



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:16 PM GMT

PDB ID : 3CCL  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535C. Density for Anisomycin is visible but not included in model.  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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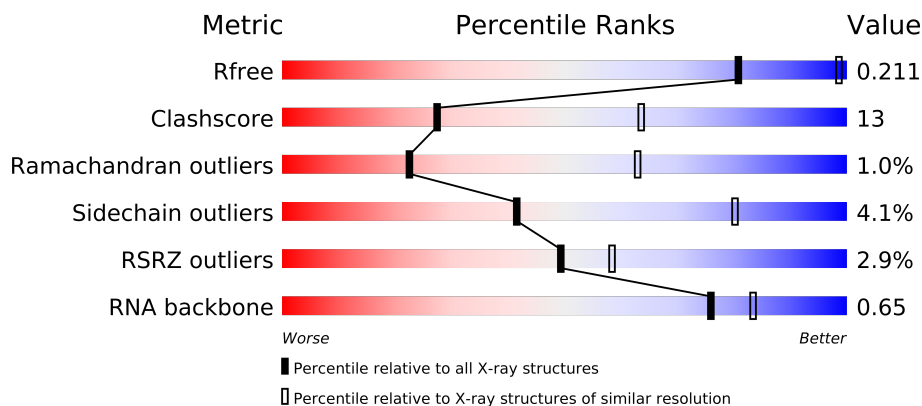
The following versions of software and data (see [references](#)) were used in the production of this report:

|                                |   |                          |
|--------------------------------|---|--------------------------|
| 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 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1053 (2.90-2.90)                                      |
| Clashscore            | 79885                       | 1326 (2.90-2.90)                                      |
| Ramachandran outliers | 78287                       | 1290 (2.90-2.90)                                      |
| Sidechain outliers    | 78261                       | 1292 (2.90-2.90)                                      |
| RSRZ outliers         | 66119                       | 1054 (2.90-2.90)                                      |
| RNA backbone          | 1838                        | 1055 (3.40-2.40)                                      |

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  $\geq 3$ , 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   | A     | 240    |                  |
| 2   | B     | 338    |                  |
| 3   | C     | 246    |                  |
| 4   | D     | 177    |                  |
| 5   | E     | 178    |                  |
| 6   | F     | 120    |                  |
| 7   | G     | 348    |                  |
| 8   | H     | 177    |                  |
| 9   | I     | 162    |                  |
| 10  | J     | 145    |                  |
| 11  | K     | 132    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 12  | L     | 165    |                  |
| 13  | M     | 196    |                  |
| 14  | N     | 187    |                  |
| 15  | O     | 116    |                  |
| 16  | P     | 149    |                  |
| 17  | Q     | 96     |                  |
| 18  | R     | 155    |                  |
| 19  | S     | 85     |                  |
| 20  | T     | 120    |                  |
| 21  | U     | 67     |                  |
| 22  | V     | 71     |                  |
| 23  | W     | 154    |                  |
| 24  | X     | 92     |                  |
| 25  | Y     | 241    |                  |
| 26  | Z     | 116    |                  |
| 27  | 1     | 57     |                  |
| 28  | 2     | 50     |                  |
| 29  | 3     | 92     |                  |
| 30  | 0     | 2923   |                  |
| 31  | 9     | 122    |                  |

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

| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 32  | MG   | 0     | 8008 | -        | X                |
| 32  | MG   | 0     | 8009 | -        | X                |
| 32  | MG   | 0     | 8014 | -        | X                |
| 32  | MG   | 0     | 8015 | -        | X                |
| 32  | MG   | 0     | 8016 | -        | X                |
| 32  | MG   | 0     | 8017 | -        | X                |
| 32  | MG   | 0     | 8018 | -        | X                |
| 32  | MG   | 0     | 8029 | -        | X                |
| 32  | MG   | 0     | 8030 | -        | X                |
| 32  | MG   | 0     | 8031 | -        | X                |
| 32  | MG   | 0     | 8037 | -        | X                |
| 32  | MG   | 0     | 8041 | -        | X                |
| 32  | MG   | 0     | 8047 | -        | X                |
| 32  | MG   | 0     | 8048 | -        | X                |
| 32  | MG   | 0     | 8055 | -        | X                |
| 32  | MG   | 0     | 8061 | -        | X                |
| 32  | MG   | 0     | 8063 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 32  | MG   | 0     | 8067 | -        | X                |
| 32  | MG   | 0     | 8071 | -        | X                |
| 32  | MG   | 0     | 8078 | -        | X                |
| 32  | MG   | 0     | 8080 | -        | X                |
| 32  | MG   | 0     | 8081 | -        | X                |
| 32  | MG   | 0     | 8082 | -        | X                |
| 32  | MG   | 0     | 8090 | -        | X                |
| 32  | MG   | 0     | 8092 | -        | X                |
| 32  | MG   | A     | 8051 | -        | X                |
| 34  | NA   | 0     | 8501 | -        | X                |
| 34  | NA   | 0     | 8505 | -        | X                |
| 34  | NA   | 0     | 8506 | -        | X                |
| 34  | NA   | 0     | 8509 | -        | X                |
| 34  | NA   | 0     | 8512 | -        | X                |
| 34  | NA   | 0     | 8514 | -        | X                |
| 34  | NA   | 0     | 8517 | -        | X                |
| 34  | NA   | 0     | 8518 | -        | X                |
| 34  | NA   | 0     | 8522 | -        | X                |
| 34  | NA   | 0     | 8524 | -        | X                |
| 34  | NA   | 0     | 8525 | -        | X                |
| 34  | NA   | 0     | 8527 | -        | X                |
| 34  | NA   | 0     | 8528 | -        | X                |
| 34  | NA   | 0     | 8530 | -        | X                |
| 34  | NA   | 0     | 8534 | -        | X                |
| 34  | NA   | 0     | 8535 | -        | X                |
| 34  | NA   | 0     | 8541 | -        | X                |
| 34  | NA   | 0     | 8542 | -        | X                |
| 34  | NA   | 0     | 8544 | -        | X                |
| 34  | NA   | 0     | 8545 | -        | X                |
| 34  | NA   | 0     | 8546 | -        | X                |
| 34  | NA   | 0     | 8547 | -        | X                |
| 34  | NA   | 0     | 8548 | -        | X                |
| 34  | NA   | 0     | 8549 | -        | X                |
| 34  | NA   | 0     | 8550 | -        | X                |
| 34  | NA   | 0     | 8551 | -        | X                |
| 34  | NA   | 0     | 8552 | -        | X                |
| 34  | NA   | 0     | 8554 | -        | X                |
| 34  | NA   | 0     | 8555 | -        | X                |
| 34  | NA   | 0     | 8556 | -        | X                |
| 34  | NA   | 0     | 8558 | -        | X                |
| 34  | NA   | 0     | 8559 | -        | X                |
| 34  | NA   | 0     | 8560 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 34  | NA   | 0     | 8561 | -        | X                |
| 34  | NA   | 0     | 8562 | -        | X                |
| 34  | NA   | 0     | 8563 | -        | X                |
| 34  | NA   | 0     | 8564 | -        | X                |
| 34  | NA   | 0     | 8565 | -        | X                |
| 34  | NA   | 0     | 8566 | -        | X                |
| 34  | NA   | 0     | 8567 | -        | X                |
| 34  | NA   | 0     | 8568 | -        | X                |
| 34  | NA   | 0     | 8569 | -        | X                |
| 34  | NA   | 0     | 8573 | -        | X                |
| 34  | NA   | 0     | 8574 | -        | X                |
| 34  | NA   | 9     | 8572 | -        | X                |
| 35  | CL   | 0     | 8816 | -        | X                |
| 35  | CL   | 0     | 8822 | -        | X                |
| 35  | CL   | Y     | 8820 | -        | X                |
| 36  | SR   | 0     | 8903 | -        | X                |
| 36  | SR   | 0     | 8904 | -        | X                |
| 36  | SR   | 0     | 8905 | -        | X                |
| 36  | SR   | 0     | 8909 | -        | X                |
| 36  | SR   | 0     | 8914 | -        | X                |
| 36  | SR   | 0     | 8922 | -        | X                |
| 36  | SR   | 0     | 8924 | -        | X                |
| 36  | SR   | 0     | 8925 | -        | X                |
| 36  | SR   | 0     | 8926 | -        | X                |
| 36  | SR   | 0     | 8937 | -        | X                |
| 36  | SR   | 0     | 8938 | -        | X                |
| 36  | SR   | 0     | 8946 | -        | X                |
| 36  | SR   | 0     | 8947 | -        | X                |
| 36  | SR   | 0     | 8959 | -        | X                |
| 36  | SR   | 0     | 8976 | -        | X                |
| 36  | SR   | 0     | 8979 | -        | X                |
| 36  | SR   | 0     | 8982 | -        | X                |
| 36  | SR   | 0     | 8983 | -        | X                |
| 36  | SR   | 0     | 8986 | -        | X                |
| 36  | SR   | 0     | 8994 | -        | X                |
| 36  | SR   | 0     | 8996 | -        | X                |
| 36  | SR   | 0     | 8997 | -        | X                |
| 36  | SR   | 0     | 9004 | -        | X                |
| 36  | SR   | 0     | 9007 | -        | X                |
| 36  | SR   | B     | 8987 | -        | X                |
| 36  | SR   | S     | 8961 | -        | X                |

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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 protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1753  | 1072 | 352 | 324 | 5 |         |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 337      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2625  | 1616 | 493 | 511 | 5 |         |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L4P.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 246      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1860  | 1130 | 345 | 384 | 1 |         |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1357  | 840 | 224 | 289 | 4 |         |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 890   | 551 | 141 | 197 | 1 |         |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L10E.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | G     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 240   | 149 | 39 | 51 | 1 |         |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L10e.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1282  | 798 | 240 | 238 | 6 |         |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L11P.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 9   | I     | 70       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 519   | 323 | 81 | 114 | 1 |         |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1120  | 696 | 199 | 222 | 3 |         |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 994   | 609 | 189 | 192 | 4 |         |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 12  | L     | 145      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1118  | 670 | 222 | 226 |         |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 194      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1558  | 943 | 333 | 281 | 1 |         |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | N     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 895 | 262 | 286 | 2 |         |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15  | O     | 115      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 865   | 529 | 161 | 175 |  |         |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L19e.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 16  | P     | 143      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1136  | 683 | 229 | 224 |  |         |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17  | Q     | 95       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 735   | 450 | 141 | 144 |  |         |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | R     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1149  | 713 | 209 | 223 | 4 |         |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 641   | 389 | 111 | 138 | 3 |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L24P.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 20  | T     | 119      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 950   | 568 | 180 | 202 |  |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L24e.



| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21  | U     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 410   | 244 | 75 | 86 | 5 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 22  | V     | 65       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 499   | 304 | 94 | 100 | 1 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | W     | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1196  | 737 | 209 | 244 | 6 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | X     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 654   | 402 | 129 | 122 | 1 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L32e.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 25  | Y     | 142      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1130  | 686 | 228 | 216 |  |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | Z     | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 573   | 343 | 113 | 112 | 5 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | 1     | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 431   | 258 | 86 | 83 | 4 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | 2     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 396   | 239 | 89 | 67 | 1 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | 3     | 92       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 458 | 153 | 137 | 7 |         |         |       |

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 30  | 0     | 2754     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 59020 | 26349 | 10874 | 19052 | 2745 |         |         |       |

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 31  | 9     | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2599  | 1160 | 471 | 847 | 121 |         |         |       |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 32  | 0     | 87       | Total | Mg | 0       | 0       |
|     |       |          | 87    | 87 |         |         |
| 32  | Y     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 32  | K     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 32  | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 32  | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 32  | T     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 32  | 9     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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

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

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

| Mol | Chain | Residues | Atoms             | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 34  | 0     | 67       | Total Na<br>67 67 | 0       | 0       |
| 34  | J     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | Q     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | C     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | R     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | 9     | 2        | Total Na<br>2 2   | 0       | 0       |
| 34  | S     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | M     | 1        | Total Na<br>1 1   | 0       | 0       |

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

| Mol | Chain | Residues | Atoms             | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 35  | 0     | 10       | Total Cl<br>10 10 | 0       | 0       |
| 35  | J     | 3        | Total Cl<br>3 3   | 0       | 0       |
| 35  | B     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | A     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | N     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | O     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | R     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | Y     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | L     | 1        | Total Cl<br>1 1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35  | 3     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |
| 35  | M     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 36  | 0     | 93       | Total<br>93 | Sr<br>93 | 0       | 0       |
| 36  | 1     | 2        | Total<br>2  | Sr<br>2  | 0       | 0       |
| 36  | B     | 2        | Total<br>2  | Sr<br>2  | 0       | 0       |
| 36  | 3     | 2        | Total<br>2  | Sr<br>2  | 0       | 0       |
| 36  | A     | 3        | Total<br>3  | Sr<br>3  | 0       | 0       |
| 36  | R     | 1        | Total<br>1  | Sr<br>1  | 0       | 0       |
| 36  | 9     | 3        | Total<br>3  | Sr<br>3  | 0       | 0       |
| 36  | S     | 1        | Total<br>1  | Sr<br>1  | 0       | 0       |
| 36  | F     | 1        | Total<br>1  | Sr<br>1  | 0       | 0       |

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

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

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 38  | 0     | 5929     | Total<br>5929 | O<br>5929 | 0       | 0       |
| 38  | 9     | 147      | Total<br>147  | O<br>147  | 0       | 0       |
| 38  | A     | 116      | Total<br>116  | O<br>116  | 0       | 0       |
| 38  | B     | 141      | Total<br>141  | O<br>141  | 0       | 0       |
| 38  | C     | 170      | Total<br>170  | O<br>170  | 0       | 0       |
| 38  | D     | 44       | Total<br>44   | O<br>44   | 0       | 0       |
| 38  | E     | 45       | Total<br>45   | O<br>45   | 0       | 0       |
| 38  | F     | 27       | Total<br>27   | O<br>27   | 0       | 0       |
| 38  | G     | 19       | Total<br>19   | O<br>19   | 0       | 0       |
| 38  | H     | 63       | Total<br>63   | O<br>63   | 0       | 0       |
| 38  | I     | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 38  | J     | 53       | Total<br>53   | O<br>53   | 0       | 0       |
| 38  | K     | 56       | Total<br>56   | O<br>56   | 0       | 0       |
| 38  | L     | 85       | Total<br>85   | O<br>85   | 0       | 0       |
| 38  | M     | 123      | Total<br>123  | O<br>123  | 0       | 0       |
| 38  | N     | 55       | Total<br>55   | O<br>55   | 0       | 0       |
| 38  | O     | 43       | Total<br>43   | O<br>43   | 0       | 0       |
| 38  | P     | 67       | Total<br>67   | O<br>67   | 0       | 0       |
| 38  | Q     | 50       | Total<br>50   | O<br>50   | 0       | 0       |
| 38  | R     | 85       | Total<br>85   | O<br>85   | 0       | 0       |
| 38  | S     | 33       | Total<br>33   | O<br>33   | 0       | 0       |
| 38  | T     | 34       | Total<br>34   | O<br>34   | 0       | 0       |

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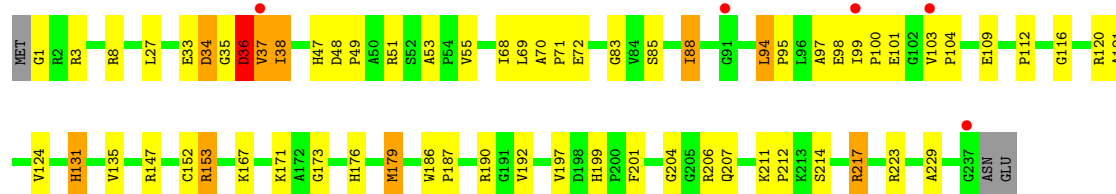
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 38  | U     | 27       | Total<br>27 | O<br>27 | 0       | 0       |
| 38  | V     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 38  | W     | 69       | Total<br>69 | O<br>69 | 0       | 0       |
| 38  | X     | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 38  | Y     | 95       | Total<br>95 | O<br>95 | 0       | 0       |
| 38  | Z     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 38  | 1     | 63       | Total<br>63 | O<br>63 | 0       | 0       |
| 38  | 2     | 50       | Total<br>50 | O<br>50 | 0       | 0       |
| 38  | 3     | 62       | Total<br>62 | O<br>62 | 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 ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

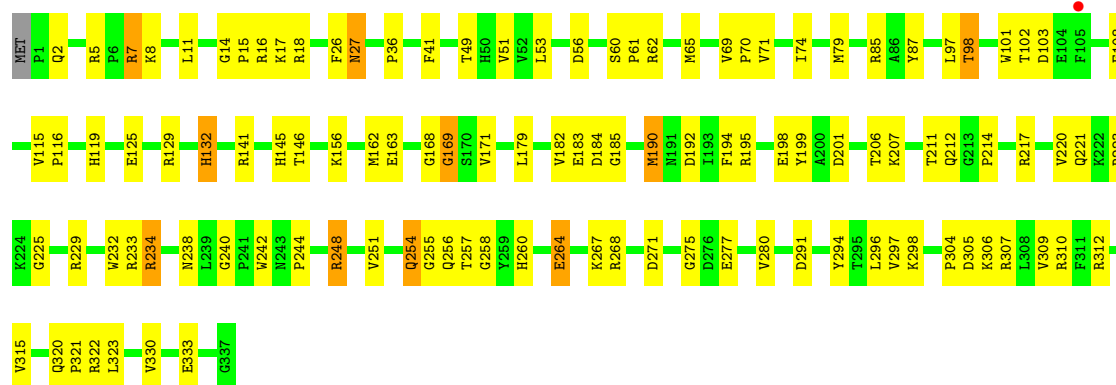
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



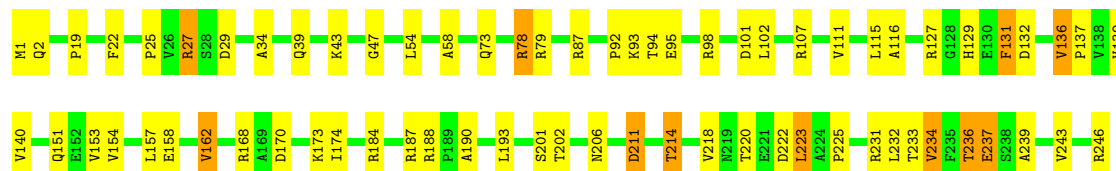
- Molecule 2: 50S ribosomal protein L3P

Chain B: 



- Molecule 3: 50S ribosomal protein L4P

Chain C: 



- Molecule 4: 50S ribosomal protein L5P

Chain D: 





- Molecule 9: 50S ribosomal protein L11P

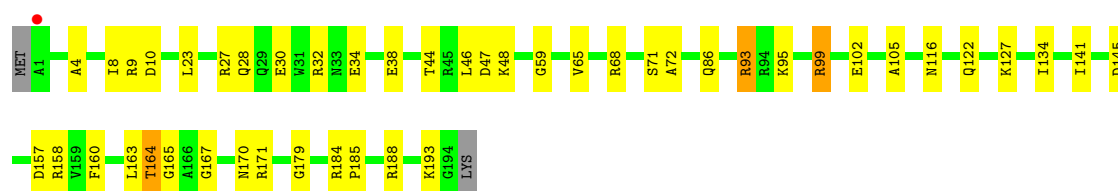
- Molecule 10: 50S ribosomal protein L13P

- Molecule 11: 50S ribosomal protein L14P

- Molecule 12: 50S ribosomal protein L15P

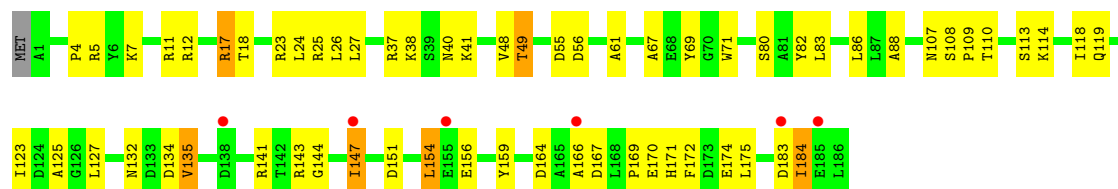
- Molecule 13: 50S ribosomal protein L15e





- Molecule 14: 50S ribosomal protein L18P

Chain N:



- Molecule 15: 50S ribosomal protein L18e

Chain O:



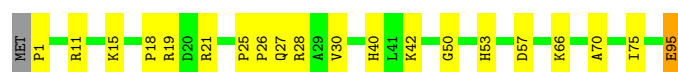
- Molecule 16: 50S ribosomal protein L19e

Chain P:



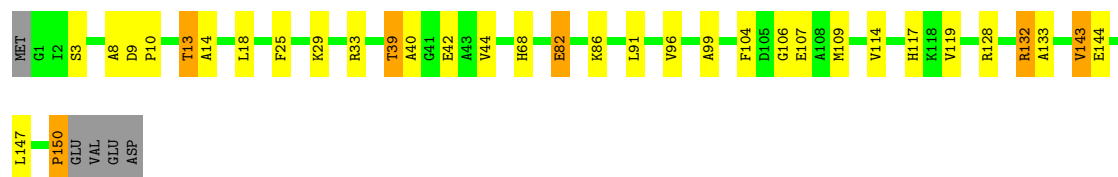
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



- Molecule 18: 50S ribosomal protein L22P

Chain R:

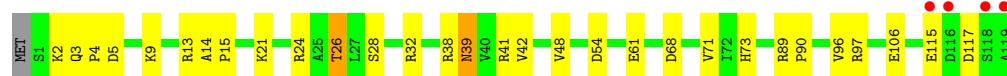


- Molecule 19: 50S ribosomal protein L23P

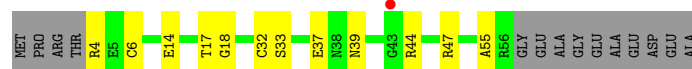
Chain S:



- Chain T: 



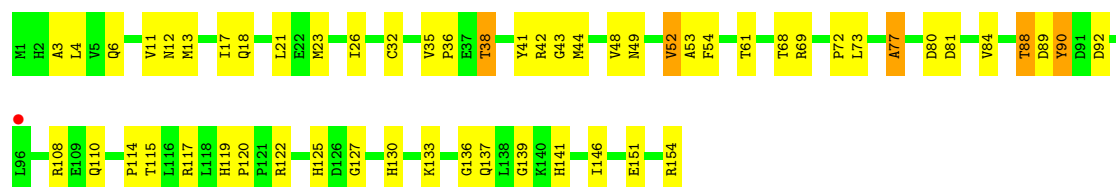
- Chain U: 



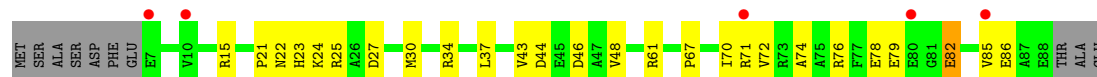
- Chain V:



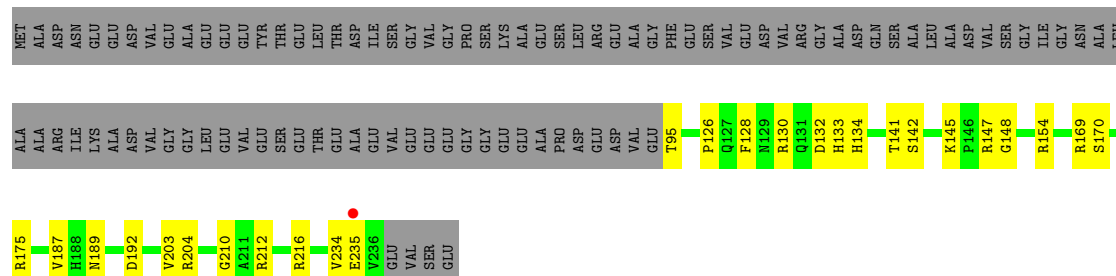
- Chain W: 



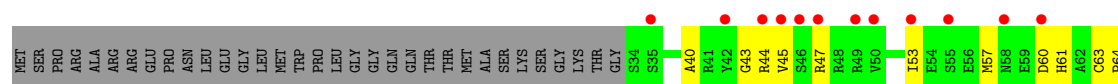
- Chain X:



- Chain Y: 



- Chain Z:



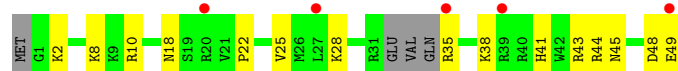
• Molecule 27: 50S ribosomal protein L37e

Chain 1:



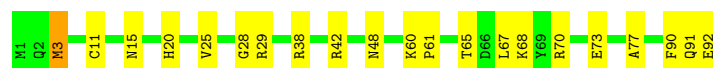
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



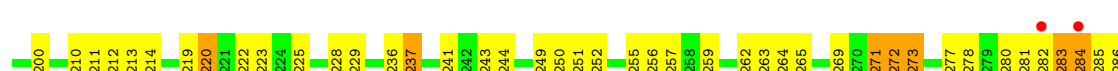
• Molecule 29: 50S ribosomal protein L44E

Chain 3:



• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:



|       |       |       |       |       |       |       |       |       |       |       |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|
| G2073 | C1853 | G1743 | C1652 | G1546 | A1434 | C1343 | A1242 | C1168 | C1068 | C880  | A790 | G684 |
| A2074 | C1854 | C1750 | A1653 | G1552 | C1436 | G1344 | A1243 | U1169 | C1069 | C     | A791 | C885 |
| A2081 | C1855 | C1751 | U1654 | C1553 | C1435 | U1350 | U1244 | A1171 | G1071 | C     | G792 | C886 |
| G2082 | C1856 | G1752 | A1655 | C1554 | G1441 | G1351 | C1245 | A1172 | G1072 | A     | U800 | G687 |
| A2083 | A1857 | A1759 | A1656 | C1555 | A1442 | C1352 | A1246 | A1173 | A1078 | G     | G801 | G688 |
| G2088 | A1858 | C1760 | A1657 | C1556 | U1446 | C1353 | U1249 | A1174 | A1079 | A     | U807 | G689 |
| A2089 | G1863 | U1761 | A1658 | U     | U1447 | A1358 | U1250 | G1176 | A1080 | G     | A808 | A694 |
| G2090 | C1866 | C1762 | G1665 | C1561 | U1447 | U1359 | C1268 | A1177 | A1081 | A     | G809 | C695 |
| C2091 | A1969 | C1763 | A1667 | U1562 | C1450 | C1360 | C1269 | U1180 | A1088 | G     | U900 | C696 |
| G2092 | G1868 | U1766 | U1668 | A1573 | C1451 | C1366 | G1269 | U1181 | U     | U     | A812 | G697 |
| A2096 | C1872 | A1767 | U1677 | U1573 | U1461 | U     | C1273 | C1182 | A1097 | C     | C905 | A698 |
| A2101 | G1873 | C1768 | U1677 | G1586 | C1462 | A1372 | U1278 | C1183 | A1098 | G     | C912 | C899 |
| C2102 | C1877 | C1769 | A1678 | U1587 | C1462 | G1373 | A1278 | C1184 | U     | C     | A912 | U701 |
| A2103 | G1877 | U1770 | C1679 | G1588 | U1482 | C1374 | U1279 | U1185 | G1099 | G     | C920 | G702 |
| C2104 | C1878 | U1771 | C1679 | G1589 | C1483 | A1375 | A1280 | C1186 | A     | C     | G921 | G703 |
| A2105 | U1879 | G1772 | A1682 | C1592 | C1477 | G1376 | U1291 | U1187 | C1104 | A     | A922 | C704 |
| C2106 | U1883 | C1773 | A1683 | C1593 | U1478 | C1377 | A1287 | U1188 | U1109 | C999  | A923 | C705 |
| G2110 | G1884 | G1774 | A1684 | C1593 | U1478 | G1378 | U1288 | A1189 | G1110 | C1000 | C822 | G709 |
| A2111 | A1885 | A1778 | A1685 | C1594 | C1482 | U1380 | C1289 | G1190 | U1115 | U1001 | U823 | G710 |
| C2112 | A1886 | A1779 | G1686 | G1595 | C1483 | U1381 | G1290 | A1191 | U1116 | G1002 | G824 | G711 |
| C2113 | G1896 | C1787 | C1687 | U1596 | C1484 | G1382 | A1291 | A1192 | U1117 | U     | U826 | C712 |
| C2114 | U1897 | U1788 | C1688 | A1597 | A1485 | U1383 | A1294 | A1193 | A1005 | A1006 | A827 | U713 |
| G2115 | U1903 | G1789 | G1697 | A1603 | A1486 | C1384 | G1295 | G1195 | A1007 | A1007 | C834 | U    |
| U2116 | C1904 | U1791 | C1700 | G1604 | U1487 | G1385 | A1296 | U1120 | C1008 | C     | U835 | G716 |
| C2121 | U1905 | G1795 | A1701 | G1605 | U1488 | C1386 | U1297 | U1198 | U1009 | U942  | G836 | C717 |
| C2122 | A1909 | A1796 | U1702 | A1606 | C1495 | G1387 | U1299 | A1199 | C1010 | G944  | U840 | C718 |
| G2128 | A1919 | C1797 | G1706 | A1615 | U1503 | G1391 | G1300 | A1200 | A1014 | U945  | A841 | G724 |
| C2134 | C1921 | G1805 | A1710 | C1617 | A1504 | A1394 | U1304 | C1201 | C1015 | U946  | A842 | C725 |
| A2135 | A1921 | G1806 | A1711 | C1617 | U1505 | C1395 | C1305 | A1207 | U1016 | U947  | U843 | G738 |
| G2136 | A1922 | G1806 | A1712 | C1617 | U1506 | C1396 | U1306 | U1205 | A1020 | U949  | U844 | U734 |
| A     | G1925 | C1818 | C1714 | G1622 | C1513 | C1397 | A1308 | U1206 | C1025 | A951  | A846 | C735 |
| C     | G1926 | G1819 | C1715 | G1623 | C1514 | G1398 | U1311 | A1207 | U1026 | G952  | C847 | A736 |
| A     | A1927 | G1820 | A1717 | A1624 | A1516 | A1399 | G1312 | C1208 | G1027 | G953  | C848 | G738 |
| C     | C1940 | U1825 | U1722 | U1625 | G1520 | G1401 | U1314 | C1209 | U1028 | C     | C853 | U741 |
| C     | A1941 | C1826 | G1723 | G1627 | C1521 | A1407 | A1321 | G1211 | U1029 | G958  | U854 | C741 |
| A     | C1942 | A1829 | U1724 | G1627 | A1522 | U1408 | G1322 | C1212 | C1044 | C959  | A857 | G744 |
| C     | C1943 | C1830 | C1725 | A1630 | G1523 | G1409 | G1322 | G1216 | G1045 | A961  | U858 | G745 |
| A     | G1947 | G1834 | G1730 | A1631 | U1524 | A1413 | G1325 | G1221 | G1052 | C962  | A861 | G746 |
| C     | G1948 | U1835 | C1731 | C1633 | A1525 | A1414 | A1328 | A1154 | G1053 | C963  | A867 | C748 |
| C     | G1949 | U1836 | A1732 | G1634 | A1527 | G1415 | U1331 | G1155 | G1054 | G968  | G868 | C749 |
| A     | G1950 | U1838 | A1733 | U1635 | A1528 | U1419 | C1332 | G1159 | U1056 | G969  | C869 | A750 |
| G     | G1951 | A1839 | C1735 | A1637 | G1535 | U1422 | U1333 | G1160 | A1057 | U     | G870 | C759 |
| U     | U     | A1840 | A1736 | U1637 | C1536 | C1423 | C1334 | A1161 | U     | G     | U872 | C764 |
| G     | A     | A     | A1736 | A1641 | C1537 | A1424 | G1339 | G1163 | C1060 | U     | A875 | G765 |
| C     | A     | A     | A1642 | A1642 | C1538 | G1425 | A1340 | U1164 | G1063 | C     | A876 | G775 |
| A     | C     | A     | C1643 | U1645 | U1539 | C1426 | A1341 | G1165 | U1066 | G     | G877 | A776 |
| G     | U     | A     | U1644 | U1645 | U1539 | C1426 | A1341 | G1166 | A1067 | C     | G878 | U777 |
| A     | U     | A     | U1645 | U1645 | U1545 | G1430 | C1342 | G1239 | A1067 | C     | C879 | C    |



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 213.16Å 300.03Å 576.13Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.98 – 2.90<br>85.91 – 2.41                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.2 (49.98-2.90)<br>92.3 (85.91-2.41)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.13  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.00 (at 2.40Å)   | Xtriage          |
| Refinement program  | CNS 1.0   | Depositor        |
| R, $R_{free}$   | 0.171 , 0.220<br>0.167 , 0.211                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3626 reflections (0.99%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.0  | Xtriage          |
| Anisotropy  | 0.314   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 47.3   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Outliers  | 0 of 667133 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 99122   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | A     | 0.32         | 0/1786         | 0.64        | 0/2408           |
| 2   | B     | 0.32         | 0/2690         | 0.64        | 0/3652           |
| 3   | C     | 0.36         | 0/1885         | 0.63        | 0/2552           |
| 4   | D     | 0.32         | 0/1111         | 0.56        | 0/1498           |
| 5   | E     | 0.33         | 0/1382         | 0.56        | 0/1880           |
| 6   | F     | 0.34         | 0/901          | 0.58        | 0/1224           |
| 7   | G     | 0.31         | 0/241          | 0.49        | 0/324            |
| 8   | H     | 0.33         | 0/1302         | 0.63        | 0/1743           |
| 9   | I     | 0.29         | 0/526          | 0.51        | 0/716            |
| 10  | J     | 0.36         | 0/1136         | 0.60        | 0/1530           |
| 11  | K     | 0.35         | 0/1004         | 0.67        | 0/1351           |
| 12  | L     | 0.33         | 0/1130         | 0.63        | 0/1509           |
| 13  | M     | 0.35         | 0/1582         | 0.61        | 0/2116           |
| 14  | N     | 0.30         | 0/1474         | 0.62        | 0/1999           |
| 15  | O     | 0.34         | 0/874          | 0.59        | 0/1181           |
| 16  | P     | 0.32         | 0/1147         | 0.51        | 0/1528           |
| 17  | Q     | 0.33         | 0/749          | 0.65        | 0/1005           |
| 18  | R     | 1.26         | 7/1172 (0.6%)  | 1.10        | 6/1578 (0.4%)    |
| 19  | S     | 0.32         | 0/648          | 0.55        | 0/875            |
| 20  | T     | 0.33         | 0/958          | 0.64        | 0/1289           |
| 21  | U     | 0.33         | 0/417          | 0.59        | 0/562            |
| 22  | V     | 0.33         | 0/502          | 0.52        | 0/675            |
| 23  | W     | 0.34         | 0/1219         | 0.63        | 0/1655           |
| 24  | X     | 0.35         | 0/664          | 0.60        | 0/895            |
| 25  | Y     | 0.36         | 0/1146         | 0.62        | 0/1536           |
| 26  | Z     | 0.37         | 0/584          | 0.60        | 0/781            |
| 27  | 1     | 0.39         | 0/438          | 0.59        | 0/578            |
| 28  | 2     | 0.34         | 0/401          | 0.60        | 0/529            |
| 29  | 3     | 0.36         | 0/771          | 0.55        | 0/1024           |
| 30  | 0     | 0.37         | 0/65957        | 0.68        | 13/102867 (0.0%) |
| 31  | 9     | 0.32         | 0/2904         | 0.68        | 1/4526 (0.0%)    |
| All | All   | 0.38         | 7/98701 (0.0%) | 0.67        | 20/147586 (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 |
|-----|-------|---------------------|---------------------|
| 18  | R     | 1                   | 0                   |
| 23  | W     | 0                   | 1                   |
| 30  | 0     | 0                   | 28                  |
| 31  | 9     | 0                   | 1                   |
| All | All   | 1                   | 30                  |

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

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 18  | R     | 150 | PRO  | CB-CG | 27.29  | 2.86        | 1.50     |
| 18  | R     | 150 | PRO  | CA-C  | -18.25 | 1.16        | 1.52     |
| 18  | R     | 150 | PRO  | CG-CD | 13.93  | 1.96        | 1.50     |
| 18  | R     | 150 | PRO  | C-O   | 11.88  | 1.47        | 1.23     |
| 18  | R     | 150 | PRO  | N-CA  | 11.37  | 1.66        | 1.47     |

The worst 5 of 20 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 18  | R     | 150 | PRO  | CB-CA-C | -22.47 | 55.83       | 112.00   |
| 18  | R     | 150 | PRO  | N-CA-C  | -19.40 | 61.65       | 112.10   |
| 18  | R     | 150 | PRO  | CA-N-CD | 12.30  | 128.92      | 111.70   |
| 18  | R     | 150 | PRO  | N-CA-CB | 10.97  | 116.46      | 103.30   |
| 18  | R     | 150 | PRO  | CA-C-O  | -8.51  | 99.79       | 120.20   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 18  | R     | 150 | PRO  | CA   |

5 of 30 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 30  | 0     | 131 | A    | Sidechain |
| 30  | 0     | 220 | C    | Sidechain |
| 30  | 0     | 333 | G    | Sidechain |
| 30  | 0     | 48  | A    | Sidechain |
| 23  | W     | 90  | TYR  | 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   | A     | 1753  | 0        | 1766     | 63      | 0            |
| 2   | B     | 2625  | 0        | 2533     | 89      | 0            |
| 3   | C     | 1860  | 0        | 1813     | 59      | 0            |
| 4   | D     | 1094  | 0        | 1085     | 45      | 0            |
| 5   | E     | 1357  | 0        | 1266     | 29      | 0            |
| 6   | F     | 890   | 0        | 843      | 26      | 0            |
| 7   | G     | 240   | 0        | 231      | 8       | 0            |
| 8   | H     | 1282  | 0        | 1292     | 33      | 0            |
| 9   | I     | 519   | 0        | 500      | 23      | 0            |
| 10  | J     | 1120  | 0        | 1098     | 32      | 0            |
| 11  | K     | 994   | 0        | 1027     | 32      | 0            |
| 12  | L     | 1118  | 0        | 1076     | 29      | 0            |
| 13  | M     | 1558  | 0        | 1573     | 42      | 0            |
| 14  | N     | 1445  | 0        | 1401     | 51      | 0            |
| 15  | O     | 865   | 0        | 873      | 18      | 0            |
| 16  | P     | 1136  | 0        | 1123     | 24      | 0            |
| 17  | Q     | 735   | 0        | 729      | 21      | 0            |
| 18  | R     | 1149  | 0        | 1122     | 37      | 0            |
| 19  | S     | 641   | 0        | 605      | 10      | 0            |
| 20  | T     | 950   | 0        | 924      | 21      | 0            |
| 21  | U     | 410   | 0        | 364      | 8       | 0            |
| 22  | V     | 499   | 0        | 511      | 17      | 0            |
| 23  | W     | 1196  | 0        | 1137     | 56      | 0            |
| 24  | X     | 654   | 0        | 653      | 18      | 0            |
| 25  | Y     | 1130  | 0        | 1133     | 23      | 0            |
| 26  | Z     | 573   | 0        | 532      | 15      | 0            |
| 27  | 1     | 431   | 0        | 426      | 23      | 0            |
| 28  | 2     | 396   | 0        | 413      | 15      | 0            |
| 29  | 3     | 755   | 0        | 728      | 18      | 0            |
| 30  | 0     | 59020 | 0        | 29811    | 1159    | 0            |
| 31  | 9     | 2599  | 0        | 1325     | 100     | 0            |
| 32  | 0     | 87    | 0        | 0        | 0       | 0            |
| 32  | 9     | 1     | 0        | 0        | 0       | 0            |
| 32  | A     | 1     | 0        | 0        | 0       | 0            |
| 32  | B     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | K     | 1     | 0        | 0        | 0       | 0            |
| 32  | T     | 1     | 0        | 0        | 0       | 0            |
| 32  | Y     | 1     | 0        | 0        | 0       | 0            |
| 33  | 0     | 2     | 0        | 0        | 0       | 0            |
| 34  | 0     | 67    | 0        | 0        | 0       | 0            |
| 34  | 9     | 2     | 0        | 0        | 0       | 0            |
| 34  | C     | 1     | 0        | 0        | 0       | 0            |
| 34  | J     | 1     | 0        | 0        | 0       | 0            |
| 34  | M     | 1     | 0        | 0        | 0       | 0            |
| 34  | Q     | 1     | 0        | 0        | 0       | 0            |
| 34  | R     | 1     | 0        | 0        | 0       | 0            |
| 34  | S     | 1     | 0        | 0        | 0       | 0            |
| 35  | 0     | 10    | 0        | 0        | 4       | 0            |
| 35  | 3     | 1     | 0        | 0        | 0       | 0            |
| 35  | A     | 1     | 0        | 0        | 0       | 0            |
| 35  | B     | 1     | 0        | 0        | 0       | 0            |
| 35  | J     | 3     | 0        | 0        | 2       | 0            |
| 35  | L     | 1     | 0        | 0        | 0       | 0            |
| 35  | M     | 1     | 0        | 0        | 0       | 0            |
| 35  | N     | 1     | 0        | 0        | 1       | 0            |
| 35  | O     | 1     | 0        | 0        | 0       | 0            |
| 35  | R     | 1     | 0        | 0        | 0       | 0            |
| 35  | Y     | 1     | 0        | 0        | 0       | 0            |
| 36  | 0     | 93    | 0        | 0        | 0       | 0            |
| 36  | 1     | 2     | 0        | 0        | 0       | 0            |
| 36  | 3     | 2     | 0        | 0        | 0       | 0            |
| 36  | 9     | 3     | 0        | 0        | 0       | 0            |
| 36  | A     | 3     | 0        | 0        | 0       | 0            |
| 36  | B     | 2     | 0        | 0        | 0       | 0            |
| 36  | F     | 1     | 0        | 0        | 0       | 0            |
| 36  | R     | 1     | 0        | 0        | 0       | 0            |
| 36  | S     | 1     | 0        | 0        | 0       | 0            |
| 37  | 1     | 1     | 0        | 0        | 0       | 0            |
| 37  | 3     | 1     | 0        | 0        | 0       | 0            |
| 37  | O     | 1     | 0        | 0        | 0       | 0            |
| 37  | U     | 1     | 0        | 0        | 0       | 0            |
| 37  | Z     | 1     | 0        | 0        | 0       | 0            |
| 38  | 0     | 5929  | 0        | 0        | 185     | 0            |
| 38  | 1     | 63    | 0        | 0        | 4       | 0            |
| 38  | 2     | 50    | 0        | 0        | 1       | 0            |
| 38  | 3     | 62    | 0        | 0        | 3       | 0            |
| 38  | 9     | 147   | 0        | 0        | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38  | A     | 116   | 0        | 0        | 5       | 0            |
| 38  | B     | 141   | 0        | 0        | 13      | 0            |
| 38  | C     | 170   | 0        | 0        | 13      | 0            |
| 38  | D     | 44    | 0        | 0        | 3       | 0            |
| 38  | E     | 45    | 0        | 0        | 2       | 0            |
| 38  | F     | 27    | 0        | 0        | 2       | 0            |
| 38  | G     | 19    | 0        | 0        | 1       | 0            |
| 38  | H     | 63    | 0        | 0        | 7       | 0            |
| 38  | I     | 8     | 0        | 0        | 3       | 0            |
| 38  | J     | 53    | 0        | 0        | 1       | 0            |
| 38  | K     | 56    | 0        | 0        | 5       | 0            |
| 38  | L     | 85    | 0        | 0        | 6       | 0            |
| 38  | M     | 123   | 0        | 0        | 2       | 0            |
| 38  | N     | 55    | 0        | 0        | 5       | 0            |
| 38  | O     | 43    | 0        | 0        | 3       | 0            |
| 38  | P     | 67    | 0        | 0        | 2       | 0            |
| 38  | Q     | 50    | 0        | 0        | 3       | 0            |
| 38  | R     | 85    | 0        | 0        | 1       | 0            |
| 38  | S     | 33    | 0        | 0        | 2       | 0            |
| 38  | T     | 34    | 0        | 0        | 2       | 0            |
| 38  | U     | 27    | 0        | 0        | 2       | 0            |
| 38  | V     | 13    | 0        | 0        | 2       | 0            |
| 38  | W     | 69    | 0        | 0        | 4       | 0            |
| 38  | X     | 25    | 0        | 0        | 2       | 0            |
| 38  | Y     | 95    | 0        | 0        | 5       | 0            |
| 38  | Z     | 26    | 0        | 0        | 3       | 0            |
| All | All   | 99122 | 0        | 59913    | 1941    | 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 13.

The worst 5 of 1941 close contacts within the same asymmetric unit are listed below.

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 18:R:150:PRO:CG | 18:R:150:PRO:CD | 1.96        | 1.43     |
| 30:0:1160:G:C5' | 30:0:1161:A:H5' | 1.77        | 1.12     |
| 30:0:871:G:C8   | 30:0:871:G:H5'  | 1.84        | 1.11     |
| 30:0:871:G:H8   | 30:0:871:G:H5'  | 1.09        | 1.10     |
| 31:9:56:A:H2'   | 31:9:57:A:H5''  | 1.31        | 1.10     |

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 |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 1   | A     | 235/240 (98%) | 211 (90%)  | 18 (8%)  | 6 (3%)   | 8           | 32  |
| 2   | B     | 335/338 (99%) | 306 (91%)  | 25 (8%)  | 4 (1%)   | 19          | 57  |
| 3   | C     | 244/246 (99%) | 224 (92%)  | 19 (8%)  | 1 (0%)   | 43          | 82  |
| 4   | D     | 134/177 (76%) | 113 (84%)  | 16 (12%) | 5 (4%)   | 5           | 20  |
| 5   | E     | 170/178 (96%) | 161 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 6   | F     | 117/120 (98%) | 106 (91%)  | 8 (7%)   | 3 (3%)   | 8           | 32  |
| 7   | G     | 25/348 (7%)   | 25 (100%)  | 0        | 0        | 100         | 100 |
| 8   | H     | 156/177 (88%) | 147 (94%)  | 8 (5%)   | 1 (1%)   | 33          | 76  |
| 9   | I     | 68/162 (42%)  | 54 (79%)   | 13 (19%) | 1 (2%)   | 15          | 50  |
| 10  | J     | 140/145 (97%) | 130 (93%)  | 9 (6%)   | 1 (1%)   | 30          | 72  |
| 11  | K     | 130/132 (98%) | 124 (95%)  | 5 (4%)   | 1 (1%)   | 27          | 68  |
| 12  | L     | 141/165 (86%) | 125 (89%)  | 14 (10%) | 2 (1%)   | 16          | 52  |
| 13  | M     | 192/196 (98%) | 182 (95%)  | 9 (5%)   | 1 (0%)   | 38          | 79  |
| 14  | N     | 184/187 (98%) | 169 (92%)  | 12 (6%)  | 3 (2%)   | 14          | 47  |
| 15  | O     | 113/116 (97%) | 108 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 16  | P     | 141/149 (95%) | 141 (100%) | 0        | 0        | 100         | 100 |
| 17  | Q     | 93/96 (97%)   | 88 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 18  | R     | 148/155 (96%) | 141 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 19  | S     | 79/85 (93%)   | 75 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 20  | T     | 117/120 (98%) | 110 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 21  | U     | 51/67 (76%)   | 45 (88%)   | 5 (10%)  | 1 (2%)   | 11          | 40  |
| 22  | V     | 63/71 (89%)   | 60 (95%)   | 2 (3%)   | 1 (2%)   | 14          | 47  |
| 23  | W     | 152/154 (99%) | 146 (96%)  | 4 (3%)   | 2 (1%)   | 18          | 54  |
| 24  | X     | 80/92 (87%)   | 75 (94%)   | 4 (5%)   | 1 (1%)   | 18          | 54  |
| 25  | Y     | 140/241 (58%) | 138 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 26  | Z     | 71/116 (61%)  | 62 (87%)   | 7 (10%)  | 2 (3%)   | 8           | 29  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 27  | 1     | 54/57 (95%)     | 52 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 28  | 2     | 42/50 (84%)     | 41 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 29  | 3     | 90/92 (98%)     | 88 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 3705/4472 (83%) | 3447 (93%) | 222 (6%) | 36 (1%)  | 22          | 63  |

5 of 36 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | VAL  |
| 4   | D     | 137 | PRO  |
| 6   | F     | 101 | ALA  |
| 14  | N     | 154 | LEU  |
| 14  | N     | 183 | ASP  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | A     | 179/182 (98%)  | 170 (95%) | 9 (5%)   | 34          | 73  |
| 2   | B     | 282/283 (100%) | 263 (93%) | 19 (7%)  | 23          | 56  |
| 3   | C     | 193/193 (100%) | 176 (91%) | 17 (9%)  | 14          | 40  |
| 4   | D     | 117/148 (79%)  | 110 (94%) | 7 (6%)   | 27          | 63  |
| 5   | E     | 152/156 (97%)  | 149 (98%) | 3 (2%)   | 68          | 92  |
| 6   | F     | 93/94 (99%)    | 91 (98%)  | 2 (2%)   | 64          | 92  |
| 7   | G     | 27/282 (10%)   | 27 (100%) | 0        | 100         | 100 |
| 8   | H     | 134/145 (92%)  | 129 (96%) | 5 (4%)   | 45          | 84  |
| 9   | I     | 58/130 (45%)   | 57 (98%)  | 1 (2%)   | 73          | 94  |
| 10  | J     | 118/121 (98%)  | 110 (93%) | 8 (7%)   | 22          | 55  |
| 11  | K     | 106/106 (100%) | 104 (98%) | 2 (2%)   | 69          | 93  |
| 12  | L     | 113/127 (89%)  | 110 (97%) | 3 (3%)   | 57          | 90  |
| 13  | M     | 158/160 (99%)  | 151 (96%) | 7 (4%)   | 39          | 77  |
| 14  | N     | 149/150 (99%)  | 142 (95%) | 7 (5%)   | 36          | 75  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 15  | O     | 93/94 (99%)     | 92 (99%)   | 1 (1%)   | 84          | 97  |
| 16  | P     | 113/117 (97%)   | 111 (98%)  | 2 (2%)   | 71          | 94  |
| 17  | Q     | 79/80 (99%)     | 76 (96%)   | 3 (4%)   | 44          | 83  |
| 18  | R     | 117/122 (96%)   | 111 (95%)  | 6 (5%)   | 33          | 72  |
| 19  | S     | 71/74 (96%)     | 70 (99%)   | 1 (1%)   | 78          | 96  |
| 20  | T     | 105/106 (99%)   | 97 (92%)   | 8 (8%)   | 19          | 48  |
| 21  | U     | 44/53 (83%)     | 43 (98%)   | 1 (2%)   | 63          | 92  |
| 22  | V     | 51/57 (90%)     | 50 (98%)   | 1 (2%)   | 68          | 92  |
| 23  | W     | 130/130 (100%)  | 126 (97%)  | 4 (3%)   | 52          | 88  |
| 24  | X     | 66/74 (89%)     | 62 (94%)   | 4 (6%)   | 26          | 62  |
| 25  | Y     | 120/196 (61%)   | 116 (97%)  | 4 (3%)   | 50          | 87  |
| 26  | Z     | 60/94 (64%)     | 60 (100%)  | 0        | 100         | 100 |
| 27  | 1     | 46/47 (98%)     | 46 (100%)  | 0        | 100         | 100 |
| 28  | 2     | 42/46 (91%)     | 41 (98%)   | 1 (2%)   | 61          | 91  |
| 29  | 3     | 79/79 (100%)    | 78 (99%)   | 1 (1%)   | 80          | 96  |
| All | All   | 3095/3646 (85%) | 2968 (96%) | 127 (4%) | 41          | 80  |

5 of 127 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 62  | HIS  |
| 11  | K     | 10  | GLN  |
| 24  | X     | 27  | ASP  |
| 8   | H     | 87  | LYS  |
| 10  | J     | 46  | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 58  | GLN  |
| 16  | P     | 66  | GLN  |
| 27  | 1     | 28  | HIS  |
| 13  | M     | 77  | HIS  |
| 14  | N     | 107 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 30  | 0     | 2745/2923 (93%) | 242 (8%)          | 27 (0%)         |
| 31  | 9     | 121/122 (99%)   | 15 (12%)          | 1 (0%)          |
| All | All   | 2866/3045 (94%) | 257 (8%)          | 28 (0%)         |

5 of 257 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | 0     | 31  | C    |
| 30  | 0     | 67  | A    |
| 30  | 0     | 69  | A    |
| 30  | 0     | 70  | A    |
| 30  | 0     | 71  | G    |

5 of 28 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 30  | 0     | 1237 | U    |
| 30  | 0     | 1377 | C    |
| 30  | 0     | 2718 | C    |
| 30  | 0     | 1246 | A    |
| 30  | 0     | 1352 | A    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 30  | OMU  | 0     | 2587 | 30   | 20,22,23     | 0.69 | 0        | 24,31,34    | 0.73 | 0        |
| 30  | OMG  | 0     | 2588 | 30   | 24,26,27     | 0.79 | 1 (4%)   | 32,38,41    | 5.06 | 3 (9%)   |
| 30  | UR3  | 0     | 2619 | 30   | 20,22,23     | 0.72 | 0        | 23,32,35    | 0.87 | 0        |
| 30  | PSU  | 0     | 2621 | 30   | 19,21,22     | 1.19 | 3 (15%)  | 23,30,33    | 1.13 | 2 (8%)   |
| 30  | 1MA  | 0     | 628  | 30   | 23,25,26     | 0.83 | 0        | 32,37,40    | 0.92 | 1 (3%)   |



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   |
|-----|------|-------|------|------|---------|------------|---------|
| 30  | OMU  | 0     | 2587 | 30   | -       | 0/8/27/28  | 0/2/2/2 |
| 30  | OMG  | 0     | 2588 | 30   | -       | 0/10/27/28 | 0/1/3/3 |
| 30  | UR3  | 0     | 2619 | 30   | -       | 0/6/25/26  | 0/2/2/2 |
| 30  | PSU  | 0     | 2621 | 30   | -       | 0/8/25/26  | 0/2/2/2 |
| 30  | 1MA  | 0     | 628  | 30   | -       | 1/8/25/26  | 0/1/3/3 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 30  | 0     | 2621 | PSU  | C2-N1 | 2.91 | 1.43        | 1.37     |
| 30  | 0     | 2621 | PSU  | C6-N1 | 2.23 | 1.34        | 1.32     |
| 30  | 0     | 2621 | PSU  | P-OP1 | 2.19 | 1.49        | 1.46     |
| 30  | 0     | 2588 | OMG  | P-OP1 | 2.03 | 1.49        | 1.46     |

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

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 30  | 0     | 2588 | OMG  | C6-C5-N7   | -28.02 | 130.37      | 134.14   |
| 30  | 0     | 628  | 1MA  | C2-N3-C4   | -3.20  | 110.76      | 116.23   |
| 30  | 0     | 2588 | OMG  | C6-N1-C2   | 3.20   | 125.11      | 119.51   |
| 30  | 0     | 2588 | OMG  | C2-N3-C4   | -2.35  | 111.79      | 115.09   |
| 30  | 0     | 2621 | PSU  | C5-C1'-C2' | -2.28  | 111.59      | 115.61   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 30  | 0     | 628 | 1MA  | C2'-C1'-N9-C8 |

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 305 ligands modelled in this entry, 305 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, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | A     | 237/240 (98%)  | -0.36  | 5 (2%) 60 69 | 35, 59, 97, 117       | 0     |
| 2   | B     | 337/338 (99%)  | -0.57  | 1 (0%) 91 95 | 36, 60, 90, 100       | 0     |
| 3   | C     | 246/246 (100%) | -0.57  | 0 100 100    | 30, 51, 75, 89        | 0     |
| 4   | D     | 140/177 (79%)  | 1.20   | 33 (23%) 1 2 | 73, 108, 135, 146     | 0     |
| 5   | E     | 172/178 (96%)  | -0.48  | 1 (0%) 86 91 | 51, 74, 96, 104       | 0     |
| 6   | F     | 119/120 (99%)  | 0.22   | 9 (7%) 14 17 | 55, 78, 111, 125      | 0     |
| 7   | G     | 29/348 (8%)    | 0.72   | 2 (6%) 17 20 | 83, 103, 109, 112     | 0     |
| 8   | H     | 160/177 (90%)  | 0.15   | 9 (5%) 24 28 | 50, 73, 106, 113      | 0     |
| 9   | I     | 70/162 (43%)   | 3.35   | 49 (70%) 0 0 | 137, 156, 173, 174    | 0     |
| 10  | J     | 142/145 (97%)  | -0.51  | 1 (0%) 84 90 | 41, 58, 78, 97        | 0     |
| 11  | K     | 132/132 (100%) | -0.74  | 0 100 100    | 40, 55, 79, 82        | 0     |
| 12  | L     | 145/165 (87%)  | 0.16   | 9 (6%) 20 23 | 34, 73, 123, 136      | 0     |
| 13  | M     | 194/196 (98%)  | -0.70  | 1 (0%) 88 93 | 35, 50, 66, 73        | 0     |
| 14  | N     | 186/187 (99%)  | 0.02   | 6 (3%) 45 54 | 52, 75, 123, 135      | 0     |
| 15  | O     | 115/116 (99%)  | -0.51  | 0 100 100    | 45, 61, 78, 84        | 0     |
| 16  | P     | 143/149 (95%)  | -0.60  | 0 100 100    | 46, 61, 77, 84        | 0     |
| 17  | Q     | 95/96 (98%)    | -0.52  | 0 100 100    | 44, 55, 71, 86        | 0     |
| 18  | R     | 150/155 (96%)  | -0.72  | 0 100 100    | 39, 52, 71, 86        | 0     |
| 19  | S     | 81/85 (95%)    | -0.41  | 2 (2%) 54 64 | 49, 65, 86, 98        | 0     |
| 20  | T     | 119/120 (99%)  | -0.35  | 4 (3%) 43 51 | 47, 62, 89, 123       | 0     |
| 21  | U     | 53/67 (79%)    | -0.61  | 1 (1%) 64 72 | 48, 62, 79, 88        | 0     |
| 22  | V     | 65/71 (91%)    | 0.89   | 10 (15%) 3 4 | 55, 80, 129, 134      | 0     |
| 23  | W     | 154/154 (100%) | -0.45  | 1 (0%) 86 91 | 41, 57, 74, 88        | 0     |
| 24  | X     | 82/92 (89%)    | -0.11  | 5 (6%) 21 24 | 49, 67, 90, 108       | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25  | Y     | 142/241 (58%)   | -0.72  | 1 (0%) 84 90   | 31, 50, 73, 94        | 0     |
| 26  | Z     | 73/116 (62%)    | 0.92   | 14 (19%) 2 2   | 63, 87, 101, 106      | 0     |
| 27  | 1     | 56/57 (98%)     | -0.69  | 0 100 100      | 32, 39, 45, 53        | 0     |
| 28  | 2     | 46/50 (92%)     | -0.01  | 5 (10%) 6 8    | 41, 69, 104, 115      | 0     |
| 29  | 3     | 92/92 (100%)    | -0.36  | 0 100 100      | 44, 68, 81, 91        | 0     |
| 30  | 0     | 2754/2923 (94%) | -0.49  | 22 (0%) 83 89  | 28, 53, 96, 172       | 0     |
| 31  | 9     | 122/122 (100%)  | -0.67  | 2 (1%) 68 78   | 45, 74, 96, 153       | 0     |
| All | All   | 6651/7517 (88%) | -0.34  | 193 (2%) 49 58 | 28, 58, 108, 174      | 0     |

The worst 5 of 193 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 22  | V     | 39  | ALA  | 11.1 |
| 9   | I     | 74  | ILE  | 9.9  |
| 9   | I     | 66  | GLY  | 9.0  |
| 22  | V     | 1   | THR  | 8.7  |
| 4   | D     | 63  | ILE  | 8.3  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 30  | UR3  | 0     | 2619 | 21/22 | 0.14 | 1.46  | 43,45,48,49                | 0     |
| 30  | OMU  | 0     | 2587 | 21/22 | 0.12 | 0.40  | 40,43,46,49                | 0     |
| 30  | 1MA  | 0     | 628  | 23/24 | 0.14 | -0.08 | 35,38,38,39                | 0     |
| 30  | PSU  | 0     | 2621 | 20/21 | 0.13 | -0.83 | 35,38,47,48                | 0     |
| 30  | OMG  | 0     | 2588 | 24/25 | 0.12 | -0.98 | 38,42,43,43                | 0     |

## 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, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|----------------------------|-------|
| 35  | CL   | 0     | 8822 | 1/1   | 0.53 | 189.49 | 106,106,106,106            | 0     |
| 36  | SR   | 0     | 9007 | 1/1   | 1.21 | 128.93 | 200,200,200,200            | 0     |
| 34  | NA   | 0     | 8505 | 1/1   | 1.03 | 106.45 | 49,49,49,49                | 0     |
| 36  | SR   | 0     | 8994 | 1/1   | 1.02 | 97.03  | 200,200,200,200            | 0     |
| 34  | NA   | 0     | 8509 | 1/1   | 0.15 | 90.51  | 69,69,69,69                | 0     |
| 34  | NA   | 0     | 8554 | 1/1   | 0.89 | 76.13  | 78,78,78,78                | 0     |
| 34  | NA   | 0     | 8562 | 1/1   | 0.76 | 65.01  | 74,74,74,74                | 0     |
| 36  | SR   | 0     | 8996 | 1/1   | 0.95 | 63.49  | 200,200,200,200            | 0     |
| 32  | MG   | 0     | 8037 | 1/1   | 0.33 | 62.43  | 90,90,90,90                | 0     |
| 34  | NA   | 0     | 8561 | 1/1   | 0.53 | 55.50  | 78,78,78,78                | 0     |
| 36  | SR   | 0     | 8997 | 1/1   | 0.61 | 54.45  | 200,200,200,200            | 0     |
| 36  | SR   | 0     | 8982 | 1/1   | 1.13 | 52.45  | 200,200,200,200            | 0     |
| 34  | NA   | 0     | 8546 | 1/1   | 1.23 | 48.86  | 112,112,112,112            | 0     |
| 34  | NA   | 0     | 8565 | 1/1   | 0.66 | 48.44  | 68,68,68,68                | 0     |
| 32  | MG   | 0     | 8031 | 1/1   | 0.32 | 36.26  | 72,72,72,72                | 0     |
| 34  | NA   | 0     | 8574 | 1/1   | 0.36 | 34.69  | 55,55,55,55                | 0     |
| 36  | SR   | 0     | 8983 | 1/1   | 0.37 | 34.60  | 195,195,195,195            | 0     |
| 36  | SR   | 0     | 9004 | 1/1   | 0.67 | 33.92  | 200,200,200,200            | 0     |
| 34  | NA   | 0     | 8514 | 1/1   | 0.47 | 28.92  | 48,48,48,48                | 0     |
| 34  | NA   | 0     | 8550 | 1/1   | 0.48 | 28.31  | 61,61,61,61                | 0     |
| 34  | NA   | 0     | 8564 | 1/1   | 0.40 | 26.17  | 81,81,81,81                | 0     |
| 34  | NA   | 0     | 8522 | 1/1   | 0.38 | 25.28  | 83,83,83,83                | 0     |
| 34  | NA   | 0     | 8566 | 1/1   | 0.29 | 23.78  | 60,60,60,60                | 0     |
| 34  | NA   | 0     | 8547 | 1/1   | 0.56 | 23.39  | 54,54,54,54                | 0     |
| 34  | NA   | 0     | 8568 | 1/1   | 0.51 | 21.84  | 50,50,50,50                | 0     |
| 36  | SR   | 0     | 8914 | 1/1   | 0.26 | 21.37  | 110,110,110,110            | 0     |
| 32  | MG   | 0     | 8092 | 1/1   | 0.16 | 21.00  | 67,67,67,67                | 0     |
| 36  | SR   | 0     | 8979 | 1/1   | 0.20 | 20.21  | 198,198,198,198            | 0     |
| 34  | NA   | 0     | 8573 | 1/1   | 0.28 | 19.38  | 77,77,77,77                | 0     |
| 32  | MG   | 0     | 8030 | 1/1   | 0.49 | 18.95  | 69,69,69,69                | 0     |
| 34  | NA   | 0     | 8512 | 1/1   | 0.44 | 17.70  | 56,56,56,56                | 0     |
| 32  | MG   | 0     | 8090 | 1/1   | 0.31 | 17.24  | 62,62,62,62                | 0     |
| 34  | NA   | 0     | 8555 | 1/1   | 0.45 | 15.53  | 51,51,51,51                | 0     |
| 34  | NA   | 0     | 8549 | 1/1   | 0.33 | 14.15  | 58,58,58,58                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 34  | NA   | 0     | 8525 | 1/1   | 0.20 | 13.78 | 78,78,78,78                | 0     |
| 36  | SR   | 0     | 8959 | 1/1   | 0.19 | 13.35 | 174,174,174,174            | 0     |
| 34  | NA   | 0     | 8535 | 1/1   | 0.24 | 12.75 | 53,53,53,53                | 0     |
| 32  | MG   | 0     | 8080 | 1/1   | 0.35 | 12.73 | 69,69,69,69                | 0     |
| 34  | NA   | 0     | 8530 | 1/1   | 0.43 | 12.58 | 55,55,55,55                | 0     |
| 36  | SR   | B     | 8987 | 1/1   | 0.49 | 12.06 | 200,200,200,200            | 0     |
| 34  | NA   | 0     | 8560 | 1/1   | 0.39 | 12.03 | 83,83,83,83                | 0     |
| 36  | SR   | 0     | 8905 | 1/1   | 0.27 | 12.00 | 68,68,68,68                | 0     |
| 34  | NA   | 0     | 8556 | 1/1   | 0.51 | 11.34 | 49,49,49,49                | 0     |
| 34  | NA   | 0     | 8544 | 1/1   | 0.22 | 11.32 | 75,75,75,75                | 0     |
| 32  | MG   | 0     | 8082 | 1/1   | 0.24 | 11.24 | 69,69,69,69                | 0     |
| 32  | MG   | 0     | 8071 | 1/1   | 0.17 | 11.04 | 71,71,71,71                | 0     |
| 34  | NA   | 0     | 8563 | 1/1   | 0.34 | 10.58 | 94,94,94,94                | 0     |
| 34  | NA   | 0     | 8506 | 1/1   | 0.23 | 10.38 | 68,68,68,68                | 0     |
| 34  | NA   | 0     | 8552 | 1/1   | 0.33 | 9.72  | 72,72,72,72                | 0     |
| 34  | NA   | 0     | 8548 | 1/1   | 0.18 | 9.57  | 55,55,55,55                | 0     |
| 34  | NA   | 0     | 8528 | 1/1   | 0.26 | 8.98  | 58,58,58,58                | 0     |
| 34  | NA   | 0     | 8551 | 1/1   | 0.30 | 8.42  | 59,59,59,59                | 0     |
| 34  | NA   | 0     | 8518 | 1/1   | 0.38 | 8.40  | 94,94,94,94                | 0     |
| 32  | MG   | 0     | 8078 | 1/1   | 0.32 | 7.86  | 61,61,61,61                | 0     |
| 34  | NA   | 0     | 8542 | 1/1   | 0.30 | 7.77  | 66,66,66,66                | 0     |
| 36  | SR   | 0     | 8903 | 1/1   | 0.18 | 7.48  | 58,58,58,58                | 0     |
| 34  | NA   | 9     | 8572 | 1/1   | 0.23 | 6.99  | 111,111,111,111            | 0     |
| 34  | NA   | 0     | 8501 | 1/1   | 0.20 | 6.97  | 44,44,44,44                | 0     |
| 35  | CL   | Y     | 8820 | 1/1   | 0.24 | 6.67  | 51,51,51,51                | 0     |
| 32  | MG   | 0     | 8063 | 1/1   | 0.17 | 6.27  | 71,71,71,71                | 0     |
| 34  | NA   | 0     | 8541 | 1/1   | 0.26 | 6.18  | 69,69,69,69                | 0     |
| 32  | MG   | 0     | 8081 | 1/1   | 0.16 | 5.96  | 74,74,74,74                | 0     |
| 36  | SR   | 0     | 8976 | 1/1   | 0.26 | 5.80  | 200,200,200,200            | 0     |
| 32  | MG   | 0     | 8047 | 1/1   | 0.29 | 5.79  | 65,65,65,65                | 0     |
| 36  | SR   | 0     | 8938 | 1/1   | 0.13 | 5.77  | 192,192,192,192            | 0     |
| 34  | NA   | 0     | 8545 | 1/1   | 0.20 | 5.74  | 41,41,41,41                | 0     |
| 36  | SR   | 0     | 8922 | 1/1   | 0.24 | 5.35  | 170,170,170,170            | 0     |
| 34  | NA   | 0     | 8569 | 1/1   | 0.24 | 5.19  | 54,54,54,54                | 0     |
| 34  | NA   | 0     | 8534 | 1/1   | 0.26 | 5.15  | 42,42,42,42                | 0     |
| 34  | NA   | 0     | 8559 | 1/1   | 0.14 | 4.94  | 76,76,76,76                | 0     |
| 35  | CL   | 0     | 8816 | 1/1   | 0.27 | 4.91  | 85,85,85,85                | 0     |
| 34  | NA   | 0     | 8517 | 1/1   | 0.18 | 4.75  | 36,36,36,36                | 0     |
| 32  | MG   | 0     | 8029 | 1/1   | 0.17 | 4.73  | 48,48,48,48                | 0     |
| 34  | NA   | 0     | 8527 | 1/1   | 0.23 | 4.67  | 71,71,71,71                | 0     |
| 32  | MG   | A     | 8051 | 1/1   | 0.45 | 4.66  | 72,72,72,72                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 36  | SR   | 0     | 8925 | 1/1   | 0.12 | 4.63 | 91,91,91,91                 | 0     |
| 36  | SR   | 0     | 8924 | 1/1   | 0.15 | 4.45 | 135,135,135,135             | 0     |
| 36  | SR   | 0     | 8947 | 1/1   | 0.26 | 4.44 | 200,200,200,200             | 0     |
| 32  | MG   | 0     | 8017 | 1/1   | 0.20 | 4.36 | 25,25,25,25                 | 0     |
| 32  | MG   | 0     | 8041 | 1/1   | 0.20 | 4.19 | 31,31,31,31                 | 0     |
| 32  | MG   | 0     | 8015 | 1/1   | 0.15 | 4.12 | 36,36,36,36                 | 0     |
| 36  | SR   | 0     | 8926 | 1/1   | 0.11 | 3.93 | 127,127,127,127             | 0     |
| 34  | NA   | 0     | 8567 | 1/1   | 0.19 | 3.86 | 80,80,80,80                 | 0     |
| 32  | MG   | 0     | 8016 | 1/1   | 0.20 | 3.76 | 60,60,60,60                 | 0     |
| 32  | MG   | 0     | 8014 | 1/1   | 0.17 | 3.67 | 35,35,35,35                 | 0     |
| 32  | MG   | 0     | 8048 | 1/1   | 0.19 | 3.63 | 26,26,26,26                 | 0     |
| 36  | SR   | 0     | 8946 | 1/1   | 0.21 | 3.54 | 122,122,122,122             | 0     |
| 32  | MG   | 0     | 8009 | 1/1   | 0.20 | 3.46 | 29,29,29,29                 | 0     |
| 32  | MG   | 0     | 8008 | 1/1   | 0.15 | 3.37 | 27,27,27,27                 | 0     |
| 32  | MG   | 0     | 8018 | 1/1   | 0.18 | 3.29 | 46,46,46,46                 | 0     |
| 36  | SR   | 0     | 8909 | 1/1   | 0.15 | 3.20 | 85,85,85,85                 | 0     |
| 32  | MG   | 0     | 8067 | 1/1   | 0.22 | 2.98 | 34,34,34,34                 | 0     |
| 34  | NA   | 0     | 8524 | 1/1   | 0.16 | 2.89 | 58,58,58,58                 | 0     |
| 34  | NA   | 0     | 8558 | 1/1   | 0.23 | 2.86 | 50,50,50,50                 | 0     |
| 36  | SR   | 0     | 8904 | 1/1   | 0.18 | 2.85 | 66,66,66,66                 | 0     |
| 32  | MG   | 0     | 8055 | 1/1   | 0.19 | 2.78 | 46,46,46,46                 | 0     |
| 36  | SR   | S     | 8961 | 1/1   | 0.09 | 2.67 | 122,122,122,122             | 0     |
| 36  | SR   | 0     | 8937 | 1/1   | 0.21 | 2.51 | 115,115,115,115             | 0     |
| 36  | SR   | 0     | 8986 | 1/1   | 0.15 | 2.37 | 200,200,200,200             | 0     |
| 32  | MG   | 0     | 8061 | 1/1   | 0.21 | 2.01 | 30,30,30,30                 | 0     |
| 32  | MG   | 0     | 8040 | 1/1   | 0.16 | 1.97 | 96,96,96,96                 | 0     |
| 34  | NA   | 0     | 8511 | 1/1   | 0.14 | 1.95 | 59,59,59,59                 | 0     |
| 36  | SR   | 0     | 8918 | 1/1   | 0.13 | 1.93 | 85,85,85,85                 | 0     |
| 32  | MG   | 0     | 8028 | 1/1   | 0.16 | 1.90 | 27,27,27,27                 | 0     |
| 32  | MG   | 0     | 8084 | 1/1   | 0.14 | 1.81 | 37,37,37,37                 | 0     |
| 32  | MG   | 0     | 8003 | 1/1   | 0.17 | 1.76 | 34,34,34,34                 | 0     |
| 34  | NA   | 0     | 8553 | 1/1   | 0.17 | 1.61 | 68,68,68,68                 | 0     |
| 36  | SR   | 0     | 8906 | 1/1   | 0.20 | 1.56 | 60,60,60,60                 | 0     |
| 32  | MG   | 0     | 8066 | 1/1   | 0.15 | 1.46 | 76,76,76,76                 | 0     |
| 32  | MG   | 0     | 8019 | 1/1   | 0.19 | 1.45 | 27,27,27,27                 | 0     |
| 36  | SR   | 0     | 8944 | 1/1   | 0.12 | 1.43 | 182,182,182,182             | 0     |
| 34  | NA   | 0     | 8570 | 1/1   | 0.12 | 1.42 | 60,60,60,60                 | 0     |
| 36  | SR   | 9     | 8980 | 1/1   | 0.12 | 1.40 | 200,200,200,200             | 0     |
| 34  | NA   | 0     | 8502 | 1/1   | 0.13 | 1.37 | 65,65,65,65                 | 0     |
| 32  | MG   | 0     | 8007 | 1/1   | 0.18 | 1.33 | 38,38,38,38                 | 0     |
| 32  | MG   | 0     | 8062 | 1/1   | 0.18 | 1.25 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 36  | SR   | 0     | 8948 | 1/1   | 0.12 | 1.16  | 102,102,102,102             | 0     |
| 35  | CL   | J     | 8801 | 1/1   | 0.19 | 1.14  | 79,79,79,79                 | 0     |
| 34  | NA   | 0     | 8533 | 1/1   | 0.14 | 1.11  | 67,67,67,67                 | 0     |
| 32  | MG   | 0     | 8004 | 1/1   | 0.17 | 1.06  | 30,30,30,30                 | 0     |
| 36  | SR   | 0     | 8958 | 1/1   | 0.11 | 1.05  | 123,123,123,123             | 0     |
| 36  | SR   | R     | 8912 | 1/1   | 0.15 | 0.97  | 86,86,86,86                 | 0     |
| 32  | MG   | 0     | 8022 | 1/1   | 0.12 | 0.93  | 32,32,32,32                 | 0     |
| 36  | SR   | A     | 8929 | 1/1   | 0.16 | 0.90  | 137,137,137,137             | 0     |
| 36  | SR   | 0     | 8921 | 1/1   | 0.12 | 0.87  | 92,92,92,92                 | 0     |
| 32  | MG   | 0     | 8023 | 1/1   | 0.14 | 0.82  | 32,32,32,32                 | 0     |
| 34  | NA   | 0     | 8575 | 1/1   | 0.15 | 0.76  | 86,86,86,86                 | 0     |
| 36  | SR   | 0     | 8915 | 1/1   | 0.12 | 0.71  | 131,131,131,131             | 0     |
| 34  | NA   | 0     | 8531 | 1/1   | 0.11 | 0.67  | 44,44,44,44                 | 0     |
| 36  | SR   | 0     | 8995 | 1/1   | 0.17 | 0.64  | 140,140,140,140             | 0     |
| 34  | NA   | 0     | 8537 | 1/1   | 0.12 | 0.61  | 41,41,41,41                 | 0     |
| 36  | SR   | 0     | 8955 | 1/1   | 0.11 | 0.57  | 200,200,200,200             | 0     |
| 32  | MG   | 0     | 8036 | 1/1   | 0.10 | 0.57  | 50,50,50,50                 | 0     |
| 35  | CL   | 0     | 8815 | 1/1   | 0.10 | 0.56  | 78,78,78,78                 | 0     |
| 32  | MG   | 0     | 8020 | 1/1   | 0.10 | 0.56  | 43,43,43,43                 | 0     |
| 36  | SR   | 0     | 8989 | 1/1   | 0.13 | 0.54  | 185,185,185,185             | 0     |
| 34  | NA   | 0     | 8507 | 1/1   | 0.14 | 0.48  | 42,42,42,42                 | 0     |
| 34  | NA   | 0     | 8508 | 1/1   | 0.12 | 0.42  | 39,39,39,39                 | 0     |
| 36  | SR   | 0     | 8981 | 1/1   | 0.14 | 0.28  | 153,153,153,153             | 0     |
| 32  | MG   | 0     | 8070 | 1/1   | 0.13 | 0.10  | 45,45,45,45                 | 0     |
| 32  | MG   | K     | 8054 | 1/1   | 0.14 | 0.08  | 50,50,50,50                 | 0     |
| 36  | SR   | 0     | 8907 | 1/1   | 0.12 | 0.06  | 56,56,56,56                 | 0     |
| 37  | CD   | U     | 8701 | 1/1   | 0.11 | 0.03  | 72,72,72,72                 | 0     |
| 36  | SR   | 0     | 8933 | 1/1   | 0.14 | -0.06 | 150,150,150,150             | 0     |
| 32  | MG   | 0     | 8011 | 1/1   | 0.16 | -0.12 | 33,33,33,33                 | 0     |
| 32  | MG   | 0     | 8043 | 1/1   | 0.11 | -0.18 | 49,49,49,49                 | 0     |
| 34  | NA   | 0     | 8504 | 1/1   | 0.15 | -0.18 | 37,37,37,37                 | 0     |
| 34  | NA   | 0     | 8513 | 1/1   | 0.16 | -0.29 | 58,58,58,58                 | 0     |
| 36  | SR   | 0     | 8972 | 1/1   | 0.14 | -0.30 | 141,141,141,141             | 0     |
| 32  | MG   | B     | 8042 | 1/1   | 0.09 | -0.30 | 50,50,50,50                 | 0     |
| 32  | MG   | 0     | 8069 | 1/1   | 0.16 | -0.32 | 72,72,72,72                 | 0     |
| 32  | MG   | 0     | 8045 | 1/1   | 0.10 | -0.33 | 35,35,35,35                 | 0     |
| 32  | MG   | 0     | 8006 | 1/1   | 0.12 | -0.36 | 30,30,30,30                 | 0     |
| 34  | NA   | J     | 8538 | 1/1   | 0.15 | -0.39 | 60,60,60,60                 | 0     |
| 34  | NA   | 0     | 8523 | 1/1   | 0.11 | -0.39 | 45,45,45,45                 | 0     |
| 32  | MG   | 0     | 8064 | 1/1   | 0.13 | -0.40 | 37,37,37,37                 | 0     |
| 36  | SR   | 0     | 9001 | 1/1   | 0.11 | -0.42 | 173,173,173,173             | 0     |
| 35  | CL   | J     | 8821 | 1/1   | 0.13 | -0.49 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 34  | NA   | 9     | 8543 | 1/1   | 0.16 | -0.53 | 49,49,49,49                 | 0     |
| 35  | CL   | 0     | 8817 | 1/1   | 0.11 | -0.57 | 65,65,65,65                 | 0     |
| 33  | K    | 0     | 8401 | 1/1   | 0.12 | -0.57 | 74,74,74,74                 | 0     |
| 32  | MG   | 0     | 8039 | 1/1   | 0.15 | -0.60 | 77,77,77,77                 | 0     |
| 32  | MG   | 0     | 8021 | 1/1   | 0.10 | -0.65 | 30,30,30,30                 | 0     |
| 32  | MG   | 0     | 8083 | 1/1   | 0.10 | -0.66 | 73,73,73,73                 | 0     |
| 36  | SR   | 0     | 9008 | 1/1   | 0.14 | -0.70 | 89,89,89,89                 | 0     |
| 36  | SR   | 3     | 8932 | 1/1   | 0.11 | -0.71 | 79,79,79,79                 | 0     |
| 34  | NA   | 0     | 8520 | 1/1   | 0.09 | -0.75 | 53,53,53,53                 | 0     |
| 32  | MG   | 0     | 8012 | 1/1   | 0.15 | -0.78 | 25,25,25,25                 | 0     |
| 36  | SR   | 0     | 8957 | 1/1   | 0.10 | -0.78 | 196,196,196,196             | 0     |
| 36  | SR   | 0     | 8964 | 1/1   | 0.09 | -0.83 | 139,139,139,139             | 0     |
| 36  | SR   | 0     | 8993 | 1/1   | 0.08 | -0.88 | 182,182,182,182             | 0     |
| 36  | SR   | 0     | 8954 | 1/1   | 0.11 | -0.90 | 112,112,112,112             | 0     |
| 36  | SR   | 0     | 8936 | 1/1   | 0.10 | -0.97 | 94,94,94,94                 | 0     |
| 35  | CL   | J     | 8802 | 1/1   | 0.09 | -0.99 | 76,76,76,76                 | 0     |
| 34  | NA   | C     | 8503 | 1/1   | 0.11 | -0.99 | 44,44,44,44                 | 0     |
| 32  | MG   | 0     | 8035 | 1/1   | 0.10 | -1.02 | 68,68,68,68                 | 0     |
| 36  | SR   | 0     | 8935 | 1/1   | 0.09 | -1.02 | 80,80,80,80                 | 0     |
| 32  | MG   | 0     | 8050 | 1/1   | 0.12 | -1.04 | 37,37,37,37                 | 0     |
| 36  | SR   | 0     | 8956 | 1/1   | 0.08 | -1.05 | 155,155,155,155             | 0     |
| 32  | MG   | 0     | 8088 | 1/1   | 0.12 | -1.09 | 42,42,42,42                 | 0     |
| 34  | NA   | 0     | 8571 | 1/1   | 0.07 | -1.16 | 77,77,77,77                 | 0     |
| 36  | SR   | 0     | 8941 | 1/1   | 0.14 | -1.17 | 116,116,116,116             | 0     |
| 36  | SR   | F     | 9005 | 1/1   | 0.07 | -1.18 | 134,134,134,134             | 0     |
| 35  | CL   | M     | 8818 | 1/1   | 0.09 | -1.19 | 47,47,47,47                 | 0     |
| 35  | CL   | O     | 8808 | 1/1   | 0.10 | -1.21 | 81,81,81,81                 | 0     |
| 36  | SR   | 0     | 8934 | 1/1   | 0.12 | -1.22 | 130,130,130,130             | 0     |
| 34  | NA   | M     | 8539 | 1/1   | 0.09 | -1.22 | 34,34,34,34                 | 0     |
| 32  | MG   | 0     | 8005 | 1/1   | 0.16 | -1.24 | 33,33,33,33                 | 0     |
| 36  | SR   | 0     | 8992 | 1/1   | 0.11 | -1.25 | 137,137,137,137             | 0     |
| 37  | CD   | Z     | 8703 | 1/1   | 0.09 | -1.25 | 91,91,91,91                 | 0     |
| 32  | MG   | 0     | 8058 | 1/1   | 0.07 | -1.28 | 23,23,23,23                 | 0     |
| 36  | SR   | 0     | 8991 | 1/1   | 0.09 | -1.28 | 197,197,197,197             | 0     |
| 35  | CL   | L     | 8810 | 1/1   | 0.09 | -1.33 | 61,61,61,61                 | 0     |
| 32  | MG   | 0     | 8010 | 1/1   | 0.12 | -1.34 | 35,35,35,35                 | 0     |
| 36  | SR   | 0     | 8931 | 1/1   | 0.09 | -1.35 | 117,117,117,117             | 0     |
| 36  | SR   | 0     | 8911 | 1/1   | 0.06 | -1.41 | 85,85,85,85                 | 0     |
| 37  | CD   | 1     | 8702 | 1/1   | 0.10 | -1.51 | 65,65,65,65                 | 0     |
| 36  | SR   | 0     | 8988 | 1/1   | 0.10 | -1.56 | 173,173,173,173             | 0     |
| 34  | NA   | 0     | 8515 | 1/1   | 0.11 | -1.59 | 37,37,37,37                 | 0     |
| 36  | SR   | B     | 8950 | 1/1   | 0.15 | -1.60 | 132,132,132,132             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 36  | SR   | 0     | 9000 | 1/1   | 0.10 | -1.61 | 177,177,177,177             | 0     |
| 34  | NA   | Q     | 8540 | 1/1   | 0.07 | -1.61 | 60,60,60,60                 | 0     |
| 35  | CL   | 0     | 8811 | 1/1   | 0.09 | -1.62 | 68,68,68,68                 | 0     |
| 35  | CL   | N     | 8807 | 1/1   | 0.10 | -1.62 | 71,71,71,71                 | 0     |
| 36  | SR   | 0     | 8969 | 1/1   | 0.10 | -1.62 | 160,160,160,160             | 0     |
| 35  | CL   | R     | 8806 | 1/1   | 0.12 | -1.63 | 52,52,52,52                 | 0     |
| 32  | MG   | 9     | 8074 | 1/1   | 0.11 | -1.65 | 77,77,77,77                 | 0     |
| 36  | SR   | 0     | 8917 | 1/1   | 0.10 | -1.65 | 111,111,111,111             | 0     |
| 36  | SR   | A     | 8977 | 1/1   | 0.07 | -1.65 | 161,161,161,161             | 0     |
| 37  | CD   | 3     | 8704 | 1/1   | 0.07 | -1.68 | 81,81,81,81                 | 0     |
| 36  | SR   | 0     | 8975 | 1/1   | 0.07 | -1.72 | 135,135,135,135             | 0     |
| 36  | SR   | 0     | 9002 | 1/1   | 0.07 | -1.72 | 184,184,184,184             | 0     |
| 32  | MG   | 0     | 8046 | 1/1   | 0.10 | -1.77 | 41,41,41,41                 | 0     |
| 32  | MG   | T     | 8057 | 1/1   | 0.08 | -1.78 | 65,65,65,65                 | 0     |
| 34  | NA   | 0     | 8516 | 1/1   | 0.12 | -1.78 | 42,42,42,42                 | 0     |
| 36  | SR   | 0     | 8951 | 1/1   | 0.07 | -1.86 | 142,142,142,142             | 0     |
| 32  | MG   | 0     | 8001 | 1/1   | 0.10 | -1.87 | 33,33,33,33                 | 0     |
| 36  | SR   | A     | 8930 | 1/1   | 0.04 | -1.87 | 104,104,104,104             | 0     |
| 35  | CL   | A     | 8809 | 1/1   | 0.10 | -1.90 | 74,74,74,74                 | 0     |
| 36  | SR   | 1     | 8952 | 1/1   | 0.13 | -1.92 | 91,91,91,91                 | 0     |
| 34  | NA   | R     | 8532 | 1/1   | 0.06 | -1.98 | 46,46,46,46                 | 0     |
| 36  | SR   | 0     | 8967 | 1/1   | 0.06 | -1.98 | 132,132,132,132             | 0     |
| 33  | K    | 0     | 8402 | 1/1   | 0.12 | -2.02 | 87,87,87,87                 | 0     |
| 36  | SR   | 0     | 8949 | 1/1   | 0.09 | -2.04 | 119,119,119,119             | 0     |
| 36  | SR   | 0     | 8985 | 1/1   | 0.07 | -2.05 | 143,143,143,143             | 0     |
| 32  | MG   | 0     | 8079 | 1/1   | 0.09 | -2.08 | 55,55,55,55                 | 0     |
| 36  | SR   | 0     | 8943 | 1/1   | 0.07 | -2.13 | 117,117,117,117             | 0     |
| 35  | CL   | 0     | 8813 | 1/1   | 0.06 | -2.38 | 61,61,61,61                 | 0     |
| 36  | SR   | 0     | 8998 | 1/1   | 0.12 | -2.45 | 175,175,175,175             | 0     |
| 32  | MG   | 0     | 8073 | 1/1   | 0.07 | -2.54 | 83,83,83,83                 | 0     |
| 36  | SR   | 0     | 8901 | 1/1   | 0.11 | -2.68 | 85,85,85,85                 | 0     |
| 32  | MG   | 0     | 8068 | 1/1   | 0.07 | -2.73 | 54,54,54,54                 | 0     |
| 37  | CD   | O     | 8705 | 1/1   | 0.05 | -2.74 | 94,94,94,94                 | 0     |
| 36  | SR   | 9     | 8978 | 1/1   | 0.06 | -2.75 | 133,133,133,133             | 0     |
| 36  | SR   | 0     | 8928 | 1/1   | 0.06 | -2.76 | 135,135,135,135             | 0     |
| 36  | SR   | 3     | 8999 | 1/1   | 0.04 | -2.78 | 106,106,106,106             | 0     |
| 36  | SR   | 0     | 8960 | 1/1   | 0.04 | -2.79 | 150,150,150,150             | 0     |
| 34  | NA   | 0     | 8519 | 1/1   | 0.13 | -2.81 | 50,50,50,50                 | 0     |
| 36  | SR   | 0     | 8908 | 1/1   | 0.08 | -2.86 | 110,110,110,110             | 0     |
| 36  | SR   | 0     | 8940 | 1/1   | 0.07 | -2.93 | 93,93,93,93                 | 0     |
| 32  | MG   | 0     | 8027 | 1/1   | 0.08 | -3.03 | 49,49,49,49                 | 0     |
| 36  | SR   | 0     | 8923 | 1/1   | 0.08 | -3.08 | 116,116,116,116             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 36  | SR   | 0     | 8990 | 1/1   | 0.09 | -3.13 | 137,137,137,137            | 0     |
| 34  | NA   | 0     | 8557 | 1/1   | 0.06 | -3.16 | 52,52,52,52                | 0     |
| 32  | MG   | 0     | 8065 | 1/1   | 0.08 | -3.17 | 49,49,49,49                | 0     |
| 34  | NA   | S     | 8510 | 1/1   | 0.10 | -3.36 | 49,49,49,49                | 0     |
| 34  | NA   | 0     | 8521 | 1/1   | 0.09 | -3.39 | 65,65,65,65                | 0     |
| 35  | CL   | 0     | 8805 | 1/1   | 0.05 | -3.41 | 67,67,67,67                | 0     |
| 35  | CL   | 3     | 8804 | 1/1   | 0.08 | -3.43 | 67,67,67,67                | 0     |
| 32  | MG   | 0     | 8053 | 1/1   | 0.03 | -3.43 | 59,59,59,59                | 0     |
| 32  | MG   | 0     | 8025 | 1/1   | 0.08 | -3.46 | 35,35,35,35                | 0     |
| 36  | SR   | 0     | 8910 | 1/1   | 0.06 | -3.47 | 101,101,101,101            | 0     |
| 34  | NA   | 0     | 8529 | 1/1   | 0.03 | -3.52 | 45,45,45,45                | 0     |
| 36  | SR   | 0     | 8902 | 1/1   | 0.11 | -3.54 | 66,66,66,66                | 0     |
| 32  | MG   | 0     | 8044 | 1/1   | 0.08 | -3.55 | 53,53,53,53                | 0     |
| 36  | SR   | 0     | 8945 | 1/1   | 0.07 | -3.60 | 112,112,112,112            | 0     |
| 32  | MG   | 0     | 8085 | 1/1   | 0.07 | -3.61 | 73,73,73,73                | 0     |
| 35  | CL   | 0     | 8812 | 1/1   | 0.06 | -3.61 | 54,54,54,54                | 0     |
| 36  | SR   | 0     | 8968 | 1/1   | 0.07 | -3.73 | 165,165,165,165            | 0     |
| 32  | MG   | 0     | 8026 | 1/1   | 0.07 | -3.75 | 37,37,37,37                | 0     |
| 32  | MG   | 0     | 8060 | 1/1   | 0.06 | -3.81 | 61,61,61,61                | 0     |
| 34  | NA   | 0     | 8536 | 1/1   | 0.06 | -3.86 | 65,65,65,65                | 0     |
| 32  | MG   | 0     | 8052 | 1/1   | 0.04 | -3.86 | 52,52,52,52                | 0     |
| 36  | SR   | 0     | 8939 | 1/1   | 0.04 | -3.87 | 160,160,160,160            | 0     |
| 32  | MG   | 0     | 8038 | 1/1   | 0.10 | -3.88 | 75,75,75,75                | 0     |
| 32  | MG   | Y     | 8086 | 1/1   | 0.06 | -3.90 | 46,46,46,46                | 0     |
| 32  | MG   | 0     | 8032 | 1/1   | 0.05 | -3.92 | 46,46,46,46                | 0     |
| 36  | SR   | 0     | 8919 | 1/1   | 0.12 | -4.02 | 192,192,192,192            | 0     |
| 32  | MG   | 0     | 8056 | 1/1   | 0.10 | -4.10 | 51,51,51,51                | 0     |
| 35  | CL   | 0     | 8803 | 1/1   | 0.07 | -4.16 | 62,62,62,62                | 0     |
| 32  | MG   | 0     | 8002 | 1/1   | 0.09 | -4.20 | 32,32,32,32                | 0     |
| 36  | SR   | 0     | 8920 | 1/1   | 0.04 | -4.23 | 134,134,134,134            | 0     |
| 32  | MG   | 0     | 8077 | 1/1   | 0.07 | -4.31 | 49,49,49,49                | 0     |
| 36  | SR   | 0     | 8974 | 1/1   | 0.10 | -4.34 | 149,149,149,149            | 0     |
| 36  | SR   | 1     | 8913 | 1/1   | 0.08 | -4.36 | 96,96,96,96                | 0     |
| 36  | SR   | 0     | 8927 | 1/1   | 0.06 | -4.42 | 151,151,151,151            | 0     |
| 32  | MG   | 0     | 8076 | 1/1   | 0.07 | -4.57 | 42,42,42,42                | 0     |
| 35  | CL   | 0     | 8814 | 1/1   | 0.09 | -4.67 | 60,60,60,60                | 0     |
| 32  | MG   | 0     | 8093 | 1/1   | 0.07 | -4.96 | 35,35,35,35                | 0     |
| 36  | SR   | 0     | 8916 | 1/1   | 0.05 | -5.21 | 113,113,113,113            | 0     |
| 32  | MG   | 0     | 8072 | 1/1   | 0.10 | -5.28 | 53,53,53,53                | 0     |
| 32  | MG   | 0     | 8075 | 1/1   | 0.04 | -5.34 | 46,46,46,46                | 0     |
| 32  | MG   | 0     | 8033 | 1/1   | 0.06 | -5.40 | 49,49,49,49                | 0     |
| 32  | MG   | 0     | 8024 | 1/1   | 0.11 | -5.46 | 55,55,55,55                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|-----------------------------|-------|
| 35  | CL   | B     | 8819 | 1/1   | 0.07 | -5.53  | 54,54,54,54                 | 0     |
| 36  | SR   | 0     | 8953 | 1/1   | 0.07 | -5.68  | 157,157,157,157             | 0     |
| 36  | SR   | 0     | 8966 | 1/1   | 0.07 | -5.70  | 111,111,111,111             | 0     |
| 36  | SR   | 0     | 8984 | 1/1   | 0.05 | -5.76  | 123,123,123,123             | 0     |
| 36  | SR   | 0     | 8970 | 1/1   | 0.03 | -6.19  | 128,128,128,128             | 0     |
| 34  | NA   | 0     | 8526 | 1/1   | 0.04 | -6.46  | 57,57,57,57                 | 0     |
| 36  | SR   | 0     | 8965 | 1/1   | 0.04 | -6.52  | 124,124,124,124             | 0     |
| 36  | SR   | 0     | 8963 | 1/1   | 0.07 | -8.27  | 134,134,134,134             | 0     |
| 32  | MG   | 0     | 8087 | 1/1   | 0.09 | -8.41  | 47,47,47,47                 | 0     |
| 36  | SR   | 9     | 9003 | 1/1   | 0.02 | -9.21  | 170,170,170,170             | 0     |
| 36  | SR   | 0     | 8962 | 1/1   | 0.05 | -9.32  | 175,175,175,175             | 0     |
| 32  | MG   | 0     | 8013 | 1/1   | 0.03 | -9.50  | 30,30,30,30                 | 0     |
| 32  | MG   | 0     | 8034 | 1/1   | 0.04 | -9.64  | 45,45,45,45                 | 0     |
| 36  | SR   | 0     | 8942 | 1/1   | 0.06 | -10.05 | 133,133,133,133             | 0     |
| 32  | MG   | 0     | 8089 | 1/1   | 0.10 | -11.73 | 57,57,57,57                 | 0     |
| 36  | SR   | 0     | 8973 | 1/1   | 0.06 | -17.80 | 137,137,137,137             | 0     |
| 36  | SR   | 0     | 8971 | 1/1   | 0.06 | -19.50 | 180,180,180,180             | 0     |
| 32  | MG   | 0     | 8059 | 1/1   | 0.04 | -19.52 | 59,59,59,59                 | 0     |
| 32  | MG   | 0     | 8091 | 1/1   | 0.04 | -26.50 | 62,62,62,62                 | 0     |
| 32  | MG   | 0     | 8049 | 1/1   | 0.45 | -      | 68,68,68,68                 | 0     |
| 36  | SR   | 0     | 9006 | 1/1   | 1.02 | -      | 200,200,200,200             | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.