



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:48 am BST

PDB ID : 1RXU  
Title : E. coli uridine phosphorylase: thymidine phosphate complex  
Authors : Caradoc-Davies, T.T.; Cutfield, S.M.; Lamont, I.L.; Cutfield, J.F.  
Deposited on : 2003-12-18  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

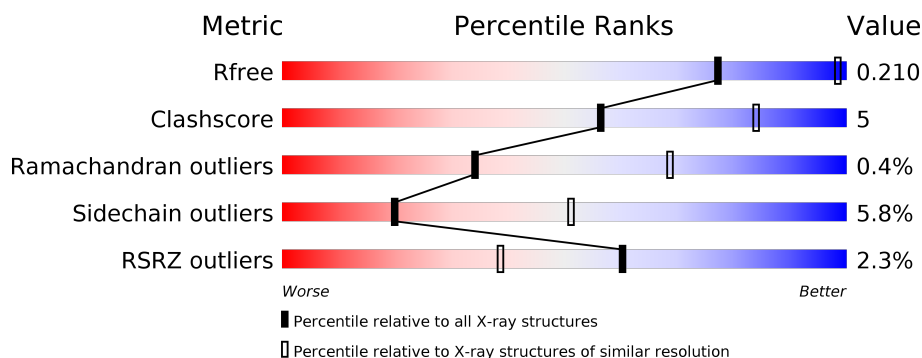
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1094 (3.10-3.10)                                      |
| Clashscore            | 141614                      | 1184 (3.10-3.10)                                      |
| Ramachandran outliers | 138981                      | 1141 (3.10-3.10)                                      |
| Sidechain outliers    | 138945                      | 1141 (3.10-3.10)                                      |
| RSRZ outliers         | 127900                      | 1067 (3.10-3.10)                                      |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 253    | <div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div> |
| 1   | B     | 253    | <div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div> |
| 1   | C     | 253    | <div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>  |
| 1   | D     | 253    | <div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div> |
| 1   | E     | 253    | <div> <div>3%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>  |
| 1   | F     | 253    | <div> <div>4%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 253    |                  |
| 1   | H     | 253    |                  |
| 1   | I     | 253    |                  |
| 1   | J     | 253    |                  |
| 1   | K     | 253    |                  |
| 1   | L     | 253    |                  |
| 1   | M     | 253    |                  |
| 1   | N     | 253    |                  |
| 1   | O     | 253    |                  |
| 1   | P     | 253    |                  |
| 1   | Q     | 253    |                  |
| 1   | R     | 253    |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | PO4  | D     | 2041 | -         | -        | X       | -                |
| 2   | PO4  | E     | 2051 | -         | -        | X       | -                |
| 2   | PO4  | F     | 2061 | -         | -        | X       | -                |
| 2   | PO4  | K     | 2111 | -         | -        | X       | -                |
| 2   | PO4  | O     | 2151 | -         | -        | X       | -                |
| 4   | THM  | A     | 2012 | X         | -        | -       | -                |
| 4   | THM  | B     | 2022 | X         | -        | -       | -                |
| 4   | THM  | C     | 2032 | X         | -        | -       | -                |
| 4   | THM  | D     | 2042 | X         | -        | -       | -                |
| 4   | THM  | E     | 2052 | X         | -        | -       | -                |
| 4   | THM  | F     | 2062 | X         | -        | -       | -                |
| 4   | THM  | G     | 2072 | X         | -        | -       | -                |
| 4   | THM  | H     | 2082 | X         | -        | -       | -                |
| 4   | THM  | I     | 2092 | X         | -        | -       | -                |
| 4   | THM  | J     | 2102 | X         | -        | -       | -                |
| 4   | THM  | K     | 2112 | X         | -        | -       | -                |
| 4   | THM  | L     | 2122 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | THM  | M     | 2132 | X         | -        | -       | -                |
| 4   | THM  | N     | 2142 | X         | -        | -       | -                |
| 4   | THM  | O     | 2152 | X         | -        | -       | -                |
| 4   | THM  | P     | 2162 | X         | -        | -       | -                |
| 4   | THM  | Q     | 2172 | X         | -        | -       | -                |
| 4   | THM  | R     | 2182 | X         | -        | -       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Uridine phosphorylase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | B     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | C     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | D     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | E     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | F     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | G     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | H     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | I     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | J     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | K     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | L     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | M     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | N     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | O     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | P     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | Q     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |
| 1   | R     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1880  | 1178 | 328 | 363 | 11 |         |         |       |

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | I     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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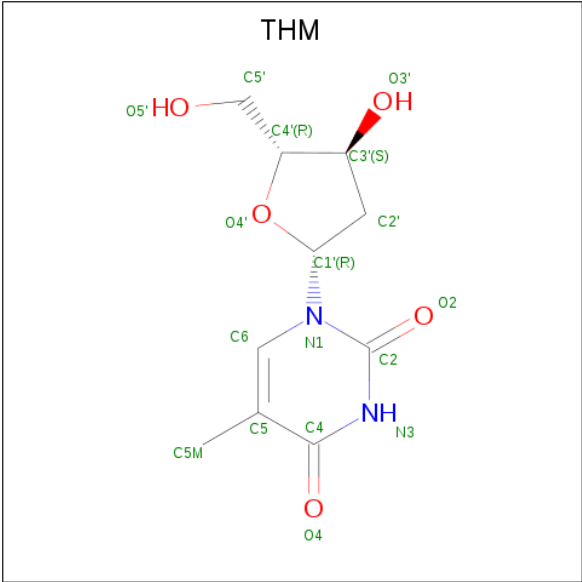
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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | K     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | L     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | M     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | N     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | O     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Q     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | R     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | G     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | Q     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | K     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | I     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | C     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | A     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | O     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | F     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | M     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 4 is THYMIDINE (three-letter code: THM) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | O     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | Q     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |
| 4   | R     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 17    | 10 | 2 | 5 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 59       | Total | O  | 0       | 0       |
|     |       |          | 59    | 59 |         |         |
| 5   | B     | 57       | Total | O  | 0       | 0       |
|     |       |          | 57    | 57 |         |         |
| 5   | C     | 62       | Total | O  | 0       | 0       |
|     |       |          | 62    | 62 |         |         |
| 5   | D     | 57       | Total | O  | 0       | 0       |
|     |       |          | 57    | 57 |         |         |
| 5   | E     | 59       | Total | O  | 0       | 0       |
|     |       |          | 59    | 59 |         |         |
| 5   | F     | 58       | Total | O  | 0       | 0       |
|     |       |          | 58    | 58 |         |         |
| 5   | G     | 59       | Total | O  | 0       | 0       |
|     |       |          | 59    | 59 |         |         |
| 5   | H     | 57       | Total | O  | 0       | 0       |
|     |       |          | 57    | 57 |         |         |
| 5   | I     | 60       | Total | O  | 0       | 0       |
|     |       |          | 60    | 60 |         |         |
| 5   | J     | 59       | Total | O  | 0       | 0       |
|     |       |          | 59    | 59 |         |         |
| 5   | K     | 58       | Total | O  | 0       | 0       |
|     |       |          | 58    | 58 |         |         |
| 5   | L     | 61       | Total | O  | 0       | 0       |
|     |       |          | 61    | 61 |         |         |
| 5   | M     | 60       | Total | O  | 0       | 0       |
|     |       |          | 60    | 60 |         |         |
| 5   | N     | 60       | Total | O  | 0       | 0       |
|     |       |          | 60    | 60 |         |         |
| 5   | O     | 58       | Total | O  | 0       | 0       |
|     |       |          | 58    | 58 |         |         |

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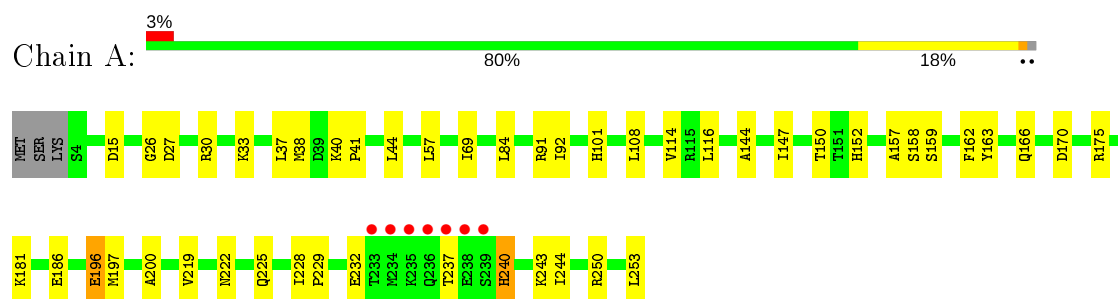
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | P     | 59       | Total | O  | 0       | 0       |
|     |       |          | 59    | 59 |         |         |
| 5   | Q     | 61       | Total | O  | 0       | 0       |
|     |       |          | 61    | 61 |         |         |
| 5   | R     | 58       | Total | O  | 0       | 0       |
|     |       |          | 58    | 58 |         |         |

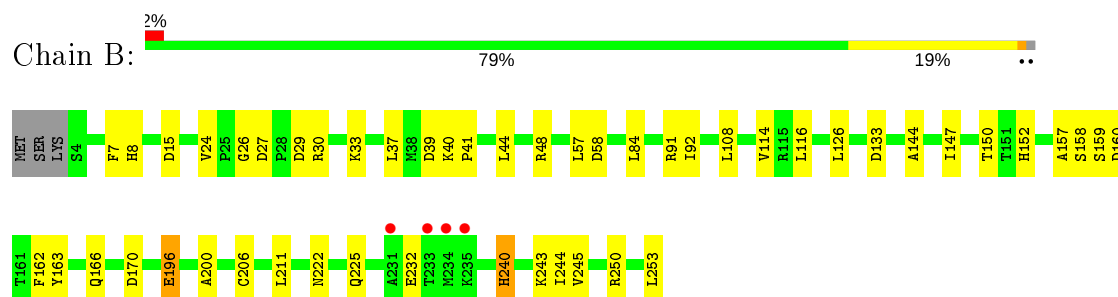
### 3 Residue-property plots [i](#)

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

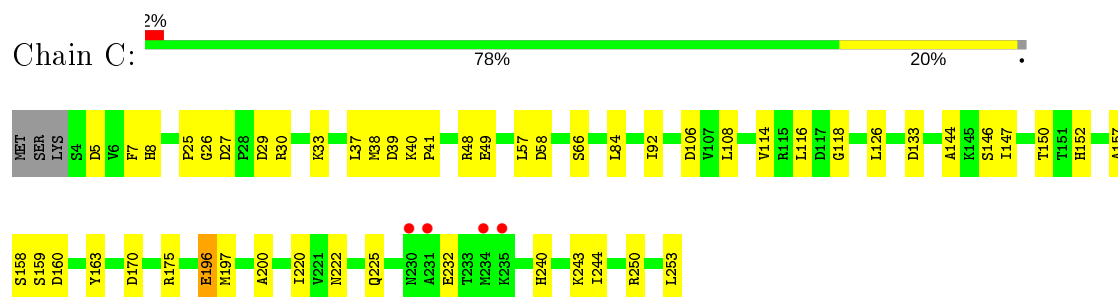
#### • Molecule 1: Uridine phosphorylase



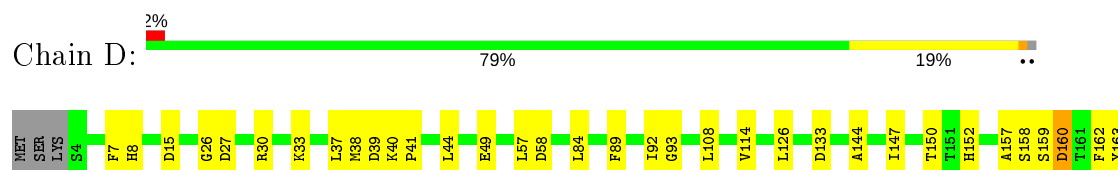
#### • Molecule 1: Uridine phosphorylase



#### • Molecule 1: Uridine phosphorylase

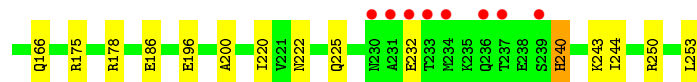
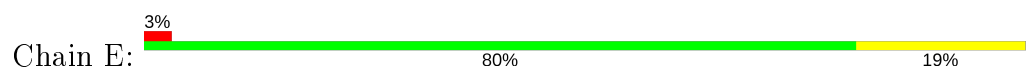


#### • Molecule 1: Uridine phosphorylase

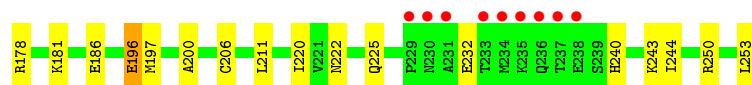
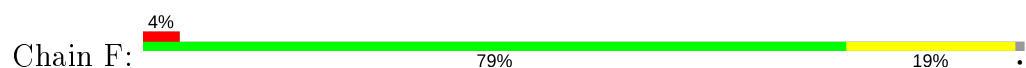




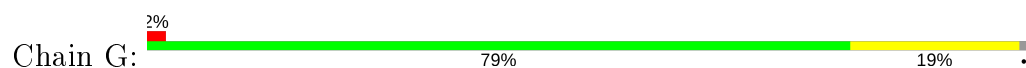
- Molecule 1: Uridine phosphorylase



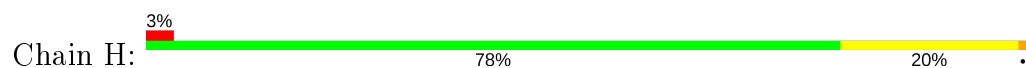
- Molecule 1: Uridine phosphorylase



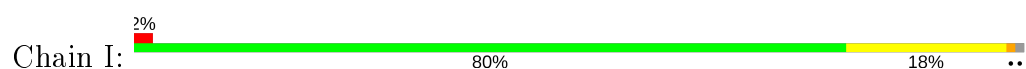
- Molecule 1: Uridine phosphorylase

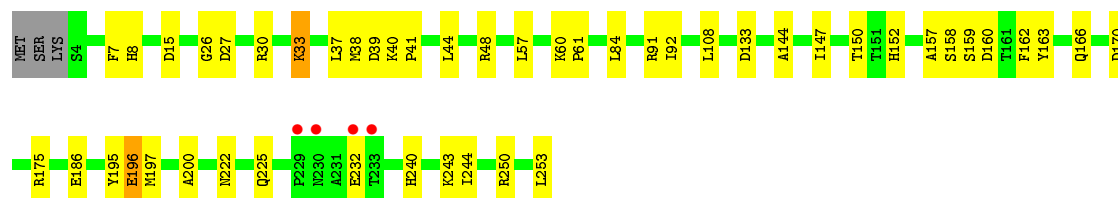


- Molecule 1: Uridine phosphorylase

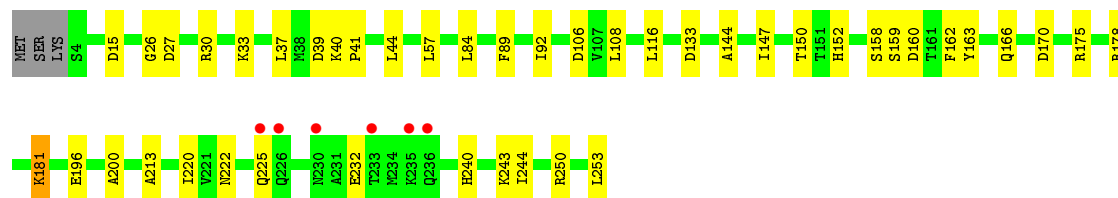
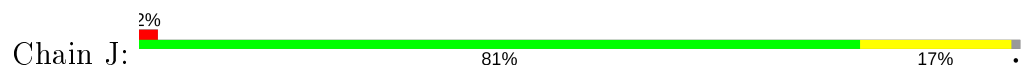


- Molecule 1: Uridine phosphorylase

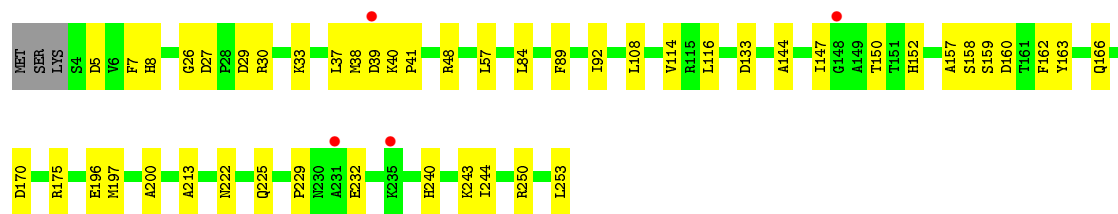
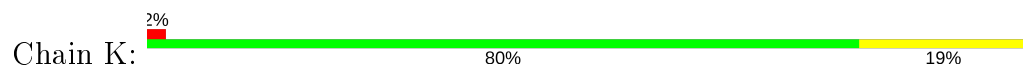




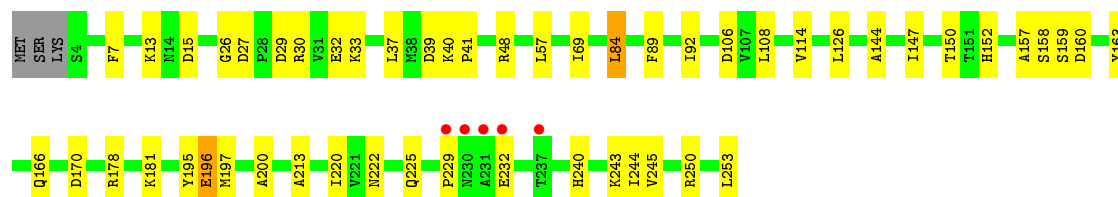
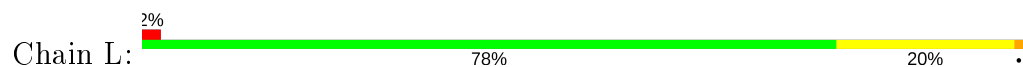
- Molecule 1: Uridine phosphorylase



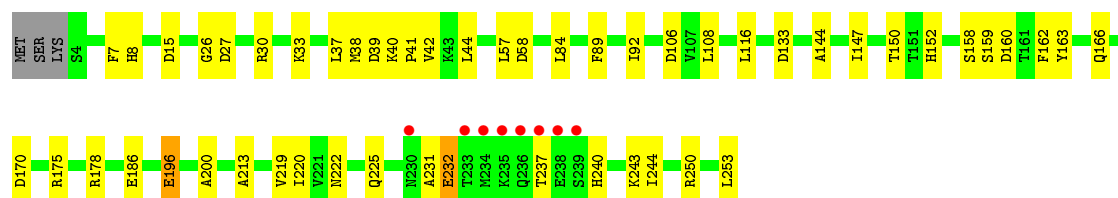
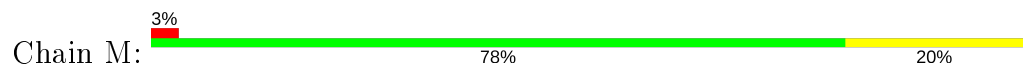
- Molecule 1: Uridine phosphorylase



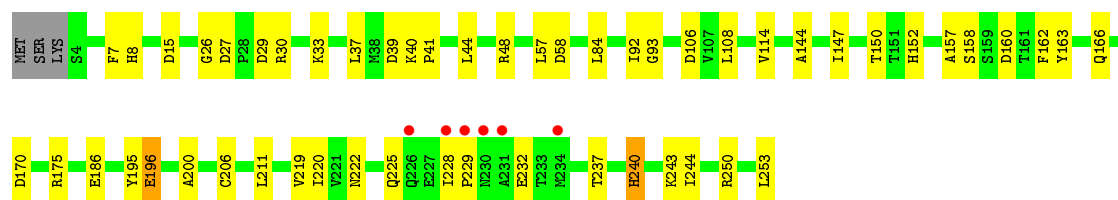
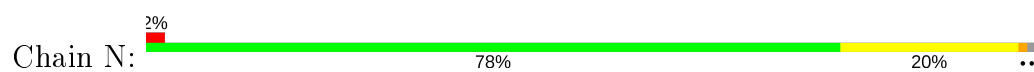
- Molecule 1: Uridine phosphorylase



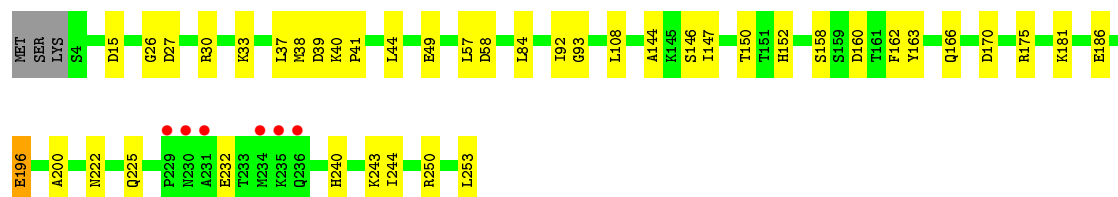
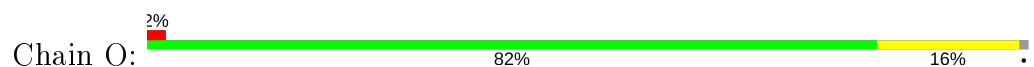
- Molecule 1: Uridine phosphorylase



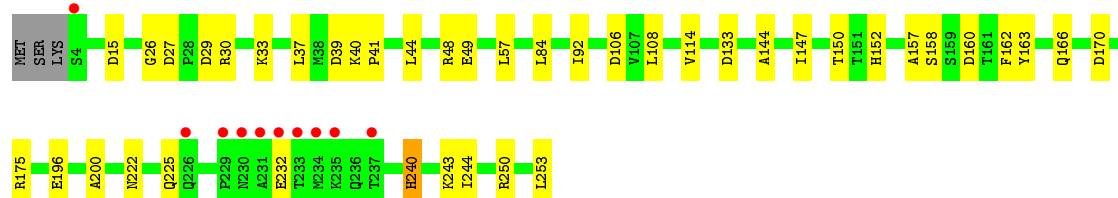
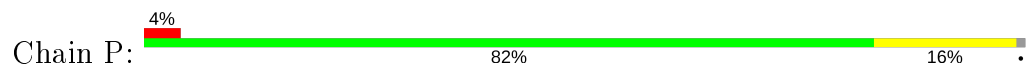
- Molecule 1: Uridine phosphorylase



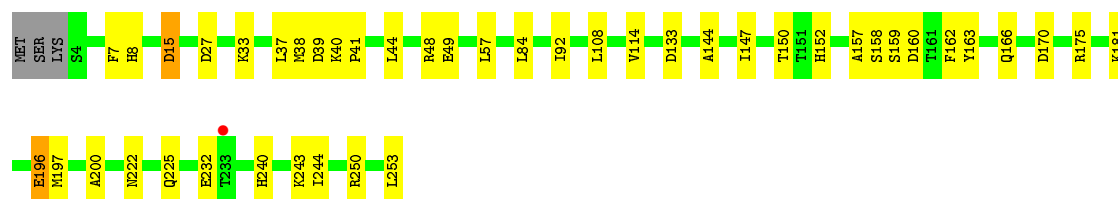
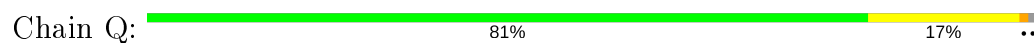
- Molecule 1: Uridine phosphorylase



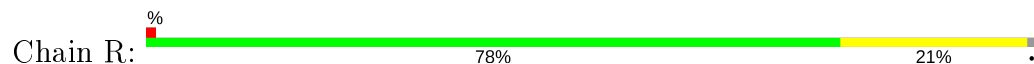
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase





## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 1 21 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 156.24Å 97.66Å 161.45Å<br>90.00° 118.23° 90.00°  | Depositor        |
| Resolution (Å)  | 25.00 – 3.10<br>24.92 – 3.10   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.5 (25.00-3.10)<br>97.5 (24.92-3.10)   | Depositor<br>EDS |
| $R_{merge}$   | 0.16   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.87 (at 3.11Å)  | Xtriage          |
| Refinement program  | REFMAC 5.1.24  | Depositor        |
| R, $R_{free}$   | 0.212 , 0.229<br>0.193 , 0.210   | Depositor<br>DCC |
| $R_{free}$ test set   | 3824 reflections (5.03%)   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.7   | Xtriage          |
| Anisotropy  | 0.046  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 61.1  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$  | Xtriage          |
| Estimated twinning fraction   | 0.001 for -h-l,k,h<br>0.001 for l,k,-h-l<br>0.021 for h,-k,-h-l<br>0.006 for -h-l,-k,l<br>0.006 for l,-k,h | Xtriage          |
| $F_o, F_c$ correlation  | 0.92   | EDS              |
| Total number of atoms   | 35307  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 26.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4850e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, THM

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     | 0.48         | 0/1912  | 0.74        | 3/2595 (0.1%)    |
| 1   | B     | 0.51         | 0/1912  | 0.75        | 7/2595 (0.3%)    |
| 1   | C     | 0.55         | 0/1912  | 0.77        | 8/2595 (0.3%)    |
| 1   | D     | 0.49         | 0/1912  | 0.75        | 5/2595 (0.2%)    |
| 1   | E     | 0.48         | 0/1912  | 0.74        | 6/2595 (0.2%)    |
| 1   | F     | 0.45         | 0/1912  | 0.73        | 5/2595 (0.2%)    |
| 1   | G     | 0.51         | 0/1912  | 0.75        | 7/2595 (0.3%)    |
| 1   | H     | 0.51         | 0/1912  | 0.76        | 7/2595 (0.3%)    |
| 1   | I     | 0.47         | 0/1912  | 0.74        | 6/2595 (0.2%)    |
| 1   | J     | 0.48         | 0/1912  | 0.73        | 6/2595 (0.2%)    |
| 1   | K     | 0.55         | 0/1912  | 0.75        | 6/2595 (0.2%)    |
| 1   | L     | 0.56         | 0/1912  | 0.79        | 7/2595 (0.3%)    |
| 1   | M     | 0.50         | 0/1912  | 0.75        | 6/2595 (0.2%)    |
| 1   | N     | 0.49         | 0/1912  | 0.73        | 6/2595 (0.2%)    |
| 1   | O     | 0.43         | 0/1912  | 0.72        | 4/2595 (0.2%)    |
| 1   | P     | 0.42         | 0/1912  | 0.72        | 7/2595 (0.3%)    |
| 1   | Q     | 0.47         | 0/1912  | 0.74        | 6/2595 (0.2%)    |
| 1   | R     | 0.48         | 0/1912  | 0.76        | 8/2595 (0.3%)    |
| All | All   | 0.49         | 0/34416 | 0.75        | 110/46710 (0.2%) |

There are no bond length outliers.

All (110) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1   | R     | 27  | ASP  | CB-CG-OD2 | 9.17 | 126.55      | 118.30   |
| 1   | L     | 27  | ASP  | CB-CG-OD2 | 8.77 | 126.19      | 118.30   |
| 1   | O     | 27  | ASP  | CB-CG-OD2 | 8.64 | 126.07      | 118.30   |
| 1   | I     | 27  | ASP  | CB-CG-OD2 | 8.41 | 125.87      | 118.30   |
| 1   | A     | 27  | ASP  | CB-CG-OD2 | 8.38 | 125.84      | 118.30   |
| 1   | J     | 27  | ASP  | CB-CG-OD2 | 8.16 | 125.65      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | P     | 27  | ASP  | CB-CG-OD2 | 8.08  | 125.58      | 118.30   |
| 1   | D     | 27  | ASP  | CB-CG-OD2 | 7.92  | 125.42      | 118.30   |
| 1   | L     | 160 | ASP  | CB-CG-OD2 | 7.76  | 125.28      | 118.30   |
| 1   | M     | 27  | ASP  | CB-CG-OD2 | 7.75  | 125.28      | 118.30   |
| 1   | E     | 27  | ASP  | CB-CG-OD2 | 7.57  | 125.11      | 118.30   |
| 1   | F     | 27  | ASP  | CB-CG-OD2 | 7.54  | 125.09      | 118.30   |
| 1   | N     | 27  | ASP  | CB-CG-OD2 | 7.53  | 125.07      | 118.30   |
| 1   | Q     | 27  | ASP  | CB-CG-OD2 | 7.39  | 124.95      | 118.30   |
| 1   | G     | 27  | ASP  | CB-CG-OD2 | 7.20  | 124.78      | 118.30   |
| 1   | R     | 133 | ASP  | CB-CG-OD2 | 7.08  | 124.67      | 118.30   |
| 1   | D     | 170 | ASP  | CB-CG-OD2 | 6.87  | 124.48      | 118.30   |
| 1   | K     | 27  | ASP  | CB-CG-OD2 | 6.74  | 124.36      | 118.30   |
| 1   | M     | 133 | ASP  | CB-CG-OD2 | 6.72  | 124.35      | 118.30   |
| 1   | C     | 27  | ASP  | CB-CG-OD2 | 6.71  | 124.34      | 118.30   |
| 1   | G     | 160 | ASP  | CB-CG-OD2 | 6.71  | 124.34      | 118.30   |
| 1   | F     | 160 | ASP  | CB-CG-OD2 | 6.71  | 124.34      | 118.30   |
| 1   | H     | 27  | ASP  | CB-CG-OD2 | 6.69  | 124.32      | 118.30   |
| 1   | H     | 91  | ARG  | NE-CZ-NH2 | -6.63 | 116.98      | 120.30   |
| 1   | D     | 160 | ASP  | CB-CG-OD2 | 6.60  | 124.24      | 118.30   |
| 1   | B     | 133 | ASP  | CB-CG-OD2 | 6.59  | 124.23      | 118.30   |
| 1   | E     | 133 | ASP  | CB-CG-OD2 | 6.50  | 124.15      | 118.30   |
| 1   | B     | 27  | ASP  | CB-CG-OD2 | 6.49  | 124.14      | 118.30   |
| 1   | P     | 170 | ASP  | CB-CG-OD2 | 6.35  | 124.01      | 118.30   |
| 1   | H     | 39  | ASP  | CB-CG-OD2 | 6.32  | 123.98      | 118.30   |
| 1   | I     | 160 | ASP  | CB-CG-OD2 | 6.31  | 123.98      | 118.30   |
| 1   | C     | 160 | ASP  | CB-CG-OD2 | 6.29  | 123.96      | 118.30   |
| 1   | C     | 29  | ASP  | CB-CG-OD2 | 6.27  | 123.94      | 118.30   |
| 1   | J     | 133 | ASP  | CB-CG-OD2 | 6.26  | 123.94      | 118.30   |
| 1   | I     | 170 | ASP  | CB-CG-OD2 | 6.24  | 123.92      | 118.30   |
| 1   | B     | 160 | ASP  | CB-CG-OD2 | 6.22  | 123.89      | 118.30   |
| 1   | C     | 133 | ASP  | CB-CG-OD2 | 6.19  | 123.87      | 118.30   |
| 1   | L     | 170 | ASP  | CB-CG-OD2 | 6.12  | 123.81      | 118.30   |
| 1   | M     | 39  | ASP  | CB-CG-OD2 | 6.12  | 123.80      | 118.30   |
| 1   | F     | 133 | ASP  | CB-CG-OD2 | 6.09  | 123.78      | 118.30   |
| 1   | N     | 160 | ASP  | CB-CG-OD2 | 6.08  | 123.78      | 118.30   |
| 1   | K     | 170 | ASP  | CB-CG-OD2 | 6.08  | 123.77      | 118.30   |
| 1   | G     | 170 | ASP  | CB-CG-OD2 | 6.02  | 123.72      | 118.30   |
| 1   | Q     | 39  | ASP  | CB-CG-OD2 | 6.00  | 123.70      | 118.30   |
| 1   | Q     | 170 | ASP  | CB-CG-OD2 | 6.00  | 123.70      | 118.30   |
| 1   | I     | 133 | ASP  | CB-CG-OD2 | 5.98  | 123.68      | 118.30   |
| 1   | G     | 133 | ASP  | CB-CG-OD2 | 5.96  | 123.66      | 118.30   |
| 1   | P     | 106 | ASP  | CB-CG-OD2 | 5.93  | 123.63      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | P     | 160 | ASP  | CB-CG-OD2 | 5.92  | 123.63      | 118.30   |
| 1   | B     | 170 | ASP  | CB-CG-OD2 | 5.92  | 123.63      | 118.30   |
| 1   | M     | 170 | ASP  | CB-CG-OD2 | 5.92  | 123.63      | 118.30   |
| 1   | B     | 39  | ASP  | CB-CG-OD2 | 5.92  | 123.62      | 118.30   |
| 1   | J     | 170 | ASP  | CB-CG-OD2 | 5.92  | 123.62      | 118.30   |
| 1   | N     | 106 | ASP  | CB-CG-OD2 | 5.91  | 123.61      | 118.30   |
| 1   | J     | 39  | ASP  | CB-CG-OD2 | 5.90  | 123.61      | 118.30   |
| 1   | E     | 39  | ASP  | CB-CG-OD2 | 5.88  | 123.59      | 118.30   |
| 1   | F     | 170 | ASP  | CB-CG-OD2 | 5.88  | 123.59      | 118.30   |
| 1   | N     | 170 | ASP  | CB-CG-OD2 | 5.85  | 123.57      | 118.30   |
| 1   | P     | 133 | ASP  | CB-CG-OD2 | 5.82  | 123.54      | 118.30   |
| 1   | Q     | 133 | ASP  | CB-CG-OD2 | 5.82  | 123.54      | 118.30   |
| 1   | Q     | 160 | ASP  | CB-CG-OD2 | 5.78  | 123.50      | 118.30   |
| 1   | K     | 133 | ASP  | CB-CG-OD2 | 5.75  | 123.47      | 118.30   |
| 1   | M     | 160 | ASP  | CB-CG-OD2 | 5.75  | 123.47      | 118.30   |
| 1   | G     | 106 | ASP  | CB-CG-OD2 | 5.74  | 123.46      | 118.30   |
| 1   | Q     | 15  | ASP  | CB-CG-OD2 | 5.71  | 123.44      | 118.30   |
| 1   | R     | 39  | ASP  | CB-CG-OD2 | 5.69  | 123.42      | 118.30   |
| 1   | K     | 160 | ASP  | CB-CG-OD2 | 5.68  | 123.41      | 118.30   |
| 1   | L     | 39  | ASP  | CB-CG-OD2 | 5.66  | 123.40      | 118.30   |
| 1   | E     | 106 | ASP  | CB-CG-OD2 | 5.60  | 123.34      | 118.30   |
| 1   | O     | 39  | ASP  | CB-CG-OD2 | 5.58  | 123.32      | 118.30   |
| 1   | J     | 160 | ASP  | CB-CG-OD2 | 5.57  | 123.31      | 118.30   |
| 1   | I     | 39  | ASP  | CB-CG-OD2 | 5.57  | 123.31      | 118.30   |
| 1   | C     | 106 | ASP  | CB-CG-OD2 | 5.55  | 123.30      | 118.30   |
| 1   | D     | 39  | ASP  | CB-CG-OD2 | 5.53  | 123.27      | 118.30   |
| 1   | R     | 160 | ASP  | CB-CG-OD2 | 5.52  | 123.27      | 118.30   |
| 1   | C     | 39  | ASP  | CB-CG-OD2 | 5.51  | 123.26      | 118.30   |
| 1   | N     | 29  | ASP  | CB-CG-OD2 | 5.51  | 123.26      | 118.30   |
| 1   | E     | 160 | ASP  | CB-CG-OD2 | 5.48  | 123.23      | 118.30   |
| 1   | P     | 39  | ASP  | CB-CG-OD2 | 5.48  | 123.23      | 118.30   |
| 1   | A     | 91  | ARG  | NE-CZ-NH2 | -5.47 | 117.56      | 120.30   |
| 1   | R     | 170 | ASP  | CB-CG-OD2 | 5.47  | 123.22      | 118.30   |
| 1   | A     | 170 | ASP  | CB-CG-OD2 | 5.38  | 123.14      | 118.30   |
| 1   | J     | 106 | ASP  | CB-CG-OD2 | 5.35  | 123.11      | 118.30   |
| 1   | E     | 91  | ARG  | NE-CZ-NH2 | -5.33 | 117.64      | 120.30   |
| 1   | K     | 29  | ASP  | CB-CG-OD2 | 5.31  | 123.08      | 118.30   |
| 1   | I     | 91  | ARG  | NE-CZ-NH2 | -5.30 | 117.65      | 120.30   |
| 1   | F     | 39  | ASP  | CB-CG-OD2 | 5.30  | 123.07      | 118.30   |
| 1   | C     | 5   | ASP  | CB-CG-OD2 | 5.29  | 123.06      | 118.30   |
| 1   | H     | 29  | ASP  | CB-CG-OD2 | 5.28  | 123.05      | 118.30   |
| 1   | L     | 106 | ASP  | CB-CG-OD2 | 5.27  | 123.04      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 91  | ARG  | NE-CZ-NH2 | -5.25 | 117.67      | 120.30   |
| 1   | L     | 15  | ASP  | CB-CG-OD2 | 5.24  | 123.02      | 118.30   |
| 1   | N     | 39  | ASP  | CB-CG-OD2 | 5.23  | 123.01      | 118.30   |
| 1   | R     | 106 | ASP  | CB-CG-OD2 | 5.21  | 122.99      | 118.30   |
| 1   | H     | 170 | ASP  | CB-CG-OD2 | 5.20  | 122.98      | 118.30   |
| 1   | P     | 29  | ASP  | CB-CG-OD2 | 5.19  | 122.97      | 118.30   |
| 1   | M     | 106 | ASP  | CB-CG-OD2 | 5.18  | 122.96      | 118.30   |
| 1   | B     | 29  | ASP  | CB-CG-OD2 | 5.17  | 122.95      | 118.30   |
| 1   | D     | 133 | ASP  | CB-CG-OD2 | 5.16  | 122.94      | 118.30   |
| 1   | L     | 29  | ASP  | CB-CG-OD2 | 5.15  | 122.94      | 118.30   |
| 1   | O     | 170 | ASP  | CB-CG-OD2 | 5.15  | 122.93      | 118.30   |
| 1   | G     | 15  | ASP  | CB-CG-OD2 | 5.14  | 122.92      | 118.30   |
| 1   | O     | 160 | ASP  | CB-CG-OD2 | 5.11  | 122.90      | 118.30   |
| 1   | G     | 39  | ASP  | CB-CG-OD2 | 5.10  | 122.89      | 118.30   |
| 1   | H     | 58  | ASP  | CB-CG-OD2 | 5.08  | 122.87      | 118.30   |
| 1   | K     | 5   | ASP  | CB-CG-OD2 | 5.08  | 122.87      | 118.30   |
| 1   | H     | 106 | ASP  | CB-CG-OD2 | 5.06  | 122.85      | 118.30   |
| 1   | R     | 117 | ASP  | CB-CG-OD2 | 5.06  | 122.85      | 118.30   |
| 1   | C     | 170 | ASP  | CB-CG-OD2 | 5.05  | 122.85      | 118.30   |
| 1   | R     | 29  | ASP  | CB-CG-OD2 | 5.05  | 122.84      | 118.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1880  | 0        | 1884     | 22      | 2            |
| 1   | B     | 1880  | 0        | 1884     | 21      | 0            |
| 1   | C     | 1880  | 0        | 1884     | 22      | 1            |
| 1   | D     | 1880  | 0        | 1884     | 23      | 1            |
| 1   | E     | 1880  | 0        | 1884     | 19      | 0            |
| 1   | F     | 1880  | 0        | 1884     | 28      | 0            |
| 1   | G     | 1880  | 0        | 1884     | 20      | 1            |
| 1   | H     | 1880  | 0        | 1884     | 19      | 9            |
| 1   | I     | 1880  | 0        | 1884     | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | J     | 1880  | 0        | 1884     | 16      | 0            |
| 1   | K     | 1880  | 0        | 1884     | 23      | 0            |
| 1   | L     | 1880  | 0        | 1885     | 21      | 9            |
| 1   | M     | 1880  | 0        | 1884     | 24      | 1            |
| 1   | N     | 1880  | 0        | 1884     | 22      | 0            |
| 1   | O     | 1880  | 0        | 1884     | 23      | 0            |
| 1   | P     | 1880  | 0        | 1884     | 14      | 0            |
| 1   | Q     | 1880  | 0        | 1884     | 17      | 0            |
| 1   | R     | 1880  | 0        | 1884     | 19      | 0            |
| 2   | A     | 5     | 0        | 0        | 1       | 0            |
| 2   | B     | 5     | 0        | 0        | 1       | 0            |
| 2   | C     | 5     | 0        | 0        | 1       | 0            |
| 2   | D     | 5     | 0        | 0        | 3       | 0            |
| 2   | E     | 5     | 0        | 0        | 2       | 0            |
| 2   | F     | 5     | 0        | 0        | 2       | 0            |
| 2   | G     | 5     | 0        | 0        | 1       | 0            |
| 2   | H     | 5     | 0        | 0        | 1       | 0            |
| 2   | I     | 5     | 0        | 0        | 0       | 0            |
| 2   | J     | 5     | 0        | 0        | 1       | 0            |
| 2   | K     | 5     | 0        | 0        | 3       | 0            |
| 2   | L     | 5     | 0        | 0        | 0       | 0            |
| 2   | M     | 5     | 0        | 0        | 1       | 0            |
| 2   | N     | 5     | 0        | 0        | 1       | 0            |
| 2   | O     | 5     | 0        | 0        | 3       | 0            |
| 2   | P     | 5     | 0        | 0        | 0       | 0            |
| 2   | Q     | 5     | 0        | 0        | 0       | 0            |
| 2   | R     | 5     | 0        | 0        | 1       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 3   | K     | 1     | 0        | 0        | 0       | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 0       | 0            |
| 3   | Q     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 17    | 0        | 13       | 0       | 0            |
| 4   | B     | 17    | 0        | 13       | 0       | 0            |
| 4   | C     | 17    | 0        | 13       | 2       | 0            |
| 4   | D     | 17    | 0        | 13       | 0       | 0            |
| 4   | E     | 17    | 0        | 13       | 1       | 0            |
| 4   | F     | 17    | 0        | 13       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | G     | 17    | 0        | 13       | 0       | 0            |
| 4   | H     | 17    | 0        | 13       | 0       | 0            |
| 4   | I     | 17    | 0        | 13       | 0       | 0            |
| 4   | J     | 17    | 0        | 13       | 1       | 0            |
| 4   | K     | 17    | 0        | 13       | 0       | 0            |
| 4   | L     | 17    | 0        | 13       | 1       | 0            |
| 4   | M     | 17    | 0        | 13       | 1       | 0            |
| 4   | N     | 17    | 0        | 13       | 1       | 0            |
| 4   | O     | 17    | 0        | 13       | 1       | 0            |
| 4   | P     | 17    | 0        | 13       | 0       | 0            |
| 4   | Q     | 17    | 0        | 13       | 1       | 0            |
| 4   | R     | 17    | 0        | 13       | 0       | 0            |
| 5   | A     | 59    | 0        | 0        | 0       | 0            |
| 5   | B     | 57    | 0        | 0        | 0       | 0            |
| 5   | C     | 62    | 0        | 0        | 0       | 1            |
| 5   | D     | 57    | 0        | 0        | 0       | 0            |
| 5   | E     | 59    | 0        | 0        | 0       | 0            |
| 5   | F     | 58    | 0        | 0        | 0       | 1            |
| 5   | G     | 59    | 0        | 0        | 0       | 0            |
| 5   | H     | 57    | 0        | 0        | 0       | 0            |
| 5   | I     | 60    | 0        | 0        | 1       | 0            |
| 5   | J     | 59    | 0        | 0        | 0       | 0            |
| 5   | K     | 58    | 0        | 0        | 0       | 0            |
| 5   | L     | 61    | 0        | 0        | 0       | 0            |
| 5   | M     | 60    | 0        | 0        | 1       | 0            |
| 5   | N     | 60    | 0        | 0        | 1       | 2            |
| 5   | O     | 58    | 0        | 0        | 0       | 0            |
| 5   | P     | 59    | 0        | 0        | 0       | 0            |
| 5   | Q     | 61    | 0        | 0        | 0       | 0            |
| 5   | R     | 58    | 0        | 0        | 1       | 0            |
| All | All   | 35307 | 0        | 34147    | 342     | 14           |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:K:39:ASP:OD2 | 1:M:42:VAL:CG1 | 1.76                     | 1.34              |
| 1:F:32:GLU:OE2 | 1:O:146:SER:HA | 1.25                     | 1.33              |
| 1:F:32:GLU:OE2 | 1:O:146:SER:CA | 1.78                     | 1.32              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:32:GLU:OE2   | 1:O:146:SER:C     | 1.76                     | 1.24              |
| 1:K:39:ASP:OD2   | 1:M:42:VAL:HG11   | 1.09                     | 1.21              |
| 1:F:32:GLU:OE2   | 1:O:146:SER:O     | 1.80                     | 1.00              |
| 1:F:32:GLU:CD    | 1:O:146:SER:O     | 2.03                     | 0.96              |
| 1:G:30:ARG:NH2   | 2:G:2071:PO4:O2   | 2.09                     | 0.86              |
| 1:H:93:GLY:HA2   | 2:H:2081:PO4:O2   | 1.79                     | 0.82              |
| 1:K:39:ASP:OD2   | 1:M:42:VAL:HG13   | 1.79                     | 0.82              |
| 1:F:32:GLU:OE1   | 1:O:146:SER:O     | 1.97                     | 0.82              |
| 1:M:30:ARG:NH2   | 2:M:2131:PO4:O2   | 2.15                     | 0.79              |
| 1:F:30:ARG:NH2   | 2:F:2061:PO4:O2   | 2.29                     | 0.66              |
| 1:O:30:ARG:NH2   | 2:O:2151:PO4:O2   | 2.30                     | 0.64              |
| 1:A:158:SER:HB3  | 1:A:200:ALA:HB2   | 1.80                     | 0.63              |
| 1:F:158:SER:HB3  | 1:F:200:ALA:HB2   | 1.81                     | 0.63              |
| 1:C:48:ARG:NH2   | 2:D:2041:PO4:O3   | 2.25                     | 0.63              |
| 1:H:158:SER:HB3  | 1:H:200:ALA:HB2   | 1.81                     | 0.63              |
| 1:I:158:SER:HB3  | 1:I:200:ALA:HB2   | 1.81                     | 0.62              |
| 1:R:158:SER:HB3  | 1:R:200:ALA:HB2   | 1.81                     | 0.62              |
| 1:B:30:ARG:NH2   | 2:B:2021:PO4:O2   | 2.30                     | 0.62              |
| 1:O:158:SER:HB3  | 1:O:200:ALA:HB2   | 1.82                     | 0.61              |
| 1:D:30:ARG:NH2   | 2:D:2041:PO4:O2   | 2.33                     | 0.61              |
| 1:C:30:ARG:NH2   | 2:C:2031:PO4:O2   | 2.34                     | 0.61              |
| 1:D:158:SER:HB3  | 1:D:200:ALA:HB2   | 1.83                     | 0.61              |
| 1:L:158:SER:HB3  | 1:L:200:ALA:HB2   | 1.82                     | 0.60              |
| 1:M:158:SER:HB3  | 1:M:200:ALA:HB2   | 1.83                     | 0.60              |
| 1:J:158:SER:HB3  | 1:J:200:ALA:HB2   | 1.83                     | 0.59              |
| 1:L:220:ILE:HD11 | 4:L:2122:THM:HM51 | 1.85                     | 0.59              |
| 1:K:158:SER:HB3  | 1:K:200:ALA:HB2   | 1.84                     | 0.59              |
| 1:N:158:SER:HB3  | 1:N:200:ALA:HB2   | 1.84                     | 0.59              |
| 1:E:158:SER:HB3  | 1:E:200:ALA:HB2   | 1.86                     | 0.58              |
| 1:C:158:SER:HB3  | 1:C:200:ALA:HB2   | 1.85                     | 0.58              |
| 1:B:158:SER:HB3  | 1:B:200:ALA:HB2   | 1.86                     | 0.57              |
| 1:Q:158:SER:HB3  | 1:Q:200:ALA:HB2   | 1.86                     | 0.57              |
| 1:P:158:SER:HB3  | 1:P:200:ALA:HB2   | 1.85                     | 0.57              |
| 1:G:158:SER:HB3  | 1:G:200:ALA:HB2   | 1.86                     | 0.56              |
| 1:J:220:ILE:HD11 | 4:J:2102:THM:HM51 | 1.89                     | 0.54              |
| 1:G:57:LEU:HB3   | 1:G:253:LEU:HD11  | 1.91                     | 0.53              |
| 1:E:162:PHE:HA   | 1:E:166:GLN:NE2   | 2.24                     | 0.53              |
| 1:K:48:ARG:HD3   | 1:L:69:ILE:HD11   | 1.91                     | 0.52              |
| 1:E:57:LEU:HB3   | 1:E:253:LEU:HD11  | 1.92                     | 0.52              |
| 1:B:162:PHE:HA   | 1:B:166:GLN:NE2   | 2.25                     | 0.52              |
| 1:O:222:ASN:HB3  | 1:O:225:GLN:HE21  | 1.74                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:144:ALA:HA   | 1:E:244:ILE:HG12 | 1.92                     | 0.52              |
| 1:F:57:LEU:HB3   | 1:F:253:LEU:HD11 | 1.92                     | 0.52              |
| 2:E:2051:PO4:O3  | 1:F:48:ARG:NH2   | 2.40                     | 0.52              |
| 1:B:57:LEU:HB3   | 1:B:253:LEU:HD11 | 1.92                     | 0.51              |
| 1:L:57:LEU:HB3   | 1:L:253:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:57:LEU:HB3   | 1:A:253:LEU:HD11 | 1.91                     | 0.51              |
| 1:R:7:PHE:HD1    | 1:R:8:HIS:CE1    | 2.27                     | 0.51              |
| 1:L:222:ASN:HB3  | 1:L:225:GLN:HE21 | 1.76                     | 0.51              |
| 1:E:222:ASN:HB3  | 1:E:225:GLN:HE21 | 1.76                     | 0.51              |
| 1:E:49:GLU:HB3   | 1:F:49:GLU:HB3   | 1.91                     | 0.51              |
| 1:H:57:LEU:HG    | 1:H:250:ARG:HG3  | 1.93                     | 0.51              |
| 1:M:144:ALA:HA   | 1:M:244:ILE:HG12 | 1.92                     | 0.51              |
| 1:K:7:PHE:CZ     | 1:L:229:PRO:HG2  | 2.45                     | 0.51              |
| 1:F:108:LEU:HD22 | 1:F:152:HIS:HB2  | 1.93                     | 0.51              |
| 1:Q:144:ALA:HA   | 1:Q:244:ILE:HG12 | 1.93                     | 0.51              |
| 1:K:57:LEU:HB3   | 1:K:253:LEU:HD11 | 1.92                     | 0.51              |
| 1:C:57:LEU:HB3   | 1:C:253:LEU:HD11 | 1.93                     | 0.50              |
| 1:C:222:ASN:HB3  | 1:C:225:GLN:HE21 | 1.76                     | 0.50              |
| 1:G:162:PHE:HA   | 1:G:166:GLN:NE2  | 2.26                     | 0.50              |
| 1:I:162:PHE:HA   | 1:I:166:GLN:NE2  | 2.26                     | 0.50              |
| 1:K:108:LEU:HD22 | 1:K:152:HIS:HB2  | 1.93                     | 0.50              |
| 1:B:144:ALA:HA   | 1:B:244:ILE:HG12 | 1.93                     | 0.50              |
| 1:H:26:GLY:H     | 1:H:30:ARG:NH2   | 2.09                     | 0.50              |
| 1:R:57:LEU:HB3   | 1:R:253:LEU:HD11 | 1.93                     | 0.50              |
| 1:J:144:ALA:HA   | 1:J:244:ILE:HG12 | 1.93                     | 0.50              |
| 1:K:144:ALA:HA   | 1:K:244:ILE:HG12 | 1.94                     | 0.50              |
| 1:E:40:LYS:N     | 1:E:41:PRO:HD3   | 2.27                     | 0.50              |
| 1:C:38:MET:SD    | 1:C:57:LEU:HD13  | 2.51                     | 0.49              |
| 1:G:144:ALA:HA   | 1:G:244:ILE:HG12 | 1.93                     | 0.49              |
| 1:N:144:ALA:HA   | 1:N:244:ILE:HG12 | 1.94                     | 0.49              |
| 1:J:30:ARG:NH2   | 2:J:2101:PO4:O2  | 2.43                     | 0.49              |
| 1:A:40:LYS:N     | 1:A:41:PRO:HD3   | 2.28                     | 0.49              |
| 1:I:57:LEU:HG    | 1:I:250:ARG:HG3  | 1.94                     | 0.49              |
| 1:K:38:MET:SD    | 1:K:57:LEU:HD13  | 2.53                     | 0.49              |
| 1:D:162:PHE:HA   | 1:D:166:GLN:NE2  | 2.28                     | 0.49              |
| 1:I:57:LEU:HB3   | 1:I:253:LEU:HD11 | 1.95                     | 0.49              |
| 1:M:108:LEU:HD22 | 1:M:152:HIS:HB2  | 1.95                     | 0.49              |
| 1:R:40:LYS:N     | 1:R:41:PRO:HD3   | 2.27                     | 0.49              |
| 1:C:108:LEU:HD22 | 1:C:152:HIS:HB2  | 1.93                     | 0.49              |
| 1:E:57:LEU:HG    | 1:E:250:ARG:HG3  | 1.95                     | 0.49              |
| 1:M:40:LYS:N     | 1:M:41:PRO:HD3   | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:144:ALA:HA   | 1:O:244:ILE:HG12 | 1.94                     | 0.49              |
| 1:P:144:ALA:HA   | 1:P:244:ILE:HG12 | 1.94                     | 0.49              |
| 1:R:57:LEU:HG    | 1:R:250:ARG:HG3  | 1.95                     | 0.49              |
| 1:K:7:PHE:HD1    | 1:K:8:HIS:CE1    | 2.31                     | 0.49              |
| 1:A:144:ALA:HA   | 1:A:244:ILE:HG12 | 1.95                     | 0.49              |
| 1:H:159:SER:O    | 1:H:197:MET:HG2  | 2.13                     | 0.49              |
| 1:I:158:SER:HA   | 1:I:196:GLU:O    | 2.13                     | 0.49              |
| 1:J:222:ASN:HB3  | 1:J:225:GLN:HE21 | 1.75                     | 0.49              |
| 1:O:57:LEU:HB3   | 1:O:253:LEU:HD11 | 1.95                     | 0.49              |
| 1:D:158:SER:HA   | 1:D:196:GLU:O    | 2.13                     | 0.49              |
| 1:D:144:ALA:HA   | 1:D:244:ILE:HG12 | 1.95                     | 0.49              |
| 1:F:144:ALA:HA   | 1:F:244:ILE:HG12 | 1.95                     | 0.49              |
| 1:H:57:LEU:HB3   | 1:H:253:LEU:HD11 | 1.94                     | 0.49              |
| 1:C:144:ALA:HA   | 1:C:244:ILE:HG12 | 1.95                     | 0.48              |
| 1:N:57:LEU:HG    | 1:N:250:ARG:HG3  | 1.95                     | 0.48              |
| 1:I:144:ALA:HA   | 1:I:244:ILE:HG12 | 1.95                     | 0.48              |
| 1:J:40:LYS:N     | 1:J:41:PRO:HD3   | 2.28                     | 0.48              |
| 1:Q:196:GLU:HA   | 4:Q:2172:THM:O2  | 2.14                     | 0.48              |
| 1:D:40:LYS:N     | 1:D:41:PRO:HD3   | 2.28                     | 0.48              |
| 1:J:108:LEU:HD22 | 1:J:152:HIS:HB2  | 1.95                     | 0.48              |
| 1:F:40:LYS:N     | 1:F:41:PRO:HD3   | 2.29                     | 0.48              |
| 1:G:57:LEU:HG    | 1:G:250:ARG:HG3  | 1.95                     | 0.48              |
| 1:G:40:LYS:N     | 1:G:41:PRO:HD3   | 2.29                     | 0.48              |
| 1:I:40:LYS:N     | 1:I:41:PRO:HD3   | 2.29                     | 0.48              |
| 1:D:57:LEU:HG    | 1:D:250:ARG:HG3  | 1.95                     | 0.48              |
| 1:F:222:ASN:HB3  | 1:F:225:GLN:HE21 | 1.79                     | 0.48              |
| 1:N:93:GLY:HA2   | 2:N:2141:PO4:O2  | 2.14                     | 0.48              |
| 1:J:57:LEU:HG    | 1:J:250:ARG:HG3  | 1.96                     | 0.48              |
| 1:L:40:LYS:N     | 1:L:41:PRO:HD3   | 2.29                     | 0.48              |
| 1:Q:57:LEU:HB3   | 1:Q:253:LEU:HD11 | 1.95                     | 0.48              |
| 1:N:40:LYS:N     | 1:N:41:PRO:HD3   | 2.28                     | 0.47              |
| 1:A:116:LEU:HB2  | 1:A:159:SER:HA   | 1.97                     | 0.47              |
| 1:H:144:ALA:HA   | 1:H:244:ILE:HG12 | 1.95                     | 0.47              |
| 1:O:57:LEU:HG    | 1:O:250:ARG:HG3  | 1.96                     | 0.47              |
| 1:P:57:LEU:HG    | 1:P:250:ARG:HG3  | 1.96                     | 0.47              |
| 1:K:30:ARG:NH2   | 2:K:2111:PO4:O2  | 2.47                     | 0.47              |
| 1:O:108:LEU:HD22 | 1:O:152:HIS:HB2  | 1.96                     | 0.47              |
| 1:P:57:LEU:HB3   | 1:P:253:LEU:HD11 | 1.96                     | 0.47              |
| 1:D:38:MET:SD    | 1:D:57:LEU:HD13  | 2.54                     | 0.47              |
| 1:Q:162:PHE:HA   | 1:Q:166:GLN:NE2  | 2.29                     | 0.47              |
| 1:C:57:LEU:HG    | 1:C:250:ARG:HG3  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:57:LEU:HB3   | 1:N:253:LEU:HD11 | 1.95                     | 0.47              |
| 1:L:57:LEU:HG    | 1:L:250:ARG:HG3  | 1.96                     | 0.47              |
| 1:M:38:MET:SD    | 1:M:57:LEU:HD13  | 2.54                     | 0.47              |
| 1:N:162:PHE:HA   | 1:N:166:GLN:NE2  | 2.30                     | 0.47              |
| 1:K:114:VAL:HB   | 1:K:157:ALA:HA   | 1.96                     | 0.47              |
| 1:A:219:VAL:O    | 1:A:237:THR:HG21 | 2.15                     | 0.47              |
| 1:K:40:LYS:N     | 1:K:41:PRO:HD3   | 2.29                     | 0.47              |
| 1:A:108:LEU:HD22 | 1:A:152:HIS:HB2  | 1.95                     | 0.47              |
| 1:I:222:ASN:HB3  | 1:I:225:GLN:HE21 | 1.80                     | 0.47              |
| 1:R:222:ASN:HB3  | 1:R:225:GLN:HE21 | 1.80                     | 0.47              |
| 1:B:206:CYS:HB3  | 1:B:211:LEU:O    | 2.15                     | 0.47              |
| 1:I:159:SER:O    | 1:I:197:MET:HG2  | 2.14                     | 0.47              |
| 1:B:40:LYS:N     | 1:B:41:PRO:HD3   | 2.30                     | 0.47              |
| 1:A:26:GLY:H     | 1:A:30:ARG:NH2   | 2.13                     | 0.46              |
| 1:A:57:LEU:HG    | 1:A:250:ARG:HG3  | 1.96                     | 0.46              |
| 1:E:15:ASP:HB3   | 1:E:44:LEU:HD13  | 1.97                     | 0.46              |
| 1:G:26:GLY:H     | 1:G:30:ARG:NH2   | 2.11                     | 0.46              |
| 1:H:40:LYS:N     | 1:H:41:PRO:HD3   | 2.29                     | 0.46              |
| 1:I:108:LEU:HD22 | 1:I:152:HIS:HB2  | 1.97                     | 0.46              |
| 1:J:57:LEU:HB3   | 1:J:253:LEU:HD11 | 1.97                     | 0.46              |
| 1:M:57:LEU:HB3   | 1:M:253:LEU:HD11 | 1.96                     | 0.46              |
| 1:O:26:GLY:H     | 1:O:30:ARG:NH2   | 2.13                     | 0.46              |
| 1:N:26:GLY:H     | 1:N:30:ARG:NH2   | 2.12                     | 0.46              |
| 1:Q:108:LEU:HD22 | 1:Q:152:HIS:HB2  | 1.97                     | 0.46              |
| 1:C:40:LYS:N     | 1:C:41:PRO:HD3   | 2.31                     | 0.46              |
| 1:F:57:LEU:HG    | 1:F:250:ARG:HG3  | 1.97                     | 0.46              |
| 1:H:114:VAL:HB   | 1:H:157:ALA:HA   | 1.97                     | 0.46              |
| 1:B:108:LEU:HD22 | 1:B:152:HIS:HB2  | 1.96                     | 0.46              |
| 1:B:222:ASN:HB3  | 1:B:225:GLN:HE21 | 1.80                     | 0.46              |
| 1:E:58:ASP:OD2   | 1:E:250:ARG:HG2  | 2.15                     | 0.46              |
| 1:H:181:LYS:O    | 1:J:178:ARG:NH2  | 2.47                     | 0.46              |
| 1:Q:38:MET:SD    | 1:Q:57:LEU:HD13  | 2.56                     | 0.46              |
| 1:L:144:ALA:HA   | 1:L:244:ILE:HG12 | 1.96                     | 0.46              |
| 1:N:222:ASN:HB3  | 1:N:225:GLN:HE21 | 1.81                     | 0.46              |
| 1:R:144:ALA:HA   | 1:R:244:ILE:HG12 | 1.97                     | 0.46              |
| 1:D:89:PHE:O     | 1:D:213:ALA:HA   | 2.16                     | 0.46              |
| 1:L:159:SER:O    | 1:L:197:MET:HG2  | 2.15                     | 0.46              |
| 1:B:58:ASP:OD2   | 1:B:250:ARG:HG2  | 2.16                     | 0.46              |
| 1:D:26:GLY:H     | 1:D:30:ARG:NH2   | 2.13                     | 0.46              |
| 1:P:162:PHE:HA   | 1:P:166:GLN:NE2  | 2.30                     | 0.46              |
| 1:B:26:GLY:H     | 1:B:30:ARG:NH2   | 2.13                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:26:GLY:H     | 1:E:30:ARG:NH2    | 2.14                     | 0.46              |
| 1:B:7:PHE:HD1    | 1:B:8:HIS:CE1     | 2.33                     | 0.45              |
| 1:D:57:LEU:HB3   | 1:D:253:LEU:HD11  | 1.97                     | 0.45              |
| 2:K:2111:PO4:P   | 1:L:48:ARG:HH22   | 2.39                     | 0.45              |
| 1:P:26:GLY:H     | 1:P:30:ARG:NH2    | 2.14                     | 0.45              |
| 1:P:40:LYS:N     | 1:P:41:PRO:HD3    | 2.30                     | 0.45              |
| 1:Q:49:GLU:HB3   | 1:R:49:GLU:HB3    | 1.97                     | 0.45              |
| 1:J:15:ASP:HB3   | 1:J:44:LEU:HD13   | 1.99                     | 0.45              |
| 1:P:108:LEU:HD22 | 1:P:152:HIS:HB2   | 1.98                     | 0.45              |
| 1:A:30:ARG:NH2   | 2:A:2011:PO4:O2   | 2.47                     | 0.45              |
| 1:A:222:ASN:HB3  | 1:A:225:GLN:HE21  | 1.81                     | 0.45              |
| 1:F:206:CYS:HB3  | 1:F:211:LEU:O     | 2.16                     | 0.45              |
| 1:G:108:LEU:HD22 | 1:G:152:HIS:HB2   | 1.98                     | 0.45              |
| 1:M:222:ASN:HB3  | 1:M:225:GLN:HE21  | 1.79                     | 0.45              |
| 1:J:116:LEU:HB2  | 1:J:159:SER:HA    | 1.98                     | 0.45              |
| 1:L:158:SER:HA   | 1:L:196:GLU:O     | 2.16                     | 0.45              |
| 1:M:116:LEU:HB2  | 1:M:159:SER:HA    | 1.98                     | 0.45              |
| 1:O:38:MET:SD    | 1:O:57:LEU:HD13   | 2.57                     | 0.45              |
| 1:D:108:LEU:HD22 | 1:D:152:HIS:HB2   | 1.97                     | 0.45              |
| 2:O:2151:PO4:O3  | 1:P:48:ARG:NH2    | 2.48                     | 0.45              |
| 1:K:222:ASN:HB3  | 1:K:225:GLN:HE21  | 1.82                     | 0.45              |
| 1:L:114:VAL:HB   | 1:L:157:ALA:HA    | 1.99                     | 0.45              |
| 1:R:108:LEU:HD22 | 1:R:152:HIS:HB2   | 1.98                     | 0.45              |
| 1:R:162:PHE:HA   | 1:R:166:GLN:NE2   | 2.31                     | 0.45              |
| 1:R:30:ARG:HH22  | 2:R:2181:PO4:P    | 2.40                     | 0.45              |
| 1:B:240:HIS:O    | 1:B:244:ILE:HD12  | 2.16                     | 0.45              |
| 1:G:222:ASN:HB3  | 1:G:225:GLN:HE21  | 1.81                     | 0.45              |
| 1:M:57:LEU:HG    | 1:M:250:ARG:HG3   | 1.99                     | 0.45              |
| 1:P:222:ASN:HB3  | 1:P:225:GLN:HE21  | 1.81                     | 0.45              |
| 1:F:26:GLY:H     | 1:F:30:ARG:NH2    | 2.15                     | 0.44              |
| 1:N:158:SER:HA   | 1:N:196:GLU:O     | 2.18                     | 0.44              |
| 1:Q:48:ARG:HD3   | 1:R:69:ILE:HD11   | 1.99                     | 0.44              |
| 1:A:162:PHE:HA   | 1:A:166:GLN:NE2   | 2.32                     | 0.44              |
| 1:D:181:LYS:O    | 1:F:178:ARG:NH2   | 2.48                     | 0.44              |
| 1:G:126:LEU:HB3  | 1:L:126:LEU:HD23  | 2.00                     | 0.44              |
| 1:Q:40:LYS:N     | 1:Q:41:PRO:HD3    | 2.32                     | 0.44              |
| 1:R:25:PRO:O     | 1:R:66:SER:HA     | 2.17                     | 0.44              |
| 1:A:38:MET:SD    | 1:A:57:LEU:HD13   | 2.57                     | 0.44              |
| 1:E:108:LEU:HD22 | 1:E:152:HIS:HB2   | 1.98                     | 0.44              |
| 1:E:220:ILE:HD11 | 4:E:2052:THM:HM51 | 2.00                     | 0.44              |
| 1:N:166:GLN:HG2  | 1:N:195:TYR:CD1   | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:178:ARG:NH2  | 1:O:181:LYS:O    | 2.46                     | 0.44              |
| 1:Q:57:LEU:HG    | 1:Q:250:ARG:HG3  | 1.98                     | 0.44              |
| 1:K:57:LEU:HG    | 1:K:250:ARG:HG3  | 1.98                     | 0.44              |
| 1:C:196:GLU:HA   | 4:C:2032:THM:O2  | 2.18                     | 0.44              |
| 1:M:231:ALA:HB3  | 5:M:538:HOH:O    | 2.17                     | 0.44              |
| 1:O:40:LYS:N     | 1:O:41:PRO:HD3   | 2.33                     | 0.44              |
| 1:A:159:SER:O    | 1:A:197:MET:HG2  | 2.18                     | 0.44              |
| 1:M:26:GLY:H     | 1:M:30:ARG:NH2   | 2.15                     | 0.44              |
| 1:M:7:PHE:HD1    | 1:M:8:HIS:CE1    | 2.35                     | 0.44              |
| 1:C:26:GLY:H     | 1:C:30:ARG:NH2   | 2.15                     | 0.44              |
| 1:J:162:PHE:HA   | 1:J:166:GLN:NE2  | 2.32                     | 0.44              |
| 1:L:26:GLY:H     | 1:L:30:ARG:NH2   | 2.16                     | 0.44              |
| 1:C:114:VAL:HB   | 1:C:157:ALA:HA   | 1.99                     | 0.44              |
| 1:G:126:LEU:HD23 | 1:L:126:LEU:HB3  | 2.00                     | 0.44              |
| 1:H:162:PHE:HA   | 1:H:166:GLN:NE2  | 2.33                     | 0.44              |
| 1:I:26:GLY:H     | 1:I:30:ARG:NH2   | 2.15                     | 0.44              |
| 1:C:118:GLY:HA3  | 1:D:160:ASP:OD2  | 2.17                     | 0.44              |
| 1:C:159:SER:O    | 1:C:197:MET:HG2  | 2.17                     | 0.44              |
| 1:N:114:VAL:HB   | 1:N:157:ALA:HA   | 2.00                     | 0.43              |
| 1:B:57:LEU:HG    | 1:B:250:ARG:HG3  | 1.99                     | 0.43              |
| 1:D:58:ASP:OD2   | 1:D:250:ARG:HG2  | 2.18                     | 0.43              |
| 1:K:162:PHE:HA   | 1:K:166:GLN:NE2  | 2.33                     | 0.43              |
| 1:K:89:PHE:O     | 1:K:213:ALA:HA   | 2.18                     | 0.43              |
| 1:M:162:PHE:HA   | 1:M:166:GLN:NE2  | 2.33                     | 0.43              |
| 1:N:108:LEU:HD22 | 1:N:152:HIS:HB2  | 1.99                     | 0.43              |
| 1:N:58:ASP:OD2   | 1:N:250:ARG:HG2  | 2.18                     | 0.43              |
| 1:O:196:GLU:HA   | 4:O:2152:THM:O2  | 2.18                     | 0.43              |
| 1:P:240:HIS:O    | 1:P:244:ILE:HD12 | 2.18                     | 0.43              |
| 1:Q:222:ASN:HB3  | 1:Q:225:GLN:HE21 | 1.84                     | 0.43              |
| 1:B:126:LEU:HD23 | 1:C:126:LEU:HB3  | 1.99                     | 0.43              |
| 2:E:2051:PO4:P   | 1:F:48:ARG:HH22  | 2.41                     | 0.43              |
| 1:G:48:ARG:HD3   | 1:H:69:ILE:HD11  | 2.00                     | 0.43              |
| 1:I:38:MET:SD    | 1:I:57:LEU:HD13  | 2.59                     | 0.43              |
| 1:L:108:LEU:HD22 | 1:L:152:HIS:HB2  | 2.00                     | 0.43              |
| 1:Q:114:VAL:HB   | 1:Q:157:ALA:HA   | 2.00                     | 0.43              |
| 1:Q:158:SER:HA   | 1:Q:196:GLU:O    | 2.18                     | 0.43              |
| 1:D:126:LEU:HD23 | 1:E:126:LEU:HD23 | 2.00                     | 0.43              |
| 1:I:7:PHE:HD1    | 1:I:8:HIS:CE1    | 2.37                     | 0.43              |
| 1:G:240:HIS:O    | 1:G:244:ILE:HD12 | 2.18                     | 0.43              |
| 1:K:159:SER:O    | 1:K:197:MET:HG2  | 2.17                     | 0.43              |
| 1:N:48:ARG:NH1   | 5:N:1328:HOH:O   | 2.50                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:15:ASP:HB3   | 1:D:44:LEU:HD13   | 2.01                     | 0.43              |
| 1:E:114:VAL:HB   | 1:E:157:ALA:HA    | 2.00                     | 0.43              |
| 1:O:49:GLU:HB3   | 1:P:49:GLU:HB3    | 1.99                     | 0.43              |
| 1:H:108:LEU:HD22 | 1:H:152:HIS:HB2   | 2.00                     | 0.43              |
| 1:H:7:PHE:HD1    | 1:H:8:HIS:CE1     | 2.37                     | 0.42              |
| 1:A:40:LYS:HE2   | 1:I:33:LYS:HE2    | 2.01                     | 0.42              |
| 1:D:222:ASN:HB3  | 1:D:225:GLN:HE21  | 1.84                     | 0.42              |
| 1:E:240:HIS:O    | 1:E:244:ILE:HD12  | 2.19                     | 0.42              |
| 1:M:220:ILE:HD11 | 4:M:2132:THM:HM51 | 2.00                     | 0.42              |
| 1:E:38:MET:SD    | 1:E:57:LEU:HD13   | 2.59                     | 0.42              |
| 1:A:69:ILE:HD11  | 1:B:48:ARG:HD3    | 2.01                     | 0.42              |
| 1:H:89:PHE:O     | 1:H:213:ALA:HA    | 2.19                     | 0.42              |
| 1:O:162:PHE:HA   | 1:O:166:GLN:NE2   | 2.34                     | 0.42              |
| 1:C:220:ILE:HD11 | 4:C:2032:THM:HM51 | 2.01                     | 0.42              |
| 1:D:114:VAL:HB   | 1:D:157:ALA:HA    | 2.01                     | 0.42              |
| 1:G:116:LEU:HB2  | 1:G:159:SER:HA    | 2.00                     | 0.42              |
| 1:J:181:LYS:O    | 1:L:178:ARG:NH2   | 2.50                     | 0.42              |
| 1:M:158:SER:HA   | 1:M:196:GLU:O     | 2.20                     | 0.42              |
| 1:O:93:GLY:HA2   | 2:O:2151:PO4:O2   | 2.19                     | 0.42              |
| 1:C:49:GLU:HB3   | 1:D:49:GLU:HB3    | 2.02                     | 0.42              |
| 1:F:15:ASP:HB3   | 1:F:44:LEU:HD13   | 2.02                     | 0.42              |
| 1:G:228:ILE:HA   | 1:G:229:PRO:HD3   | 1.96                     | 0.42              |
| 1:H:206:CYS:HB3  | 1:H:211:LEU:O     | 2.20                     | 0.42              |
| 1:K:26:GLY:H     | 1:K:30:ARG:NH2    | 2.17                     | 0.42              |
| 1:Q:159:SER:O    | 1:Q:197:MET:HG2   | 2.19                     | 0.42              |
| 1:B:158:SER:HA   | 1:B:196:GLU:O     | 2.20                     | 0.42              |
| 1:F:116:LEU:HB2  | 1:F:159:SER:HA    | 2.02                     | 0.42              |
| 1:R:129:PRO:O    | 1:R:131:VAL:HG12  | 2.20                     | 0.42              |
| 1:D:93:GLY:HA2   | 2:D:2041:PO4:O2   | 2.19                     | 0.42              |
| 1:N:206:CYS:HB3  | 1:N:211:LEU:O     | 2.20                     | 0.42              |
| 1:N:7:PHE:HD1    | 1:N:8:HIS:CE1     | 2.38                     | 0.42              |
| 1:O:58:ASP:OD2   | 1:O:250:ARG:HG2   | 2.20                     | 0.42              |
| 1:P:114:VAL:HB   | 1:P:157:ALA:HA    | 2.01                     | 0.42              |
| 1:F:196:GLU:HA   | 4:F:2062:THM:O2   | 2.20                     | 0.42              |
| 1:B:114:VAL:HB   | 1:B:157:ALA:HA    | 2.01                     | 0.41              |
| 1:C:58:ASP:OD2   | 1:C:250:ARG:HG2   | 2.20                     | 0.41              |
| 1:D:159:SER:O    | 1:D:197:MET:HG2   | 2.20                     | 0.41              |
| 1:E:60:LYS:HA    | 1:E:61:PRO:HD3    | 1.91                     | 0.41              |
| 1:F:60:LYS:HA    | 1:F:61:PRO:HD3    | 1.94                     | 0.41              |
| 1:H:222:ASN:HB3  | 1:H:225:GLN:HE21  | 1.85                     | 0.41              |
| 1:I:157:ALA:O    | 1:I:195:TYR:HA    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:166:GLN:HG2  | 1:I:195:TYR:CD1   | 2.55                     | 0.41              |
| 1:G:206:CYS:HB3  | 1:G:211:LEU:O     | 2.20                     | 0.41              |
| 1:I:15:ASP:HB3   | 1:I:44:LEU:HD13   | 2.02                     | 0.41              |
| 1:J:26:GLY:H     | 1:J:30:ARG:NH2    | 2.18                     | 0.41              |
| 1:N:219:VAL:O    | 1:N:237:THR:HG21  | 2.20                     | 0.41              |
| 1:G:60:LYS:HA    | 1:G:61:PRO:HD3    | 1.92                     | 0.41              |
| 1:N:220:ILE:HD11 | 4:N:2142:THM:HM51 | 2.03                     | 0.41              |
| 1:B:116:LEU:HB2  | 1:B:159:SER:HA    | 2.01                     | 0.41              |
| 1:A:240:HIS:O    | 1:A:244:ILE:HD12  | 2.20                     | 0.41              |
| 1:I:60:LYS:HA    | 1:I:61:PRO:HD3    | 1.91                     | 0.41              |
| 1:K:116:LEU:HB2  | 1:K:159:SER:HA    | 2.01                     | 0.41              |
| 1:N:15:ASP:HB3   | 1:N:44:LEU:HD13   | 2.01                     | 0.41              |
| 1:R:48:ARG:NH1   | 5:R:1728:HOH:O    | 2.49                     | 0.41              |
| 1:H:116:LEU:HB2  | 1:H:159:SER:HA    | 2.02                     | 0.41              |
| 1:H:240:HIS:O    | 1:H:244:ILE:HD12  | 2.20                     | 0.41              |
| 1:A:114:VAL:HB   | 1:A:157:ALA:HA    | 2.01                     | 0.41              |
| 1:C:116:LEU:HB2  | 1:C:159:SER:HA    | 2.01                     | 0.41              |
| 1:D:7:PHE:HD1    | 1:D:8:HIS:CE1     | 2.38                     | 0.41              |
| 1:N:228:ILE:HA   | 1:N:229:PRO:HD3   | 1.92                     | 0.41              |
| 1:A:181:LYS:O    | 1:E:178:ARG:NH2   | 2.49                     | 0.41              |
| 1:A:228:ILE:HA   | 1:A:229:PRO:HD3   | 1.96                     | 0.41              |
| 1:C:7:PHE:HD1    | 1:C:8:HIS:CE1     | 2.38                     | 0.41              |
| 1:M:89:PHE:O     | 1:M:213:ALA:HA    | 2.21                     | 0.41              |
| 1:B:24:VAL:HG23  | 1:B:24:VAL:O      | 2.21                     | 0.41              |
| 1:F:159:SER:O    | 1:F:197:MET:HG2   | 2.21                     | 0.41              |
| 1:G:114:VAL:HB   | 1:G:157:ALA:HA    | 2.02                     | 0.41              |
| 1:I:48:ARG:NH1   | 5:I:828:HOH:O     | 2.48                     | 0.41              |
| 1:J:89:PHE:O     | 1:J:213:ALA:HA    | 2.20                     | 0.41              |
| 1:M:219:VAL:O    | 1:M:237:THR:HG21  | 2.21                     | 0.41              |
| 1:A:15:ASP:HB3   | 1:A:44:LEU:HD13   | 2.02                     | 0.41              |
| 1:F:30:ARG:HH22  | 2:F:2061:PO4:P    | 2.43                     | 0.41              |
| 1:M:58:ASP:OD2   | 1:M:250:ARG:HG2   | 2.21                     | 0.41              |
| 1:O:15:ASP:HB3   | 1:O:44:LEU:HD13   | 2.02                     | 0.41              |
| 1:N:240:HIS:O    | 1:N:244:ILE:HD12  | 2.21                     | 0.40              |
| 1:R:114:VAL:HB   | 1:R:157:ALA:HA    | 2.03                     | 0.40              |
| 1:R:206:CYS:HB3  | 1:R:211:LEU:O     | 2.21                     | 0.40              |
| 1:G:166:GLN:HG2  | 1:G:195:TYR:CD1   | 2.56                     | 0.40              |
| 1:K:229:PRO:HG2  | 1:L:7:PHE:CZ      | 2.56                     | 0.40              |
| 1:K:30:ARG:HH22  | 2:K:2111:PO4:P    | 2.44                     | 0.40              |
| 1:P:15:ASP:HB3   | 1:P:44:LEU:HD13   | 2.03                     | 0.40              |
| 1:Q:15:ASP:HB3   | 1:Q:44:LEU:HD13   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:Q:7:PHE:HD1    | 1:Q:8:HIS:CE1     | 2.39                     | 0.40              |
| 1:A:158:SER:HA   | 1:A:196:GLU:O     | 2.22                     | 0.40              |
| 1:B:15:ASP:HB3   | 1:B:44:LEU:HD13   | 2.04                     | 0.40              |
| 1:C:25:PRO:O     | 1:C:66:SER:HA     | 2.21                     | 0.40              |
| 1:F:7:PHE:HD1    | 1:F:8:HIS:CE1     | 2.38                     | 0.40              |
| 1:L:166:GLN:HG2  | 1:L:195:TYR:CD1   | 2.56                     | 0.40              |
| 1:L:89:PHE:O     | 1:L:213:ALA:HA    | 2.21                     | 0.40              |
| 1:R:38:MET:SD    | 1:R:57:LEU:HD13   | 2.61                     | 0.40              |
| 1:R:89:PHE:O     | 1:R:213:ALA:HA    | 2.22                     | 0.40              |
| 1:M:15:ASP:HB3   | 1:M:44:LEU:HD13   | 2.02                     | 0.40              |
| 1:F:220:ILE:HD11 | 4:F:2062:THM:HM51 | 2.03                     | 0.40              |

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:H:232:GLU:CG  | 1:L:13:LYS:CE[2_657]  | 1.02                     | 1.18              |
| 1:H:232:GLU:CG  | 1:L:13:LYS:NZ[2_657]  | 1.34                     | 0.86              |
| 1:H:232:GLU:CB  | 1:L:13:LYS:CD[2_657]  | 1.35                     | 0.85              |
| 1:H:232:GLU:CG  | 1:L:13:LYS:CD[2_657]  | 1.47                     | 0.73              |
| 1:H:232:GLU:CB  | 1:L:13:LYS:CE[2_657]  | 1.68                     | 0.52              |
| 1:H:232:GLU:CD  | 1:L:13:LYS:NZ[2_657]  | 1.85                     | 0.35              |
| 1:M:232:GLU:OE1 | 5:F:3035:HOH:O[2_646] | 2.06                     | 0.14              |
| 1:A:101:HIS:N   | 5:N:1338:HOH:O[2_646] | 2.08                     | 0.12              |
| 1:H:232:GLU:OE2 | 1:L:13:LYS:NZ[2_657]  | 2.09                     | 0.11              |
| 1:C:146:SER:OG  | 1:L:32:GLU:OE2[1_454] | 2.10                     | 0.10              |
| 1:D:232:GLU:CB  | 5:C:3051:HOH:O[2_555] | 2.11                     | 0.09              |
| 1:H:232:GLU:OE1 | 1:L:84:LEU:O[2_657]   | 2.13                     | 0.07              |
| 1:G:103:ASN:OD1 | 1:H:181:LYS:NZ[2_647] | 2.17                     | 0.03              |
| 1:A:101:HIS:CB  | 5:N:1338:HOH:O[2_646] | 2.19                     | 0.01              |

## 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     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | B     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | C     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | D     | 248/253 (98%)   | 242 (98%)  | 5 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | E     | 248/253 (98%)   | 241 (97%)  | 6 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | F     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | G     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | H     | 248/253 (98%)   | 242 (98%)  | 5 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | I     | 248/253 (98%)   | 241 (97%)  | 6 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | J     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | K     | 248/253 (98%)   | 242 (98%)  | 5 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | L     | 248/253 (98%)   | 242 (98%)  | 5 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | M     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | N     | 248/253 (98%)   | 241 (97%)  | 6 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | O     | 248/253 (98%)   | 244 (98%)  | 3 (1%)  | 1 (0%)   | 34          | 69 |
| 1   | P     | 248/253 (98%)   | 241 (97%)  | 6 (2%)  | 1 (0%)   | 34          | 69 |
| 1   | Q     | 248/253 (98%)   | 244 (98%)  | 3 (1%)  | 1 (0%)   | 34          | 69 |
| 1   | R     | 248/253 (98%)   | 243 (98%)  | 4 (2%)  | 1 (0%)   | 34          | 69 |
| All | All   | 4464/4554 (98%) | 4364 (98%) | 82 (2%) | 18 (0%)  | 34          | 69 |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 163 | TYR  |
| 1   | L     | 163 | TYR  |
| 1   | A     | 163 | TYR  |
| 1   | C     | 163 | TYR  |
| 1   | D     | 163 | TYR  |
| 1   | E     | 163 | TYR  |
| 1   | F     | 163 | TYR  |
| 1   | G     | 163 | TYR  |
| 1   | H     | 163 | TYR  |
| 1   | I     | 163 | TYR  |
| 1   | J     | 163 | TYR  |
| 1   | K     | 163 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 163 | TYR  |
| 1   | N     | 163 | TYR  |
| 1   | O     | 163 | TYR  |
| 1   | P     | 163 | TYR  |
| 1   | Q     | 163 | TYR  |
| 1   | R     | 163 | TYR  |

### 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     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | B     | 201/204 (98%)   | 190 (94%)  | 11 (6%)  | 21          | 53 |
| 1   | C     | 201/204 (98%)   | 190 (94%)  | 11 (6%)  | 21          | 53 |
| 1   | D     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | E     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | F     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | G     | 201/204 (98%)   | 191 (95%)  | 10 (5%)  | 24          | 57 |
| 1   | H     | 201/204 (98%)   | 188 (94%)  | 13 (6%)  | 17          | 47 |
| 1   | I     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | J     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | K     | 201/204 (98%)   | 190 (94%)  | 11 (6%)  | 21          | 53 |
| 1   | L     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | M     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | N     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | O     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | P     | 201/204 (98%)   | 190 (94%)  | 11 (6%)  | 21          | 53 |
| 1   | Q     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| 1   | R     | 201/204 (98%)   | 189 (94%)  | 12 (6%)  | 19          | 49 |
| All | All   | 3618/3672 (98%) | 3407 (94%) | 211 (6%) | 20          | 51 |

All (211) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | LYS  |
| 1   | A     | 37  | LEU  |
| 1   | A     | 84  | LEU  |
| 1   | A     | 92  | ILE  |
| 1   | A     | 147 | ILE  |
| 1   | A     | 150 | THR  |
| 1   | A     | 175 | ARG  |
| 1   | A     | 186 | GLU  |
| 1   | A     | 196 | GLU  |
| 1   | A     | 232 | GLU  |
| 1   | A     | 240 | HIS  |
| 1   | A     | 243 | LYS  |
| 1   | B     | 33  | LYS  |
| 1   | B     | 37  | LEU  |
| 1   | B     | 84  | LEU  |
| 1   | B     | 92  | ILE  |
| 1   | B     | 147 | ILE  |
| 1   | B     | 150 | THR  |
| 1   | B     | 196 | GLU  |
| 1   | B     | 232 | GLU  |
| 1   | B     | 240 | HIS  |
| 1   | B     | 243 | LYS  |
| 1   | B     | 245 | VAL  |
| 1   | C     | 33  | LYS  |
| 1   | C     | 37  | LEU  |
| 1   | C     | 84  | LEU  |
| 1   | C     | 92  | ILE  |
| 1   | C     | 147 | ILE  |
| 1   | C     | 150 | THR  |
| 1   | C     | 175 | ARG  |
| 1   | C     | 196 | GLU  |
| 1   | C     | 232 | GLU  |
| 1   | C     | 240 | HIS  |
| 1   | C     | 243 | LYS  |
| 1   | D     | 33  | LYS  |
| 1   | D     | 37  | LEU  |
| 1   | D     | 84  | LEU  |
| 1   | D     | 92  | ILE  |
| 1   | D     | 147 | ILE  |
| 1   | D     | 150 | THR  |
| 1   | D     | 175 | ARG  |
| 1   | D     | 196 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 232 | GLU  |
| 1   | D     | 240 | HIS  |
| 1   | D     | 243 | LYS  |
| 1   | D     | 245 | VAL  |
| 1   | E     | 33  | LYS  |
| 1   | E     | 37  | LEU  |
| 1   | E     | 84  | LEU  |
| 1   | E     | 92  | ILE  |
| 1   | E     | 147 | ILE  |
| 1   | E     | 150 | THR  |
| 1   | E     | 175 | ARG  |
| 1   | E     | 186 | GLU  |
| 1   | E     | 196 | GLU  |
| 1   | E     | 232 | GLU  |
| 1   | E     | 240 | HIS  |
| 1   | E     | 243 | LYS  |
| 1   | F     | 33  | LYS  |
| 1   | F     | 37  | LEU  |
| 1   | F     | 84  | LEU  |
| 1   | F     | 92  | ILE  |
| 1   | F     | 147 | ILE  |
| 1   | F     | 150 | THR  |
| 1   | F     | 181 | LYS  |
| 1   | F     | 186 | GLU  |
| 1   | F     | 196 | GLU  |
| 1   | F     | 232 | GLU  |
| 1   | F     | 240 | HIS  |
| 1   | F     | 243 | LYS  |
| 1   | G     | 33  | LYS  |
| 1   | G     | 37  | LEU  |
| 1   | G     | 84  | LEU  |
| 1   | G     | 92  | ILE  |
| 1   | G     | 147 | ILE  |
| 1   | G     | 150 | THR  |
| 1   | G     | 196 | GLU  |
| 1   | G     | 232 | GLU  |
| 1   | G     | 240 | HIS  |
| 1   | G     | 243 | LYS  |
| 1   | H     | 33  | LYS  |
| 1   | H     | 37  | LEU  |
| 1   | H     | 84  | LEU  |
| 1   | H     | 92  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 147 | ILE  |
| 1   | H     | 150 | THR  |
| 1   | H     | 175 | ARG  |
| 1   | H     | 186 | GLU  |
| 1   | H     | 196 | GLU  |
| 1   | H     | 232 | GLU  |
| 1   | H     | 239 | SER  |
| 1   | H     | 240 | HIS  |
| 1   | H     | 243 | LYS  |
| 1   | I     | 33  | LYS  |
| 1   | I     | 37  | LEU  |
| 1   | I     | 84  | LEU  |
| 1   | I     | 92  | ILE  |
| 1   | I     | 147 | ILE  |
| 1   | I     | 150 | THR  |
| 1   | I     | 175 | ARG  |
| 1   | I     | 186 | GLU  |
| 1   | I     | 196 | GLU  |
| 1   | I     | 232 | GLU  |
| 1   | I     | 240 | HIS  |
| 1   | I     | 243 | LYS  |
| 1   | J     | 33  | LYS  |
| 1   | J     | 37  | LEU  |
| 1   | J     | 84  | LEU  |
| 1   | J     | 92  | ILE  |
| 1   | J     | 147 | ILE  |
| 1   | J     | 150 | THR  |
| 1   | J     | 175 | ARG  |
| 1   | J     | 181 | LYS  |
| 1   | J     | 196 | GLU  |
| 1   | J     | 232 | GLU  |
| 1   | J     | 240 | HIS  |
| 1   | J     | 243 | LYS  |
| 1   | K     | 33  | LYS  |
| 1   | K     | 37  | LEU  |
| 1   | K     | 84  | LEU  |
| 1   | K     | 92  | ILE  |
| 1   | K     | 147 | ILE  |
| 1   | K     | 150 | THR  |
| 1   | K     | 175 | ARG  |
| 1   | K     | 196 | GLU  |
| 1   | K     | 232 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 240 | HIS  |
| 1   | K     | 243 | LYS  |
| 1   | L     | 33  | LYS  |
| 1   | L     | 37  | LEU  |
| 1   | L     | 84  | LEU  |
| 1   | L     | 92  | ILE  |
| 1   | L     | 147 | ILE  |
| 1   | L     | 150 | THR  |
| 1   | L     | 181 | LYS  |
| 1   | L     | 196 | GLU  |
| 1   | L     | 232 | GLU  |
| 1   | L     | 240 | HIS  |
| 1   | L     | 243 | LYS  |
| 1   | L     | 245 | VAL  |
| 1   | M     | 33  | LYS  |
| 1   | M     | 37  | LEU  |
| 1   | M     | 84  | LEU  |
| 1   | M     | 92  | ILE  |
| 1   | M     | 147 | ILE  |
| 1   | M     | 150 | THR  |
| 1   | M     | 175 | ARG  |
| 1   | M     | 186 | GLU  |
| 1   | M     | 196 | GLU  |
| 1   | M     | 232 | GLU  |
| 1   | M     | 240 | HIS  |
| 1   | M     | 243 | LYS  |
| 1   | N     | 33  | LYS  |
| 1   | N     | 37  | LEU  |
| 1   | N     | 84  | LEU  |
| 1   | N     | 92  | ILE  |
| 1   | N     | 147 | ILE  |
| 1   | N     | 150 | THR  |
| 1   | N     | 175 | ARG  |
| 1   | N     | 186 | GLU  |
| 1   | N     | 196 | GLU  |
| 1   | N     | 232 | GLU  |
| 1   | N     | 240 | HIS  |
| 1   | N     | 243 | LYS  |
| 1   | O     | 33  | LYS  |
| 1   | O     | 37  | LEU  |
| 1   | O     | 84  | LEU  |
| 1   | O     | 92  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 147 | ILE  |
| 1   | O     | 150 | THR  |
| 1   | O     | 175 | ARG  |
| 1   | O     | 186 | GLU  |
| 1   | O     | 196 | GLU  |
| 1   | O     | 232 | GLU  |
| 1   | O     | 240 | HIS  |
| 1   | O     | 243 | LYS  |
| 1   | P     | 33  | LYS  |
| 1   | P     | 37  | LEU  |
| 1   | P     | 84  | LEU  |
| 1   | P     | 92  | ILE  |
| 1   | P     | 147 | ILE  |
| 1   | P     | 150 | THR  |
| 1   | P     | 175 | ARG  |
| 1   | P     | 196 | GLU  |
| 1   | P     | 232 | GLU  |
| 1   | P     | 240 | HIS  |
| 1   | P     | 243 | LYS  |
| 1   | Q     | 33  | LYS  |
| 1   | Q     | 37  | LEU  |
| 1   | Q     | 84  | LEU  |
| 1   | Q     | 92  | ILE  |
| 1   | Q     | 147 | ILE  |
| 1   | Q     | 150 | THR  |
| 1   | Q     | 175 | ARG  |
| 1   | Q     | 181 | LYS  |
| 1   | Q     | 196 | GLU  |
| 1   | Q     | 232 | GLU  |
| 1   | Q     | 240 | HIS  |
| 1   | Q     | 243 | LYS  |
| 1   | R     | 33  | LYS  |
| 1   | R     | 37  | LEU  |
| 1   | R     | 84  | LEU  |
| 1   | R     | 92  | ILE  |
| 1   | R     | 147 | ILE  |
| 1   | R     | 150 | THR  |
| 1   | R     | 175 | ARG  |
| 1   | R     | 181 | LYS  |
| 1   | R     | 196 | GLU  |
| 1   | R     | 232 | GLU  |
| 1   | R     | 240 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 243 | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 225 | GLN  |
| 1   | A     | 226 | GLN  |
| 1   | A     | 230 | ASN  |
| 1   | B     | 225 | GLN  |
| 1   | B     | 226 | GLN  |
| 1   | B     | 230 | ASN  |
| 1   | C     | 225 | GLN  |
| 1   | C     | 226 | GLN  |
| 1   | C     | 230 | ASN  |
| 1   | D     | 225 | GLN  |
| 1   | D     | 226 | GLN  |
| 1   | D     | 230 | ASN  |
| 1   | E     | 225 | GLN  |
| 1   | E     | 226 | GLN  |
| 1   | E     | 230 | ASN  |
| 1   | F     | 225 | GLN  |
| 1   | F     | 226 | GLN  |
| 1   | F     | 230 | ASN  |
| 1   | G     | 225 | GLN  |
| 1   | G     | 226 | GLN  |
| 1   | G     | 230 | ASN  |
| 1   | H     | 225 | GLN  |
| 1   | H     | 226 | GLN  |
| 1   | H     | 230 | ASN  |
| 1   | I     | 225 | GLN  |
| 1   | I     | 226 | GLN  |
| 1   | I     | 230 | ASN  |
| 1   | J     | 225 | GLN  |
| 1   | J     | 226 | GLN  |
| 1   | J     | 230 | ASN  |
| 1   | K     | 225 | GLN  |
| 1   | K     | 226 | GLN  |
| 1   | K     | 230 | ASN  |
| 1   | L     | 225 | GLN  |
| 1   | L     | 226 | GLN  |
| 1   | L     | 230 | ASN  |
| 1   | M     | 225 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 226 | GLN  |
| 1   | M     | 230 | ASN  |
| 1   | N     | 225 | GLN  |
| 1   | N     | 226 | GLN  |
| 1   | N     | 230 | ASN  |
| 1   | O     | 225 | GLN  |
| 1   | O     | 226 | GLN  |
| 1   | O     | 230 | ASN  |
| 1   | P     | 225 | GLN  |
| 1   | P     | 226 | GLN  |
| 1   | P     | 230 | ASN  |
| 1   | Q     | 225 | GLN  |
| 1   | Q     | 226 | GLN  |
| 1   | Q     | 230 | ASN  |
| 1   | R     | 225 | GLN  |
| 1   | R     | 226 | GLN  |
| 1   | R     | 230 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 9 are monoatomic - leaving 36 for Mogul analysis.

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



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PO4  | E     | 2051 | -    | 4,4,4        | 0.80 | 0        | 6,6,6       | 0.58 | 0        |
| 2   | PO4  | M     | 2131 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | D     | 2041 | -    | 4,4,4        | 1.08 | 0        | 6,6,6       | 0.44 | 0        |
| 4   | THM  | L     | 2122 | -    | 15,18,18     | 2.16 | 3 (20%)  | 16,26,26    | 4.53 | 6 (37%)  |
| 4   | THM  | C     | 2032 | -    | 15,18,18     | 2.41 | 3 (20%)  | 16,26,26    | 4.67 | 6 (37%)  |
| 4   | THM  | O     | 2152 | -    | 15,18,18     | 2.23 | 3 (20%)  | 16,26,26    | 4.20 | 4 (25%)  |
| 4   | THM  | A     | 2012 | -    | 15,18,18     | 2.26 | 3 (20%)  | 16,26,26    | 4.41 | 4 (25%)  |
| 2   | PO4  | B     | 2021 | -    | 4,4,4        | 1.07 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | C     | 2031 | -    | 4,4,4        | 0.84 | 0        | 6,6,6       | 0.59 | 0        |
| 4   | THM  | J     | 2102 | -    | 15,18,18     | 2.56 | 3 (20%)  | 16,26,26    | 4.71 | 5 (31%)  |
| 4   | THM  | D     | 2042 | -    | 15,18,18     | 2.36 | 3 (20%)  | 16,26,26    | 4.20 | 5 (31%)  |
| 4   | THM  | G     | 2072 | -    | 15,18,18     | 2.32 | 3 (20%)  | 16,26,26    | 4.19 | 5 (31%)  |
| 4   | THM  | N     | 2142 | -    | 15,18,18     | 2.30 | 3 (20%)  | 16,26,26    | 4.27 | 6 (37%)  |
| 2   | PO4  | L     | 2121 | -    | 4,4,4        | 0.88 | 0        | 6,6,6       | 0.54 | 0        |
| 4   | THM  | Q     | 2172 | -    | 15,18,18     | 2.15 | 3 (20%)  | 16,26,26    | 4.49 | 5 (31%)  |
| 2   | PO4  | K     | 2111 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.60 | 0        |
| 4   | THM  | H     | 2082 | -    | 15,18,18     | 2.35 | 3 (20%)  | 16,26,26    | 4.39 | 6 (37%)  |
| 2   | PO4  | I     | 2091 | -    | 4,4,4        | 0.97 | 0        | 6,6,6       | 0.61 | 0        |
| 4   | THM  | P     | 2162 | -    | 15,18,18     | 2.25 | 3 (20%)  | 16,26,26    | 4.37 | 6 (37%)  |
| 2   | PO4  | G     | 2071 | -    | 4,4,4        | 0.88 | 0        | 6,6,6       | 0.61 | 0        |
| 2   | PO4  | R     | 2181 | -    | 4,4,4        | 0.88 | 0        | 6,6,6       | 0.67 | 0        |
| 2   | PO4  | F     | 2061 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.78 | 0        |
| 4   | THM  | R     | 2182 | -    | 15,18,18     | 2.34 | 3 (20%)  | 16,26,26    | 4.67 | 5 (31%)  |
| 2   | PO4  | A     | 2011 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.38 | 0        |
| 2   | PO4  | P     | 2161 | -    | 4,4,4        | 0.87 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | J     | 2101 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.40 | 0        |
| 2   | PO4  | N     | 2141 | -    | 4,4,4        | 0.83 | 0        | 6,6,6       | 0.59 | 0        |
| 4   | THM  | B     | 2022 | -    | 15,18,18     | 2.15 | 3 (20%)  | 16,26,26    | 4.62 | 5 (31%)  |
| 4   | THM  | M     | 2132 | -    | 15,18,18     | 2.30 | 3 (20%)  | 16,26,26    | 4.43 | 5 (31%)  |
| 4   | THM  | E     | 2052 | -    | 15,18,18     | 2.17 | 3 (20%)  | 16,26,26    | 4.18 | 4 (25%)  |
| 4   | THM  | F     | 2062 | -    | 15,18,18     | 2.13 | 3 (20%)  | 16,26,26    | 4.42 | 5 (31%)  |
| 4   | THM  | K     | 2112 | -    | 15,18,18     | 2.29 | 3 (20%)  | 16,26,26    | 4.29 | 5 (31%)  |
| 2   | PO4  | Q     | 2171 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.50 | 0        |
| 4   | THM  | I     | 2092 | -    | 15,18,18     | 2.56 | 3 (20%)  | 16,26,26    | 4.23 | 4 (25%)  |
| 2   | PO4  | H     | 2081 | -    | 4,4,4        | 0.93 | 0        | 6,6,6       | 0.79 | 0        |
| 2   | PO4  | O     | 2151 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.49 | 0        |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 4   | THM  | P     | 2162 | -    | 1/1/3/3 | 1/3/18/18 | 0/2/2/2 |
| 4   | THM  | A     | 2012 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | J     | 2102 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | Q     | 2172 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | D     | 2042 | -    | 1/1/3/3 | 1/3/18/18 | 0/2/2/2 |
| 4   | THM  | G     | 2072 | -    | 1/1/3/3 | 0/3/18/18 | 0/2/2/2 |
| 4   | THM  | N     | 2142 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | B     | 2022 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | O     | 2152 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | L     | 2122 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | C     | 2032 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | F     | 2062 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | K     | 2112 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | H     | 2082 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | R     | 2182 | -    | 1/1/3/3 | 0/3/18/18 | 0/2/2/2 |
| 4   | THM  | I     | 2092 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | M     | 2132 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |
| 4   | THM  | E     | 2052 | -    | 1/1/3/3 | 2/3/18/18 | 0/2/2/2 |

All (54) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 4   | J     | 2102 | THM  | C4-N3 | 7.58 | 1.46        | 1.33     |
| 4   | I     | 2092 | THM  | C4-N3 | 7.36 | 1.45        | 1.33     |
| 4   | D     | 2042 | THM  | C4-N3 | 6.95 | 1.45        | 1.33     |
| 4   | R     | 2182 | THM  | C4-N3 | 6.93 | 1.45        | 1.33     |
| 4   | C     | 2032 | THM  | C4-N3 | 6.87 | 1.45        | 1.33     |
| 4   | H     | 2082 | THM  | C4-N3 | 6.83 | 1.44        | 1.33     |
| 4   | G     | 2072 | THM  | C4-N3 | 6.77 | 1.44        | 1.33     |
| 4   | N     | 2142 | THM  | C4-N3 | 6.74 | 1.44        | 1.33     |
| 4   | M     | 2132 | THM  | C4-N3 | 6.74 | 1.44        | 1.33     |
| 4   | P     | 2162 | THM  | C4-N3 | 6.50 | 1.44        | 1.33     |
| 4   | K     | 2112 | THM  | C4-N3 | 6.49 | 1.44        | 1.33     |
| 4   | A     | 2012 | THM  | C4-N3 | 6.48 | 1.44        | 1.33     |
| 4   | L     | 2122 | THM  | C4-N3 | 6.31 | 1.44        | 1.33     |
| 4   | O     | 2152 | THM  | C4-N3 | 6.25 | 1.43        | 1.33     |
| 4   | F     | 2062 | THM  | C4-N3 | 6.21 | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 4   | B     | 2022 | THM  | C4-N3 | 6.19 | 1.43        | 1.33     |
| 4   | E     | 2052 | THM  | C4-N3 | 6.18 | 1.43        | 1.33     |
| 4   | Q     | 2172 | THM  | C4-N3 | 5.95 | 1.43        | 1.33     |
| 4   | I     | 2092 | THM  | C4-C5 | 4.82 | 1.51        | 1.41     |
| 4   | D     | 2042 | THM  | C4-C5 | 4.53 | 1.51        | 1.41     |
| 4   | J     | 2102 | THM  | C4-C5 | 4.38 | 1.50        | 1.41     |
| 4   | O     | 2152 | THM  | C4-C5 | 4.29 | 1.50        | 1.41     |
| 4   | A     | 2012 | THM  | C4-C5 | 4.26 | 1.50        | 1.41     |
| 4   | C     | 2032 | THM  | C4-C5 | 4.25 | 1.50        | 1.41     |
| 4   | E     | 2052 | THM  | C4-C5 | 4.18 | 1.50        | 1.41     |
| 4   | P     | 2162 | THM  | C4-C5 | 4.15 | 1.50        | 1.41     |
| 4   | G     | 2072 | THM  | C4-C5 | 4.07 | 1.50        | 1.41     |
| 4   | R     | 2182 | THM  | C4-C5 | 4.03 | 1.50        | 1.41     |
| 4   | B     | 2022 | THM  | C4-C5 | 4.02 | 1.50        | 1.41     |
| 4   | H     | 2082 | THM  | C4-C5 | 4.01 | 1.50        | 1.41     |
| 4   | J     | 2102 | THM  | C2-N3 | 3.95 | 1.46        | 1.38     |
| 4   | Q     | 2172 | THM  | C4-C5 | 3.95 | 1.49        | 1.41     |
| 4   | C     | 2032 | THM  | C2-N3 | 3.94 | 1.46        | 1.38     |
| 4   | K     | 2112 | THM  | C4-C5 | 3.92 | 1.49        | 1.41     |
| 4   | I     | 2092 | THM  | C2-N3 | 3.86 | 1.45        | 1.38     |
| 4   | K     | 2112 | THM  | C2-N3 | 3.86 | 1.45        | 1.38     |
| 4   | F     | 2062 | THM  | C4-C5 | 3.85 | 1.49        | 1.41     |
| 4   | N     | 2142 | THM  | C4-C5 | 3.82 | 1.49        | 1.41     |
| 4   | M     | 2132 | THM  | C2-N3 | 3.71 | 1.45        | 1.38     |
| 4   | H     | 2082 | THM  | C2-N3 | 3.71 | 1.45        | 1.38     |
| 4   | M     | 2132 | THM  | C4-C5 | 3.64 | 1.49        | 1.41     |
| 4   | N     | 2142 | THM  | C2-N3 | 3.53 | 1.45        | 1.38     |
| 4   | Q     | 2172 | THM  | C2-N3 | 3.50 | 1.45        | 1.38     |
| 4   | R     | 2182 | THM  | C2-N3 | 3.47 | 1.45        | 1.38     |
| 4   | L     | 2122 | THM  | C2-N3 | 3.41 | 1.44        | 1.38     |
| 4   | G     | 2072 | THM  | C2-N3 | 3.39 | 1.44        | 1.38     |
| 4   | L     | 2122 | THM  | C4-C5 | 3.37 | 1.48        | 1.41     |
| 4   | A     | 2012 | THM  | C2-N3 | 3.32 | 1.44        | 1.38     |
| 4   | O     | 2152 | THM  | C2-N3 | 3.31 | 1.44        | 1.38     |
| 4   | B     | 2022 | THM  | C2-N3 | 3.10 | 1.44        | 1.38     |
| 4   | F     | 2062 | THM  | C2-N3 | 3.01 | 1.44        | 1.38     |
| 4   | P     | 2162 | THM  | C2-N3 | 3.01 | 1.44        | 1.38     |
| 4   | D     | 2042 | THM  | C2-N3 | 3.00 | 1.44        | 1.38     |
| 4   | E     | 2052 | THM  | C2-N3 | 2.86 | 1.43        | 1.38     |

All (91) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | R     | 2182 | THM  | C2'-C1'-N1  | 15.17 | 149.27      | 114.27   |
| 4   | J     | 2102 | THM  | C2'-C1'-N1  | 14.97 | 148.80      | 114.27   |
| 4   | A     | 2012 | THM  | C2'-C1'-N1  | 14.71 | 148.19      | 114.27   |
| 4   | L     | 2122 | THM  | C2'-C1'-N1  | 14.60 | 147.95      | 114.27   |
| 4   | B     | 2022 | THM  | C2'-C1'-N1  | 14.60 | 147.94      | 114.27   |
| 4   | C     | 2032 | THM  | C2'-C1'-N1  | 14.56 | 147.86      | 114.27   |
| 4   | M     | 2132 | THM  | C2'-C1'-N1  | 14.54 | 147.82      | 114.27   |
| 4   | Q     | 2172 | THM  | C2'-C1'-N1  | 14.51 | 147.74      | 114.27   |
| 4   | K     | 2112 | THM  | C2'-C1'-N1  | 14.22 | 147.07      | 114.27   |
| 4   | G     | 2072 | THM  | C2'-C1'-N1  | 14.17 | 146.95      | 114.27   |
| 4   | E     | 2052 | THM  | C2'-C1'-N1  | 14.03 | 146.63      | 114.27   |
| 4   | P     | 2162 | THM  | C2'-C1'-N1  | 13.98 | 146.52      | 114.27   |
| 4   | F     | 2062 | THM  | C2'-C1'-N1  | 13.98 | 146.50      | 114.27   |
| 4   | N     | 2142 | THM  | C2'-C1'-N1  | 13.97 | 146.49      | 114.27   |
| 4   | O     | 2152 | THM  | C2'-C1'-N1  | 13.94 | 146.42      | 114.27   |
| 4   | H     | 2082 | THM  | C2'-C1'-N1  | 13.92 | 146.38      | 114.27   |
| 4   | I     | 2092 | THM  | C2'-C1'-N1  | 13.58 | 145.60      | 114.27   |
| 4   | D     | 2042 | THM  | C2'-C1'-N1  | 13.49 | 145.39      | 114.27   |
| 4   | C     | 2032 | THM  | C4-N3-C2    | 8.71  | 122.49      | 115.14   |
| 4   | J     | 2102 | THM  | C4-N3-C2    | 8.33  | 122.17      | 115.14   |
| 4   | H     | 2082 | THM  | C4-N3-C2    | 8.14  | 122.01      | 115.14   |
| 4   | B     | 2022 | THM  | C4-N3-C2    | 8.01  | 121.91      | 115.14   |
| 4   | F     | 2062 | THM  | C4-N3-C2    | 7.94  | 121.85      | 115.14   |
| 4   | Q     | 2172 | THM  | C4-N3-C2    | 7.72  | 121.66      | 115.14   |
| 4   | I     | 2092 | THM  | C4-N3-C2    | 7.59  | 121.55      | 115.14   |
| 4   | D     | 2042 | THM  | C4-N3-C2    | 7.51  | 121.48      | 115.14   |
| 4   | P     | 2162 | THM  | C4-N3-C2    | 7.49  | 121.47      | 115.14   |
| 4   | R     | 2182 | THM  | C4-N3-C2    | 7.27  | 121.28      | 115.14   |
| 4   | N     | 2142 | THM  | C4-N3-C2    | 7.17  | 121.20      | 115.14   |
| 4   | L     | 2122 | THM  | C4-N3-C2    | 6.79  | 120.87      | 115.14   |
| 4   | E     | 2052 | THM  | C4-N3-C2    | 6.78  | 120.87      | 115.14   |
| 4   | M     | 2132 | THM  | C4-N3-C2    | 6.76  | 120.85      | 115.14   |
| 4   | O     | 2152 | THM  | C4-N3-C2    | 6.66  | 120.77      | 115.14   |
| 4   | K     | 2112 | THM  | C4-N3-C2    | 6.63  | 120.74      | 115.14   |
| 4   | A     | 2012 | THM  | C4-N3-C2    | 6.60  | 120.72      | 115.14   |
| 4   | J     | 2102 | THM  | C5-C6-N1    | 5.54  | 128.16      | 122.19   |
| 4   | G     | 2072 | THM  | C4-N3-C2    | 5.36  | 119.67      | 115.14   |
| 4   | R     | 2182 | THM  | O4'-C1'-C2' | -5.09 | 96.64       | 106.25   |
| 4   | B     | 2022 | THM  | C5-C6-N1    | 5.09  | 127.68      | 122.19   |
| 4   | F     | 2062 | THM  | C5-C6-N1    | 5.01  | 127.60      | 122.19   |
| 4   | G     | 2072 | THM  | O4'-C1'-C2' | -4.80 | 97.19       | 106.25   |
| 4   | L     | 2122 | THM  | C5-C6-N1    | 4.76  | 127.33      | 122.19   |
| 4   | B     | 2022 | THM  | O4'-C1'-C2' | -4.70 | 97.38       | 106.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | C     | 2032 | THM  | C5-C6-N1    | 4.67  | 127.23      | 122.19   |
| 4   | M     | 2132 | THM  | O4'-C1'-C2' | -4.63 | 97.50       | 106.25   |
| 4   | R     | 2182 | THM  | C5-C6-N1    | 4.62  | 127.18      | 122.19   |
| 4   | P     | 2162 | THM  | C5-C6-N1    | 4.57  | 127.12      | 122.19   |
| 4   | A     | 2012 | THM  | O4'-C1'-C2' | -4.48 | 97.79       | 106.25   |
| 4   | A     | 2012 | THM  | C5-C6-N1    | 4.35  | 126.89      | 122.19   |
| 4   | Q     | 2172 | THM  | O4'-C1'-C2' | -4.35 | 98.04       | 106.25   |
| 4   | I     | 2092 | THM  | C5-C6-N1    | 4.34  | 126.87      | 122.19   |
| 4   | H     | 2082 | THM  | C5-C6-N1    | 4.32  | 126.85      | 122.19   |
| 4   | N     | 2142 | THM  | C5-C6-N1    | 4.30  | 126.83      | 122.19   |
| 4   | Q     | 2172 | THM  | C5-C6-N1    | 4.18  | 126.70      | 122.19   |
| 4   | M     | 2132 | THM  | C5-C6-N1    | 4.15  | 126.67      | 122.19   |
| 4   | K     | 2112 | THM  | O4'-C1'-C2' | -4.02 | 98.65       | 106.25   |
| 4   | C     | 2032 | THM  | O4'-C1'-C2' | -4.00 | 98.69       | 106.25   |
| 4   | D     | 2042 | THM  | C5-C6-N1    | 3.99  | 126.49      | 122.19   |
| 4   | E     | 2052 | THM  | C5-C6-N1    | 3.96  | 126.47      | 122.19   |
| 4   | J     | 2102 | THM  | O4'-C1'-C2' | -3.95 | 98.79       | 106.25   |
| 4   | O     | 2152 | THM  | O4'-C1'-C2' | -3.87 | 98.93       | 106.25   |
| 4   | P     | 2162 | THM  | O4'-C1'-C2' | -3.85 | 98.99       | 106.25   |
| 4   | L     | 2122 | THM  | O4'-C1'-C2' | -3.74 | 99.18       | 106.25   |
| 4   | I     | 2092 | THM  | O4'-C1'-C2' | -3.71 | 99.24       | 106.25   |
| 4   | K     | 2112 | THM  | C5-C6-N1    | 3.69  | 126.17      | 122.19   |
| 4   | O     | 2152 | THM  | C5-C6-N1    | 3.55  | 126.02      | 122.19   |
| 4   | L     | 2122 | THM  | O4'-C4'-C5' | -3.54 | 101.55      | 109.21   |
| 4   | D     | 2042 | THM  | O4'-C1'-C2' | -3.44 | 99.76       | 106.25   |
| 4   | H     | 2082 | THM  | O4'-C1'-C2' | -3.39 | 99.85       | 106.25   |
| 4   | G     | 2072 | THM  | C5-C6-N1    | 3.14  | 125.58      | 122.19   |
| 4   | F     | 2062 | THM  | O4'-C1'-C2' | -3.07 | 100.44      | 106.25   |
| 4   | L     | 2122 | THM  | C5'-C4'-C3' | 3.03  | 122.47      | 114.81   |
| 4   | N     | 2142 | THM  | O4'-C1'-C2' | -3.00 | 100.58      | 106.25   |
| 4   | E     | 2052 | THM  | O4'-C1'-C2' | -2.69 | 101.17      | 106.25   |
| 4   | C     | 2032 | THM  | O4'-C4'-C5' | -2.61 | 103.57      | 109.21   |
| 4   | K     | 2112 | THM  | C6-N1-C1'   | 2.35  | 124.52      | 119.24   |
| 4   | C     | 2032 | THM  | C5'-C4'-C3' | 2.34  | 120.72      | 114.81   |
| 4   | M     | 2132 | THM  | C5M-C5-C4   | -2.31 | 117.24      | 121.37   |
| 4   | Q     | 2172 | THM  | O3'-C3'-C2' | 2.24  | 118.92      | 110.90   |
| 4   | D     | 2042 | THM  | C6-N1-C1'   | 2.21  | 124.19      | 119.24   |
| 4   | R     | 2182 | THM  | C5M-C5-C4   | -2.18 | 117.47      | 121.37   |
| 4   | H     | 2082 | THM  | C5M-C5-C4   | -2.17 | 117.49      | 121.37   |
| 4   | B     | 2022 | THM  | O3'-C3'-C2' | 2.15  | 118.60      | 110.90   |
| 4   | J     | 2102 | THM  | C5'-C4'-C3' | 2.14  | 120.22      | 114.81   |
| 4   | N     | 2142 | THM  | C5M-C5-C4   | -2.11 | 117.59      | 121.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | N     | 2142 | THM  | C5'-C4'-C3' | 2.07  | 120.04      | 114.81   |
| 4   | P     | 2162 | THM  | C5'-C4'-C3' | 2.06  | 120.03      | 114.81   |
| 4   | P     | 2162 | THM  | C6-N1-C1'   | 2.06  | 123.86      | 119.24   |
| 4   | F     | 2062 | THM  | C5'-C4'-C3' | 2.04  | 119.96      | 114.81   |
| 4   | H     | 2082 | THM  | C6-N1-C1'   | 2.04  | 123.81      | 119.24   |
| 4   | G     | 2072 | THM  | C5M-C5-C4   | -2.03 | 117.74      | 121.37   |

All (18) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 4   | B     | 2022 | THM  | C1'  |
| 4   | L     | 2122 | THM  | C1'  |
| 4   | C     | 2032 | THM  | C1'  |
| 4   | A     | 2012 | THM  | C1'  |
| 4   | J     | 2102 | THM  | C1'  |
| 4   | D     | 2042 | THM  | C1'  |
| 4   | G     | 2072 | THM  | C1'  |
| 4   | N     | 2142 | THM  | C1'  |
| 4   | H     | 2082 | THM  | C1'  |
| 4   | O     | 2152 | THM  | C1'  |
| 4   | P     | 2162 | THM  | C1'  |
| 4   | Q     | 2172 | THM  | C1'  |
| 4   | R     | 2182 | THM  | C1'  |
| 4   | I     | 2092 | THM  | C1'  |
| 4   | M     | 2132 | THM  | C1'  |
| 4   | E     | 2052 | THM  | C1'  |
| 4   | F     | 2062 | THM  | C1'  |
| 4   | K     | 2112 | THM  | C1'  |

All (30) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | Q     | 2172 | THM  | C3'-C4'-C5'-O5' |
| 4   | E     | 2052 | THM  | C3'-C4'-C5'-O5' |
| 4   | B     | 2022 | THM  | O4'-C4'-C5'-O5' |
| 4   | Q     | 2172 | THM  | O4'-C4'-C5'-O5' |
| 4   | E     | 2052 | THM  | O4'-C4'-C5'-O5' |
| 4   | B     | 2022 | THM  | C3'-C4'-C5'-O5' |
| 4   | K     | 2112 | THM  | C3'-C4'-C5'-O5' |
| 4   | L     | 2122 | THM  | C3'-C4'-C5'-O5' |
| 4   | A     | 2012 | THM  | C3'-C4'-C5'-O5' |
| 4   | N     | 2142 | THM  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | I     | 2092 | THM  | C3'-C4'-C5'-O5' |
| 4   | A     | 2012 | THM  | O4'-C4'-C5'-O5' |
| 4   | K     | 2112 | THM  | O4'-C4'-C5'-O5' |
| 4   | N     | 2142 | THM  | O4'-C4'-C5'-O5' |
| 4   | H     | 2082 | THM  | O4'-C4'-C5'-O5' |
| 4   | H     | 2082 | THM  | C3'-C4'-C5'-O5' |
| 4   | L     | 2122 | THM  | O4'-C4'-C5'-O5' |
| 4   | I     | 2092 | THM  | O4'-C4'-C5'-O5' |
| 4   | O     | 2152 | THM  | C3'-C4'-C5'-O5' |
| 4   | O     | 2152 | THM  | O4'-C4'-C5'-O5' |
| 4   | J     | 2102 | THM  | C3'-C4'-C5'-O5' |
| 4   | F     | 2062 | THM  | O4'-C4'-C5'-O5' |
| 4   | J     | 2102 | THM  | O4'-C4'-C5'-O5' |
| 4   | C     | 2032 | THM  | O4'-C4'-C5'-O5' |
| 4   | F     | 2062 | THM  | C3'-C4'-C5'-O5' |
| 4   | C     | 2032 | THM  | C3'-C4'-C5'-O5' |
| 4   | M     | 2132 | THM  | O4'-C4'-C5'-O5' |
| 4   | M     | 2132 | THM  | C3'-C4'-C5'-O5' |
| 4   | D     | 2042 | THM  | O4'-C4'-C5'-O5' |
| 4   | P     | 2162 | THM  | O4'-C4'-C5'-O5' |

There are no ring outliers.

23 monomers are involved in 33 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | E     | 2051 | PO4  | 2       | 0            |
| 2   | M     | 2131 | PO4  | 1       | 0            |
| 2   | D     | 2041 | PO4  | 3       | 0            |
| 4   | L     | 2122 | THM  | 1       | 0            |
| 4   | C     | 2032 | THM  | 2       | 0            |
| 4   | O     | 2152 | THM  | 1       | 0            |
| 2   | B     | 2021 | PO4  | 1       | 0            |
| 2   | C     | 2031 | PO4  | 1       | 0            |
| 4   | J     | 2102 | THM  | 1       | 0            |
| 4   | N     | 2142 | THM  | 1       | 0            |
| 4   | Q     | 2172 | THM  | 1       | 0            |
| 2   | K     | 2111 | PO4  | 3       | 0            |
| 2   | G     | 2071 | PO4  | 1       | 0            |
| 2   | R     | 2181 | PO4  | 1       | 0            |
| 2   | F     | 2061 | PO4  | 2       | 0            |
| 2   | A     | 2011 | PO4  | 1       | 0            |
| 2   | J     | 2101 | PO4  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | N     | 2141 | PO4  | 1       | 0            |
| 4   | M     | 2132 | THM  | 1       | 0            |
| 4   | E     | 2052 | THM  | 1       | 0            |
| 4   | F     | 2062 | THM  | 2       | 0            |
| 2   | H     | 2081 | PO4  | 1       | 0            |
| 2   | O     | 2151 | PO4  | 3       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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     | 250/253 (98%)   | -0.40  | 7 (2%)   | 53 | 30 | 7, 22, 47, 73         | 0     |
| 1   | B     | 250/253 (98%)   | -0.53  | 4 (1%)   | 72 | 51 | 7, 22, 47, 73         | 0     |
| 1   | C     | 250/253 (98%)   | -0.46  | 4 (1%)   | 72 | 51 | 7, 22, 47, 73         | 0     |
| 1   | D     | 250/253 (98%)   | -0.46  | 6 (2%)   | 59 | 37 | 7, 22, 47, 73         | 0     |
| 1   | E     | 250/253 (98%)   | -0.38  | 8 (3%)   | 47 | 25 | 7, 22, 47, 73         | 0     |
| 1   | F     | 250/253 (98%)   | -0.32  | 9 (3%)   | 42 | 22 | 7, 22, 47, 73         | 0     |
| 1   | G     | 250/253 (98%)   | -0.47  | 6 (2%)   | 59 | 37 | 7, 22, 47, 73         | 0     |
| 1   | H     | 250/253 (98%)   | -0.47  | 7 (2%)   | 53 | 30 | 7, 22, 47, 73         | 0     |
| 1   | I     | 250/253 (98%)   | -0.41  | 4 (1%)   | 72 | 51 | 7, 22, 47, 73         | 0     |
| 1   | J     | 250/253 (98%)   | -0.33  | 6 (2%)   | 59 | 37 | 7, 22, 47, 73         | 0     |
| 1   | K     | 250/253 (98%)   | -0.56  | 4 (1%)   | 72 | 51 | 7, 22, 47, 73         | 0     |
| 1   | L     | 250/253 (98%)   | -0.49  | 5 (2%)   | 65 | 44 | 7, 22, 47, 73         | 0     |
| 1   | M     | 250/253 (98%)   | -0.35  | 8 (3%)   | 47 | 25 | 7, 22, 47, 73         | 0     |
| 1   | N     | 250/253 (98%)   | -0.35  | 6 (2%)   | 59 | 37 | 7, 22, 47, 73         | 0     |
| 1   | O     | 250/253 (98%)   | -0.29  | 6 (2%)   | 59 | 37 | 7, 22, 47, 73         | 0     |
| 1   | P     | 250/253 (98%)   | -0.22  | 10 (4%)  | 38 | 19 | 7, 22, 47, 73         | 0     |
| 1   | Q     | 250/253 (98%)   | -0.40  | 1 (0%)   | 92 | 84 | 7, 22, 47, 73         | 0     |
| 1   | R     | 250/253 (98%)   | -0.41  | 3 (1%)   | 79 | 61 | 7, 22, 47, 73         | 0     |
| All | All   | 4500/4554 (98%) | -0.41  | 104 (2%) | 60 | 39 | 7, 22, 48, 73         | 0     |

All (104) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 229 | PRO  | 7.4  |
| 1   | M     | 238 | GLU  | 5.6  |
| 1   | H     | 236 | GLN  | 5.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 239 | SER  | 5.2  |
| 1   | N     | 231 | ALA  | 5.1  |
| 1   | D     | 236 | GLN  | 4.9  |
| 1   | M     | 235 | LYS  | 4.9  |
| 1   | A     | 239 | SER  | 4.8  |
| 1   | E     | 231 | ALA  | 4.8  |
| 1   | H     | 233 | THR  | 4.8  |
| 1   | M     | 234 | MET  | 4.4  |
| 1   | G     | 237 | THR  | 4.3  |
| 1   | M     | 233 | THR  | 4.3  |
| 1   | P     | 237 | THR  | 4.2  |
| 1   | L     | 231 | ALA  | 4.1  |
| 1   | D     | 234 | MET  | 4.0  |
| 1   | O     | 230 | ASN  | 4.0  |
| 1   | D     | 233 | THR  | 4.0  |
| 1   | C     | 230 | ASN  | 4.0  |
| 1   | P     | 234 | MET  | 3.9  |
| 1   | H     | 235 | LYS  | 3.8  |
| 1   | P     | 231 | ALA  | 3.8  |
| 1   | F     | 229 | PRO  | 3.8  |
| 1   | H     | 232 | GLU  | 3.7  |
| 1   | G     | 235 | LYS  | 3.7  |
| 1   | B     | 234 | MET  | 3.5  |
| 1   | H     | 237 | THR  | 3.5  |
| 1   | A     | 235 | LYS  | 3.5  |
| 1   | E     | 234 | MET  | 3.5  |
| 1   | M     | 237 | THR  | 3.4  |
| 1   | O     | 231 | ALA  | 3.4  |
| 1   | A     | 238 | GLU  | 3.4  |
| 1   | I     | 230 | ASN  | 3.3  |
| 1   | G     | 236 | GLN  | 3.3  |
| 1   | A     | 237 | THR  | 3.3  |
| 1   | M     | 236 | GLN  | 3.3  |
| 1   | L     | 229 | PRO  | 3.3  |
| 1   | J     | 230 | ASN  | 3.2  |
| 1   | B     | 233 | THR  | 3.2  |
| 1   | I     | 229 | PRO  | 3.2  |
| 1   | H     | 238 | GLU  | 3.2  |
| 1   | O     | 229 | PRO  | 3.2  |
| 1   | I     | 233 | THR  | 3.1  |
| 1   | G     | 234 | MET  | 3.1  |
| 1   | N     | 228 | ILE  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 237 | THR  | 3.1  |
| 1   | H     | 234 | MET  | 3.1  |
| 1   | E     | 232 | GLU  | 3.0  |
| 1   | A     | 234 | MET  | 3.0  |
| 1   | Q     | 233 | THR  | 3.0  |
| 1   | F     | 231 | ALA  | 3.0  |
| 1   | B     | 235 | LYS  | 3.0  |
| 1   | K     | 231 | ALA  | 3.0  |
| 1   | F     | 230 | ASN  | 3.0  |
| 1   | N     | 234 | MET  | 2.9  |
| 1   | A     | 233 | THR  | 2.9  |
| 1   | P     | 226 | GLN  | 2.9  |
| 1   | C     | 235 | LYS  | 2.9  |
| 1   | O     | 235 | LYS  | 2.8  |
| 1   | L     | 232 | GLU  | 2.8  |
| 1   | P     | 233 | THR  | 2.8  |
| 1   | N     | 226 | GLN  | 2.7  |
| 1   | C     | 231 | ALA  | 2.7  |
| 1   | R     | 235 | LYS  | 2.7  |
| 1   | F     | 235 | LYS  | 2.6  |
| 1   | J     | 225 | GLN  | 2.6  |
| 1   | F     | 238 | GLU  | 2.6  |
| 1   | P     | 235 | LYS  | 2.6  |
| 1   | G     | 238 | GLU  | 2.6  |
| 1   | E     | 230 | ASN  | 2.5  |
| 1   | J     | 233 | THR  | 2.5  |
| 1   | O     | 234 | MET  | 2.5  |
| 1   | L     | 237 | THR  | 2.5  |
| 1   | K     | 235 | LYS  | 2.5  |
| 1   | N     | 230 | ASN  | 2.5  |
| 1   | I     | 232 | GLU  | 2.4  |
| 1   | F     | 237 | THR  | 2.3  |
| 1   | B     | 231 | ALA  | 2.3  |
| 1   | E     | 239 | SER  | 2.3  |
| 1   | J     | 235 | LYS  | 2.3  |
| 1   | P     | 232 | GLU  | 2.3  |
| 1   | P     | 229 | PRO  | 2.3  |
| 1   | F     | 233 | THR  | 2.3  |
| 1   | G     | 231 | ALA  | 2.3  |
| 1   | D     | 238 | GLU  | 2.3  |
| 1   | R     | 237 | THR  | 2.3  |
| 1   | F     | 236 | GLN  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 226 | GLN  | 2.2  |
| 1   | J     | 236 | GLN  | 2.2  |
| 1   | F     | 234 | MET  | 2.2  |
| 1   | M     | 230 | ASN  | 2.2  |
| 1   | E     | 236 | GLN  | 2.2  |
| 1   | O     | 236 | GLN  | 2.2  |
| 1   | K     | 148 | GLY  | 2.2  |
| 1   | P     | 230 | ASN  | 2.2  |
| 1   | C     | 234 | MET  | 2.2  |
| 1   | K     | 39  | ASP  | 2.2  |
| 1   | L     | 230 | ASN  | 2.2  |
| 1   | E     | 237 | THR  | 2.1  |
| 1   | R     | 234 | MET  | 2.1  |
| 1   | A     | 236 | GLN  | 2.1  |
| 1   | P     | 4   | SER  | 2.1  |
| 1   | E     | 233 | THR  | 2.1  |
| 1   | D     | 235 | LYS  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | P     | 2161 | 5/5   | 0.80 | 0.34 | 72,73,73,73                 | 0     |
| 2   | PO4  | H     | 2081 | 5/5   | 0.82 | 0.33 | 76,76,77,77                 | 0     |
| 3   | K    | Q     | 3008 | 1/1   | 0.83 | 0.14 | 70,70,70,70                 | 0     |
| 2   | PO4  | E     | 2051 | 5/5   | 0.87 | 0.27 | 73,73,75,75                 | 0     |
| 3   | K    | F     | 3003 | 1/1   | 0.89 | 0.07 | 54,54,54,54                 | 0     |
| 3   | K    | O     | 3009 | 1/1   | 0.89 | 0.09 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | THM  | C     | 2032 | 17/17 | 0.90 | 0.24 | 45,47,48,48                 | 0     |
| 4   | THM  | P     | 2162 | 17/17 | 0.90 | 0.25 | 43,45,46,46                 | 0     |
| 2   | PO4  | R     | 2181 | 5/5   | 0.90 | 0.24 | 69,70,70,71                 | 0     |
| 4   | THM  | J     | 2102 | 17/17 | 0.91 | 0.24 | 37,43,44,45                 | 0     |
| 2   | PO4  | N     | 2141 | 5/5   | 0.91 | 0.22 | 63,63,64,64                 | 0     |
| 2   | PO4  | C     | 2031 | 5/5   | 0.91 | 0.27 | 74,74,74,75                 | 0     |
| 4   | THM  | I     | 2092 | 17/17 | 0.92 | 0.22 | 45,46,48,48                 | 0     |
| 2   | PO4  | J     | 2101 | 5/5   | 0.92 | 0.26 | 59,59,60,60                 | 0     |
| 2   | PO4  | G     | 2071 | 5/5   | 0.92 | 0.26 | 77,77,77,77                 | 0     |
| 4   | THM  | Q     | 2172 | 17/17 | 0.92 | 0.26 | 42,45,46,46                 | 0     |
| 3   | K    | K     | 3006 | 1/1   | 0.93 | 0.05 | 28,28,28,28                 | 0     |
| 4   | THM  | O     | 2152 | 17/17 | 0.93 | 0.26 | 44,47,48,50                 | 0     |
| 3   | K    | C     | 3002 | 1/1   | 0.93 | 0.10 | 37,37,37,37                 | 0     |
| 4   | THM  | M     | 2132 | 17/17 | 0.93 | 0.21 | 37,39,40,42                 | 0     |
| 2   | PO4  | M     | 2131 | 5/5   | 0.93 | 0.29 | 77,77,77,78                 | 0     |
| 4   | THM  | N     | 2142 | 17/17 | 0.93 | 0.22 | 53,54,54,55                 | 0     |
| 2   | PO4  | O     | 2151 | 5/5   | 0.93 | 0.16 | 61,62,62,62                 | 0     |
| 4   | THM  | F     | 2062 | 17/17 | 0.94 | 0.22 | 43,44,45,45                 | 0     |
| 2   | PO4  | Q     | 2171 | 5/5   | 0.94 | 0.22 | 67,67,67,68                 | 0     |
| 4   | THM  | L     | 2122 | 17/17 | 0.94 | 0.22 | 35,41,42,43                 | 0     |
| 3   | K    | M     | 3007 | 1/1   | 0.94 | 0.08 | 50,50,50,50                 | 0     |
| 4   | THM  | H     | 2082 | 17/17 | 0.94 | 0.20 | 40,42,44,45                 | 0     |
| 4   | THM  | A     | 2012 | 17/17 | 0.95 | 0.23 | 41,42,43,45                 | 0     |
| 4   | THM  | E     | 2052 | 17/17 | 0.95 | 0.23 | 38,40,44,45                 | 0     |
| 4   | THM  | D     | 2042 | 17/17 | 0.95 | 0.16 | 44,46,49,51                 | 0     |
| 4   | THM  | K     | 2112 | 17/17 | 0.95 | 0.21 | 36,43,44,45                 | 0     |
| 3   | K    | I     | 3005 | 1/1   | 0.95 | 0.08 | 49,49,49,49                 | 0     |
| 4   | THM  | G     | 2072 | 17/17 | 0.95 | 0.19 | 44,47,51,53                 | 0     |
| 2   | PO4  | I     | 2091 | 5/5   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 3   | K    | G     | 3004 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 4   | THM  | R     | 2182 | 17/17 | 0.96 | 0.23 | 37,40,41,42                 | 0     |
| 2   | PO4  | L     | 2121 | 5/5   | 0.96 | 0.14 | 61,61,61,61                 | 0     |
| 4   | THM  | B     | 2022 | 17/17 | 0.96 | 0.16 | 42,44,45,45                 | 0     |
| 2   | PO4  | F     | 2061 | 5/5   | 0.96 | 0.14 | 51,51,51,51                 | 0     |
| 3   | K    | A     | 3001 | 1/1   | 0.97 | 0.05 | 40,40,40,40                 | 0     |
| 2   | PO4  | B     | 2021 | 5/5   | 0.97 | 0.13 | 58,59,59,59                 | 0     |
| 2   | PO4  | K     | 2111 | 5/5   | 0.97 | 0.15 | 65,65,65,65                 | 0     |
| 2   | PO4  | D     | 2041 | 5/5   | 0.97 | 0.12 | 55,55,56,56                 | 0     |
| 2   | PO4  | A     | 2011 | 5/5   | 0.97 | 0.13 | 69,69,69,70                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.