1809 | A1463 | G1453 | G1340 | U1237 | |
| G2577 | U2476 | C | G2292 | C | C | G | U2016 | C1940 | C1699 | A1470 | C1342 | C1238 | U1237 | |
| G2578 | U2477 | C | U2273 | C | A | U | G | C1940 | C1700 | C1342 | C1342 | G1239 | G1239 | |
| G2582 | U2478 | C | A2274 | C | G | C | G2033 | | A1315 | A1701 | G1595 | C1343 | | |



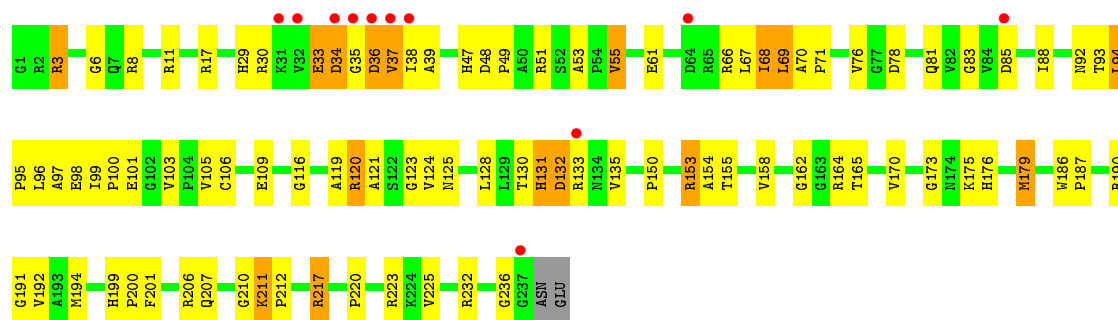
• Molecule 2: 5S RRNA



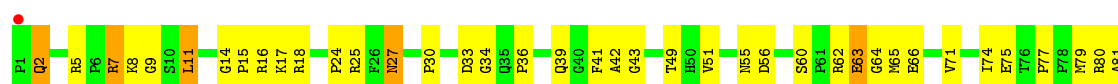
• Molecule 3: CCA

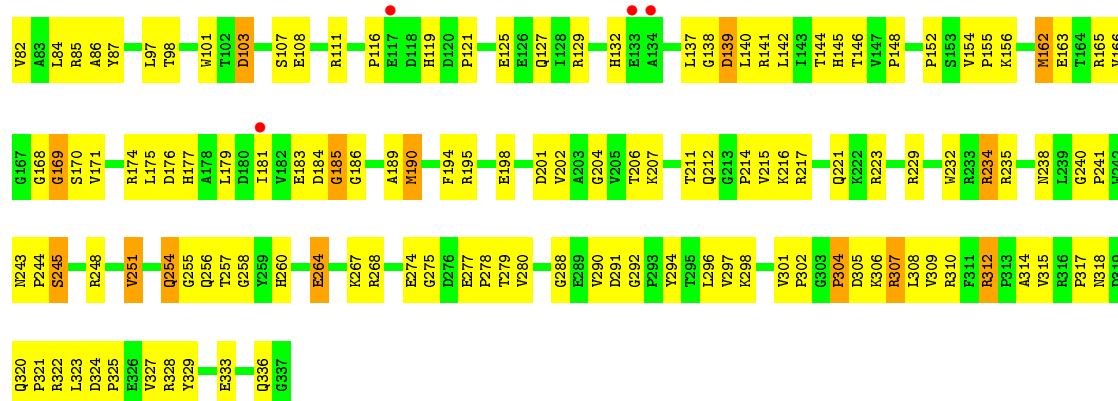


• Molecule 4: RIBOSOMAL PROTEIN L2

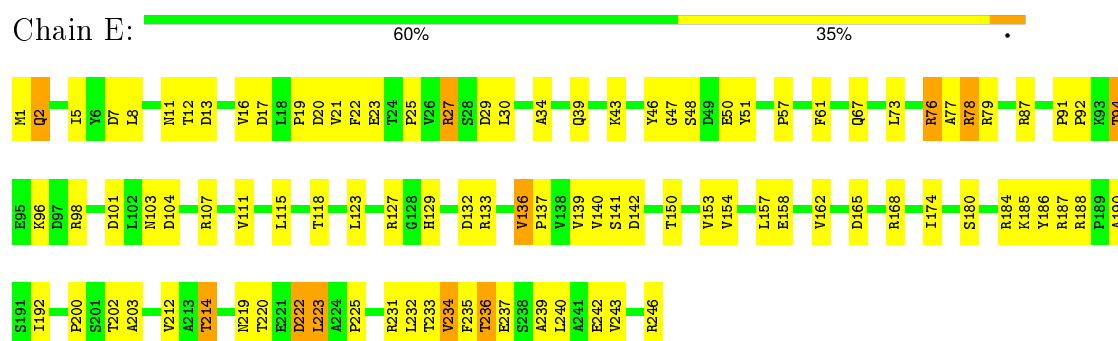


• Molecule 5: RIBOSOMAL PROTEIN L3

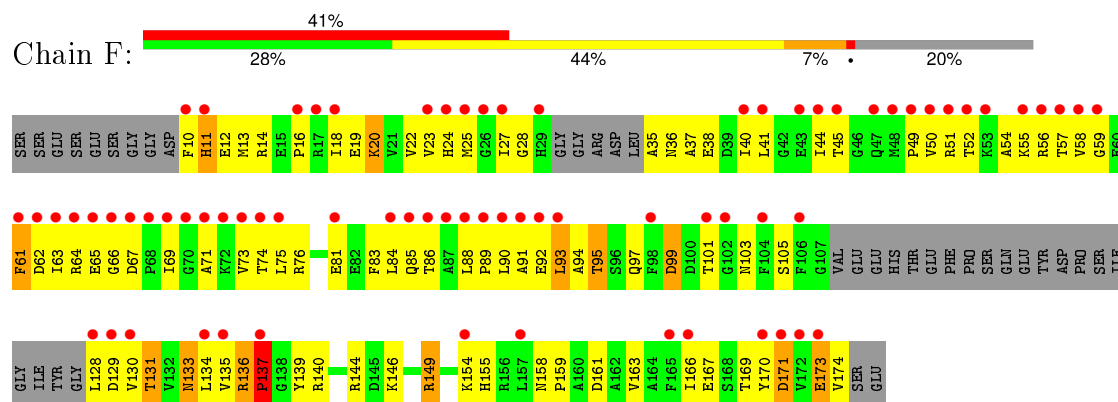




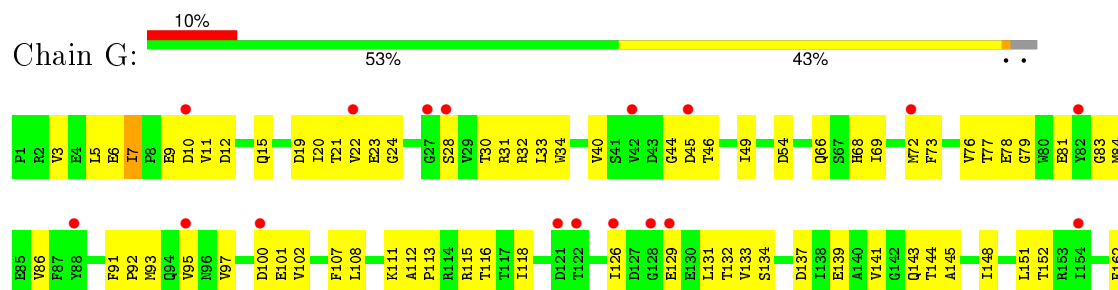
• Molecule 6: RIBOSOMAL PROTEIN L4



• Molecule 7: RIBOSOMAL PROTEIN L5

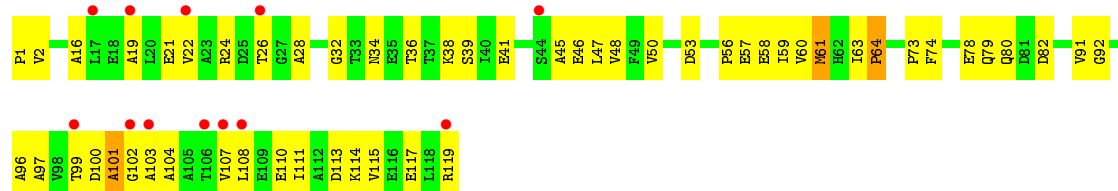


• Molecule 8: RIBOSOMAL PROTEIN L6

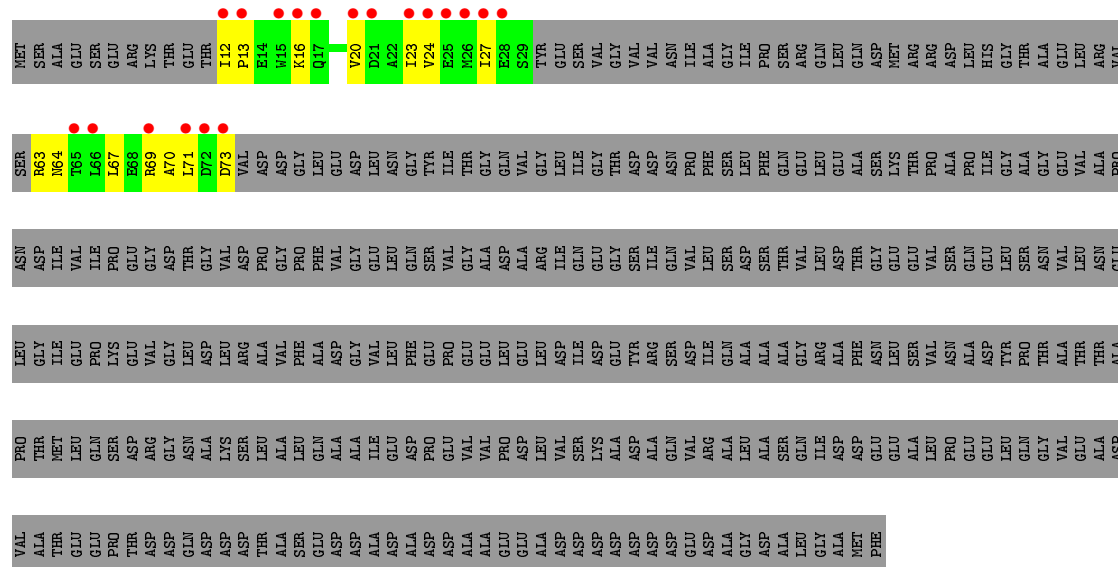




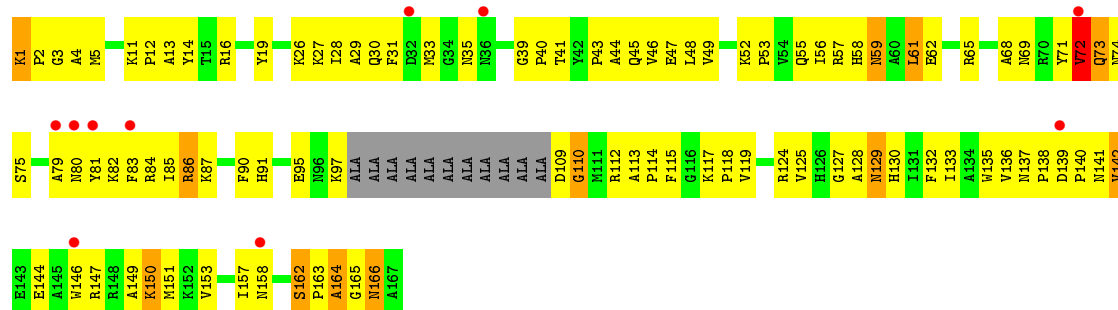
• Molecule 9: RIBOSOMAL PROTEIN L7AE



• Molecule 10: RIBOSOMAL PROTEIN L10

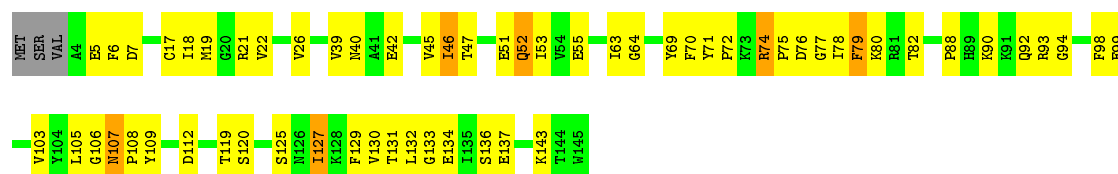


• Molecule 11: RIBOSOMAL PROTEIN L10E



• Molecule 12: RIBOSOMAL PROTEIN L13

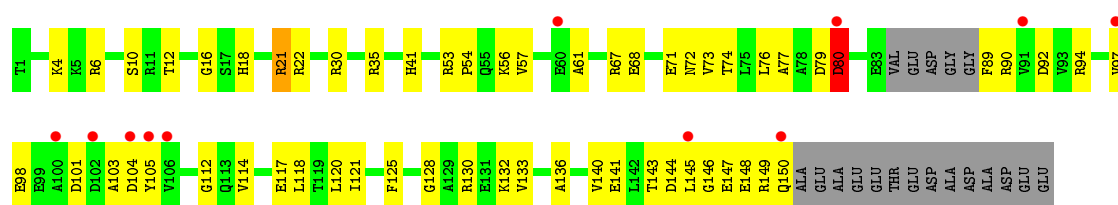




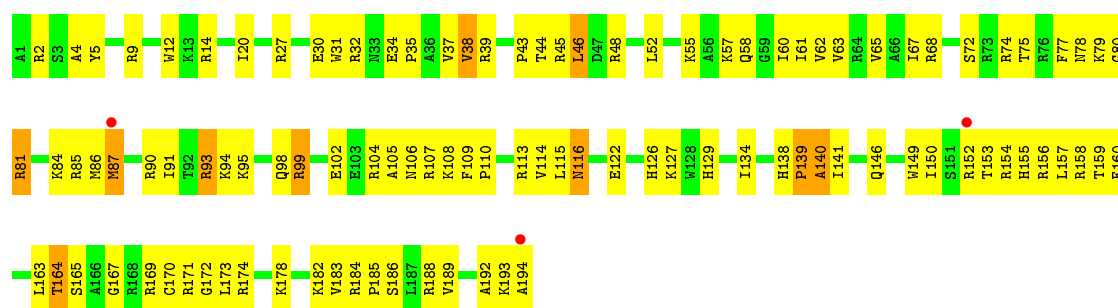
• Molecule 13: RIBOSOMAL PROTEIN L14



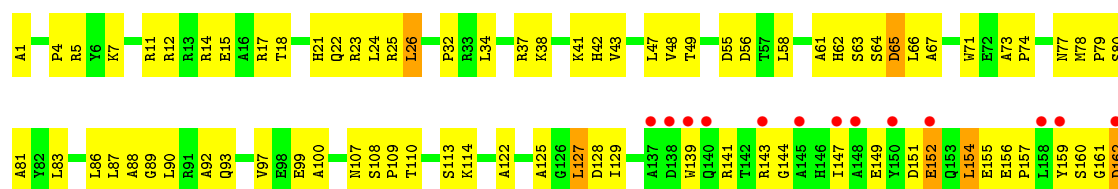
• Molecule 14: RIBOSOMAL PROTEIN L15

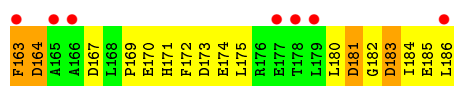


• Molecule 15: RIBOSOMAL PROTEIN L15E

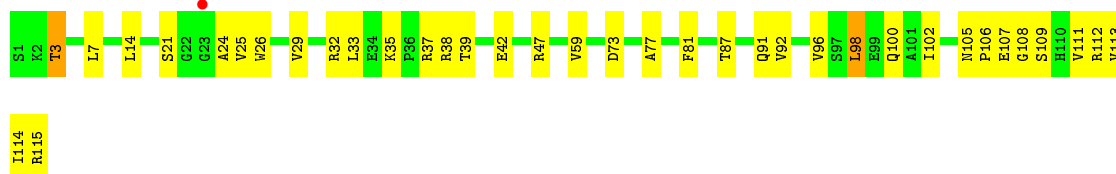


• Molecule 16: RIBOSOMAL PROTEIN L18

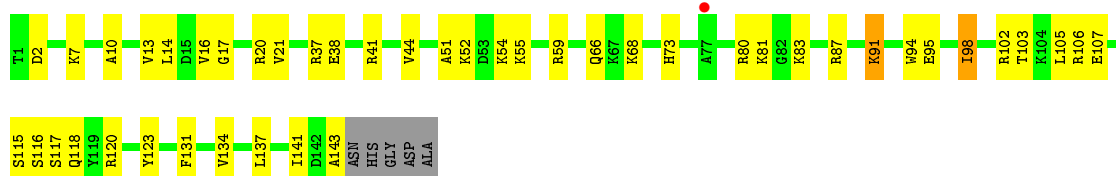




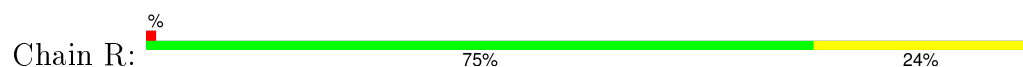
• Molecule 17: RIBOSOMAL PROTEIN L18E



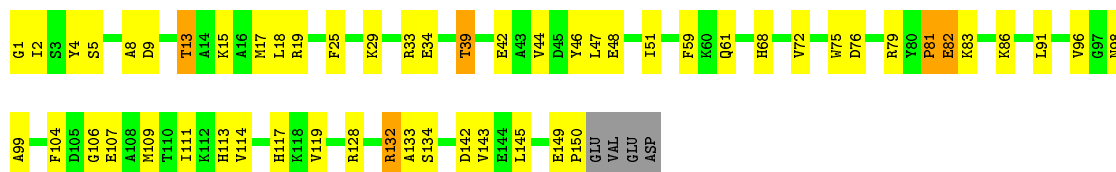
• Molecule 18: RIBOSOMAL PROTEIN L19E



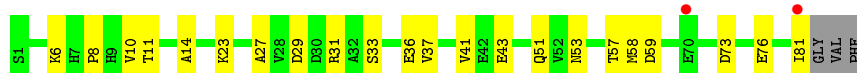
• Molecule 19: RIBOSOMAL PROTEIN L21E



• Molecule 20: RIBOSOMAL PROTEIN L22



• Molecule 21: RIBOSOMAL PROTEIN L23

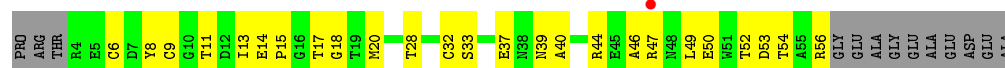
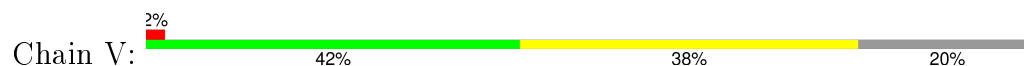


• Molecule 22: RIBOSOMAL PROTEIN L24

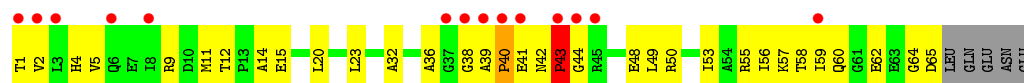




• Molecule 23: RIBOSOMAL PROTEIN L24E



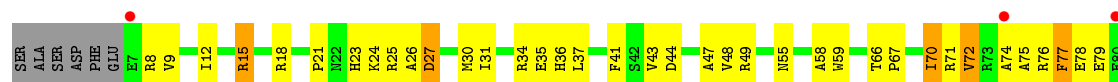
• Molecule 24: RIBOSOMAL PROTEIN L29



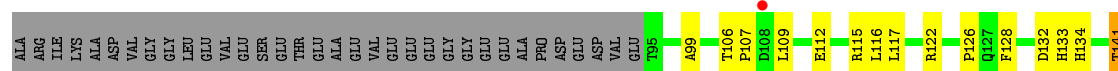
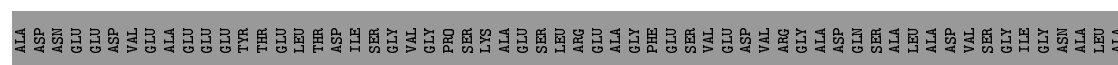
• Molecule 25: RIBOSOMAL PROTEIN L30

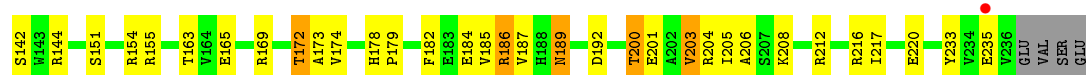


• Molecule 26: RIBOSOMAL PROTEIN L31E

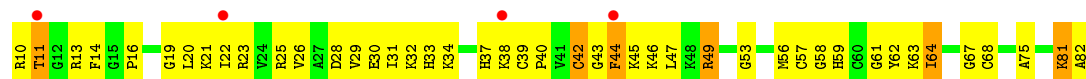


• Molecule 27: RIBOSOMAL PROTEIN L32E





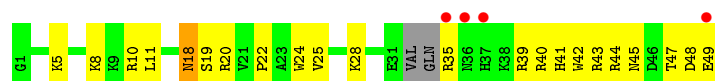
• Molecule 28: RIBOSOMAL PROTEIN L37Ae



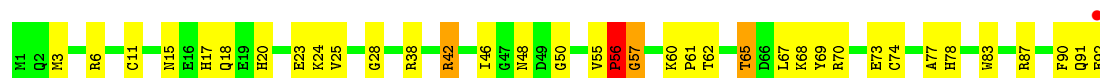
• Molecule 29: RIBOSOMAL PROTEIN L37E



• Molecule 30: RIBOSOMAL PROTEIN L39E



• Molecule 31: RIBOSOMAL PROTEIN L44E



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 299.77Å 573.68Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 2.80 49.96 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 94.3 (20.00-2.80) 94.4 (49.96-2.80) | Depositor EDS |
| R_{merge} | 0.14 | Depositor |
| R_{sym} | 0.14 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.21 (at 2.81Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.181 , 0.222 0.181 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 44.1 | Xtriage |
| Anisotropy | 0.207 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 57.9 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 0 of 442473 reflections | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 98611 | wwPDB-VP |
| Average B, all atoms (Å ²) | 49.0 | 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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, CL, NA, K, SPS, ACA, CD, PHA

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.42 | 1/66076 (0.0%) | 0.70 | 27/103052 (0.0%) |
| 2 | B | 0.50 | 0/2905 | 0.79 | 4/4528 (0.1%) |
| 3 | 5 | 0.74 | 0/65 | 1.17 | 1/99 (1.0%) |
| 4 | C | 0.34 | 0/1787 | 0.66 | 0/2409 |
| 5 | D | 0.34 | 0/2689 | 0.65 | 0/3652 |
| 6 | E | 0.40 | 0/1883 | 0.66 | 0/2551 |
| 7 | F | 0.33 | 0/1111 | 0.60 | 0/1498 |
| 8 | G | 0.34 | 0/1382 | 0.59 | 0/1880 |
| 9 | H | 0.33 | 0/896 | 0.58 | 0/1219 |
| 10 | I | 0.27 | 0/241 | 0.47 | 0/324 |
| 11 | J | 0.39 | 0/1246 | 0.75 | 2/1686 (0.1%) |
| 12 | K | 0.37 | 0/1135 | 0.61 | 0/1530 |
| 13 | L | 0.35 | 0/1003 | 0.67 | 0/1351 |
| 14 | M | 0.34 | 0/1126 | 0.67 | 0/1504 |
| 15 | N | 0.41 | 0/1633 | 0.70 | 1/2180 (0.0%) |
| 16 | O | 0.31 | 0/1473 | 0.64 | 0/1999 |
| 17 | P | 0.38 | 0/873 | 0.63 | 0/1181 |
| 18 | Q | 0.37 | 0/1143 | 0.56 | 0/1521 |
| 19 | R | 0.38 | 0/748 | 0.67 | 0/1005 |
| 20 | S | 0.38 | 0/1172 | 0.67 | 0/1578 |
| 21 | T | 0.34 | 0/648 | 0.60 | 0/875 |
| 22 | U | 0.32 | 0/957 | 0.63 | 0/1289 |
| 23 | V | 0.35 | 0/417 | 0.57 | 0/562 |
| 24 | W | 0.32 | 0/502 | 0.56 | 0/675 |
| 25 | X | 0.36 | 0/1218 | 0.64 | 0/1655 |
| 26 | Y | 0.36 | 0/664 | 0.61 | 0/895 |
| 27 | Z | 0.39 | 0/1146 | 0.67 | 0/1536 |
| 28 | 1 | 0.39 | 0/575 | 0.71 | 0/763 |
| 29 | 2 | 0.44 | 0/437 | 0.67 | 0/578 |
| 30 | 3 | 0.34 | 0/398 | 0.56 | 0/527 |
| 31 | 4 | 0.40 | 0/771 | 0.62 | 0/1024 |
| All | All | 0.41 | 1/98320 (0.0%) | 0.69 | 35/147126 (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 | A | 1 | 58 |
| 2 | B | 0 | 3 |
| All | All | 1 | 61 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 2474 | A | C5-C6 | -5.43 | 1.36 | 1.41 |

The worst 5 of 35 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | A | 1164 | U | OP1-P-O3' | -17.46 | 66.80 | 105.20 |
| 1 | A | 1164 | U | OP2-P-O3' | -16.54 | 68.82 | 105.20 |
| 1 | A | 1563 | G | C2'-C3'-O3' | 9.62 | 130.67 | 109.50 |
| 1 | A | 1979 | G | C2'-C3'-O3' | 7.74 | 126.52 | 109.50 |
| 1 | A | 1942 | A | C5'-C4'-C3' | 7.39 | 127.82 | 116.00 |

All (1) chirality outliers are listed below:

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

5 of 61 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 221 | G | Sidechain |
| 1 | A | 246 | G | Sidechain |
| 1 | A | 270 | U | Sidechain |
| 1 | A | 332 | G | Sidechain |
| 1 | A | 333 | G | Sidechain |

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 59017 | 0 | 29805 | 894 | 0 |
| 2 | B | 2600 | 0 | 1326 | 73 | 0 |
| 3 | 5 | 59 | 0 | 34 | 2 | 0 |
| 4 | C | 1754 | 0 | 1763 | 129 | 0 |
| 5 | D | 2624 | 0 | 2533 | 176 | 0 |
| 6 | E | 1858 | 0 | 1816 | 114 | 0 |
| 7 | F | 1094 | 0 | 1085 | 127 | 0 |
| 8 | G | 1357 | 0 | 1266 | 77 | 0 |
| 9 | H | 885 | 0 | 854 | 62 | 0 |
| 10 | I | 240 | 0 | 231 | 21 | 0 |
| 11 | J | 1215 | 0 | 1215 | 152 | 0 |
| 12 | K | 1119 | 0 | 1098 | 67 | 0 |
| 13 | L | 993 | 0 | 1027 | 55 | 0 |
| 14 | M | 1114 | 0 | 1072 | 61 | 0 |
| 15 | N | 1605 | 0 | 1676 | 159 | 0 |
| 16 | O | 1444 | 0 | 1401 | 128 | 0 |
| 17 | P | 864 | 0 | 873 | 41 | 0 |
| 18 | Q | 1133 | 0 | 1127 | 49 | 0 |
| 19 | R | 734 | 0 | 728 | 21 | 0 |
| 20 | S | 1149 | 0 | 1122 | 65 | 0 |
| 21 | T | 641 | 0 | 605 | 19 | 0 |
| 22 | U | 949 | 0 | 923 | 48 | 0 |
| 23 | V | 410 | 0 | 364 | 32 | 0 |
| 24 | W | 499 | 0 | 511 | 34 | 0 |
| 25 | X | 1195 | 0 | 1137 | 101 | 0 |
| 26 | Y | 654 | 0 | 653 | 47 | 0 |
| 27 | Z | 1130 | 0 | 1133 | 61 | 0 |
| 28 | 1 | 563 | 0 | 597 | 59 | 0 |
| 29 | 2 | 430 | 0 | 426 | 24 | 0 |
| 30 | 3 | 393 | 0 | 406 | 28 | 0 |
| 31 | 4 | 755 | 0 | 728 | 36 | 0 |
| 32 | 1 | 1 | 0 | 0 | 0 | 0 |
| 32 | 4 | 1 | 0 | 0 | 0 | 0 |
| 32 | 5 | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 111 | 0 | 0 | 0 | 0 |
| 32 | B | 1 | 0 | 0 | 0 | 0 |
| 32 | C | 1 | 0 | 0 | 0 | 0 |
| 32 | L | 1 | 0 | 0 | 0 | 0 |
| 32 | U | 1 | 0 | 0 | 0 | 0 |
| 32 | Z | 1 | 0 | 0 | 0 | 0 |
| 33 | A | 73 | 0 | 0 | 0 | 0 |
| 33 | B | 2 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33 | C | 1 | 0 | 0 | 0 | 0 |
| 33 | E | 1 | 0 | 0 | 0 | 0 |
| 33 | J | 1 | 0 | 0 | 0 | 0 |
| 33 | K | 1 | 0 | 0 | 0 | 0 |
| 33 | M | 1 | 0 | 0 | 0 | 0 |
| 33 | N | 1 | 0 | 0 | 0 | 0 |
| 33 | R | 1 | 0 | 0 | 0 | 0 |
| 33 | S | 2 | 0 | 0 | 0 | 0 |
| 33 | T | 1 | 0 | 0 | 0 | 0 |
| 33 | U | 1 | 0 | 0 | 0 | 0 |
| 34 | A | 2 | 0 | 0 | 0 | 0 |
| 35 | 4 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 10 | 0 | 0 | 0 | 0 |
| 35 | C | 1 | 0 | 0 | 0 | 0 |
| 35 | D | 1 | 0 | 0 | 0 | 0 |
| 35 | K | 3 | 0 | 0 | 1 | 0 |
| 35 | M | 1 | 0 | 0 | 0 | 0 |
| 35 | N | 1 | 0 | 0 | 1 | 0 |
| 35 | O | 1 | 0 | 0 | 0 | 0 |
| 35 | P | 1 | 0 | 0 | 0 | 0 |
| 35 | S | 1 | 0 | 0 | 0 | 0 |
| 35 | Z | 1 | 0 | 0 | 0 | 0 |
| 36 | 5 | 23 | 0 | 19 | 4 | 0 |
| 37 | 5 | 11 | 0 | 8 | 0 | 0 |
| 38 | 5 | 8 | 0 | 12 | 0 | 0 |
| 39 | 1 | 1 | 0 | 0 | 0 | 0 |
| 39 | 2 | 1 | 0 | 0 | 0 | 0 |
| 39 | 4 | 1 | 0 | 0 | 0 | 0 |
| 39 | P | 1 | 0 | 0 | 0 | 0 |
| 39 | V | 1 | 0 | 0 | 0 | 0 |
| 40 | 1 | 36 | 0 | 0 | 8 | 0 |
| 40 | 2 | 55 | 0 | 0 | 3 | 0 |
| 40 | 3 | 40 | 0 | 0 | 4 | 0 |
| 40 | 4 | 73 | 0 | 0 | 10 | 0 |
| 40 | 5 | 1 | 0 | 0 | 0 | 0 |
| 40 | A | 5920 | 0 | 0 | 193 | 0 |
| 40 | B | 136 | 0 | 0 | 11 | 0 |
| 40 | C | 119 | 0 | 0 | 23 | 0 |
| 40 | D | 142 | 0 | 0 | 30 | 0 |
| 40 | E | 172 | 0 | 0 | 27 | 0 |
| 40 | F | 51 | 0 | 0 | 23 | 0 |
| 40 | G | 44 | 0 | 0 | 8 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | H | 28 | 0 | 0 | 8 | 0 |
| 40 | I | 21 | 0 | 0 | 6 | 0 |
| 40 | J | 75 | 0 | 0 | 23 | 0 |
| 40 | K | 56 | 0 | 0 | 5 | 0 |
| 40 | L | 61 | 0 | 0 | 16 | 0 |
| 40 | M | 86 | 0 | 0 | 19 | 0 |
| 40 | N | 125 | 0 | 0 | 21 | 0 |
| 40 | O | 69 | 0 | 0 | 17 | 0 |
| 40 | P | 43 | 0 | 0 | 7 | 0 |
| 40 | Q | 67 | 0 | 0 | 1 | 0 |
| 40 | R | 49 | 0 | 0 | 3 | 0 |
| 40 | S | 83 | 0 | 0 | 11 | 0 |
| 40 | T | 35 | 0 | 0 | 5 | 0 |
| 40 | U | 37 | 0 | 0 | 4 | 0 |
| 40 | V | 24 | 0 | 0 | 5 | 0 |
| 40 | W | 16 | 0 | 0 | 2 | 0 |
| 40 | X | 71 | 0 | 0 | 12 | 0 |
| 40 | Y | 31 | 0 | 0 | 5 | 0 |
| 40 | Z | 92 | 0 | 0 | 14 | 0 |
| All | All | 98611 | 0 | 59574 | 2699 | 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 18.

The worst 5 of 2699 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) |
|------------------|-------------------|--------------------------|-------------------|
| 6:E:236:THR:HG22 | 6:E:239:ALA:H | 1.04 | 1.16 |
| 1:A:1160:G:H5' | 1:A:1161:A:H5' | 1.22 | 1.15 |
| 11:J:86:ARG:NH1 | 11:J:133:ILE:HG13 | 1.63 | 1.13 |
| 11:J:45:GLN:HB3 | 11:J:163:PRO:HD2 | 1.30 | 1.12 |
| 24:W:12:THR:HG22 | 24:W:15:GLU:HG3 | 1.31 | 1.12 |

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4 | C | 235/239 (98%) | 209 (89%) | 21 (9%) | 5 (2%) | 9 | 29 |
| 5 | D | 335/337 (99%) | 303 (90%) | 25 (8%) | 7 (2%) | 9 | 29 |
| 6 | E | 244/246 (99%) | 218 (89%) | 25 (10%) | 1 (0%) | 39 | 74 |
| 7 | F | 134/176 (76%) | 98 (73%) | 28 (21%) | 8 (6%) | 2 | 5 |
| 8 | G | 170/177 (96%) | 159 (94%) | 10 (6%) | 1 (1%) | 30 | 65 |
| 9 | H | 117/119 (98%) | 102 (87%) | 12 (10%) | 3 (3%) | 7 | 22 |
| 10 | I | 25/348 (7%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 11 | J | 152/167 (91%) | 133 (88%) | 13 (9%) | 6 (4%) | 4 | 12 |
| 12 | K | 140/145 (97%) | 126 (90%) | 11 (8%) | 3 (2%) | 9 | 29 |
| 13 | L | 130/132 (98%) | 118 (91%) | 10 (8%) | 2 (2%) | 13 | 40 |
| 14 | M | 141/164 (86%) | 120 (85%) | 19 (14%) | 2 (1%) | 14 | 42 |
| 15 | N | 192/194 (99%) | 174 (91%) | 16 (8%) | 2 (1%) | 19 | 52 |
| 16 | O | 184/186 (99%) | 167 (91%) | 11 (6%) | 6 (3%) | 5 | 16 |
| 17 | P | 113/115 (98%) | 110 (97%) | 3 (3%) | 0 | 100 | 100 |
| 18 | Q | 141/148 (95%) | 137 (97%) | 3 (2%) | 1 (1%) | 26 | 62 |
| 19 | R | 93/95 (98%) | 85 (91%) | 8 (9%) | 0 | 100 | 100 |
| 20 | S | 148/154 (96%) | 140 (95%) | 7 (5%) | 1 (1%) | 26 | 62 |
| 21 | T | 79/84 (94%) | 75 (95%) | 4 (5%) | 0 | 100 | 100 |
| 22 | U | 117/119 (98%) | 111 (95%) | 5 (4%) | 1 (1%) | 21 | 55 |
| 23 | V | 51/66 (77%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 24 | W | 63/70 (90%) | 58 (92%) | 3 (5%) | 2 (3%) | 5 | 17 |
| 25 | X | 152/154 (99%) | 147 (97%) | 3 (2%) | 2 (1%) | 15 | 44 |
| 26 | Y | 80/91 (88%) | 70 (88%) | 8 (10%) | 2 (2%) | 7 | 24 |
| 27 | Z | 140/240 (58%) | 139 (99%) | 1 (1%) | 0 | 100 | 100 |
| 28 | 1 | 71/73 (97%) | 63 (89%) | 7 (10%) | 1 (1%) | 14 | 42 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 29 | 2 | 54/56 (96%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | 3 | 42/48 (88%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 31 | 4 | 90/92 (98%) | 85 (94%) | 3 (3%) | 2 (2%) | 8 | 28 |
| All | All | 3633/4235 (86%) | 3313 (91%) | 262 (7%) | 58 (2%) | 12 | 38 |

5 of 58 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | D | 139 | ASP |
| 7 | F | 20 | LYS |
| 7 | F | 93 | LEU |
| 7 | F | 95 | THR |
| 7 | F | 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 | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4 | C | 179/181 (99%) | 166 (93%) | 13 (7%) | 17 | 44 |
| 5 | D | 282/282 (100%) | 264 (94%) | 18 (6%) | 22 | 52 |
| 6 | E | 193/193 (100%) | 177 (92%) | 16 (8%) | 14 | 38 |
| 7 | F | 117/147 (80%) | 109 (93%) | 8 (7%) | 20 | 49 |
| 8 | G | 152/155 (98%) | 148 (97%) | 4 (3%) | 54 | 86 |
| 9 | H | 92/92 (100%) | 91 (99%) | 1 (1%) | 80 | 95 |
| 10 | I | 27/283 (10%) | 27 (100%) | 0 | 100 | 100 |
| 11 | J | 122/122 (100%) | 110 (90%) | 12 (10%) | 10 | 28 |
| 12 | K | 118/121 (98%) | 109 (92%) | 9 (8%) | 16 | 42 |
| 13 | L | 106/106 (100%) | 103 (97%) | 3 (3%) | 51 | 84 |
| 14 | M | 112/126 (89%) | 109 (97%) | 3 (3%) | 52 | 85 |
| 15 | N | 166/166 (100%) | 157 (95%) | 9 (5%) | 27 | 60 |
| 16 | O | 149/149 (100%) | 144 (97%) | 5 (3%) | 44 | 78 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 17 | P | 93/93 (100%) | 91 (98%) | 2 (2%) | 60 | 89 |
| 18 | Q | 113/116 (97%) | 110 (97%) | 3 (3%) | 52 | 85 |
| 19 | R | 79/79 (100%) | 75 (95%) | 4 (5%) | 29 | 63 |
| 20 | S | 117/121 (97%) | 113 (97%) | 4 (3%) | 44 | 78 |
| 21 | T | 71/73 (97%) | 71 (100%) | 0 | 100 | 100 |
| 22 | U | 105/105 (100%) | 104 (99%) | 1 (1%) | 82 | 96 |
| 23 | V | 44/52 (85%) | 44 (100%) | 0 | 100 | 100 |
| 24 | W | 51/56 (91%) | 50 (98%) | 1 (2%) | 63 | 90 |
| 25 | X | 130/130 (100%) | 123 (95%) | 7 (5%) | 27 | 60 |
| 26 | Y | 66/73 (90%) | 62 (94%) | 4 (6%) | 23 | 55 |
| 27 | Z | 120/195 (62%) | 113 (94%) | 7 (6%) | 25 | 57 |
| 28 | 1 | 56/56 (100%) | 51 (91%) | 5 (9%) | 12 | 34 |
| 29 | 2 | 46/46 (100%) | 46 (100%) | 0 | 100 | 100 |
| 30 | 3 | 42/44 (96%) | 41 (98%) | 1 (2%) | 57 | 87 |
| 31 | 4 | 79/79 (100%) | 76 (96%) | 3 (4%) | 40 | 74 |
| All | All | 3027/3441 (88%) | 2884 (95%) | 143 (5%) | 32 | 67 |

5 of 143 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | J | 72 | VAL |
| 12 | K | 127 | ILE |
| 27 | Z | 200 | THR |
| 11 | J | 82 | LYS |
| 12 | K | 46 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | M | 42 | ASN |
| 18 | Q | 66 | GLN |
| 29 | 2 | 28 | HIS |
| 14 | M | 116 | HIS |
| 15 | N | 176 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2747/2922 (94%) | 237 (8%) | 38 (1%) |
| 2 | B | 121/122 (99%) | 15 (12%) | 3 (2%) |
| 3 | 5 | 2/3 (66%) | 1 (50%) | 0 |
| All | All | 2870/3047 (94%) | 253 (8%) | 41 (1%) |

5 of 253 RNA backbone outliers are listed below:

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

5 of 41 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1377 | C |
| 1 | A | 1684 | A |
| 1 | A | 2791 | U |
| 1 | A | 1450 | C |
| 1 | A | 1563 | G |

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 237 ligands modelled in this entry, 234 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 37 | PHA | 5 | 9077 | 3,38 | 10,11,11 | 0.78 | 0 | 10,13,13 | 0.40 | 0 |
| 38 | ACA | 5 | 9078 | 37 | 7,7,8 | 1.80 | 2 (28%) | 5,6,8 | 0.79 | 0 |
| 36 | SPS | 5 | 9080 | 32 | 17,23,23 | 1.97 | 5 (29%) | 15,30,30 | 2.12 | 3 (20%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 37 | PHA | 5 | 9077 | 3,38 | - | 0/4/6/6 | 0/1/1/1 |
| 38 | ACA | 5 | 9078 | 37 | - | 0/4/5/6 | 0/0/0/0 |
| 36 | SPS | 5 | 9080 | 32 | - | 0/15/18/18 | 0/1/1/1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | 5 | 9080 | SPS | C9-C10 | -3.26 | 1.41 | 1.48 |
| 36 | 5 | 9080 | SPS | O15-S15 | -2.63 | 1.41 | 1.50 |
| 38 | 5 | 9078 | ACA | C3-C2 | -2.47 | 1.42 | 1.52 |
| 36 | 5 | 9080 | SPS | C1-N2 | 2.71 | 1.38 | 1.33 |
| 36 | 5 | 9080 | SPS | C5-N4 | 2.93 | 1.38 | 1.34 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | 5 | 9080 | SPS | C7-C5-C6 | -2.43 | 120.75 | 123.69 |
| 36 | 5 | 9080 | SPS | C9-C10-N11 | 2.15 | 118.85 | 114.12 |
| 36 | 5 | 9080 | SPS | C1-N2-C3 | 6.58 | 120.94 | 115.25 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 36 | 5 | 9080 | SPS | 4 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 2754/2922 (94%) | 0.01 | 69 (2%) 61 48 | 18, 43, 87, 135 | 0 |
| 2 | B | 122/122 (100%) | 0.30 | 4 (3%) 50 38 | 35, 60, 87, 145 | 0 |
| 3 | 5 | 3/3 (100%) | -0.07 | 0 100 100 | 33, 33, 35, 36 | 0 |
| 4 | C | 237/239 (99%) | 0.13 | 11 (4%) 36 25 | 24, 47, 79, 101 | 0 |
| 5 | D | 337/337 (100%) | -0.00 | 5 (1%) 76 68 | 25, 53, 79, 88 | 0 |
| 6 | E | 246/246 (100%) | -0.28 | 0 100 100 | 21, 42, 64, 75 | 0 |
| 7 | F | 140/176 (79%) | 2.06 | 73 (52%) 0 0 | 51, 94, 112, 118 | 0 |
| 8 | G | 172/177 (97%) | 0.95 | 17 (9%) 9 4 | 44, 67, 85, 92 | 0 |
| 9 | H | 119/119 (100%) | 0.58 | 12 (10%) 9 4 | 45, 66, 91, 97 | 0 |
| 10 | I | 29/348 (8%) | 2.43 | 19 (65%) 0 0 | 66, 85, 93, 96 | 0 |
| 11 | J | 156/167 (93%) | 0.33 | 10 (6%) 23 14 | 34, 52, 77, 80 | 0 |
| 12 | K | 142/145 (97%) | 0.00 | 0 100 100 | 33, 49, 68, 86 | 0 |
| 13 | L | 132/132 (100%) | -0.10 | 2 (1%) 76 68 | 31, 50, 70, 80 | 0 |
| 14 | M | 145/164 (88%) | 0.41 | 11 (7%) 17 9 | 20, 60, 98, 111 | 0 |
| 15 | N | 194/194 (100%) | -0.14 | 3 (1%) 76 68 | 28, 39, 58, 68 | 0 |
| 16 | O | 186/186 (100%) | 0.54 | 20 (10%) 8 3 | 36, 59, 99, 111 | 0 |
| 17 | P | 115/115 (100%) | -0.05 | 1 (0%) 85 79 | 35, 49, 67, 77 | 0 |
| 18 | Q | 143/148 (96%) | 0.13 | 1 (0%) 89 84 | 36, 52, 64, 74 | 0 |
| 19 | R | 95/95 (100%) | -0.11 | 1 (1%) 82 74 | 29, 40, 54, 70 | 0 |
| 20 | S | 150/154 (97%) | -0.22 | 0 100 100 | 29, 41, 61, 70 | 0 |
| 21 | T | 81/84 (96%) | 0.10 | 2 (2%) 61 48 | 40, 54, 73, 80 | 0 |
| 22 | U | 119/119 (100%) | 0.34 | 10 (8%) 14 6 | 36, 52, 76, 90 | 0 |
| 23 | V | 53/66 (80%) | 0.22 | 1 (1%) 70 59 | 39, 53, 69, 77 | 0 |
| 24 | W | 65/70 (92%) | 1.29 | 14 (21%) 1 1 | 49, 68, 105, 110 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | X | 154/154 (100%) | -0.25 | 0 100 100 | 32, 45, 63, 72 | 0 |
| 26 | Y | 82/91 (90%) | 0.15 | 4 (4%) 33 22 | 40, 57, 79, 99 | 0 |
| 27 | Z | 142/240 (59%) | -0.09 | 2 (1%) 78 69 | 24, 41, 65, 82 | 0 |
| 28 | 1 | 73/73 (100%) | 0.24 | 4 (5%) 29 18 | 46, 60, 71, 79 | 0 |
| 29 | 2 | 56/56 (100%) | -0.60 | 0 100 100 | 24, 29, 35, 43 | 0 |
| 30 | 3 | 46/48 (95%) | 0.41 | 4 (8%) 13 6 | 31, 57, 84, 98 | 0 |
| 31 | 4 | 92/92 (100%) | 0.10 | 1 (1%) 82 74 | 31, 51, 64, 78 | 0 |
| All | All | 6580/7282 (90%) | 0.13 | 301 (4%) 36 25 | 18, 48, 88, 145 | 0 |

The worst 5 of 301 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | W | 1 | THR | 10.9 |
| 1 | A | 1172 | G | 6.8 |
| 2 | B | 3001 | U | 6.5 |
| 7 | F | 88 | LEU | 6.2 |
| 7 | F | 57 | THR | 6.1 |

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 | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 33 | NA | A | 8340 | 1/1 | 0.95 | 0.47 | 68.63 | 44,44,44,44 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 33 | NA | S | 8386 | 1/1 | 0.37 | 0.92 | 41.74 | 91,91,91,91 | 0 |
| 33 | NA | A | 8374 | 1/1 | 0.98 | 0.68 | 34.60 | 53,53,53,53 | 0 |
| 33 | NA | A | 8362 | 1/1 | 0.92 | 0.31 | 26.91 | 64,64,64,64 | 0 |
| 33 | NA | A | 8378 | 1/1 | 0.96 | 0.54 | 25.28 | 47,47,47,47 | 0 |
| 38 | ACA | 5 | 9078 | 8/9 | 0.79 | 0.38 | 24.08 | 45,53,55,55 | 0 |
| 34 | K | A | 8390 | 1/1 | 0.91 | 0.36 | 21.26 | 70,70,70,70 | 0 |
| 33 | NA | A | 8364 | 1/1 | 0.84 | 0.27 | 20.93 | 39,39,39,39 | 0 |
| 33 | NA | A | 8373 | 1/1 | 0.93 | 0.48 | 19.75 | 50,50,50,50 | 0 |
| 35 | CL | A | 8515 | 1/1 | 0.96 | 0.34 | 18.06 | 65,65,65,65 | 0 |
| 33 | NA | A | 8325 | 1/1 | 0.99 | 0.36 | 18.06 | 50,50,50,50 | 0 |
| 33 | NA | A | 8361 | 1/1 | 0.97 | 0.28 | 14.69 | 47,47,47,47 | 0 |
| 33 | NA | A | 8350 | 1/1 | 0.96 | 0.24 | 13.57 | 32,32,32,32 | 0 |
| 33 | NA | A | 8372 | 1/1 | 0.86 | 0.44 | 12.94 | 58,58,58,58 | 0 |
| 34 | K | A | 8391 | 1/1 | 0.99 | 0.24 | 12.67 | 48,48,48,48 | 0 |
| 33 | NA | A | 8371 | 1/1 | 0.85 | 0.32 | 12.36 | 61,61,61,61 | 0 |
| 33 | NA | A | 8356 | 1/1 | 0.95 | 0.28 | 12.09 | 47,47,47,47 | 0 |
| 33 | NA | A | 8359 | 1/1 | 0.84 | 0.38 | 11.56 | 40,40,40,40 | 0 |
| 33 | NA | B | 8383 | 1/1 | 0.80 | 0.61 | 11.53 | 69,69,69,69 | 0 |
| 33 | NA | M | 8380 | 1/1 | 0.89 | 0.41 | 11.49 | 64,64,64,64 | 0 |
| 37 | PHA | 5 | 9077 | 11/11 | 0.96 | 0.24 | 7.33 | 41,45,52,53 | 0 |
| 33 | NA | A | 8310 | 1/1 | 0.89 | 0.26 | 7.20 | 39,39,39,39 | 0 |
| 33 | NA | A | 8335 | 1/1 | 0.93 | 0.22 | 7.17 | 43,43,43,43 | 0 |
| 33 | NA | A | 8368 | 1/1 | 0.73 | 0.21 | 6.80 | 56,56,56,56 | 0 |
| 33 | NA | A | 8366 | 1/1 | 0.92 | 0.49 | 6.55 | 68,68,68,68 | 0 |
| 36 | SPS | 5 | 9080 | 23/23 | 0.96 | 0.21 | 5.94 | 30,33,47,49 | 0 |
| 32 | MG | A | 8060 | 1/1 | 0.99 | 0.18 | 3.76 | 42,42,42,42 | 0 |
| 33 | NA | A | 8303 | 1/1 | 0.93 | 0.18 | 3.08 | 43,43,43,43 | 0 |
| 33 | NA | A | 8331 | 1/1 | 0.96 | 0.17 | 2.47 | 31,31,31,31 | 0 |
| 33 | NA | A | 8321 | 1/1 | 0.97 | 0.18 | 2.26 | 54,54,54,54 | 0 |
| 33 | NA | A | 8382 | 1/1 | 0.90 | 0.17 | 1.72 | 72,72,72,72 | 0 |
| 32 | MG | A | 8112 | 1/1 | 0.98 | 0.18 | 1.36 | 28,28,28,28 | 0 |
| 33 | NA | A | 8314 | 1/1 | 0.89 | 0.19 | 1.34 | 38,38,38,38 | 0 |
| 32 | MG | A | 8013 | 1/1 | 0.97 | 0.17 | 1.03 | 32,32,32,32 | 0 |
| 33 | NA | A | 8302 | 1/1 | 0.97 | 0.15 | 0.98 | 46,46,46,46 | 0 |
| 33 | NA | A | 8365 | 1/1 | 0.91 | 0.24 | 0.75 | 43,43,43,43 | 0 |
| 33 | NA | S | 8337 | 1/1 | 0.95 | 0.19 | 0.69 | 28,28,28,28 | 0 |
| 32 | MG | A | 8053 | 1/1 | 0.95 | 0.14 | 0.35 | 50,50,50,50 | 0 |
| 33 | NA | A | 8324 | 1/1 | 0.71 | 0.18 | 0.17 | 55,55,55,55 | 0 |
| 32 | MG | A | 8064 | 1/1 | 0.98 | 0.14 | 0.02 | 31,31,31,31 | 0 |
| 35 | CL | A | 8505 | 1/1 | 0.97 | 0.16 | -0.07 | 49,49,49,49 | 0 |
| 33 | NA | A | 8332 | 1/1 | 0.93 | 0.14 | -0.10 | 29,29,29,29 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 32 | MG | A | 8119 | 1/1 | 0.95 | 0.14 | -0.13 | 41,41,41,41 | 0 |
| 33 | NA | A | 8333 | 1/1 | 0.79 | 0.15 | -0.20 | 33,33,33,33 | 0 |
| 32 | MG | A | 8070 | 1/1 | 0.94 | 0.15 | -0.24 | 47,47,47,47 | 0 |
| 33 | NA | A | 8353 | 1/1 | 0.94 | 0.15 | -0.42 | 23,23,23,23 | 0 |
| 33 | NA | A | 8317 | 1/1 | 0.95 | 0.17 | -0.54 | 45,45,45,45 | 0 |
| 33 | NA | U | 8343 | 1/1 | 0.92 | 0.15 | -0.69 | 33,33,33,33 | 0 |
| 33 | NA | R | 8348 | 1/1 | 0.97 | 0.17 | -0.86 | 42,42,42,42 | 0 |
| 33 | NA | A | 8339 | 1/1 | 0.97 | 0.14 | -0.97 | 22,22,22,22 | 0 |
| 35 | CL | 4 | 8504 | 1/1 | 0.94 | 0.14 | -1.04 | 67,67,67,67 | 0 |
| 33 | NA | A | 8376 | 1/1 | 0.98 | 0.14 | -1.08 | 47,47,47,47 | 0 |
| 35 | CL | A | 8516 | 1/1 | 0.97 | 0.13 | -1.13 | 56,56,56,56 | 0 |
| 33 | NA | N | 8347 | 1/1 | 0.93 | 0.12 | -1.50 | 23,23,23,23 | 0 |
| 33 | NA | A | 8309 | 1/1 | 0.95 | 0.09 | -1.62 | 32,32,32,32 | 0 |
| 32 | MG | A | 8027 | 1/1 | 0.94 | 0.08 | -1.64 | 49,49,49,49 | 0 |
| 33 | NA | A | 8379 | 1/1 | 0.97 | 0.12 | -1.67 | 45,45,45,45 | 0 |
| 32 | MG | C | 8065 | 1/1 | 0.99 | 0.11 | -1.83 | 31,31,31,31 | 0 |
| 35 | CL | A | 8512 | 1/1 | 0.97 | 0.09 | -1.98 | 47,47,47,47 | 0 |
| 39 | CD | V | 8401 | 1/1 | 1.00 | 0.07 | -2.00 | 62,62,62,62 | 0 |
| 32 | MG | A | 8108 | 1/1 | 0.94 | 0.13 | -2.00 | 60,60,60,60 | 0 |
| 35 | CL | P | 8508 | 1/1 | 0.96 | 0.10 | -2.09 | 62,62,62,62 | 0 |
| 39 | CD | 1 | 8403 | 1/1 | 0.99 | 0.08 | -2.12 | 62,62,62,62 | 0 |
| 35 | CL | N | 8518 | 1/1 | 0.98 | 0.12 | -2.13 | 39,39,39,39 | 0 |
| 39 | CD | 4 | 8404 | 1/1 | 0.99 | 0.06 | -2.20 | 57,57,57,57 | 0 |
| 33 | NA | C | 8345 | 1/1 | 0.94 | 0.13 | -2.28 | 44,44,44,44 | 0 |
| 33 | NA | A | 8305 | 1/1 | 0.94 | 0.13 | -2.36 | 35,35,35,35 | 0 |
| 32 | MG | A | 8074 | 1/1 | 0.99 | 0.03 | -2.40 | 29,29,29,29 | 0 |
| 32 | MG | A | 8033 | 1/1 | 0.97 | 0.11 | -2.62 | 28,28,28,28 | 0 |
| 39 | CD | 2 | 8402 | 1/1 | 0.99 | 0.07 | -2.62 | 56,56,56,56 | 0 |
| 32 | MG | A | 8107 | 1/1 | 0.96 | 0.05 | -2.63 | 43,43,43,43 | 0 |
| 33 | NA | K | 8346 | 1/1 | 0.96 | 0.08 | -2.64 | 40,40,40,40 | 0 |
| 32 | MG | A | 8062 | 1/1 | 0.96 | 0.10 | -2.68 | 48,48,48,48 | 0 |
| 35 | CL | K | 8521 | 1/1 | 0.93 | 0.10 | -2.68 | 50,50,50,50 | 0 |
| 32 | MG | A | 8057 | 1/1 | 0.93 | 0.13 | -2.75 | 40,40,40,40 | 0 |
| 32 | MG | A | 8058 | 1/1 | 0.97 | 0.11 | -2.85 | 37,37,37,37 | 0 |
| 32 | MG | U | 8073 | 1/1 | 0.95 | 0.09 | -2.88 | 46,46,46,46 | 0 |
| 35 | CL | D | 8519 | 1/1 | 0.98 | 0.11 | -2.97 | 40,40,40,40 | 0 |
| 33 | NA | A | 8338 | 1/1 | 0.96 | 0.09 | -3.00 | 41,41,41,41 | 0 |
| 33 | NA | A | 8327 | 1/1 | 0.98 | 0.11 | -3.29 | 41,41,41,41 | 0 |
| 32 | MG | A | 8059 | 1/1 | 0.96 | 0.13 | -3.36 | 35,35,35,35 | 0 |
| 32 | MG | A | 8003 | 1/1 | 0.99 | 0.12 | -3.48 | 26,26,26,26 | 0 |
| 32 | MG | A | 8067 | 1/1 | 0.97 | 0.12 | -3.74 | 43,43,43,43 | 0 |
| 32 | MG | A | 8055 | 1/1 | 0.96 | 0.08 | -3.77 | 43,43,43,43 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 32 | MG | A | 8001 | 1/1 | 0.98 | 0.07 | -3.87 | 27,27,27,27 | 0 |
| 32 | MG | A | 8110 | 1/1 | 0.98 | 0.11 | -4.01 | 35,35,35,35 | 0 |
| 32 | MG | A | 8018 | 1/1 | 0.99 | 0.09 | -4.19 | 31,31,31,31 | 0 |
| 32 | MG | A | 8056 | 1/1 | 0.97 | 0.06 | -4.21 | 39,39,39,39 | 0 |
| 33 | NA | A | 8320 | 1/1 | 0.98 | 0.11 | -4.22 | 38,38,38,38 | 0 |
| 32 | MG | A | 8012 | 1/1 | 0.99 | 0.09 | -4.27 | 28,28,28,28 | 0 |
| 32 | MG | 4 | 8078 | 1/1 | 0.98 | 0.04 | -4.41 | 41,41,41,41 | 0 |
| 33 | NA | A | 8308 | 1/1 | 0.90 | 0.10 | -4.47 | 43,43,43,43 | 0 |
| 32 | MG | A | 8039 | 1/1 | 0.99 | 0.08 | -4.47 | 42,42,42,42 | 0 |
| 32 | MG | A | 8021 | 1/1 | 0.98 | 0.11 | -4.56 | 33,33,33,33 | 0 |
| 32 | MG | A | 8010 | 1/1 | 0.99 | 0.09 | -4.71 | 35,35,35,35 | 0 |
| 32 | MG | 5 | 8118 | 1/1 | 0.97 | 0.11 | -4.73 | 29,29,29,29 | 0 |
| 32 | MG | A | 8015 | 1/1 | 0.98 | 0.09 | -4.87 | 29,29,29,29 | 0 |
| 33 | NA | A | 8323 | 1/1 | 1.00 | 0.11 | -5.25 | 42,42,42,42 | 0 |
| 32 | MG | A | 8019 | 1/1 | 0.98 | 0.04 | -5.46 | 29,29,29,29 | 0 |
| 32 | MG | Z | 8109 | 1/1 | 0.97 | 0.07 | -5.61 | 33,33,33,33 | 0 |
| 32 | MG | A | 8044 | 1/1 | 0.96 | 0.06 | -5.74 | 36,36,36,36 | 0 |
| 32 | MG | A | 8038 | 1/1 | 0.98 | 0.09 | -5.99 | 27,27,27,27 | 0 |
| 32 | MG | A | 8004 | 1/1 | 0.96 | 0.07 | -6.01 | 26,26,26,26 | 0 |
| 32 | MG | A | 8007 | 1/1 | 0.96 | 0.06 | -6.04 | 16,16,16,16 | 0 |
| 32 | MG | A | 8032 | 1/1 | 0.95 | 0.08 | -6.12 | 28,28,28,28 | 0 |
| 32 | MG | A | 8002 | 1/1 | 0.99 | 0.06 | -6.12 | 28,28,28,28 | 0 |
| 32 | MG | A | 8054 | 1/1 | 0.97 | 0.10 | -6.39 | 24,24,24,24 | 0 |
| 32 | MG | A | 8096 | 1/1 | 0.96 | 0.07 | -6.45 | 46,46,46,46 | 0 |
| 32 | MG | A | 8052 | 1/1 | 0.97 | 0.06 | -7.72 | 40,40,40,40 | 0 |
| 32 | MG | A | 8071 | 1/1 | 0.97 | 0.04 | -8.63 | 63,63,63,63 | 0 |
| 33 | NA | A | 8344 | 1/1 | 0.99 | 0.05 | -8.67 | 25,25,25,25 | 0 |
| 32 | MG | A | 8017 | 1/1 | 0.99 | 0.03 | -8.67 | 19,19,19,19 | 0 |
| 32 | MG | A | 8020 | 1/1 | 1.00 | 0.06 | -8.70 | 28,28,28,28 | 0 |
| 32 | MG | A | 8028 | 1/1 | 0.99 | 0.09 | -9.05 | 34,34,34,34 | 0 |
| 32 | MG | A | 8008 | 1/1 | 0.97 | 0.05 | -9.79 | 35,35,35,35 | 0 |
| 32 | MG | A | 8006 | 1/1 | 0.98 | 0.04 | -10.76 | 30,30,30,30 | 0 |
| 32 | MG | A | 8035 | 1/1 | 0.98 | 0.03 | -10.78 | 52,52,52,52 | 0 |
| 32 | MG | A | 8084 | 1/1 | 0.99 | 0.05 | -11.19 | 40,40,40,40 | 0 |
| 32 | MG | A | 8080 | 1/1 | 0.99 | 0.05 | -12.48 | 36,36,36,36 | 0 |
| 32 | MG | A | 8077 | 1/1 | 0.99 | 0.06 | -13.58 | 27,27,27,27 | 0 |
| 32 | MG | A | 8014 | 1/1 | 0.99 | 0.06 | -24.42 | 25,25,25,25 | 0 |
| 32 | MG | A | 8075 | 1/1 | 0.96 | 0.07 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 8115 | 1/1 | 0.98 | 0.06 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 8102 | 1/1 | 0.98 | 0.12 | - | 45,45,45,45 | 0 |
| 33 | NA | A | 8358 | 1/1 | 0.95 | 0.79 | - | 82,82,82,82 | 0 |
| 32 | MG | L | 8069 | 1/1 | 0.95 | 0.07 | - | 50,50,50,50 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 33 | NA | A | 8377 | 1/1 | 0.93 | 0.22 | - | 66,66,66,66 | 0 |
| 32 | MG | B | 8095 | 1/1 | 0.72 | 0.17 | - | 70,70,70,70 | 0 |
| 33 | NA | A | 8363 | 1/1 | 0.85 | 0.25 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 8079 | 1/1 | 0.96 | 0.11 | - | 27,27,27,27 | 0 |
| 32 | MG | A | 8034 | 1/1 | 0.99 | 0.07 | - | 33,33,33,33 | 0 |
| 32 | MG | A | 8101 | 1/1 | 0.91 | 0.13 | - | 52,52,52,52 | 0 |
| 33 | NA | A | 8367 | 1/1 | 0.95 | 0.10 | - | 44,44,44,44 | 0 |
| 35 | CL | A | 8514 | 1/1 | 0.97 | 0.12 | - | 46,46,46,46 | 0 |
| 33 | NA | A | 8375 | 1/1 | 0.92 | 0.60 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 8050 | 1/1 | 0.93 | 0.15 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 8088 | 1/1 | 0.95 | 0.09 | - | 30,30,30,30 | 0 |
| 32 | MG | A | 8016 | 1/1 | 0.97 | 0.11 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 8086 | 1/1 | 0.99 | 0.17 | - | 45,45,45,45 | 0 |
| 32 | MG | A | 8117 | 1/1 | 0.97 | 0.08 | - | 25,25,25,25 | 0 |
| 33 | NA | A | 8328 | 1/1 | 0.96 | 0.32 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 8098 | 1/1 | 0.96 | 0.14 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 8037 | 1/1 | 0.97 | 0.05 | - | 34,34,34,34 | 0 |
| 33 | NA | A | 8318 | 1/1 | 0.97 | 0.41 | - | 55,55,55,55 | 0 |
| 33 | NA | A | 8354 | 1/1 | 0.96 | 0.27 | - | 34,34,34,34 | 0 |
| 33 | NA | T | 8312 | 1/1 | 0.68 | 0.65 | - | 79,79,79,79 | 0 |
| 33 | NA | A | 8334 | 1/1 | 0.96 | 0.06 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 8089 | 1/1 | 0.89 | 0.08 | - | 58,58,58,58 | 0 |
| 35 | CL | O | 8507 | 1/1 | 0.84 | 0.27 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 8111 | 1/1 | 0.94 | 0.10 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 8048 | 1/1 | 0.98 | 0.16 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 8114 | 1/1 | 0.92 | 0.22 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 8093 | 1/1 | 0.98 | 0.07 | - | 49,49,49,49 | 0 |
| 33 | NA | A | 8352 | 1/1 | 0.76 | 0.41 | - | 71,71,71,71 | 0 |
| 32 | MG | A | 8066 | 1/1 | 0.93 | 0.23 | - | 84,84,84,84 | 0 |
| 32 | MG | A | 8072 | 1/1 | 0.98 | 0.10 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 8082 | 1/1 | 0.91 | 0.11 | - | 53,53,53,53 | 0 |
| 33 | NA | A | 8301 | 1/1 | 0.92 | 0.17 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 8030 | 1/1 | 0.99 | 0.10 | - | 32,32,32,32 | 0 |
| 33 | NA | A | 8329 | 1/1 | 0.75 | 0.23 | - | 54,54,54,54 | 0 |
| 33 | NA | A | 8306 | 1/1 | 0.95 | 0.52 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 8040 | 1/1 | 0.97 | 0.12 | - | 53,53,53,53 | 0 |
| 35 | CL | C | 8509 | 1/1 | 0.94 | 0.18 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 8116 | 1/1 | 0.96 | 0.11 | - | 51,51,51,51 | 0 |
| 35 | CL | Z | 8520 | 1/1 | 0.93 | 0.12 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 8031 | 1/1 | 0.99 | 0.05 | - | 27,27,27,27 | 0 |
| 32 | MG | A | 8063 | 1/1 | 0.95 | 0.05 | - | 73,73,73,73 | 0 |
| 35 | CL | A | 8503 | 1/1 | 0.95 | 0.13 | - | 46,46,46,46 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | A | 8042 | 1/1 | 0.97 | 0.12 | - | 31,31,31,31 | 0 |
| 33 | NA | B | 8351 | 1/1 | 0.59 | 0.53 | - | 78,78,78,78 | 0 |
| 33 | NA | A | 8355 | 1/1 | 0.92 | 0.55 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 8068 | 1/1 | 0.96 | 0.16 | - | 50,50,50,50 | 0 |
| 33 | NA | A | 8330 | 1/1 | 0.98 | 0.21 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 8025 | 1/1 | 0.98 | 0.07 | - | 40,40,40,40 | 0 |
| 33 | NA | A | 8315 | 1/1 | 0.99 | 0.10 | - | 32,32,32,32 | 0 |
| 35 | CL | A | 8522 | 1/1 | 0.98 | 0.17 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 8049 | 1/1 | 0.92 | 0.62 | - | 77,77,77,77 | 0 |
| 33 | NA | A | 8316 | 1/1 | 0.97 | 0.21 | - | 40,40,40,40 | 0 |
| 35 | CL | K | 8501 | 1/1 | 0.96 | 0.12 | - | 55,55,55,55 | 0 |
| 33 | NA | E | 8304 | 1/1 | 0.90 | 0.17 | - | 33,33,33,33 | 0 |
| 32 | MG | A | 8041 | 1/1 | 0.95 | 0.16 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 8076 | 1/1 | 0.80 | 0.09 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 8022 | 1/1 | 0.97 | 0.12 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 8103 | 1/1 | 0.94 | 0.18 | - | 61,61,61,61 | 0 |
| 35 | CL | A | 8513 | 1/1 | 0.98 | 0.11 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 8051 | 1/1 | 0.96 | 0.08 | - | 57,57,57,57 | 0 |
| 33 | NA | A | 8349 | 1/1 | 0.97 | 0.14 | - | 41,41,41,41 | 0 |
| 32 | MG | 1 | 8105 | 1/1 | 0.89 | 0.27 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 8104 | 1/1 | 0.95 | 0.26 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 8091 | 1/1 | 0.96 | 0.05 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 8061 | 1/1 | 0.96 | 0.08 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 8113 | 1/1 | 0.73 | 0.20 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 8094 | 1/1 | 0.94 | 0.04 | - | 63,63,63,63 | 0 |
| 33 | NA | A | 8341 | 1/1 | 0.91 | 0.13 | - | 41,41,41,41 | 0 |
| 33 | NA | A | 8370 | 1/1 | 0.97 | 0.41 | - | 57,57,57,57 | 0 |
| 35 | CL | S | 8506 | 1/1 | 0.98 | 0.11 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 8043 | 1/1 | 0.97 | 0.08 | - | 39,39,39,39 | 0 |
| 39 | CD | P | 8405 | 1/1 | 0.56 | 0.14 | - | 174,174,174,174 | 0 |
| 33 | NA | A | 8384 | 1/1 | 0.38 | 0.82 | - | 75,75,75,75 | 0 |
| 32 | MG | A | 8005 | 1/1 | 0.96 | 0.12 | - | 33,33,33,33 | 0 |
| 33 | NA | A | 8369 | 1/1 | 0.91 | 0.14 | - | 49,49,49,49 | 0 |
| 33 | NA | A | 8313 | 1/1 | 0.88 | 0.10 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 8009 | 1/1 | 0.99 | 0.04 | - | 26,26,26,26 | 0 |
| 32 | MG | A | 8011 | 1/1 | 0.98 | 0.09 | - | 26,26,26,26 | 0 |
| 32 | MG | A | 8036 | 1/1 | 0.98 | 0.05 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 8092 | 1/1 | 0.96 | 0.13 | - | 79,79,79,79 | 0 |
| 32 | MG | A | 8090 | 1/1 | 0.91 | 0.29 | - | 70,70,70,70 | 0 |
| 33 | NA | A | 8326 | 1/1 | 0.88 | 0.33 | - | 37,37,37,37 | 0 |
| 33 | NA | A | 8385 | 1/1 | 0.68 | 0.41 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 8045 | 1/1 | 0.91 | 0.09 | - | 56,56,56,56 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 33 | NA | A | 8336 | 1/1 | 0.96 | 0.06 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 8026 | 1/1 | 0.99 | 0.07 | - | 26,26,26,26 | 0 |
| 32 | MG | A | 8085 | 1/1 | 0.92 | 0.11 | - | 45,45,45,45 | 0 |
| 33 | NA | A | 8342 | 1/1 | 0.93 | 0.23 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 8106 | 1/1 | 0.92 | 0.08 | - | 52,52,52,52 | 0 |
| 33 | NA | A | 8319 | 1/1 | 0.94 | 0.10 | - | 36,36,36,36 | 0 |
| 33 | NA | A | 8357 | 1/1 | 0.89 | 0.08 | - | 53,53,53,53 | 0 |
| 33 | NA | A | 8307 | 1/1 | 0.70 | 0.27 | - | 46,46,46,46 | 0 |
| 35 | CL | K | 8502 | 1/1 | 0.87 | 0.14 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 8087 | 1/1 | 0.91 | 0.19 | - | 63,63,63,63 | 0 |
| 35 | CL | A | 8517 | 1/1 | 0.93 | 0.14 | - | 59,59,59,59 | 0 |
| 32 | MG | A | 8023 | 1/1 | 0.98 | 0.06 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 8083 | 1/1 | 0.94 | 0.09 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 8100 | 1/1 | 0.95 | 0.16 | - | 65,65,65,65 | 0 |
| 33 | NA | A | 8360 | 1/1 | 0.95 | 0.56 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 8081 | 1/1 | 0.97 | 0.12 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 8099 | 1/1 | 0.95 | 0.12 | - | 48,48,48,48 | 0 |
| 32 | MG | A | 8029 | 1/1 | 0.98 | 0.08 | - | 41,41,41,41 | 0 |
| 35 | CL | A | 8511 | 1/1 | 0.94 | 0.11 | - | 48,48,48,48 | 0 |
| 35 | CL | M | 8510 | 1/1 | 0.98 | 0.16 | - | 47,47,47,47 | 0 |
| 33 | NA | A | 8381 | 1/1 | 0.98 | 0.23 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 8097 | 1/1 | 0.98 | 0.17 | - | 28,28,28,28 | 0 |
| 32 | MG | A | 8024 | 1/1 | 0.48 | 1.23 | - | 89,89,89,89 | 0 |
| 33 | NA | J | 8322 | 1/1 | 0.70 | 0.31 | - | 61,61,61,61 | 0 |
| 33 | NA | A | 8311 | 1/1 | 0.76 | 0.30 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 8047 | 1/1 | 0.94 | 0.15 | - | 66,66,66,66 | 0 |
| 32 | MG | A | 8046 | 1/1 | 0.94 | 0.08 | - | 47,47,47,47 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.