



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:17 PM UTC

PDB ID : 2WQT / pdb\_00002wqt  
Title : Dodecahedral assembly of MhpD  
Authors : Montgomery, M.G.; Wood, S.P.  
Deposited on : 2009-08-27  
Resolution : 2.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

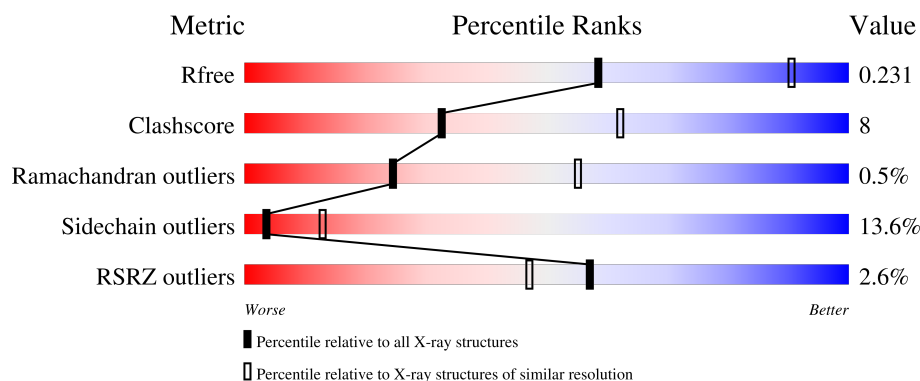
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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     | 270    | <div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• •</div> </div> </div>  |
| 1   | B     | 270    | <div> <div>2%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• •</div> </div> </div>  |
| 1   | C     | 270    | <div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>5% •</div> </div> </div> |
| 1   | D     | 270    | <div> <div>3%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>  |
| 1   | E     | 270    | <div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>5% •</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 270    |                  |
| 1   | G     | 270    |                  |
| 1   | H     | 270    |                  |
| 1   | I     | 270    |                  |
| 1   | J     | 270    |                  |
| 1   | K     | 270    |                  |
| 1   | L     | 270    |                  |
| 1   | M     | 270    |                  |
| 1   | N     | 270    |                  |
| 1   | O     | 270    |                  |
| 1   | P     | 270    |                  |
| 1   | Q     | 270    |                  |
| 1   | R     | 270    |                  |
| 1   | S     | 270    |                  |
| 1   | T     | 270    |                  |

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  | F     | 1262 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40183 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 2-KETO-4-PENTENOATE HYDRATASE.

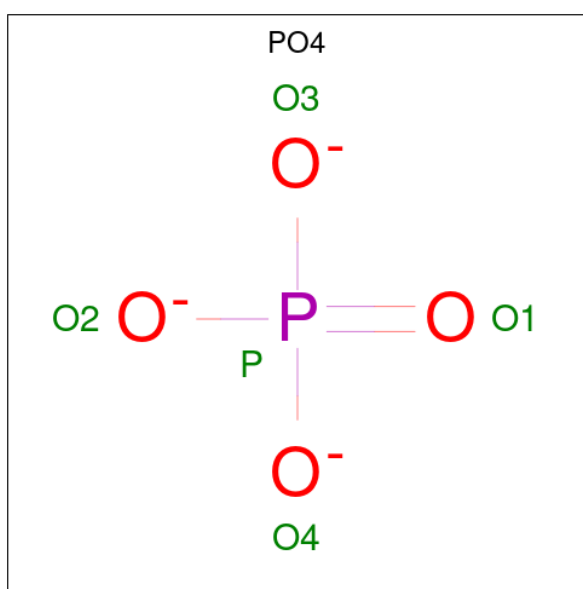
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | B     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | C     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | D     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | E     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | F     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | G     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | H     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | I     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | J     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | K     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | L     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | M     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | N     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | O     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | P     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | Q     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | R     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | S     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |
| 1   | T     | 262      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1986  | 1242 | 357 | 377 | 10 |         |         |       |

- Molecule 2 is PHOSPHATE ION (CCD ID: 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   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 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 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | D     | 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   | F     | 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   | G     | 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   | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | I     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | K     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | K     | 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   | 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 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | O     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | P     | 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   | Q     | 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 |         |         |
| 2   | S     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | T     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | F     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | G     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | I     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | K     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | L     | 2        | Total | Na | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | M     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 3   | N     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 3   | O     | 2        | Total<br>2 | Na<br>2 | 0       | 0       |
| 3   | P     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 3   | Q     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 3   | R     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 3   | S     | 2        | Total<br>2 | Na<br>2 | 0       | 0       |
| 3   | T     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 4   | A     | 2        | Total<br>2 | K<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 4   | C     | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 4   | D     | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 4   | E     | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 4   | F     | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 4   | G     | 2        | Total<br>2 | K<br>2 | 0       | 0       |
| 4   | I     | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 4   | K     | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 4   | L     | 2        | Total<br>2 | K<br>2 | 0       | 0       |
| 4   | N     | 1        | Total<br>1 | K<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4   | P     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | Q     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | R     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | S     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | T     | 1        | Total K<br>1 1 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5   | A     | 10       | Total O<br>10 10 | 0       | 0       |
| 5   | B     | 9        | Total O<br>9 9   | 0       | 0       |
| 5   | C     | 13       | Total O<br>13 13 | 0       | 0       |
| 5   | D     | 12       | Total O<br>12 12 | 0       | 0       |
| 5   | E     | 10       | Total O<br>10 10 | 0       | 0       |
| 5   | F     | 14       | Total O<br>14 14 | 0       | 0       |
| 5   | G     | 11       | Total O<br>11 11 | 0       | 0       |
| 5   | H     | 12       | Total O<br>12 12 | 0       | 0       |
| 5   | I     | 11       | Total O<br>11 11 | 0       | 0       |
| 5   | J     | 13       | Total O<br>13 13 | 0       | 0       |
| 5   | K     | 14       | Total O<br>14 14 | 0       | 0       |
| 5   | L     | 17       | Total O<br>17 17 | 0       | 0       |
| 5   | M     | 10       | Total O<br>10 10 | 0       | 0       |
| 5   | N     | 11       | Total O<br>11 11 | 0       | 0       |

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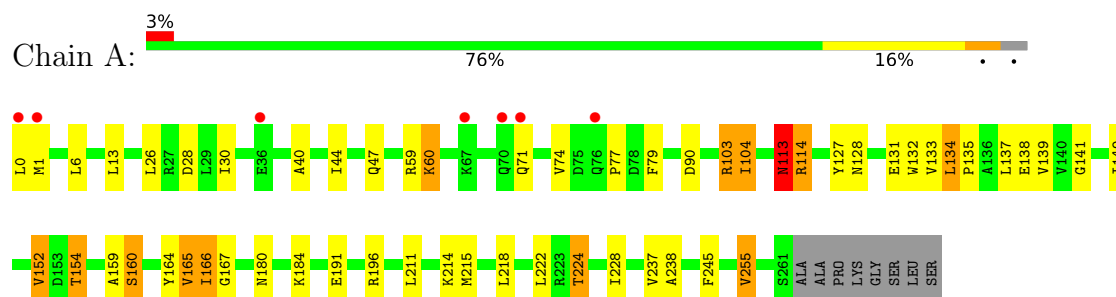
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | O     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 5   | P     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 5   | Q     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 5   | R     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 5   | S     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 5   | T     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |

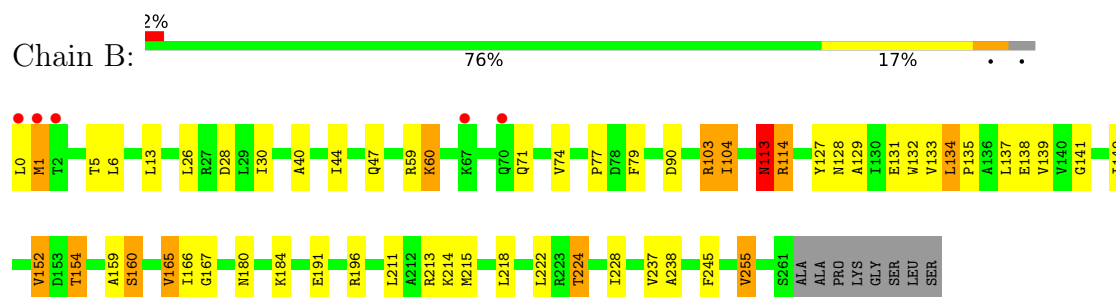
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

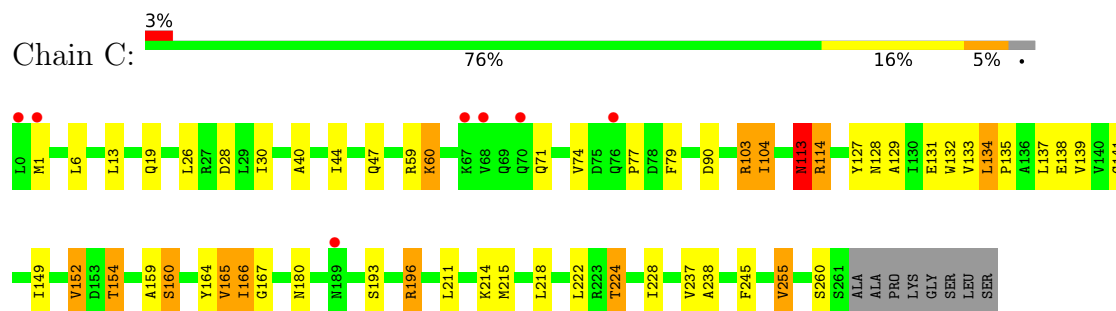
#### • Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



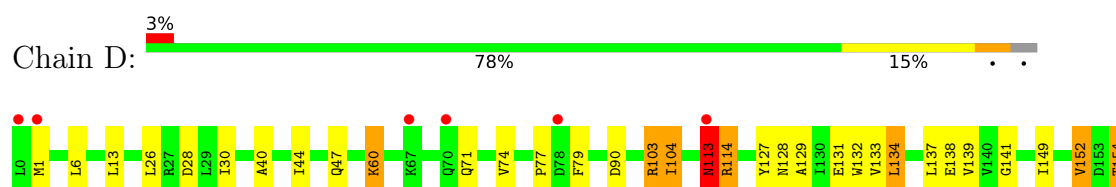
#### • Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



#### • Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

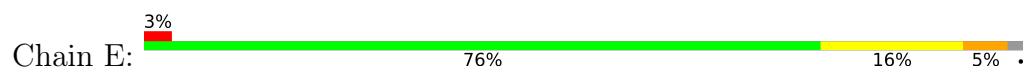


#### • Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

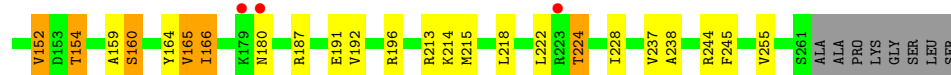
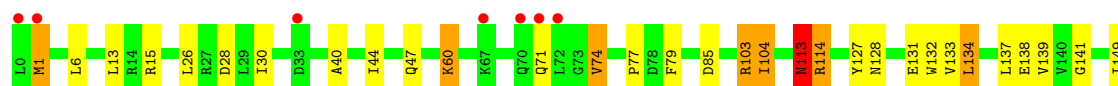
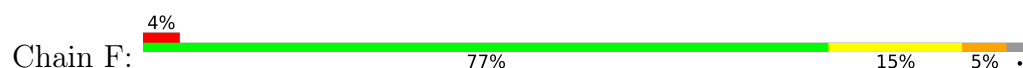




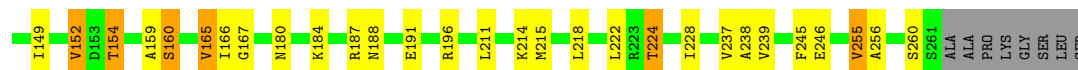
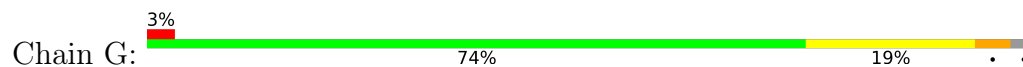
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



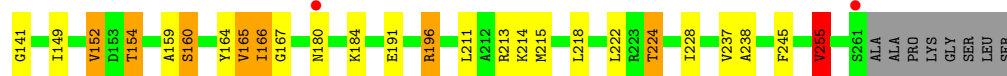
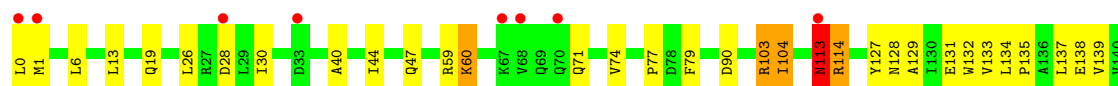
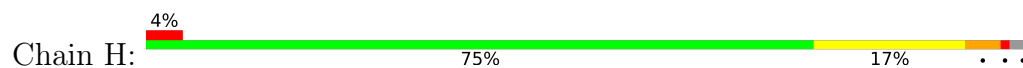
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

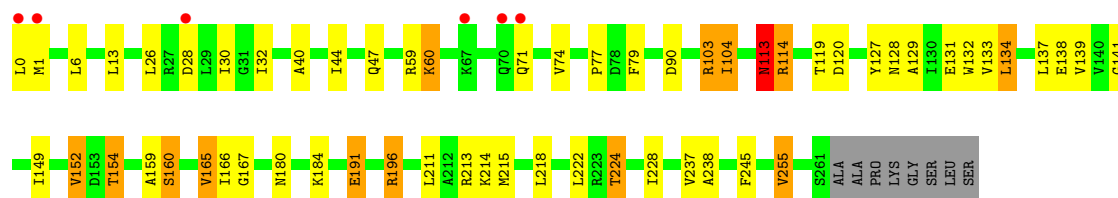


• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

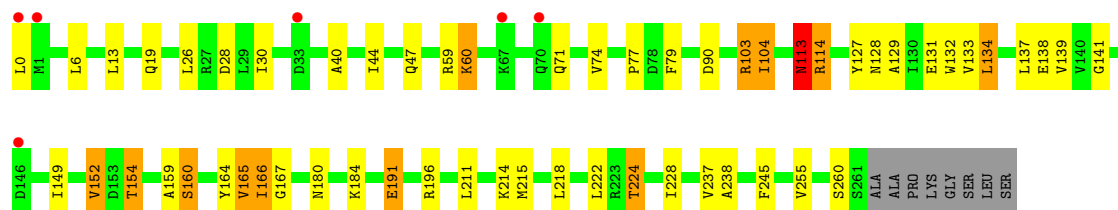
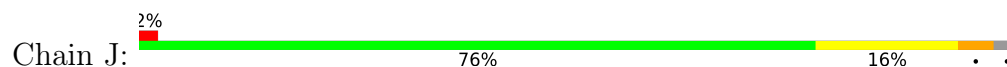


• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

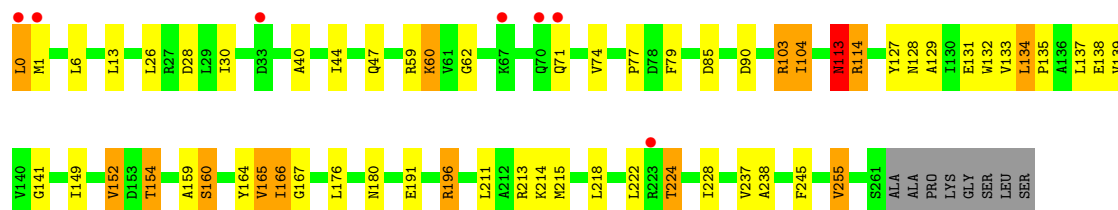
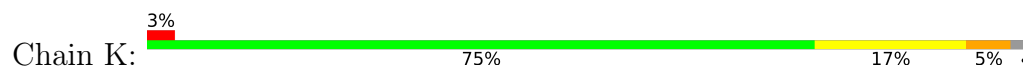




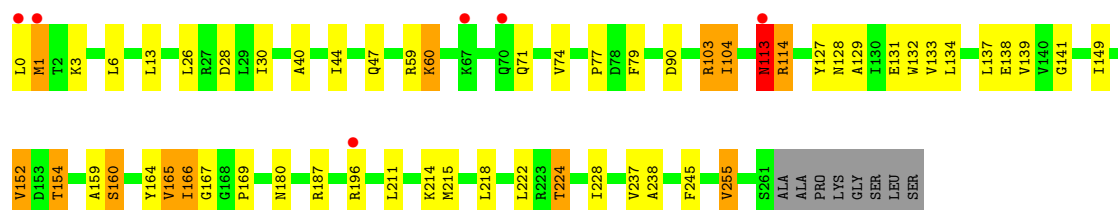
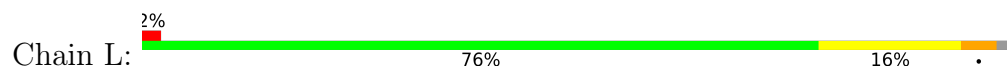
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



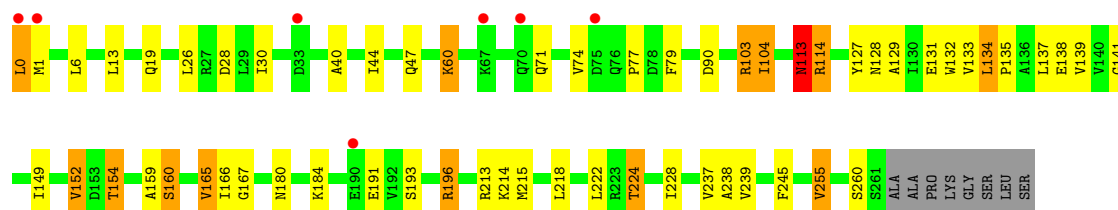
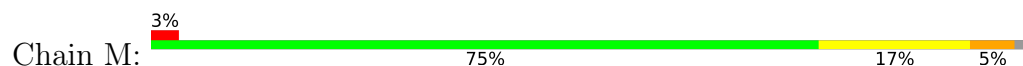
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



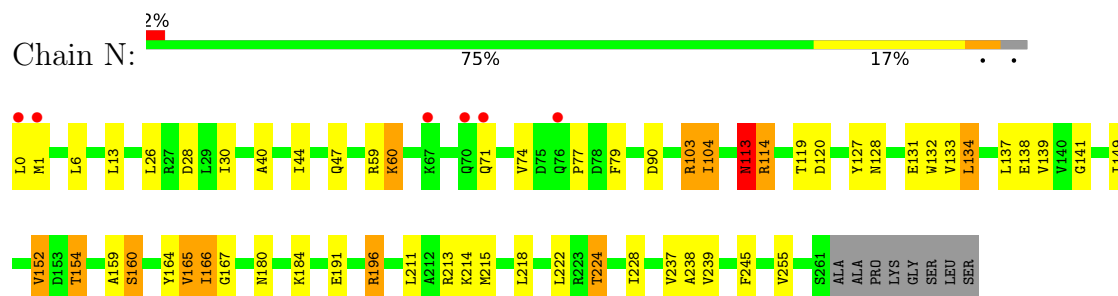
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



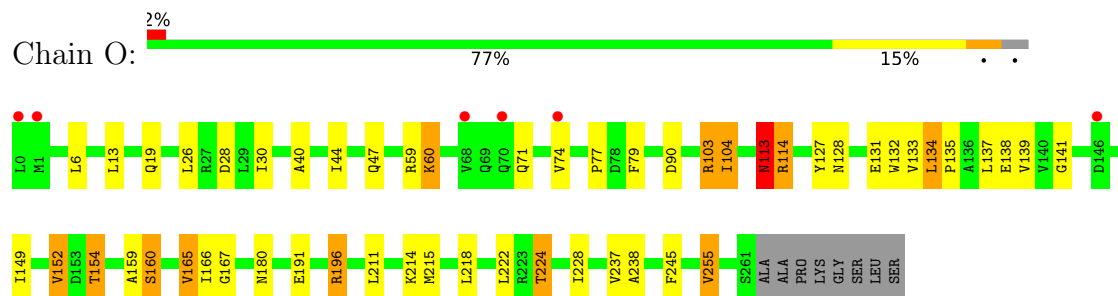
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



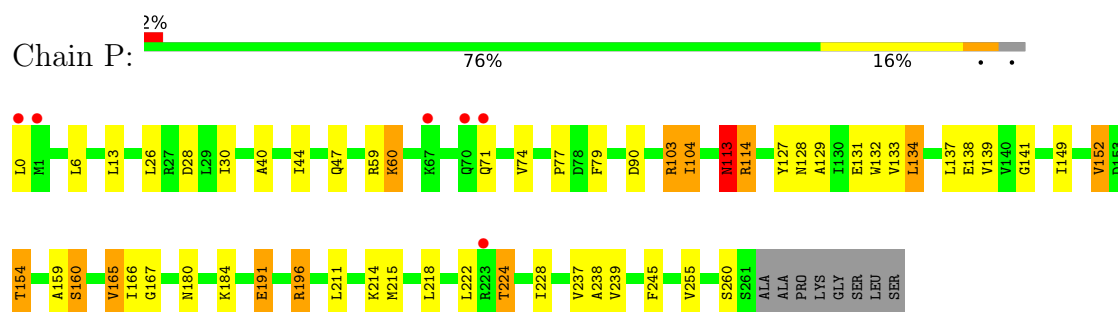
- Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



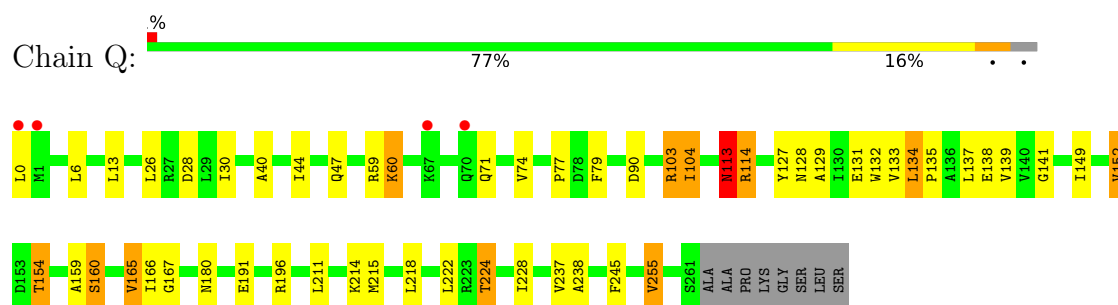
- Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



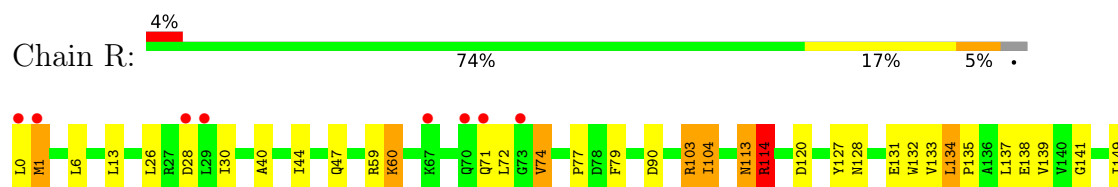
- Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

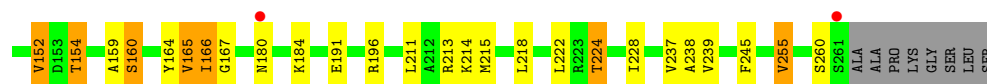


- Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

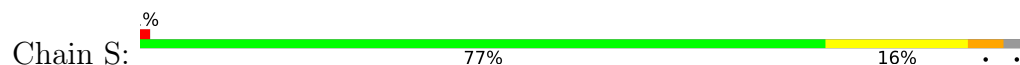


- Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

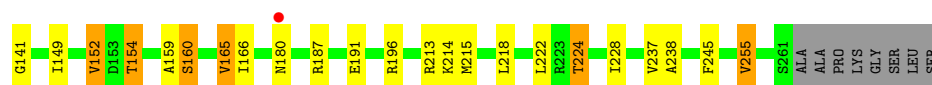
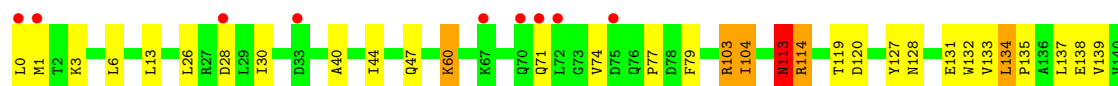
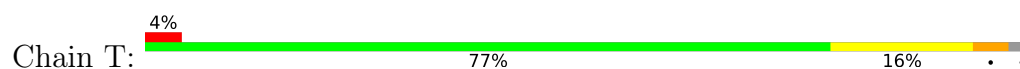




• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | H 3                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 207.35Å 207.35Å 545.47Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 35.26 – 2.80<br>35.26 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.9 (35.26-2.80)<br>94.8 (35.26-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.87 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.5.0088                                             | Depositor        |
| R, $R_{free}$                                                           | 0.222 , 0.234<br>0.220 , 0.231                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10232 reflections (4.94%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.087                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 29.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.010 for -h-k,k,-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 40183                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 35.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: K, PO4, NA

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     | 0.58         | 0/2020          | 0.89        | 2/2744 (0.1%)   |
| 1   | B     | 0.58         | 0/2020          | 0.90        | 2/2744 (0.1%)   |
| 1   | C     | 0.67         | 4/2020 (0.2%)   | 0.89        | 1/2744 (0.0%)   |
| 1   | D     | 0.59         | 0/2020          | 0.90        | 2/2744 (0.1%)   |
| 1   | E     | 0.59         | 0/2020          | 0.88        | 1/2744 (0.0%)   |
| 1   | F     | 0.60         | 0/2020          | 0.90        | 3/2744 (0.1%)   |
| 1   | G     | 0.60         | 0/2020          | 0.90        | 2/2744 (0.1%)   |
| 1   | H     | 0.65         | 2/2020 (0.1%)   | 0.90        | 2/2744 (0.1%)   |
| 1   | I     | 0.60         | 0/2020          | 0.90        | 3/2744 (0.1%)   |
| 1   | J     | 0.64         | 3/2020 (0.1%)   | 0.90        | 2/2744 (0.1%)   |
| 1   | K     | 0.59         | 0/2020          | 0.90        | 2/2744 (0.1%)   |
| 1   | L     | 0.61         | 0/2020          | 0.92        | 4/2744 (0.1%)   |
| 1   | M     | 0.63         | 2/2020 (0.1%)   | 0.89        | 2/2744 (0.1%)   |
| 1   | N     | 0.59         | 0/2020          | 0.89        | 2/2744 (0.1%)   |
| 1   | O     | 0.64         | 2/2020 (0.1%)   | 0.90        | 2/2744 (0.1%)   |
| 1   | P     | 0.57         | 0/2020          | 0.89        | 2/2744 (0.1%)   |
| 1   | Q     | 0.58         | 0/2020          | 0.88        | 2/2744 (0.1%)   |
| 1   | R     | 0.59         | 0/2020          | 0.95        | 6/2744 (0.2%)   |
| 1   | S     | 0.63         | 2/2020 (0.1%)   | 0.89        | 2/2744 (0.1%)   |
| 1   | T     | 0.59         | 0/2020          | 0.90        | 2/2744 (0.1%)   |
| All | All   | 0.61         | 15/40400 (0.0%) | 0.90        | 46/54880 (0.1%) |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | H     | 19  | GLN  | CD-NE2 | -9.75 | 1.12        | 1.33     |
| 1   | M     | 19  | GLN  | CD-NE2 | -9.50 | 1.13        | 1.33     |
| 1   | J     | 19  | GLN  | CD-NE2 | -9.47 | 1.13        | 1.33     |
| 1   | O     | 19  | GLN  | CD-NE2 | -9.45 | 1.13        | 1.33     |
| 1   | C     | 19  | GLN  | CD-NE2 | -9.18 | 1.14        | 1.33     |
| 1   | S     | 19  | GLN  | CD-NE2 | -9.08 | 1.14        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 19  | GLN  | CD-OE1 | -8.40 | 1.07        | 1.23     |
| 1   | M     | 19  | GLN  | CD-OE1 | -8.11 | 1.08        | 1.23     |
| 1   | S     | 19  | GLN  | CD-OE1 | -8.10 | 1.08        | 1.23     |
| 1   | O     | 19  | GLN  | CD-OE1 | -8.10 | 1.08        | 1.23     |
| 1   | H     | 19  | GLN  | CD-OE1 | -8.08 | 1.08        | 1.23     |
| 1   | C     | 19  | GLN  | CD-OE1 | -8.01 | 1.08        | 1.23     |
| 1   | C     | 113 | ASN  | CG-ND2 | -7.58 | 1.17        | 1.33     |
| 1   | C     | 113 | ASN  | CG-OD1 | -7.09 | 1.10        | 1.23     |
| 1   | J     | 113 | ASN  | CG-OD1 | -5.05 | 1.14        | 1.23     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | R     | 114 | ARG  | NE-CZ-NH2 | 10.97  | 129.07      | 119.20   |
| 1   | R     | 114 | ARG  | NE-CZ-NH1 | -10.73 | 110.77      | 121.50   |
| 1   | R     | 114 | ARG  | CD-NE-CZ  | 7.68   | 135.16      | 124.40   |
| 1   | L     | 1   | MET  | CB-CG-SD  | 6.31   | 131.64      | 112.70   |
| 1   | L     | 113 | ASN  | CB-CA-C   | -6.10  | 98.96       | 110.67   |
| 1   | G     | 113 | ASN  | CB-CA-C   | -6.04  | 99.08       | 110.67   |
| 1   | Q     | 113 | ASN  | CB-CA-C   | -5.97  | 99.21       | 110.67   |
| 1   | I     | 113 | ASN  | CB-CA-C   | -5.90  | 99.35       | 110.67   |
| 1   | P     | 113 | ASN  | CB-CA-C   | -5.85  | 99.43       | 110.67   |
| 1   | O     | 113 | ASN  | CB-CA-C   | -5.82  | 99.50       | 110.67   |
| 1   | R     | 113 | ASN  | CB-CA-C   | -5.81  | 99.52       | 110.67   |
| 1   | A     | 113 | ASN  | CB-CA-C   | -5.80  | 99.53       | 110.67   |
| 1   | T     | 113 | ASN  | CB-CA-C   | -5.70  | 99.73       | 110.67   |
| 1   | N     | 113 | ASN  | CB-CA-C   | -5.66  | 99.80       | 110.67   |
| 1   | F     | 113 | ASN  | CB-CA-C   | -5.65  | 99.82       | 110.67   |
| 1   | S     | 113 | ASN  | CB-CA-C   | -5.62  | 99.88       | 110.67   |
| 1   | K     | 113 | ASN  | CB-CA-C   | -5.55  | 100.02      | 110.67   |
| 1   | B     | 113 | ASN  | CB-CA-C   | -5.51  | 100.09      | 110.67   |
| 1   | G     | 134 | LEU  | CA-CB-CG  | 5.33   | 134.94      | 116.30   |
| 1   | E     | 134 | LEU  | CA-CB-CG  | 5.29   | 134.81      | 116.30   |
| 1   | D     | 134 | LEU  | CA-CB-CG  | 5.26   | 134.72      | 116.30   |
| 1   | I     | 134 | LEU  | CA-CB-CG  | 5.26   | 134.69      | 116.30   |
| 1   | P     | 134 | LEU  | CA-CB-CG  | 5.26   | 134.69      | 116.30   |
| 1   | D     | 113 | ASN  | CB-CA-C   | -5.24  | 100.61      | 110.67   |
| 1   | B     | 134 | LEU  | CA-CB-CG  | 5.22   | 134.59      | 116.30   |
| 1   | F     | 134 | LEU  | CA-CB-CG  | 5.22   | 134.56      | 116.30   |
| 1   | S     | 134 | LEU  | CA-CB-CG  | 5.22   | 134.56      | 116.30   |
| 1   | A     | 134 | LEU  | CA-CB-CG  | 5.19   | 134.46      | 116.30   |
| 1   | N     | 134 | LEU  | CA-CB-CG  | 5.19   | 134.46      | 116.30   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | L     | 1   | MET  | CG-SD-CE | 5.17  | 112.28      | 100.90   |
| 1   | J     | 134 | LEU  | CA-CB-CG | 5.17  | 134.40      | 116.30   |
| 1   | H     | 113 | ASN  | CB-CA-C  | -5.15 | 99.88       | 110.38   |
| 1   | Q     | 134 | LEU  | CA-CB-CG | 5.14  | 134.29      | 116.30   |
| 1   | J     | 113 | ASN  | CB-CA-C  | -5.14 | 100.81      | 110.67   |
| 1   | M     | 113 | ASN  | CB-CA-C  | -5.13 | 99.28       | 109.99   |
| 1   | L     | 255 | VAL  | CB-CA-C  | -5.12 | 102.61      | 110.50   |
| 1   | C     | 134 | LEU  | CA-CB-CG | 5.12  | 134.24      | 116.30   |
| 1   | R     | 134 | LEU  | CA-CB-CG | 5.11  | 134.19      | 116.30   |
| 1   | H     | 255 | VAL  | CB-CA-C  | -5.06 | 102.70      | 110.50   |
| 1   | F     | 74  | VAL  | N-CA-C   | 5.06  | 116.19      | 108.80   |
| 1   | I     | 32  | ILE  | N-CA-C   | 5.04  | 116.36      | 110.62   |
| 1   | M     | 134 | LEU  | CA-CB-CG | 5.03  | 133.89      | 116.30   |
| 1   | R     | 74  | VAL  | N-CA-C   | 5.02  | 116.13      | 108.80   |
| 1   | T     | 134 | LEU  | CA-CB-CG | 5.02  | 133.88      | 116.30   |
| 1   | O     | 134 | LEU  | CA-CB-CG | 5.01  | 133.85      | 116.30   |
| 1   | K     | 134 | LEU  | CA-CB-CG | 5.01  | 133.84      | 116.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1986  | 0        | 1979     | 31      | 0            |
| 1   | B     | 1986  | 0        | 1979     | 39      | 0            |
| 1   | C     | 1986  | 0        | 1979     | 32      | 0            |
| 1   | D     | 1986  | 0        | 1979     | 29      | 0            |
| 1   | E     | 1986  | 0        | 1979     | 40      | 0            |
| 1   | F     | 1986  | 0        | 1979     | 40      | 0            |
| 1   | G     | 1986  | 0        | 1979     | 36      | 0            |
| 1   | H     | 1986  | 0        | 1979     | 40      | 0            |
| 1   | I     | 1986  | 0        | 1979     | 42      | 0            |
| 1   | J     | 1986  | 0        | 1979     | 31      | 0            |
| 1   | K     | 1986  | 0        | 1979     | 42      | 0            |
| 1   | L     | 1986  | 0        | 1979     | 33      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | M     | 1986  | 0        | 1979     | 39      | 0            |
| 1   | N     | 1986  | 0        | 1979     | 42      | 0            |
| 1   | O     | 1986  | 0        | 1979     | 28      | 0            |
| 1   | P     | 1986  | 0        | 1979     | 31      | 0            |
| 1   | Q     | 1986  | 0        | 1979     | 32      | 0            |
| 1   | R     | 1986  | 0        | 1979     | 40      | 0            |
| 1   | S     | 1986  | 0        | 1979     | 29      | 0            |
| 1   | T     | 1986  | 0        | 1979     | 37      | 0            |
| 2   | A     | 15    | 0        | 0        | 1       | 0            |
| 2   | B     | 10    | 0        | 0        | 1       | 0            |
| 2   | C     | 5     | 0        | 0        | 0       | 0            |
| 2   | D     | 15    | 0        | 0        | 1       | 0            |
| 2   | E     | 5     | 0        | 0        | 1       | 0            |
| 2   | F     | 15    | 0        | 0        | 2       | 0            |
| 2   | G     | 15    | 0        | 0        | 2       | 0            |
| 2   | H     | 10    | 0        | 0        | 0       | 0            |
| 2   | I     | 5     | 0        | 0        | 0       | 0            |
| 2   | J     | 10    | 0        | 0        | 0       | 0            |
| 2   | K     | 15    | 0        | 0        | 1       | 0            |
| 2   | L     | 10    | 0        | 0        | 1       | 0            |
| 2   | M     | 5     | 0        | 0        | 0       | 0            |
| 2   | N     | 5     | 0        | 0        | 0       | 0            |
| 2   | O     | 5     | 0        | 0        | 0       | 0            |
| 2   | P     | 15    | 0        | 0        | 1       | 0            |
| 2   | Q     | 15    | 0        | 0        | 1       | 0            |
| 2   | R     | 5     | 0        | 0        | 1       | 0            |
| 2   | S     | 5     | 0        | 0        | 0       | 0            |
| 2   | T     | 5     | 0        | 0        | 1       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 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   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 2     | 0        | 0        | 0       | 0            |
| 3   | P     | 1     | 0        | 0        | 0       | 0            |
| 3   | Q     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | R     | 1     | 0        | 0        | 0       | 0            |
| 3   | S     | 2     | 0        | 0        | 0       | 0            |
| 3   | T     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 2     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 2     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 2     | 0        | 0        | 0       | 0            |
| 4   | N     | 1     | 0        | 0        | 0       | 0            |
| 4   | P     | 1     | 0        | 0        | 0       | 0            |
| 4   | Q     | 2     | 0        | 0        | 0       | 0            |
| 4   | R     | 1     | 0        | 0        | 0       | 0            |
| 4   | S     | 1     | 0        | 0        | 0       | 0            |
| 4   | T     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 10    | 0        | 0        | 0       | 0            |
| 5   | B     | 9     | 0        | 0        | 0       | 0            |
| 5   | C     | 13    | 0        | 0        | 1       | 0            |
| 5   | D     | 12    | 0        | 0        | 0       | 0            |
| 5   | E     | 10    | 0        | 0        | 0       | 0            |
| 5   | F     | 14    | 0        | 0        | 0       | 0            |
| 5   | G     | 11    | 0        | 0        | 0       | 0            |
| 5   | H     | 12    | 0        | 0        | 0       | 0            |
| 5   | I     | 11    | 0        | 0        | 1       | 0            |
| 5   | J     | 13    | 0        | 0        | 1       | 0            |
| 5   | K     | 14    | 0        | 0        | 0       | 0            |
| 5   | L     | 17    | 0        | 0        | 0       | 0            |
| 5   | M     | 10    | 0        | 0        | 1       | 0            |
| 5   | N     | 11    | 0        | 0        | 0       | 0            |
| 5   | O     | 10    | 0        | 0        | 0       | 0            |
| 5   | P     | 11    | 0        | 0        | 1       | 0            |
| 5   | Q     | 11    | 0        | 0        | 0       | 0            |
| 5   | R     | 12    | 0        | 0        | 0       | 0            |
| 5   | S     | 11    | 0        | 0        | 0       | 0            |
| 5   | T     | 11    | 0        | 0        | 0       | 0            |
| All | All   | 40183 | 0        | 39580    | 630     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (630) 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:H:213:ARG:NH1  | 1:R:1:MET:HE3    | 1.64                     | 1.10              |
| 1:K:213:ARG:NH1  | 1:T:1:MET:HE3    | 1.68                     | 1.09              |
| 1:P:128:ASN:HD22 | 1:Q:132:TRP:HE1  | 1.05                     | 1.00              |
| 1:B:128:ASN:HD22 | 1:E:132:TRP:HE1  | 1.02                     | 0.99              |
| 1:P:132:TRP:HE1  | 1:S:128:ASN:HD22 | 1.04                     | 0.98              |
| 1:F:132:TRP:HE1  | 1:I:128:ASN:HD22 | 1.02                     | 0.96              |
| 1:K:132:TRP:HE1  | 1:N:128:ASN:HD22 | 1.01                     | 0.96              |
| 1:A:132:TRP:HE1  | 1:D:128:ASN:HD22 | 1.15                     | 0.95              |
| 1:A:128:ASN:HD22 | 1:B:132:TRP:HE1  | 1.02                     | 0.94              |
| 1:E:213:ARG:NH1  | 1:M:1:MET:HE3    | 1.83                     | 0.94              |
| 1:Q:128:ASN:HD22 | 1:T:132:TRP:HE1  | 1.11                     | 0.94              |
| 1:F:128:ASN:HD22 | 1:G:132:TRP:HE1  | 1.14                     | 0.93              |
| 1:H:128:ASN:HD22 | 1:I:132:TRP:HE1  | 1.03                     | 0.93              |
| 1:M:132:TRP:HE1  | 1:O:128:ASN:HD22 | 1.15                     | 0.93              |
| 1:R:128:ASN:HD22 | 1:S:132:TRP:HE1  | 1.09                     | 0.92              |
| 1:H:1:MET:HE3    | 1:R:213:ARG:NH1  | 1.84                     | 0.92              |
| 1:M:128:ASN:HD22 | 1:N:132:TRP:HE1  | 1.02                     | 0.92              |
| 1:H:132:TRP:HE1  | 1:J:128:ASN:HD22 | 1.15                     | 0.92              |
| 1:C:132:TRP:HE1  | 1:E:128:ASN:HD22 | 1.12                     | 0.91              |
| 1:B:1:MET:HE3    | 1:F:213:ARG:NH1  | 1.85                     | 0.91              |
| 1:C:128:ASN:HD22 | 1:D:132:TRP:HE1  | 1.19                     | 0.89              |
| 1:K:128:ASN:HD22 | 1:L:132:TRP:HE1  | 1.21                     | 0.88              |
| 1:R:132:TRP:HE1  | 1:T:128:ASN:HD22 | 1.17                     | 0.88              |
| 1:G:60:LYS:NZ    | 2:G:1263:PO4:O1  | 2.11                     | 0.83              |
| 1:I:213:ARG:NH1  | 1:N:1:MET:HE3    | 1.96                     | 0.81              |
| 1:K:1:MET:HE3    | 1:T:213:ARG:NH1  | 1.96                     | 0.80              |
| 1:I:1:MET:HE3    | 1:N:213:ARG:NH1  | 1.97                     | 0.79              |
| 1:K:132:TRP:NE1  | 1:N:128:ASN:HD22 | 1.79                     | 0.79              |
| 1:E:60:LYS:NZ    | 2:E:1262:PO4:O3  | 2.16                     | 0.78              |
| 1:H:213:ARG:NH1  | 1:R:1:MET:CE     | 2.44                     | 0.77              |
| 1:F:104:ILE:HD11 | 1:F:245:PHE:CE2  | 2.20                     | 0.77              |
| 1:B:128:ASN:HD22 | 1:E:132:TRP:NE1  | 1.82                     | 0.76              |
| 1:F:132:TRP:NE1  | 1:I:128:ASN:HD22 | 1.82                     | 0.76              |
| 1:Q:114:ARG:HA   | 1:Q:224:THR:HB   | 1.69                     | 0.75              |
| 1:L:114:ARG:HA   | 1:L:224:THR:HB   | 1.68                     | 0.75              |
| 1:A:128:ASN:HD22 | 1:B:132:TRP:NE1  | 1.82                     | 0.74              |
| 1:G:128:ASN:HD22 | 1:J:132:TRP:HE1  | 1.34                     | 0.74              |
| 1:C:114:ARG:HA   | 1:C:224:THR:HB   | 1.69                     | 0.74              |
| 1:R:60:LYS:NZ    | 2:R:1262:PO4:O3  | 2.22                     | 0.73              |
| 1:C:104:ILE:HD11 | 1:C:245:PHE:CE2  | 2.24                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:114:ARG:HA   | 1:A:224:THR:HB   | 1.70                     | 0.73              |
| 1:G:114:ARG:HA   | 1:G:224:THR:HB   | 1.71                     | 0.73              |
| 1:P:132:TRP:NE1  | 1:S:128:ASN:HD22 | 1.83                     | 0.72              |
| 1:F:114:ARG:HA   | 1:F:224:THR:HB   | 1.71                     | 0.72              |
| 1:G:104:ILE:HD11 | 1:G:245:PHE:CE2  | 2.24                     | 0.72              |
| 1:I:119:THR:OG1  | 1:N:0:LEU:HD12   | 1.90                     | 0.72              |
| 1:B:1:MET:CE     | 1:F:213:ARG:NH1  | 2.53                     | 0.72              |
| 1:Q:154:THR:HG23 | 1:Q:160:SER:OG   | 1.91                     | 0.71              |
| 1:J:114:ARG:HA   | 1:J:224:THR:HB   | 1.73                     | 0.71              |
| 1:I:114:ARG:HA   | 1:I:224:THR:HB   | 1.72                     | 0.71              |
| 1:N:154:THR:HG23 | 1:N:160:SER:OG   | 1.91                     | 0.70              |
| 1:T:114:ARG:HA   | 1:T:224:THR:HB   | 1.73                     | 0.70              |
| 1:J:104:ILE:HD11 | 1:J:245:PHE:CE2  | 2.27                     | 0.70              |
| 1:K:114:ARG:HA   | 1:K:224:THR:HB   | 1.74                     | 0.70              |
| 1:M:154:THR:HG23 | 1:M:160:SER:OG   | 1.92                     | 0.70              |
| 1:E:114:ARG:HA   | 1:E:224:THR:HB   | 1.73                     | 0.69              |
| 1:L:128:ASN:HD22 | 1:O:132:TRP:HE1  | 1.38                     | 0.69              |
| 1:B:114:ARG:HA   | 1:B:224:THR:HB   | 1.74                     | 0.69              |
| 1:H:114:ARG:HA   | 1:H:224:THR:HB   | 1.74                     | 0.69              |
| 1:D:154:THR:HG23 | 1:D:160:SER:OG   | 1.93                     | 0.69              |
| 1:A:154:THR:HG23 | 1:A:160:SER:OG   | 1.93                     | 0.69              |
| 1:D:114:ARG:HA   | 1:D:224:THR:HB   | 1.73                     | 0.69              |
| 1:H:1:MET:HE3    | 1:R:213:ARG:HH11 | 1.56                     | 0.69              |
| 1:K:0:LEU:HD13   | 1:T:119:THR:OG1  | 1.93                     | 0.69              |
| 1:S:114:ARG:HA   | 1:S:224:THR:HB   | 1.73                     | 0.69              |
| 1:T:79:PHE:CE1   | 1:T:215:MET:HE1  | 2.28                     | 0.69              |
| 1:D:40:ALA:O     | 1:D:44:ILE:HG12  | 1.92                     | 0.69              |
| 1:S:40:ALA:O     | 1:S:44:ILE:HG12  | 1.93                     | 0.69              |
| 1:N:114:ARG:HA   | 1:N:224:THR:HB   | 1.72                     | 0.69              |
| 1:H:128:ASN:HD22 | 1:I:132:TRP:NE1  | 1.86                     | 0.69              |
| 1:O:114:ARG:HA   | 1:O:224:THR:HB   | 1.75                     | 0.68              |
| 1:H:40:ALA:O     | 1:H:44:ILE:HG12  | 1.94                     | 0.68              |
| 1:M:114:ARG:HA   | 1:M:224:THR:HB   | 1.74                     | 0.68              |
| 1:P:154:THR:HG23 | 1:P:160:SER:OG   | 1.93                     | 0.68              |
| 1:A:40:ALA:O     | 1:A:44:ILE:HG12  | 1.94                     | 0.68              |
| 1:O:154:THR:HG23 | 1:O:160:SER:OG   | 1.94                     | 0.67              |
| 1:C:40:ALA:O     | 1:C:44:ILE:HG12  | 1.94                     | 0.67              |
| 1:M:128:ASN:HD22 | 1:N:132:TRP:NE1  | 1.86                     | 0.67              |
| 1:A:60:LYS:NZ    | 2:A:1264:PO4:O1  | 2.28                     | 0.67              |
| 1:E:154:THR:HG23 | 1:E:160:SER:OG   | 1.95                     | 0.67              |
| 1:J:154:THR:HG23 | 1:J:160:SER:OG   | 1.94                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:154:THR:HG23 | 1:K:160:SER:OG   | 1.93                     | 0.67              |
| 1:S:79:PHE:CE1   | 1:S:215:MET:HE1  | 2.29                     | 0.67              |
| 1:H:79:PHE:CE1   | 1:H:215:MET:HE1  | 2.30                     | 0.67              |
| 1:I:154:THR:HG23 | 1:I:160:SER:OG   | 1.95                     | 0.67              |
| 1:P:128:ASN:HD22 | 1:Q:132:TRP:NE1  | 1.86                     | 0.67              |
| 1:Q:104:ILE:HD11 | 1:Q:245:PHE:CE2  | 2.28                     | 0.67              |
| 1:K:1:MET:HE3    | 1:T:213:ARG:HH11 | 1.58                     | 0.67              |
| 1:B:154:THR:HG23 | 1:B:160:SER:OG   | 1.95                     | 0.67              |
| 1:E:213:ARG:HH11 | 1:M:1:MET:HE3    | 1.56                     | 0.66              |
| 1:K:213:ARG:HH11 | 1:T:1:MET:HE3    | 1.55                     | 0.66              |
| 1:P:79:PHE:CE1   | 1:P:215:MET:HE1  | 2.31                     | 0.66              |
| 1:K:40:ALA:O     | 1:K:44:ILE:HG12  | 1.95                     | 0.66              |
| 1:F:154:THR:HG23 | 1:F:160:SER:OG   | 1.96                     | 0.66              |
| 1:L:154:THR:HG23 | 1:L:160:SER:OG   | 1.95                     | 0.66              |
| 1:N:79:PHE:CE1   | 1:N:215:MET:HE1  | 2.31                     | 0.66              |
| 1:R:40:ALA:O     | 1:R:44:ILE:HG12  | 1.94                     | 0.66              |
| 1:C:104:ILE:HD11 | 1:C:245:PHE:CZ   | 2.31                     | 0.66              |
| 1:I:0:LEU:HD12   | 1:N:119:THR:OG1  | 1.96                     | 0.66              |
| 1:K:132:TRP:HE1  | 1:N:128:ASN:ND2  | 1.85                     | 0.65              |
| 1:R:154:THR:HG23 | 1:R:160:SER:OG   | 1.96                     | 0.65              |
| 1:A:79:PHE:CE1   | 1:A:215:MET:HE1  | 2.31                     | 0.65              |
| 1:C:154:THR:HG23 | 1:C:160:SER:OG   | 1.96                     | 0.65              |
| 1:E:1:MET:CE     | 1:M:213:ARG:NH1  | 2.60                     | 0.65              |
| 1:B:213:ARG:NH1  | 1:F:1:MET:HE2    | 2.12                     | 0.65              |
| 1:I:40:ALA:O     | 1:I:44:ILE:HG12  | 1.97                     | 0.65              |
| 1:O:79:PHE:CE1   | 1:O:215:MET:HE1  | 2.31                     | 0.65              |
| 1:P:114:ARG:HA   | 1:P:224:THR:HB   | 1.78                     | 0.65              |
| 1:T:154:THR:HG23 | 1:T:160:SER:OG   | 1.97                     | 0.65              |
| 1:H:154:THR:HG23 | 1:H:160:SER:OG   | 1.95                     | 0.65              |
| 1:P:60:LYS:NZ    | 2:P:1263:PO4:O2  | 2.29                     | 0.65              |
| 1:E:1:MET:HE3    | 1:M:213:ARG:NH1  | 2.12                     | 0.65              |
| 1:M:40:ALA:O     | 1:M:44:ILE:HG12  | 1.97                     | 0.65              |
| 1:Q:40:ALA:O     | 1:Q:44:ILE:HG12  | 1.97                     | 0.65              |
| 1:B:40:ALA:O     | 1:B:44:ILE:HG12  | 1.97                     | 0.65              |
| 1:R:79:PHE:CE1   | 1:R:215:MET:HE1  | 2.31                     | 0.65              |
| 1:F:104:ILE:HD11 | 1:F:245:PHE:CZ   | 2.32                     | 0.64              |
| 1:Q:128:ASN:HD22 | 1:T:132:TRP:NE1  | 1.92                     | 0.64              |
| 1:E:40:ALA:O     | 1:E:44:ILE:HG12  | 1.96                     | 0.64              |
| 1:F:40:ALA:O     | 1:F:44:ILE:HG12  | 1.97                     | 0.64              |
| 1:N:40:ALA:O     | 1:N:44:ILE:HG12  | 1.97                     | 0.64              |
| 1:B:154:THR:CG2  | 1:B:160:SER:OG   | 2.45                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:79:PHE:CE1   | 1:I:215:MET:HE1  | 2.33                     | 0.64              |
| 1:H:213:ARG:HH11 | 1:R:1:MET:HE3    | 1.60                     | 0.64              |
| 1:R:114:ARG:HA   | 1:R:224:THR:HB   | 1.80                     | 0.64              |
| 1:B:79:PHE:CE1   | 1:B:215:MET:HE1  | 2.33                     | 0.64              |
| 1:J:40:ALA:O     | 1:J:44:ILE:HG12  | 1.97                     | 0.64              |
| 1:B:213:ARG:NH1  | 1:F:1:MET:CE     | 2.60                     | 0.64              |
| 1:K:104:ILE:HD11 | 1:K:245:PHE:CE2  | 2.32                     | 0.63              |
| 1:S:154:THR:HG23 | 1:S:160:SER:OG   | 1.98                     | 0.63              |
| 1:I:1:MET:HE3    | 1:N:213:ARG:HH11 | 1.62                     | 0.63              |
| 1:T:40:ALA:O     | 1:T:44:ILE:HG12  | 1.98                     | 0.63              |
| 1:L:40:ALA:O     | 1:L:44:ILE:HG12  | 1.98                     | 0.63              |
| 1:Q:79:PHE:CE1   | 1:Q:215:MET:HE1  | 2.34                     | 0.63              |
| 1:E:104:ILE:HD11 | 1:E:245:PHE:CE2  | 2.33                     | 0.63              |
| 1:M:79:PHE:CE1   | 1:M:215:MET:HE1  | 2.33                     | 0.63              |
| 1:P:40:ALA:O     | 1:P:44:ILE:HG12  | 1.99                     | 0.63              |
| 1:Q:104:ILE:HD11 | 1:Q:245:PHE:CZ   | 2.34                     | 0.63              |
| 1:O:40:ALA:O     | 1:O:44:ILE:HG12  | 1.99                     | 0.62              |
| 1:B:60:LYS:NZ    | 2:B:1263:PO4:O3  | 2.33                     | 0.62              |
| 1:E:79:PHE:CE1   | 1:E:215:MET:HE1  | 2.35                     | 0.62              |
| 1:I:213:ARG:HH11 | 1:N:1:MET:HE3    | 1.63                     | 0.62              |
| 1:Q:154:THR:CG2  | 1:Q:160:SER:OG   | 2.47                     | 0.62              |
| 1:G:79:PHE:CE1   | 1:G:215:MET:HE1  | 2.34                     | 0.62              |
| 1:J:104:ILE:HD11 | 1:J:245:PHE:CZ   | 2.34                     | 0.62              |
| 1:N:104:ILE:HD11 | 1:N:245:PHE:CE2  | 2.34                     | 0.62              |
| 1:C:79:PHE:CE1   | 1:C:215:MET:HE1  | 2.35                     | 0.62              |
| 1:T:60:LYS:NZ    | 2:T:1262:PO4:O3  | 2.33                     | 0.62              |
| 1:J:154:THR:CG2  | 1:J:160:SER:OG   | 2.48                     | 0.61              |
| 1:G:40:ALA:O     | 1:G:44:ILE:HG12  | 1.99                     | 0.61              |
| 1:S:104:ILE:HD11 | 1:S:245:PHE:CE2  | 2.36                     | 0.61              |
| 1:M:132:TRP:NE1  | 1:O:128:ASN:HD22 | 1.93                     | 0.61              |
| 1:N:154:THR:CG2  | 1:N:160:SER:OG   | 2.49                     | 0.61              |
| 1:G:30:ILE:HD11  | 1:G:152:VAL:HG13 | 1.82                     | 0.61              |
| 1:S:30:ILE:HD11  | 1:S:152:VAL:HG13 | 1.82                     | 0.61              |
| 1:B:104:ILE:HD11 | 1:B:245:PHE:CE2  | 2.36                     | 0.61              |
| 1:E:30:ILE:HD11  | 1:E:152:VAL:HG13 | 1.83                     | 0.61              |
| 1:G:113:ASN:HD22 | 1:G:114:ARG:HH11 | 1.47                     | 0.61              |
| 1:G:154:THR:HG23 | 1:G:160:SER:OG   | 2.01                     | 0.61              |
| 1:H:132:TRP:NE1  | 1:J:128:ASN:HD22 | 1.93                     | 0.60              |
| 1:L:104:ILE:HD11 | 1:L:245:PHE:CE2  | 2.36                     | 0.60              |
| 1:D:104:ILE:HD11 | 1:D:245:PHE:CE2  | 2.36                     | 0.60              |
| 1:I:154:THR:CG2  | 1:I:160:SER:OG   | 2.49                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:104:ILE:HD11 | 1:O:245:PHE:CE2  | 2.36                     | 0.60              |
| 1:J:79:PHE:CE1   | 1:J:215:MET:HE1  | 2.35                     | 0.60              |
| 1:K:154:THR:CG2  | 1:K:160:SER:OG   | 2.48                     | 0.60              |
| 1:R:30:ILE:HD11  | 1:R:152:VAL:HG13 | 1.82                     | 0.60              |
| 1:I:191:GLU:OE1  | 5:I:2008:HOH:O   | 2.16                     | 0.60              |
| 1:F:128:ASN:HD22 | 1:G:132:TRP:NE1  | 1.94                     | 0.60              |
| 1:D:113:ASN:OD1  | 1:D:129:ALA:C    | 2.45                     | 0.60              |
| 1:F:132:TRP:HE1  | 1:I:128:ASN:ND2  | 1.87                     | 0.60              |
| 1:P:104:ILE:HD11 | 1:P:245:PHE:CE2  | 2.37                     | 0.59              |
| 1:I:30:ILE:HD11  | 1:I:152:VAL:HG13 | 1.84                     | 0.59              |
| 1:T:30:ILE:HD11  | 1:T:152:VAL:HG13 | 1.84                     | 0.59              |
| 1:F:30:ILE:HD11  | 1:F:152:VAL:HG13 | 1.84                     | 0.59              |
| 1:P:191:GLU:OE1  | 5:P:2007:HOH:O   | 2.17                     | 0.59              |
| 1:L:79:PHE:CE1   | 1:L:215:MET:HE1  | 2.37                     | 0.59              |
| 1:P:79:PHE:CZ    | 1:P:215:MET:HE1  | 2.37                     | 0.59              |
| 1:F:154:THR:CG2  | 1:F:160:SER:OG   | 2.51                     | 0.59              |
| 1:K:104:ILE:HD11 | 1:K:245:PHE:CZ   | 2.36                     | 0.59              |
| 1:O:113:ASN:HD22 | 1:O:114:ARG:HH11 | 1.51                     | 0.59              |
| 1:H:154:THR:CG2  | 1:H:160:SER:OG   | 2.50                     | 0.59              |
| 1:D:154:THR:CG2  | 1:D:160:SER:OG   | 2.51                     | 0.59              |
| 1:M:154:THR:CG2  | 1:M:160:SER:OG   | 2.51                     | 0.59              |
| 1:A:30:ILE:HD11  | 1:A:152:VAL:HG13 | 1.84                     | 0.59              |
| 1:A:154:THR:CG2  | 1:A:160:SER:OG   | 2.50                     | 0.59              |
| 1:D:79:PHE:CE1   | 1:D:215:MET:HE1  | 2.38                     | 0.59              |
| 1:G:104:ILE:HD11 | 1:G:245:PHE:CZ   | 2.37                     | 0.59              |
| 1:K:30:ILE:HD11  | 1:K:152:VAL:HG13 | 1.85                     | 0.59              |
| 1:P:30:ILE:HD11  | 1:P:152:VAL:HG13 | 1.85                     | 0.59              |
| 1:T:79:PHE:CZ    | 1:T:215:MET:HE1  | 2.38                     | 0.58              |
| 1:N:30:ILE:HD11  | 1:N:152:VAL:HG13 | 1.84                     | 0.58              |
| 1:I:104:ILE:HD11 | 1:I:245:PHE:CE2  | 2.38                     | 0.58              |
| 1:K:79:PHE:CE1   | 1:K:215:MET:HE1  | 2.38                     | 0.58              |
| 1:A:79:PHE:CZ    | 1:A:215:MET:HE1  | 2.39                     | 0.58              |
| 1:F:79:PHE:CE1   | 1:F:215:MET:HE1  | 2.38                     | 0.58              |
| 1:S:154:THR:CG2  | 1:S:160:SER:OG   | 2.52                     | 0.58              |
| 1:C:132:TRP:NE1  | 1:E:128:ASN:HD22 | 1.91                     | 0.58              |
| 1:M:104:ILE:HD11 | 1:M:245:PHE:CE2  | 2.38                     | 0.58              |
| 1:O:30:ILE:HD11  | 1:O:152:VAL:HG13 | 1.83                     | 0.58              |
| 1:B:113:ASN:OD1  | 1:B:129:ALA:O    | 2.22                     | 0.58              |
| 1:C:154:THR:CG2  | 1:C:160:SER:OG   | 2.52                     | 0.58              |
| 1:O:79:PHE:CZ    | 1:O:215:MET:HE1  | 2.39                     | 0.58              |
| 1:O:154:THR:CG2  | 1:O:160:SER:OG   | 2.51                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:113:ASN:HD22 | 1:S:114:ARG:HH11 | 1.52                     | 0.58              |
| 1:B:113:ASN:OD1  | 1:B:129:ALA:C    | 2.47                     | 0.58              |
| 1:R:128:ASN:HD22 | 1:S:132:TRP:NE1  | 1.90                     | 0.58              |
| 1:E:104:ILE:HD11 | 1:E:245:PHE:CZ   | 2.39                     | 0.57              |
| 1:S:79:PHE:CZ    | 1:S:215:MET:HE1  | 2.39                     | 0.57              |
| 1:T:154:THR:CG2  | 1:T:160:SER:OG   | 2.52                     | 0.57              |
| 1:J:30:ILE:HD11  | 1:J:152:VAL:HG13 | 1.87                     | 0.57              |
| 1:N:113:ASN:HD22 | 1:N:114:ARG:HH11 | 1.52                     | 0.57              |
| 1:Q:30:ILE:HD11  | 1:Q:152:VAL:HG13 | 1.86                     | 0.57              |
| 1:B:79:PHE:CZ    | 1:B:215:MET:HE1  | 2.39                     | 0.57              |
| 1:L:30:ILE:HD11  | 1:L:152:VAL:HG13 | 1.84                     | 0.57              |
| 1:A:104:ILE:HD11 | 1:A:245:PHE:CE2  | 2.39                     | 0.57              |
| 1:P:104:ILE:HG23 | 1:P:139:VAL:HG22 | 1.85                     | 0.57              |
| 1:P:154:THR:CG2  | 1:P:160:SER:OG   | 2.52                     | 0.57              |
| 1:R:104:ILE:HD12 | 1:R:104:ILE:H    | 1.70                     | 0.57              |
| 1:R:104:ILE:HD11 | 1:R:245:PHE:CE2  | 2.39                     | 0.57              |
| 1:B:213:ARG:HH11 | 1:F:1:MET:HE2    | 1.69                     | 0.57              |
| 1:H:104:ILE:HD11 | 1:H:245:PHE:CE2  | 2.38                     | 0.57              |
| 1:E:104:ILE:HG23 | 1:E:139:VAL:HG22 | 1.87                     | 0.57              |
| 1:M:104:ILE:HG23 | 1:M:139:VAL:HG22 | 1.87                     | 0.57              |
| 1:N:104:ILE:HG23 | 1:N:139:VAL:HG22 | 1.86                     | 0.57              |
| 1:O:104:ILE:HD11 | 1:O:245:PHE:CZ   | 2.40                     | 0.57              |
| 1:R:79:PHE:CZ    | 1:R:215:MET:HE1  | 2.40                     | 0.57              |
| 1:E:104:ILE:HD12 | 1:E:104:ILE:H    | 1.70                     | 0.57              |
| 1:E:154:THR:CG2  | 1:E:160:SER:OG   | 2.53                     | 0.57              |
| 1:B:104:ILE:HD11 | 1:B:245:PHE:CZ   | 2.40                     | 0.56              |
| 1:D:104:ILE:HG23 | 1:D:139:VAL:HG22 | 1.87                     | 0.56              |
| 1:H:104:ILE:HD12 | 1:H:104:ILE:H    | 1.71                     | 0.56              |
| 1:M:128:ASN:ND2  | 1:N:132:TRP:HE1  | 1.87                     | 0.56              |
| 1:S:104:ILE:HD11 | 1:S:245:PHE:CZ   | 2.40                     | 0.56              |
| 1:B:30:ILE:HD11  | 1:B:152:VAL:HG13 | 1.86                     | 0.56              |
| 1:B:104:ILE:HG23 | 1:B:139:VAL:HG22 | 1.87                     | 0.56              |
| 1:H:79:PHE:CZ    | 1:H:215:MET:HE1  | 2.40                     | 0.56              |
| 1:N:79:PHE:CZ    | 1:N:215:MET:HE1  | 2.40                     | 0.56              |
| 1:L:154:THR:CG2  | 1:L:160:SER:OG   | 2.53                     | 0.56              |
| 1:N:104:ILE:HD11 | 1:N:245:PHE:CZ   | 2.41                     | 0.56              |
| 1:M:104:ILE:HD12 | 1:M:104:ILE:H    | 1.71                     | 0.56              |
| 1:R:104:ILE:HG23 | 1:R:139:VAL:HG22 | 1.86                     | 0.56              |
| 1:A:104:ILE:HG23 | 1:A:139:VAL:HG22 | 1.88                     | 0.56              |
| 1:H:30:ILE:HD11  | 1:H:152:VAL:HG13 | 1.88                     | 0.56              |
| 1:I:104:ILE:HD12 | 1:I:104:ILE:H    | 1.70                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:104:ILE:HG23 | 1:Q:139:VAL:HG22 | 1.88                     | 0.55              |
| 1:C:30:ILE:HD11  | 1:C:152:VAL:HG13 | 1.89                     | 0.55              |
| 1:F:104:ILE:HG23 | 1:F:139:VAL:HG22 | 1.88                     | 0.55              |
| 1:K:62:GLY:HA3   | 2:K:1264:PO4:O3  | 2.06                     | 0.55              |
| 1:T:113:ASN:HD22 | 1:T:114:ARG:HH11 | 1.53                     | 0.55              |
| 1:F:113:ASN:HD22 | 1:F:114:ARG:HH11 | 1.54                     | 0.55              |
| 1:D:30:ILE:HD11  | 1:D:152:VAL:HG13 | 1.87                     | 0.55              |
| 1:C:128:ASN:HD22 | 1:D:132:TRP:NE1  | 1.98                     | 0.55              |
| 1:J:113:ASN:OD1  | 1:J:129:ALA:C    | 2.49                     | 0.55              |
| 1:R:104:ILE:HD11 | 1:R:245:PHE:CZ   | 2.41                     | 0.55              |
| 1:K:1:MET:HE2    | 1:T:120:ASP:HB2  | 1.88                     | 0.55              |
| 1:M:30:ILE:HD11  | 1:M:152:VAL:HG13 | 1.87                     | 0.55              |
| 1:M:104:ILE:HD11 | 1:M:245:PHE:CZ   | 2.41                     | 0.55              |
| 1:I:79:PHE:CZ    | 1:I:215:MET:HE1  | 2.42                     | 0.55              |
| 1:O:104:ILE:H    | 1:O:104:ILE:HD12 | 1.72                     | 0.55              |
| 1:F:79:PHE:CZ    | 1:F:215:MET:HE1  | 2.42                     | 0.55              |
| 1:K:79:PHE:CZ    | 1:K:215:MET:HE1  | 2.42                     | 0.55              |
| 1:K:113:ASN:HD22 | 1:K:114:ARG:HH11 | 1.55                     | 0.55              |
| 1:C:104:ILE:HG23 | 1:C:139:VAL:HG22 | 1.89                     | 0.54              |
| 1:Q:79:PHE:CZ    | 1:Q:215:MET:HE1  | 2.42                     | 0.54              |
| 1:Q:113:ASN:HD22 | 1:Q:114:ARG:HH11 | 1.55                     | 0.54              |
| 1:E:79:PHE:CZ    | 1:E:215:MET:HE1  | 2.41                     | 0.54              |
| 1:K:104:ILE:HG23 | 1:K:139:VAL:HG22 | 1.89                     | 0.54              |
| 1:N:104:ILE:HD12 | 1:N:104:ILE:H    | 1.72                     | 0.54              |
| 1:B:131:GLU:HG2  | 1:B:132:TRP:CD1  | 2.42                     | 0.54              |
| 1:T:104:ILE:HG23 | 1:T:139:VAL:HG22 | 1.89                     | 0.54              |
| 1:H:104:ILE:HG23 | 1:H:139:VAL:HG22 | 1.89                     | 0.54              |
| 1:K:60:LYS:HE3   | 1:K:159:ALA:O    | 2.07                     | 0.54              |
| 1:P:104:ILE:HD11 | 1:P:245:PHE:CZ   | 2.41                     | 0.54              |
| 1:E:60:LYS:HE3   | 1:E:159:ALA:O    | 2.08                     | 0.54              |
| 1:J:79:PHE:CZ    | 1:J:215:MET:HE1  | 2.42                     | 0.54              |
| 1:J:104:ILE:H    | 1:J:104:ILE:HD12 | 1.71                     | 0.54              |
| 1:A:132:TRP:NE1  | 1:D:128:ASN:HD22 | 1.96                     | 0.54              |
| 1:P:104:ILE:HD12 | 1:P:104:ILE:H    | 1.73                     | 0.54              |
| 1:R:154:THR:CG2  | 1:R:160:SER:OG   | 2.56                     | 0.54              |
| 1:C:79:PHE:CZ    | 1:C:215:MET:HE1  | 2.43                     | 0.53              |
| 1:M:79:PHE:CZ    | 1:M:215:MET:HE1  | 2.43                     | 0.53              |
| 1:P:113:ASN:HD22 | 1:P:114:ARG:HH11 | 1.57                     | 0.53              |
| 1:D:79:PHE:CZ    | 1:D:215:MET:HE1  | 2.43                     | 0.53              |
| 1:E:113:ASN:OD1  | 1:E:129:ALA:C    | 2.52                     | 0.53              |
| 1:M:113:ASN:HD22 | 1:M:114:ARG:HH11 | 1.56                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:104:ILE:HG23 | 1:G:139:VAL:HG22 | 1.91                     | 0.53              |
| 1:I:60:LYS:HE2   | 1:I:138:GLU:OE2  | 2.09                     | 0.53              |
| 1:L:113:ASN:HD22 | 1:L:114:ARG:HH11 | 1.55                     | 0.53              |
| 1:O:60:LYS:HE3   | 1:O:159:ALA:O    | 2.09                     | 0.53              |
| 1:S:104:ILE:HG23 | 1:S:139:VAL:HG22 | 1.91                     | 0.53              |
| 1:H:104:ILE:HD11 | 1:H:245:PHE:CZ   | 2.44                     | 0.53              |
| 1:Q:131:GLU:HG2  | 1:Q:132:TRP:CD1  | 2.44                     | 0.53              |
| 1:I:113:ASN:HD22 | 1:I:114:ARG:HH11 | 1.57                     | 0.53              |
| 1:G:104:ILE:HD12 | 1:G:104:ILE:H    | 1.74                     | 0.53              |
| 1:K:128:ASN:HD22 | 1:L:132:TRP:NE1  | 2.01                     | 0.53              |
| 1:O:104:ILE:HG23 | 1:O:139:VAL:HG22 | 1.91                     | 0.53              |
| 1:D:104:ILE:HD12 | 1:D:104:ILE:H    | 1.74                     | 0.52              |
| 1:S:131:GLU:HG2  | 1:S:132:TRP:CD1  | 2.43                     | 0.52              |
| 1:A:104:ILE:HD11 | 1:A:245:PHE:CZ   | 2.45                     | 0.52              |
| 1:I:104:ILE:HD11 | 1:I:245:PHE:CZ   | 2.44                     | 0.52              |
| 1:E:131:GLU:HG2  | 1:E:132:TRP:CD1  | 2.44                     | 0.52              |
| 1:H:213:ARG:HH11 | 1:R:1:MET:CE     | 2.20                     | 0.52              |
| 1:L:103:ARG:HG3  | 1:L:238:ALA:HA   | 1.91                     | 0.52              |
| 1:L:104:ILE:HG23 | 1:L:139:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:60:LYS:HE2   | 1:A:138:GLU:OE2  | 2.09                     | 0.52              |
| 1:H:113:ASN:HD22 | 1:H:114:ARG:HH11 | 1.56                     | 0.52              |
| 1:I:131:GLU:HG2  | 1:I:132:TRP:CD1  | 2.45                     | 0.52              |
| 1:K:104:ILE:HD12 | 1:K:104:ILE:H    | 1.74                     | 0.52              |
| 1:T:104:ILE:HD11 | 1:T:245:PHE:CE2  | 2.45                     | 0.52              |
| 1:B:104:ILE:HD12 | 1:B:104:ILE:H    | 1.74                     | 0.52              |
| 1:C:104:ILE:HD12 | 1:C:104:ILE:H    | 1.74                     | 0.52              |
| 1:D:104:ILE:HD11 | 1:D:245:PHE:CZ   | 2.44                     | 0.52              |
| 1:F:103:ARG:HG3  | 1:F:238:ALA:HA   | 1.91                     | 0.52              |
| 1:L:104:ILE:HD12 | 1:L:104:ILE:H    | 1.75                     | 0.52              |
| 1:A:131:GLU:HG2  | 1:A:132:TRP:CD1  | 2.45                     | 0.52              |
| 1:J:131:GLU:HG2  | 1:J:132:TRP:CD1  | 2.45                     | 0.52              |
| 1:O:131:GLU:HG2  | 1:O:132:TRP:CD1  | 2.45                     | 0.52              |
| 1:P:60:LYS:HE3   | 1:P:159:ALA:O    | 2.09                     | 0.52              |
| 1:Q:60:LYS:HE3   | 1:Q:159:ALA:O    | 2.10                     | 0.52              |
| 1:B:60:LYS:HE2   | 1:B:138:GLU:OE2  | 2.10                     | 0.52              |
| 1:F:60:LYS:HE3   | 1:F:159:ALA:O    | 2.09                     | 0.52              |
| 1:C:60:LYS:HE3   | 1:C:159:ALA:O    | 2.10                     | 0.51              |
| 1:J:104:ILE:HG23 | 1:J:139:VAL:HG22 | 1.90                     | 0.51              |
| 1:D:131:GLU:HG2  | 1:D:132:TRP:CD1  | 2.45                     | 0.51              |
| 1:I:104:ILE:HG23 | 1:I:139:VAL:HG22 | 1.91                     | 0.51              |
| 1:R:60:LYS:HE3   | 1:R:159:ALA:O    | 2.09                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:T:104:ILE:HD12 | 1:T:104:ILE:H   | 1.75                     | 0.51              |
| 1:C:103:ARG:HG3  | 1:C:238:ALA:HA  | 1.91                     | 0.51              |
| 1:E:113:ASN:OD1  | 1:E:129:ALA:O   | 2.28                     | 0.51              |
| 1:H:141:GLY:O    | 1:H:160:SER:HB3 | 2.10                     | 0.51              |
| 1:T:60:LYS:HE2   | 1:T:138:GLU:OE2 | 2.11                     | 0.51              |
| 1:G:141:GLY:O    | 1:G:160:SER:HB3 | 2.10                     | 0.51              |
| 1:K:103:ARG:HG3  | 1:K:238:ALA:HA  | 1.93                     | 0.51              |
| 1:S:104:ILE:HD12 | 1:S:104:ILE:H   | 1.74                     | 0.51              |
| 1:F:60:LYS:HE2   | 1:F:138:GLU:OE2 | 2.11                     | 0.51              |
| 1:G:60:LYS:HE3   | 1:G:159:ALA:O   | 2.10                     | 0.51              |
| 1:C:113:ASN:OD1  | 1:C:129:ALA:HA  | 2.11                     | 0.51              |
| 1:G:154:THR:CG2  | 1:G:160:SER:OG  | 2.59                     | 0.51              |
| 1:K:131:GLU:HG2  | 1:K:132:TRP:CD1 | 2.45                     | 0.51              |
| 1:M:60:LYS:HE2   | 1:M:138:GLU:OE2 | 2.10                     | 0.51              |
| 1:N:60:LYS:HE2   | 1:N:138:GLU:OE2 | 2.10                     | 0.51              |
| 1:T:131:GLU:HG2  | 1:T:132:TRP:CD1 | 2.46                     | 0.51              |
| 1:K:60:LYS:HE2   | 1:K:138:GLU:OE2 | 2.11                     | 0.50              |
| 1:N:131:GLU:HG2  | 1:N:132:TRP:CD1 | 2.45                     | 0.50              |
| 1:F:104:ILE:CD1  | 1:F:245:PHE:CE2 | 2.93                     | 0.50              |
| 1:G:79:PHE:CZ    | 1:G:215:MET:HE1 | 2.46                     | 0.50              |
| 1:D:113:ASN:OD1  | 1:D:129:ALA:O   | 2.29                     | 0.50              |
| 1:E:1:MET:HE2    | 1:M:213:ARG:NH1 | 2.25                     | 0.50              |
| 1:C:114:ARG:CA   | 1:C:224:THR:HB  | 2.41                     | 0.50              |
| 1:J:60:LYS:HE3   | 1:J:159:ALA:O   | 2.12                     | 0.50              |
| 1:L:60:LYS:HE2   | 1:L:138:GLU:OE2 | 2.12                     | 0.50              |
| 1:L:79:PHE:CZ    | 1:L:215:MET:HE1 | 2.46                     | 0.50              |
| 1:H:60:LYS:HE3   | 1:H:159:ALA:O   | 2.11                     | 0.50              |
| 1:T:60:LYS:HE3   | 1:T:159:ALA:O   | 2.12                     | 0.50              |
| 1:E:119:THR:OG1  | 1:M:0:LEU:HG    | 2.11                     | 0.49              |
| 1:F:85:ASP:HA    | 1:N:1:MET:SD    | 2.51                     | 0.49              |
| 1:F:131:GLU:HG2  | 1:F:132:TRP:CD1 | 2.47                     | 0.49              |
| 1:J:60:LYS:HE2   | 1:J:138:GLU:OE2 | 2.12                     | 0.49              |
| 1:P:131:GLU:HG2  | 1:P:132:TRP:CD1 | 2.46                     | 0.49              |
| 1:Q:104:ILE:HD12 | 1:Q:104:ILE:H   | 1.77                     | 0.49              |
| 1:C:60:LYS:HE2   | 1:C:138:GLU:OE2 | 2.12                     | 0.49              |
| 1:G:103:ARG:HG3  | 1:G:238:ALA:HA  | 1.92                     | 0.49              |
| 1:G:131:GLU:HG2  | 1:G:132:TRP:CD1 | 2.47                     | 0.49              |
| 1:I:60:LYS:HE3   | 1:I:159:ALA:O   | 2.12                     | 0.49              |
| 1:M:131:GLU:HG2  | 1:M:132:TRP:CD1 | 2.47                     | 0.49              |
| 1:R:71:GLN:O     | 1:R:71:GLN:HG2  | 2.12                     | 0.49              |
| 1:B:60:LYS:HE3   | 1:B:159:ALA:O   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:131:GLU:HG2  | 1:C:132:TRP:CD1  | 2.47                     | 0.49              |
| 1:E:71:GLN:HG2   | 1:E:71:GLN:O     | 2.12                     | 0.49              |
| 1:T:104:ILE:HD11 | 1:T:245:PHE:CZ   | 2.48                     | 0.49              |
| 1:D:60:LYS:HE3   | 1:D:159:ALA:O    | 2.12                     | 0.49              |
| 1:M:60:LYS:HE3   | 1:M:159:ALA:O    | 2.13                     | 0.49              |
| 1:N:60:LYS:HE3   | 1:N:159:ALA:O    | 2.11                     | 0.49              |
| 1:A:104:ILE:HD12 | 1:A:104:ILE:H    | 1.77                     | 0.49              |
| 1:Q:103:ARG:HG3  | 1:Q:238:ALA:HA   | 1.95                     | 0.49              |
| 1:R:180:ASN:HD22 | 1:R:196:ARG:HH21 | 1.61                     | 0.49              |
| 1:L:180:ASN:HD22 | 1:L:196:ARG:HH21 | 1.60                     | 0.49              |
| 1:Q:114:ARG:CA   | 1:Q:224:THR:HB   | 2.40                     | 0.49              |
| 1:L:141:GLY:O    | 1:L:160:SER:HB3  | 2.13                     | 0.49              |
| 1:L:131:GLU:HG2  | 1:L:132:TRP:CD1  | 2.48                     | 0.49              |
| 1:P:60:LYS:HE2   | 1:P:138:GLU:OE2  | 2.12                     | 0.49              |
| 1:F:104:ILE:HD12 | 1:F:104:ILE:H    | 1.78                     | 0.49              |
| 1:G:180:ASN:HD22 | 1:G:196:ARG:HH21 | 1.61                     | 0.49              |
| 1:A:114:ARG:CA   | 1:A:224:THR:HB   | 2.41                     | 0.48              |
| 1:I:141:GLY:O    | 1:I:160:SER:HB3  | 2.12                     | 0.48              |
| 1:R:132:TRP:NE1  | 1:T:128:ASN:HD22 | 1.97                     | 0.48              |
| 1:T:71:GLN:HG2   | 1:T:71:GLN:O     | 2.13                     | 0.48              |
| 1:A:113:ASN:N    | 1:A:113:ASN:OD1  | 2.47                     | 0.48              |
| 1:P:103:ARG:HG3  | 1:P:238:ALA:HA   | 1.95                     | 0.48              |
| 1:G:60:LYS:HE2   | 1:G:138:GLU:OE2  | 2.12                     | 0.48              |
| 1:H:60:LYS:HE2   | 1:H:138:GLU:OE2  | 2.14                     | 0.48              |
| 1:O:180:ASN:HD22 | 1:O:196:ARG:HH21 | 1.61                     | 0.48              |
| 1:A:137:LEU:HB2  | 1:A:165:VAL:HG13 | 1.96                     | 0.48              |
| 1:D:60:LYS:HE2   | 1:D:138:GLU:OE2  | 2.12                     | 0.48              |
| 1:H:131:GLU:HG2  | 1:H:132:TRP:CD1  | 2.48                     | 0.48              |
| 1:J:141:GLY:O    | 1:J:160:SER:HB3  | 2.14                     | 0.48              |
| 1:K:176:LEU:O    | 1:L:169:PRO:HB3  | 2.13                     | 0.48              |
| 1:L:71:GLN:O     | 1:L:71:GLN:HG2   | 2.13                     | 0.48              |
| 1:S:71:GLN:O     | 1:S:71:GLN:HG2   | 2.13                     | 0.48              |
| 1:F:141:GLY:O    | 1:F:160:SER:HB3  | 2.14                     | 0.48              |
| 1:G:71:GLN:O     | 1:G:71:GLN:HG2   | 2.13                     | 0.48              |
| 1:E:113:ASN:OD1  | 1:E:113:ASN:N    | 2.47                     | 0.48              |
| 1:O:60:LYS:HE2   | 1:O:138:GLU:OE2  | 2.13                     | 0.48              |
| 1:Q:222:LEU:HD13 | 1:Q:228:ILE:HD11 | 1.96                     | 0.48              |
| 1:R:131:GLU:HG2  | 1:R:132:TRP:CD1  | 2.49                     | 0.48              |
| 1:B:213:ARG:NH1  | 1:F:1:MET:HE3    | 2.27                     | 0.48              |
| 1:B:222:LEU:HD13 | 1:B:228:ILE:HD11 | 1.94                     | 0.48              |
| 1:H:71:GLN:O     | 1:H:71:GLN:HG2   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:71:GLN:O     | 1:K:71:GLN:HG2   | 2.14                     | 0.48              |
| 1:L:60:LYS:HE3   | 1:L:159:ALA:O    | 2.13                     | 0.48              |
| 1:Q:71:GLN:O     | 1:Q:71:GLN:HG2   | 2.12                     | 0.48              |
| 1:J:71:GLN:HG2   | 1:J:71:GLN:O     | 2.14                     | 0.48              |
| 1:L:104:ILE:HD11 | 1:L:245:PHE:CZ   | 2.48                     | 0.48              |
| 1:R:141:GLY:O    | 1:R:160:SER:HB3  | 2.13                     | 0.48              |
| 1:S:60:LYS:HE2   | 1:S:138:GLU:OE2  | 2.14                     | 0.48              |
| 1:D:71:GLN:O     | 1:D:71:GLN:HG2   | 2.14                     | 0.47              |
| 1:H:128:ASN:ND2  | 1:I:132:TRP:HE1  | 1.88                     | 0.47              |
| 1:N:137:LEU:HB2  | 1:N:165:VAL:HG13 | 1.96                     | 0.47              |
| 1:T:137:LEU:HB2  | 1:T:165:VAL:HG13 | 1.97                     | 0.47              |
| 1:C:141:GLY:O    | 1:C:160:SER:HB3  | 2.14                     | 0.47              |
| 1:H:137:LEU:HB2  | 1:H:165:VAL:HG13 | 1.96                     | 0.47              |
| 1:I:103:ARG:HG3  | 1:I:238:ALA:HA   | 1.96                     | 0.47              |
| 1:F:71:GLN:O     | 1:F:71:GLN:HG2   | 2.13                     | 0.47              |
| 1:G:104:ILE:CD1  | 1:G:245:PHE:CE2  | 2.95                     | 0.47              |
| 1:L:114:ARG:CA   | 1:L:224:THR:HB   | 2.41                     | 0.47              |
| 1:O:71:GLN:HG2   | 1:O:71:GLN:O     | 2.13                     | 0.47              |
| 1:F:114:ARG:CA   | 1:F:224:THR:HB   | 2.44                     | 0.47              |
| 1:P:180:ASN:HD22 | 1:P:196:ARG:HH21 | 1.63                     | 0.47              |
| 1:R:59:ARG:HB2   | 1:R:211:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:60:LYS:HE3   | 1:A:159:ALA:O    | 2.14                     | 0.47              |
| 1:A:71:GLN:O     | 1:A:71:GLN:HG2   | 2.14                     | 0.47              |
| 1:D:103:ARG:HG3  | 1:D:238:ALA:HA   | 1.96                     | 0.47              |
| 1:I:71:GLN:O     | 1:I:71:GLN:HG2   | 2.14                     | 0.47              |
| 1:K:59:ARG:HB2   | 1:K:211:LEU:HD21 | 1.97                     | 0.47              |
| 1:T:0:LEU:HA     | 1:T:3:LYS:HB2    | 1.96                     | 0.47              |
| 1:C:104:ILE:CD1  | 1:C:245:PHE:CE2  | 2.97                     | 0.47              |
| 1:I:1:MET:SD     | 1:K:85:ASP:HA    | 2.55                     | 0.47              |
| 1:F:187:ARG:HB2  | 1:F:245:PHE:CE2  | 2.50                     | 0.47              |
| 1:M:71:GLN:O     | 1:M:71:GLN:HG2   | 2.15                     | 0.47              |
| 1:P:71:GLN:O     | 1:P:71:GLN:HG2   | 2.14                     | 0.47              |
| 1:A:141:GLY:O    | 1:A:160:SER:HB3  | 2.15                     | 0.46              |
| 1:G:137:LEU:HB2  | 1:G:165:VAL:HG13 | 1.96                     | 0.46              |
| 1:E:60:LYS:HE2   | 1:E:138:GLU:OE2  | 2.15                     | 0.46              |
| 1:H:1:MET:HE3    | 1:R:213:ARG:CZ   | 2.43                     | 0.46              |
| 1:O:141:GLY:O    | 1:O:160:SER:HB3  | 2.16                     | 0.46              |
| 1:J:113:ASN:OD1  | 1:J:129:ALA:O    | 2.33                     | 0.46              |
| 1:B:71:GLN:O     | 1:B:71:GLN:HG2   | 2.15                     | 0.46              |
| 1:A:135:PRO:HB2  | 1:A:255:VAL:HG22 | 1.97                     | 0.46              |
| 1:N:71:GLN:O     | 1:N:71:GLN:HG2   | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:103:ARG:HG3  | 1:O:238:ALA:HA   | 1.97                     | 0.46              |
| 1:Q:60:LYS:HE2   | 1:Q:138:GLU:OE2  | 2.15                     | 0.46              |
| 1:R:114:ARG:CA   | 1:R:224:THR:HB   | 2.45                     | 0.46              |
| 1:T:180:ASN:HD22 | 1:T:196:ARG:HH21 | 1.64                     | 0.46              |
| 1:I:180:ASN:HD22 | 1:I:196:ARG:HH21 | 1.62                     | 0.46              |
| 1:M:141:GLY:O    | 1:M:160:SER:HB3  | 2.16                     | 0.46              |
| 1:H:90:ASP:HB2   | 1:H:167:GLY:HA2  | 1.98                     | 0.46              |
| 1:K:141:GLY:O    | 1:K:160:SER:HB3  | 2.16                     | 0.46              |
| 1:S:60:LYS:HE3   | 1:S:159:ALA:O    | 2.16                     | 0.46              |
| 1:A:59:ARG:HB2   | 1:A:211:LEU:HD21 | 1.96                     | 0.46              |
| 1:G:114:ARG:CA   | 1:G:224:THR:HB   | 2.42                     | 0.45              |
| 1:J:103:ARG:HG3  | 1:J:238:ALA:HA   | 1.97                     | 0.45              |
| 1:M:103:ARG:HG3  | 1:M:238:ALA:HA   | 1.97                     | 0.45              |
| 1:L:59:ARG:HB2   | 1:L:211:LEU:HD21 | 1.98                     | 0.45              |
| 1:N:180:ASN:HD22 | 1:N:196:ARG:HH21 | 1.63                     | 0.45              |
| 1:Q:137:LEU:HB2  | 1:Q:165:VAL:HG13 | 1.98                     | 0.45              |
| 1:B:103:ARG:HG3  | 1:B:238:ALA:HA   | 1.98                     | 0.45              |
| 1:H:103:ARG:HG3  | 1:H:238:ALA:HA   | 1.98                     | 0.45              |
| 1:K:137:LEU:HB2  | 1:K:165:VAL:HG13 | 1.98                     | 0.45              |
| 1:E:180:ASN:HD22 | 1:E:196:ARG:HH21 | 1.63                     | 0.45              |
| 1:J:104:ILE:CD1  | 1:J:245:PHE:CE2  | 2.98                     | 0.45              |
| 1:J:191:GLU:OE1  | 5:J:2011:HOH:O   | 2.21                     | 0.45              |
| 1:P:90:ASP:HB2   | 1:P:167:GLY:HA2  | 1.99                     | 0.45              |
| 1:T:141:GLY:O    | 1:T:160:SER:HB3  | 2.16                     | 0.45              |
| 1:C:71:GLN:O     | 1:C:71:GLN:HG2   | 2.15                     | 0.45              |
| 1:F:137:LEU:HB2  | 1:F:165:VAL:HG13 | 1.99                     | 0.45              |
| 1:J:180:ASN:HD22 | 1:J:196:ARG:HH21 | 1.63                     | 0.45              |
| 1:N:141:GLY:O    | 1:N:160:SER:HB3  | 2.16                     | 0.45              |
| 1:Q:90:ASP:HB2   | 1:Q:167:GLY:HA2  | 1.99                     | 0.45              |
| 1:R:60:LYS:HE2   | 1:R:138:GLU:OE2  | 2.16                     | 0.45              |
| 1:D:141:GLY:O    | 1:D:160:SER:HB3  | 2.16                     | 0.45              |
| 1:D:180:ASN:HD22 | 1:D:196:ARG:HH21 | 1.64                     | 0.45              |
| 1:E:103:ARG:HG3  | 1:E:238:ALA:HA   | 1.98                     | 0.45              |
| 1:B:137:LEU:HB2  | 1:B:165:VAL:HG13 | 1.97                     | 0.45              |
| 1:O:90:ASP:HB2   | 1:O:167:GLY:HA2  | 1.99                     | 0.45              |
| 1:T:222:LEU:HD13 | 1:T:228:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:180:ASN:HD22 | 1:B:196:ARG:HH21 | 1.64                     | 0.45              |
| 1:B:213:ARG:HH11 | 1:F:1:MET:CE     | 2.27                     | 0.45              |
| 1:D:114:ARG:CA   | 1:D:224:THR:HB   | 2.46                     | 0.45              |
| 1:R:137:LEU:HB2  | 1:R:165:VAL:HG13 | 1.98                     | 0.45              |
| 1:S:222:LEU:HD13 | 1:S:228:ILE:HD11 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:137:LEU:HB2  | 1:C:165:VAL:HG13 | 1.97                     | 0.44              |
| 1:D:137:LEU:HB2  | 1:D:165:VAL:HG13 | 1.98                     | 0.44              |
| 1:H:1:MET:HE2    | 1:R:120:ASP:HB2  | 1.99                     | 0.44              |
| 1:M:222:LEU:HD13 | 1:M:228:ILE:HD11 | 1.99                     | 0.44              |
| 1:S:103:ARG:HG3  | 1:S:238:ALA:HA   | 1.99                     | 0.44              |
| 1:A:90:ASP:HB2   | 1:A:167:GLY:HA2  | 1.99                     | 0.44              |
| 1:G:187:ARG:HB2  | 1:G:245:PHE:CE2  | 2.51                     | 0.44              |
| 1:R:222:LEU:HD13 | 1:R:228:ILE:HD11 | 2.00                     | 0.44              |
| 1:S:114:ARG:CA   | 1:S:224:THR:HB   | 2.43                     | 0.44              |
| 1:S:141:GLY:O    | 1:S:160:SER:HB3  | 2.17                     | 0.44              |
| 1:B:135:PRO:HB2  | 1:B:255:VAL:HG22 | 2.00                     | 0.44              |
| 1:J:137:LEU:HB2  | 1:J:165:VAL:HG13 | 2.00                     | 0.44              |
| 1:E:141:GLY:O    | 1:E:160:SER:HB3  | 2.18                     | 0.44              |
| 1:N:103:ARG:HG3  | 1:N:238:ALA:HA   | 2.00                     | 0.44              |
| 1:G:222:LEU:HD13 | 1:G:228:ILE:HD11 | 1.99                     | 0.44              |
| 1:J:222:LEU:HD13 | 1:J:228:ILE:HD11 | 1.99                     | 0.44              |
| 1:N:90:ASP:HB2   | 1:N:167:GLY:HA2  | 1.98                     | 0.44              |
| 1:O:135:PRO:HB2  | 1:O:255:VAL:HG22 | 2.00                     | 0.44              |
| 1:T:114:ARG:CA   | 1:T:224:THR:HB   | 2.45                     | 0.44              |
| 1:H:114:ARG:CA   | 1:H:224:THR:HB   | 2.46                     | 0.44              |
| 1:K:114:ARG:CA   | 1:K:224:THR:HB   | 2.46                     | 0.44              |
| 1:N:222:LEU:HD13 | 1:N:228:ILE:HD11 | 2.00                     | 0.44              |
| 1:P:222:LEU:HD13 | 1:P:228:ILE:HD11 | 2.00                     | 0.44              |
| 1:H:135:PRO:HB2  | 1:H:255:VAL:HG22 | 2.00                     | 0.44              |
| 1:H:180:ASN:HD22 | 1:H:196:ARG:HH21 | 1.64                     | 0.44              |
| 1:I:222:LEU:HD13 | 1:I:228:ILE:HD11 | 2.00                     | 0.44              |
| 1:L:137:LEU:HB2  | 1:L:165:VAL:HG13 | 1.99                     | 0.44              |
| 1:I:0:LEU:HB3    | 1:N:120:ASP:HB3  | 1.98                     | 0.44              |
| 1:I:114:ARG:CA   | 1:I:224:THR:HB   | 2.44                     | 0.44              |
| 1:N:114:ARG:CA   | 1:N:224:THR:HB   | 2.44                     | 0.44              |
| 1:P:141:GLY:O    | 1:P:160:SER:HB3  | 2.17                     | 0.44              |
| 1:H:113:ASN:ND2  | 1:H:129:ALA:HA   | 2.33                     | 0.43              |
| 1:R:90:ASP:HB2   | 1:R:167:GLY:HA2  | 1.99                     | 0.43              |
| 1:C:222:LEU:HD13 | 1:C:228:ILE:HD11 | 1.99                     | 0.43              |
| 1:D:90:ASP:HB2   | 1:D:167:GLY:HA2  | 2.00                     | 0.43              |
| 1:A:180:ASN:HD22 | 1:A:196:ARG:HH21 | 1.66                     | 0.43              |
| 1:B:128:ASN:ND2  | 1:E:132:TRP:HE1  | 1.87                     | 0.43              |
| 1:F:222:LEU:HD13 | 1:F:228:ILE:HD11 | 2.00                     | 0.43              |
| 1:J:114:ARG:CA   | 1:J:224:THR:HB   | 2.45                     | 0.43              |
| 1:O:137:LEU:HB2  | 1:O:165:VAL:HG13 | 1.99                     | 0.43              |
| 1:Q:104:ILE:CD1  | 1:Q:245:PHE:CE2  | 3.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:60:LYS:NZ    | 2:L:1262:PO4:O2  | 2.51                     | 0.43              |
| 1:Q:113:ASN:ND2  | 1:Q:129:ALA:HA   | 2.34                     | 0.43              |
| 1:Q:141:GLY:O    | 1:Q:160:SER:HB3  | 2.17                     | 0.43              |
| 1:S:180:ASN:HD22 | 1:S:196:ARG:HH21 | 1.66                     | 0.43              |
| 1:I:113:ASN:ND2  | 1:I:129:ALA:HA   | 2.33                     | 0.43              |
| 1:M:114:ARG:CA   | 1:M:224:THR:HB   | 2.46                     | 0.43              |
| 1:M:180:ASN:HD22 | 1:M:196:ARG:HH21 | 1.65                     | 0.43              |
| 1:O:59:ARG:HB2   | 1:O:211:LEU:HD21 | 2.01                     | 0.43              |
| 1:Q:180:ASN:HD22 | 1:Q:196:ARG:HH21 | 1.67                     | 0.43              |
| 1:I:120:ASP:HB3  | 1:N:0:LEU:HB3    | 1.99                     | 0.43              |
| 1:J:164:TYR:HE2  | 1:J:166:ILE:CD1  | 2.32                     | 0.43              |
| 1:K:180:ASN:HD22 | 1:K:196:ARG:HH21 | 1.66                     | 0.43              |
| 1:R:104:ILE:HG13 | 1:R:239:VAL:CG2  | 2.49                     | 0.43              |
| 1:B:59:ARG:HB2   | 1:B:211:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:222:LEU:HD13 | 1:D:228:ILE:HD11 | 1.99                     | 0.43              |
| 1:L:222:LEU:HD13 | 1:L:228:ILE:HD11 | 2.01                     | 0.43              |
| 1:S:59:ARG:HB2   | 1:S:211:LEU:HD21 | 2.01                     | 0.43              |
| 1:T:135:PRO:HB2  | 1:T:255:VAL:HG22 | 2.01                     | 0.43              |
| 1:B:141:GLY:O    | 1:B:160:SER:HB3  | 2.18                     | 0.42              |
| 1:E:222:LEU:HD13 | 1:E:228:ILE:HD11 | 2.01                     | 0.42              |
| 1:G:90:ASP:HB2   | 1:G:167:GLY:HA2  | 2.00                     | 0.42              |
| 1:M:193:SER:HA   | 5:M:2008:HOH:O   | 2.19                     | 0.42              |
| 1:R:164:TYR:HE2  | 1:R:166:ILE:CD1  | 2.32                     | 0.42              |
| 1:S:137:LEU:HB2  | 1:S:165:VAL:HG13 | 2.00                     | 0.42              |
| 1:L:90:ASP:HB2   | 1:L:167:GLY:HA2  | 2.01                     | 0.42              |
| 1:N:104:ILE:HG13 | 1:N:239:VAL:CG2  | 2.49                     | 0.42              |
| 1:M:90:ASP:HB2   | 1:M:167:GLY:HA2  | 2.02                     | 0.42              |
| 1:T:187:ARG:HB2  | 1:T:245:PHE:CE2  | 2.55                     | 0.42              |
| 1:B:167:GLY:HA3  | 1:B:255:VAL:HG13 | 2.02                     | 0.42              |
| 1:I:90:ASP:HB2   | 1:I:167:GLY:HA2  | 2.01                     | 0.42              |
| 1:E:1:MET:CE     | 1:M:213:ARG:HH11 | 2.33                     | 0.42              |
| 1:F:15:ARG:NH1   | 2:F:1262:PO4:O3  | 2.53                     | 0.42              |
| 1:R:103:ARG:HG3  | 1:R:238:ALA:HA   | 2.01                     | 0.42              |
| 1:G:59:ARG:HB2   | 1:G:211:LEU:HD21 | 2.01                     | 0.42              |
| 1:T:103:ARG:HG3  | 1:T:238:ALA:HA   | 2.01                     | 0.42              |
| 1:B:90:ASP:HB2   | 1:B:167:GLY:HA2  | 2.02                     | 0.42              |
| 1:G:71:GLN:O     | 1:G:72:LEU:HD12  | 2.20                     | 0.42              |
| 1:I:137:LEU:HB2  | 1:I:165:VAL:HG13 | 2.02                     | 0.42              |
| 1:K:90:ASP:HB2   | 1:K:167:GLY:HA2  | 2.01                     | 0.42              |
| 1:C:180:ASN:HD22 | 1:C:196:ARG:HH21 | 1.67                     | 0.42              |
| 1:E:59:ARG:HB2   | 1:E:211:LEU:HD21 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:104:ILE:HG13 | 1:G:239:VAL:CG2  | 2.50                     | 0.42              |
| 1:H:222:LEU:HD13 | 1:H:228:ILE:HD11 | 2.02                     | 0.42              |
| 1:S:135:PRO:HB2  | 1:S:255:VAL:HG22 | 2.02                     | 0.42              |
| 1:F:180:ASN:HD22 | 1:F:196:ARG:HH21 | 1.68                     | 0.42              |
| 1:J:59:ARG:HB2   | 1:J:211:LEU:HD21 | 2.01                     | 0.42              |
| 1:O:114:ARG:CA   | 1:O:224:THR:HB   | 2.47                     | 0.42              |
| 1:P:137:LEU:HB2  | 1:P:165:VAL:HG13 | 2.02                     | 0.42              |
| 1:L:113:ASN:ND2  | 1:L:129:ALA:HA   | 2.35                     | 0.41              |
| 1:O:222:LEU:HD13 | 1:O:228:ILE:HD11 | 2.02                     | 0.41              |
| 1:E:90:ASP:HB2   | 1:E:167:GLY:HA2  | 2.02                     | 0.41              |
| 1:I:59:ARG:HB2   | 1:I:211:LEU:HD21 | 2.02                     | 0.41              |
| 1:R:71:GLN:O     | 1:R:72:LEU:HD12  | 2.20                     | 0.41              |
| 1:Q:60:LYS:NZ    | 2:Q:1262:PO4:O2  | 2.53                     | 0.41              |
| 1:E:137:LEU:HB2  | 1:E:165:VAL:HG13 | 2.02                     | 0.41              |
| 1:K:213:ARG:CZ   | 1:T:1:MET:HE3    | 2.43                     | 0.41              |
| 1:M:135:PRO:HB2  | 1:M:255:VAL:HG22 | 2.03                     | 0.41              |
| 1:M:137:LEU:HB2  | 1:M:165:VAL:HG13 | 2.03                     | 0.41              |
| 1:C:135:PRO:HB2  | 1:C:255:VAL:HG22 | 2.03                     | 0.41              |
| 1:I:167:GLY:HA3  | 1:I:255:VAL:HG13 | 2.03                     | 0.41              |
| 1:P:113:ASN:ND2  | 1:P:129:ALA:HA   | 2.36                     | 0.41              |
| 1:A:103:ARG:HG3  | 1:A:238:ALA:HA   | 2.02                     | 0.41              |
| 1:E:114:ARG:CA   | 1:E:224:THR:HB   | 2.45                     | 0.41              |
| 1:Q:59:ARG:HB2   | 1:Q:211:LEU:HD21 | 2.03                     | 0.41              |
| 1:F:164:TYR:HE2  | 1:F:166:ILE:CD1  | 2.34                     | 0.41              |
| 1:C:193:SER:HA   | 5:C:2010:HOH:O   | 2.19                     | 0.41              |
| 1:G:135:PRO:HB2  | 1:G:255:VAL:HG22 | 2.02                     | 0.41              |
| 1:J:90:ASP:HB2   | 1:J:167:GLY:HA2  | 2.03                     | 0.41              |
| 1:A:222:LEU:HD13 | 1:A:228:ILE:HD11 | 2.03                     | 0.41              |
| 1:C:90:ASP:HB2   | 1:C:167:GLY:HA2  | 2.03                     | 0.41              |
| 1:F:15:ARG:HD3   | 2:F:1262:PO4:O2  | 2.20                     | 0.41              |
| 1:G:187:ARG:O    | 1:G:188:ASN:C    | 2.63                     | 0.41              |
| 1:G:246:GLU:HG3  | 1:G:256:ALA:HB2  | 2.02                     | 0.41              |
| 1:H:59:ARG:HB2   | 1:H:211:LEU:HD21 | 2.03                     | 0.41              |
| 1:K:135:PRO:HB2  | 1:K:255:VAL:HG22 | 2.03                     | 0.41              |
| 1:K:164:TYR:HE2  | 1:K:166:ILE:CD1  | 2.34                     | 0.41              |
| 1:Q:135:PRO:HB2  | 1:Q:255:VAL:HG22 | 2.02                     | 0.41              |
| 1:E:164:TYR:HE2  | 1:E:166:ILE:CD1  | 2.34                     | 0.41              |
| 1:N:104:ILE:CD1  | 1:N:245:PHE:CE2  | 3.04                     | 0.41              |
| 1:P:104:ILE:HG13 | 1:P:239:VAL:CG2  | 2.51                     | 0.41              |
| 1:C:59:ARG:HB2   | 1:C:211:LEU:HD21 | 2.02                     | 0.40              |
| 1:D:60:LYS:NZ    | 2:D:1263:PO4:O4  | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:104:ILE:HG13 | 1:M:239:VAL:CG2  | 2.51                     | 0.40              |
| 1:M:113:ASN:ND2  | 1:M:129:ALA:HA   | 2.36                     | 0.40              |
| 1:R:135:PRO:HB2  | 1:R:255:VAL:HG22 | 2.03                     | 0.40              |
| 1:L:164:TYR:HE2  | 1:L:166:ILE:CD1  | 2.34                     | 0.40              |
| 1:L:187:ARG:HB2  | 1:L:245:PHE:CE2  | 2.56                     | 0.40              |
| 1:N:59:ARG:HB2   | 1:N:211:LEU:HD21 | 2.03                     | 0.40              |
| 1:S:104:ILE:HG13 | 1:S:239:VAL:CG2  | 2.51                     | 0.40              |
| 1:N:164:TYR:HE2  | 1:N:166:ILE:CD1  | 2.34                     | 0.40              |
| 1:A:164:TYR:HE2  | 1:A:166:ILE:CD1  | 2.34                     | 0.40              |
| 1:G:15:ARG:HD3   | 2:G:1262:PO4:O2  | 2.22                     | 0.40              |
| 1:L:0:LEU:HD22   | 1:L:3:LYS:HD2    | 2.03                     | 0.40              |
| 1:P:59:ARG:HB2   | 1:P:211:LEU:HD21 | 2.04                     | 0.40              |
| 1:C:164:TYR:HE2  | 1:C:166:ILE:CD1  | 2.34                     | 0.40              |
| 1:H:164:TYR:HE2  | 1:H:166:ILE:CD1  | 2.33                     | 0.40              |
| 1:K:113:ASN:ND2  | 1:K:129:ALA:HA   | 2.37                     | 0.40              |
| 1:K:222:LEU:HD13 | 1:K:228:ILE:HD11 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 260/270 (96%) | 250 (96%) | 9 (4%)  | 1 (0%)   | 30          | 60 |
| 1   | B     | 260/270 (96%) | 250 (96%) | 9 (4%)  | 1 (0%)   | 30          | 60 |
| 1   | C     | 260/270 (96%) | 253 (97%) | 5 (2%)  | 2 (1%)   | 16          | 44 |
| 1   | D     | 260/270 (96%) | 251 (96%) | 7 (3%)  | 2 (1%)   | 16          | 44 |
| 1   | E     | 260/270 (96%) | 252 (97%) | 7 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | F     | 260/270 (96%) | 251 (96%) | 8 (3%)  | 1 (0%)   | 30          | 60 |
| 1   | G     | 260/270 (96%) | 251 (96%) | 7 (3%)  | 2 (1%)   | 16          | 44 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | H     | 260/270 (96%)   | 252 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | I     | 260/270 (96%)   | 251 (96%)  | 8 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | J     | 260/270 (96%)   | 252 (97%)  | 6 (2%)   | 2 (1%)   | 16          | 44 |
| 1   | K     | 260/270 (96%)   | 251 (96%)  | 8 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | L     | 260/270 (96%)   | 251 (96%)  | 8 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | M     | 260/270 (96%)   | 252 (97%)  | 6 (2%)   | 2 (1%)   | 16          | 44 |
| 1   | N     | 260/270 (96%)   | 252 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | O     | 260/270 (96%)   | 251 (96%)  | 8 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | P     | 260/270 (96%)   | 251 (96%)  | 7 (3%)   | 2 (1%)   | 16          | 44 |
| 1   | Q     | 260/270 (96%)   | 252 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 60 |
| 1   | R     | 260/270 (96%)   | 251 (96%)  | 7 (3%)   | 2 (1%)   | 16          | 44 |
| 1   | S     | 260/270 (96%)   | 253 (97%)  | 6 (2%)   | 1 (0%)   | 30          | 60 |
| 1   | T     | 260/270 (96%)   | 252 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 60 |
| All | All   | 5200/5400 (96%) | 5029 (97%) | 144 (3%) | 27 (0%)  | 24          | 55 |

All (27) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 260 | SER  |
| 1   | J     | 260 | SER  |
| 1   | A     | 77  | PRO  |
| 1   | C     | 260 | SER  |
| 1   | D     | 260 | SER  |
| 1   | F     | 77  | PRO  |
| 1   | G     | 77  | PRO  |
| 1   | H     | 77  | PRO  |
| 1   | I     | 77  | PRO  |
| 1   | L     | 77  | PRO  |
| 1   | M     | 260 | SER  |
| 1   | N     | 77  | PRO  |
| 1   | P     | 260 | SER  |
| 1   | R     | 77  | PRO  |
| 1   | R     | 260 | SER  |
| 1   | S     | 77  | PRO  |
| 1   | B     | 77  | PRO  |
| 1   | C     | 77  | PRO  |
| 1   | D     | 77  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 77  | PRO  |
| 1   | J     | 77  | PRO  |
| 1   | K     | 77  | PRO  |
| 1   | M     | 77  | PRO  |
| 1   | O     | 77  | PRO  |
| 1   | P     | 77  | PRO  |
| 1   | Q     | 77  | PRO  |
| 1   | T     | 77  | PRO  |

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 207/212 (98%) | 178 (86%) | 29 (14%) | 3           | 12 |
| 1   | B     | 207/212 (98%) | 177 (86%) | 30 (14%) | 3           | 11 |
| 1   | C     | 207/212 (98%) | 180 (87%) | 27 (13%) | 4           | 14 |
| 1   | D     | 207/212 (98%) | 179 (86%) | 28 (14%) | 4           | 13 |
| 1   | E     | 207/212 (98%) | 179 (86%) | 28 (14%) | 4           | 13 |
| 1   | F     | 207/212 (98%) | 178 (86%) | 29 (14%) | 3           | 12 |
| 1   | G     | 207/212 (98%) | 179 (86%) | 28 (14%) | 4           | 13 |
| 1   | H     | 207/212 (98%) | 178 (86%) | 29 (14%) | 3           | 12 |
| 1   | I     | 207/212 (98%) | 179 (86%) | 28 (14%) | 4           | 13 |
| 1   | J     | 207/212 (98%) | 179 (86%) | 28 (14%) | 4           | 13 |
| 1   | K     | 207/212 (98%) | 179 (86%) | 28 (14%) | 4           | 13 |
| 1   | L     | 207/212 (98%) | 181 (87%) | 26 (13%) | 4           | 15 |
| 1   | M     | 207/212 (98%) | 178 (86%) | 29 (14%) | 3           | 12 |
| 1   | N     | 207/212 (98%) | 179 (86%) | 28 (14%) | 4           | 13 |
| 1   | O     | 207/212 (98%) | 180 (87%) | 27 (13%) | 4           | 14 |
| 1   | P     | 207/212 (98%) | 178 (86%) | 29 (14%) | 3           | 12 |
| 1   | Q     | 207/212 (98%) | 180 (87%) | 27 (13%) | 4           | 14 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | R     | 207/212 (98%)   | 178 (86%)  | 29 (14%)  | 3           | 12 |
| 1   | S     | 207/212 (98%)   | 178 (86%)  | 29 (14%)  | 3           | 12 |
| 1   | T     | 207/212 (98%)   | 181 (87%)  | 26 (13%)  | 4           | 15 |
| All | All   | 4140/4240 (98%) | 3578 (86%) | 562 (14%) | 3           | 13 |

All (562) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 0   | LEU  |
| 1   | A     | 1   | MET  |
| 1   | A     | 6   | LEU  |
| 1   | A     | 13  | LEU  |
| 1   | A     | 26  | LEU  |
| 1   | A     | 28  | ASP  |
| 1   | A     | 47  | GLN  |
| 1   | A     | 60  | LYS  |
| 1   | A     | 74  | VAL  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 104 | ILE  |
| 1   | A     | 113 | ASN  |
| 1   | A     | 114 | ARG  |
| 1   | A     | 127 | TYR  |
| 1   | A     | 133 | VAL  |
| 1   | A     | 134 | LEU  |
| 1   | A     | 149 | ILE  |
| 1   | A     | 152 | VAL  |
| 1   | A     | 154 | THR  |
| 1   | A     | 160 | SER  |
| 1   | A     | 165 | VAL  |
| 1   | A     | 166 | ILE  |
| 1   | A     | 184 | LYS  |
| 1   | A     | 191 | GLU  |
| 1   | A     | 214 | LYS  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 224 | THR  |
| 1   | A     | 237 | VAL  |
| 1   | A     | 255 | VAL  |
| 1   | B     | 0   | LEU  |
| 1   | B     | 1   | MET  |
| 1   | B     | 5   | THR  |
| 1   | B     | 6   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 13  | LEU  |
| 1   | B     | 26  | LEU  |
| 1   | B     | 28  | ASP  |
| 1   | B     | 47  | GLN  |
| 1   | B     | 60  | LYS  |
| 1   | B     | 74  | VAL  |
| 1   | B     | 103 | ARG  |
| 1   | B     | 104 | ILE  |
| 1   | B     | 113 | ASN  |
| 1   | B     | 114 | ARG  |
| 1   | B     | 127 | TYR  |
| 1   | B     | 133 | VAL  |
| 1   | B     | 134 | LEU  |
| 1   | B     | 149 | ILE  |
| 1   | B     | 152 | VAL  |
| 1   | B     | 154 | THR  |
| 1   | B     | 160 | SER  |
| 1   | B     | 165 | VAL  |
| 1   | B     | 166 | ILE  |
| 1   | B     | 184 | LYS  |
| 1   | B     | 191 | GLU  |
| 1   | B     | 214 | LYS  |
| 1   | B     | 218 | LEU  |
| 1   | B     | 224 | THR  |
| 1   | B     | 237 | VAL  |
| 1   | B     | 255 | VAL  |
| 1   | C     | 1   | MET  |
| 1   | C     | 6   | LEU  |
| 1   | C     | 13  | LEU  |
| 1   | C     | 26  | LEU  |
| 1   | C     | 28  | ASP  |
| 1   | C     | 47  | GLN  |
| 1   | C     | 60  | LYS  |
| 1   | C     | 74  | VAL  |
| 1   | C     | 103 | ARG  |
| 1   | C     | 104 | ILE  |
| 1   | C     | 113 | ASN  |
| 1   | C     | 114 | ARG  |
| 1   | C     | 127 | TYR  |
| 1   | C     | 133 | VAL  |
| 1   | C     | 134 | LEU  |
| 1   | C     | 149 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 152 | VAL  |
| 1   | C     | 154 | THR  |
| 1   | C     | 160 | SER  |
| 1   | C     | 165 | VAL  |
| 1   | C     | 166 | ILE  |
| 1   | C     | 196 | ARG  |
| 1   | C     | 214 | LYS  |
| 1   | C     | 218 | LEU  |
| 1   | C     | 224 | THR  |
| 1   | C     | 237 | VAL  |
| 1   | C     | 255 | VAL  |
| 1   | D     | 1   | MET  |
| 1   | D     | 6   | LEU  |
| 1   | D     | 13  | LEU  |
| 1   | D     | 26  | LEU  |
| 1   | D     | 28  | ASP  |
| 1   | D     | 47  | GLN  |
| 1   | D     | 60  | LYS  |
| 1   | D     | 74  | VAL  |
| 1   | D     | 103 | ARG  |
| 1   | D     | 104 | ILE  |
| 1   | D     | 113 | ASN  |
| 1   | D     | 114 | ARG  |
| 1   | D     | 127 | TYR  |
| 1   | D     | 133 | VAL  |
| 1   | D     | 134 | LEU  |
| 1   | D     | 149 | ILE  |
| 1   | D     | 152 | VAL  |
| 1   | D     | 154 | THR  |
| 1   | D     | 160 | SER  |
| 1   | D     | 165 | VAL  |
| 1   | D     | 166 | ILE  |
| 1   | D     | 191 | GLU  |
| 1   | D     | 196 | ARG  |
| 1   | D     | 214 | LYS  |
| 1   | D     | 218 | LEU  |
| 1   | D     | 224 | THR  |
| 1   | D     | 237 | VAL  |
| 1   | D     | 255 | VAL  |
| 1   | E     | 1   | MET  |
| 1   | E     | 6   | LEU  |
| 1   | E     | 13  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 26  | LEU  |
| 1   | E     | 28  | ASP  |
| 1   | E     | 60  | LYS  |
| 1   | E     | 74  | VAL  |
| 1   | E     | 103 | ARG  |
| 1   | E     | 104 | ILE  |
| 1   | E     | 113 | ASN  |
| 1   | E     | 114 | ARG  |
| 1   | E     | 127 | TYR  |
| 1   | E     | 133 | VAL  |
| 1   | E     | 134 | LEU  |
| 1   | E     | 149 | ILE  |
| 1   | E     | 152 | VAL  |
| 1   | E     | 154 | THR  |
| 1   | E     | 160 | SER  |
| 1   | E     | 165 | VAL  |
| 1   | E     | 166 | ILE  |
| 1   | E     | 184 | LYS  |
| 1   | E     | 191 | GLU  |
| 1   | E     | 196 | ARG  |
| 1   | E     | 214 | LYS  |
| 1   | E     | 218 | LEU  |
| 1   | E     | 224 | THR  |
| 1   | E     | 237 | VAL  |
| 1   | E     | 255 | VAL  |
| 1   | F     | 1   | MET  |
| 1   | F     | 6   | LEU  |
| 1   | F     | 13  | LEU  |
| 1   | F     | 26  | LEU  |
| 1   | F     | 28  | ASP  |
| 1   | F     | 47  | GLN  |
| 1   | F     | 60  | LYS  |
| 1   | F     | 74  | VAL  |
| 1   | F     | 103 | ARG  |
| 1   | F     | 104 | ILE  |
| 1   | F     | 113 | ASN  |
| 1   | F     | 114 | ARG  |
| 1   | F     | 127 | TYR  |
| 1   | F     | 133 | VAL  |
| 1   | F     | 134 | LEU  |
| 1   | F     | 149 | ILE  |
| 1   | F     | 152 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 154 | THR  |
| 1   | F     | 160 | SER  |
| 1   | F     | 165 | VAL  |
| 1   | F     | 166 | ILE  |
| 1   | F     | 191 | GLU  |
| 1   | F     | 192 | VAL  |
| 1   | F     | 214 | LYS  |
| 1   | F     | 218 | LEU  |
| 1   | F     | 224 | THR  |
| 1   | F     | 237 | VAL  |
| 1   | F     | 244 | ARG  |
| 1   | F     | 255 | VAL  |
| 1   | G     | 0   | LEU  |
| 1   | G     | 6   | LEU  |
| 1   | G     | 13  | LEU  |
| 1   | G     | 26  | LEU  |
| 1   | G     | 28  | ASP  |
| 1   | G     | 47  | GLN  |
| 1   | G     | 60  | LYS  |
| 1   | G     | 74  | VAL  |
| 1   | G     | 103 | ARG  |
| 1   | G     | 104 | ILE  |
| 1   | G     | 113 | ASN  |
| 1   | G     | 114 | ARG  |
| 1   | G     | 127 | TYR  |
| 1   | G     | 133 | VAL  |
| 1   | G     | 134 | LEU  |
| 1   | G     | 149 | ILE  |
| 1   | G     | 152 | VAL  |
| 1   | G     | 154 | THR  |
| 1   | G     | 160 | SER  |
| 1   | G     | 165 | VAL  |
| 1   | G     | 166 | ILE  |
| 1   | G     | 184 | LYS  |
| 1   | G     | 191 | GLU  |
| 1   | G     | 214 | LYS  |
| 1   | G     | 218 | LEU  |
| 1   | G     | 224 | THR  |
| 1   | G     | 237 | VAL  |
| 1   | G     | 255 | VAL  |
| 1   | H     | 0   | LEU  |
| 1   | H     | 6   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 13  | LEU  |
| 1   | H     | 26  | LEU  |
| 1   | H     | 28  | ASP  |
| 1   | H     | 47  | GLN  |
| 1   | H     | 60  | LYS  |
| 1   | H     | 74  | VAL  |
| 1   | H     | 103 | ARG  |
| 1   | H     | 104 | ILE  |
| 1   | H     | 113 | ASN  |
| 1   | H     | 114 | ARG  |
| 1   | H     | 127 | TYR  |
| 1   | H     | 133 | VAL  |
| 1   | H     | 134 | LEU  |
| 1   | H     | 149 | ILE  |
| 1   | H     | 152 | VAL  |
| 1   | H     | 154 | THR  |
| 1   | H     | 160 | SER  |
| 1   | H     | 165 | VAL  |
| 1   | H     | 166 | ILE  |
| 1   | H     | 184 | LYS  |
| 1   | H     | 191 | GLU  |
| 1   | H     | 196 | ARG  |
| 1   | H     | 214 | LYS  |
| 1   | H     | 218 | LEU  |
| 1   | H     | 224 | THR  |
| 1   | H     | 237 | VAL  |
| 1   | H     | 255 | VAL  |
| 1   | I     | 6   | LEU  |
| 1   | I     | 13  | LEU  |
| 1   | I     | 26  | LEU  |
| 1   | I     | 28  | ASP  |
| 1   | I     | 47  | GLN  |
| 1   | I     | 60  | LYS  |
| 1   | I     | 74  | VAL  |
| 1   | I     | 103 | ARG  |
| 1   | I     | 104 | ILE  |
| 1   | I     | 113 | ASN  |
| 1   | I     | 114 | ARG  |
| 1   | I     | 127 | TYR  |
| 1   | I     | 133 | VAL  |
| 1   | I     | 134 | LEU  |
| 1   | I     | 149 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 152 | VAL  |
| 1   | I     | 154 | THR  |
| 1   | I     | 160 | SER  |
| 1   | I     | 165 | VAL  |
| 1   | I     | 166 | ILE  |
| 1   | I     | 184 | LYS  |
| 1   | I     | 191 | GLU  |
| 1   | I     | 196 | ARG  |
| 1   | I     | 214 | LYS  |
| 1   | I     | 218 | LEU  |
| 1   | I     | 224 | THR  |
| 1   | I     | 237 | VAL  |
| 1   | I     | 255 | VAL  |
| 1   | J     | 0   | LEU  |
| 1   | J     | 6   | LEU  |
| 1   | J     | 13  | LEU  |
| 1   | J     | 26  | LEU  |
| 1   | J     | 28  | ASP  |
| 1   | J     | 47  | GLN  |
| 1   | J     | 60  | LYS  |
| 1   | J     | 74  | VAL  |
| 1   | J     | 103 | ARG  |
| 1   | J     | 104 | ILE  |
| 1   | J     | 113 | ASN  |
| 1   | J     | 114 | ARG  |
| 1   | J     | 127 | TYR  |
| 1   | J     | 133 | VAL  |
| 1   | J     | 134 | LEU  |
| 1   | J     | 149 | ILE  |
| 1   | J     | 152 | VAL  |
| 1   | J     | 154 | THR  |
| 1   | J     | 160 | SER  |
| 1   | J     | 165 | VAL  |
| 1   | J     | 166 | ILE  |
| 1   | J     | 184 | LYS  |
| 1   | J     | 191 | GLU  |
| 1   | J     | 214 | LYS  |
| 1   | J     | 218 | LEU  |
| 1   | J     | 224 | THR  |
| 1   | J     | 237 | VAL  |
| 1   | J     | 255 | VAL  |
| 1   | K     | 0   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 6   | LEU  |
| 1   | K     | 13  | LEU  |
| 1   | K     | 26  | LEU  |
| 1   | K     | 28  | ASP  |
| 1   | K     | 47  | GLN  |
| 1   | K     | 60  | LYS  |
| 1   | K     | 74  | VAL  |
| 1   | K     | 103 | ARG  |
| 1   | K     | 104 | ILE  |
| 1   | K     | 113 | ASN  |
| 1   | K     | 114 | ARG  |
| 1   | K     | 127 | TYR  |
| 1   | K     | 133 | VAL  |
| 1   | K     | 134 | LEU  |
| 1   | K     | 149 | ILE  |
| 1   | K     | 152 | VAL  |
| 1   | K     | 154 | THR  |
| 1   | K     | 160 | SER  |
| 1   | K     | 165 | VAL  |
| 1   | K     | 166 | ILE  |
| 1   | K     | 191 | GLU  |
| 1   | K     | 196 | ARG  |
| 1   | K     | 214 | LYS  |
| 1   | K     | 218 | LEU  |
| 1   | K     | 224 | THR  |
| 1   | K     | 237 | VAL  |
| 1   | K     | 255 | VAL  |
| 1   | L     | 1   | MET  |
| 1   | L     | 6   | LEU  |
| 1   | L     | 13  | LEU  |
| 1   | L     | 26  | LEU  |
| 1   | L     | 28  | ASP  |
| 1   | L     | 47  | GLN  |
| 1   | L     | 60  | LYS  |
| 1   | L     | 74  | VAL  |
| 1   | L     | 103 | ARG  |
| 1   | L     | 104 | ILE  |
| 1   | L     | 113 | ASN  |
| 1   | L     | 114 | ARG  |
| 1   | L     | 127 | TYR  |
| 1   | L     | 133 | VAL  |
| 1   | L     | 134 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 149 | ILE  |
| 1   | L     | 152 | VAL  |
| 1   | L     | 154 | THR  |
| 1   | L     | 160 | SER  |
| 1   | L     | 165 | VAL  |
| 1   | L     | 166 | ILE  |
| 1   | L     | 214 | LYS  |
| 1   | L     | 218 | LEU  |
| 1   | L     | 224 | THR  |
| 1   | L     | 237 | VAL  |
| 1   | L     | 255 | VAL  |
| 1   | M     | 0   | LEU  |
| 1   | M     | 6   | LEU  |
| 1   | M     | 13  | LEU  |
| 1   | M     | 26  | LEU  |
| 1   | M     | 28  | ASP  |
| 1   | M     | 47  | GLN  |
| 1   | M     | 60  | LYS  |
| 1   | M     | 74  | VAL  |
| 1   | M     | 103 | ARG  |
| 1   | M     | 104 | ILE  |
| 1   | M     | 113 | ASN  |
| 1   | M     | 114 | ARG  |
| 1   | M     | 127 | TYR  |
| 1   | M     | 133 | VAL  |
| 1   | M     | 134 | LEU  |
| 1   | M     | 149 | ILE  |
| 1   | M     | 152 | VAL  |
| 1   | M     | 154 | THR  |
| 1   | M     | 160 | SER  |
| 1   | M     | 165 | VAL  |
| 1   | M     | 166 | ILE  |
| 1   | M     | 184 | LYS  |
| 1   | M     | 191 | GLU  |
| 1   | M     | 196 | ARG  |
| 1   | M     | 214 | LYS  |
| 1   | M     | 218 | LEU  |
| 1   | M     | 224 | THR  |
| 1   | M     | 237 | VAL  |
| 1   | M     | 255 | VAL  |
| 1   | N     | 6   | LEU  |
| 1   | N     | 13  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 26  | LEU  |
| 1   | N     | 28  | ASP  |
| 1   | N     | 47  | GLN  |
| 1   | N     | 60  | LYS  |
| 1   | N     | 74  | VAL  |
| 1   | N     | 103 | ARG  |
| 1   | N     | 104 | ILE  |
| 1   | N     | 113 | ASN  |
| 1   | N     | 114 | ARG  |
| 1   | N     | 127 | TYR  |
| 1   | N     | 133 | VAL  |
| 1   | N     | 134 | LEU  |
| 1   | N     | 149 | ILE  |
| 1   | N     | 152 | VAL  |
| 1   | N     | 154 | THR  |
| 1   | N     | 160 | SER  |
| 1   | N     | 165 | VAL  |
| 1   | N     | 166 | ILE  |
| 1   | N     | 184 | LYS  |
| 1   | N     | 191 | GLU  |
| 1   | N     | 196 | ARG  |
| 1   | N     | 214 | LYS  |
| 1   | N     | 218 | LEU  |
| 1   | N     | 224 | THR  |
| 1   | N     | 237 | VAL  |
| 1   | N     | 255 | VAL  |
| 1   | O     | 6   | LEU  |
| 1   | O     | 13  | LEU  |
| 1   | O     | 26  | LEU  |
| 1   | O     | 28  | ASP  |
| 1   | O     | 47  | GLN  |
| 1   | O     | 60  | LYS  |
| 1   | O     | 74  | VAL  |
| 1   | O     | 103 | ARG  |
| 1   | O     | 104 | ILE  |
| 1   | O     | 113 | ASN  |
| 1   | O     | 114 | ARG  |
| 1   | O     | 127 | TYR  |
| 1   | O     | 133 | VAL  |
| 1   | O     | 134 | LEU  |
| 1   | O     | 149 | ILE  |
| 1   | O     | 152 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 154 | THR  |
| 1   | O     | 160 | SER  |
| 1   | O     | 165 | VAL  |
| 1   | O     | 166 | ILE  |
| 1   | O     | 191 | GLU  |
| 1   | O     | 196 | ARG  |
| 1   | O     | 214 | LYS  |
| 1   | O     | 218 | LEU  |
| 1   | O     | 224 | THR  |
| 1   | O     | 237 | VAL  |
| 1   | O     | 255 | VAL  |
| 1   | P     | 0   | LEU  |
| 1   | P     | 6   | LEU  |
| 1   | P     | 13  | LEU  |
| 1   | P     | 26  | LEU  |
| 1   | P     | 28  | ASP  |
| 1   | P     | 47  | GLN  |
| 1   | P     | 60  | LYS  |
| 1   | P     | 74  | VAL  |
| 1   | P     | 103 | ARG  |
| 1   | P     | 104 | ILE  |
| 1   | P     | 113 | ASN  |
| 1   | P     | 114 | ARG  |
| 1   | P     | 127 | TYR  |
| 1   | P     | 133 | VAL  |
| 1   | P     | 134 | LEU  |
| 1   | P     | 149 | ILE  |
| 1   | P     | 152 | VAL  |
| 1   | P     | 154 | THR  |
| 1   | P     | 160 | SER  |
| 1   | P     | 165 | VAL  |
| 1   | P     | 166 | ILE  |
| 1   | P     | 184 | LYS  |
| 1   | P     | 191 | GLU  |
| 1   | P     | 196 | ARG  |
| 1   | P     | 214 | LYS  |
| 1   | P     | 218 | LEU  |
| 1   | P     | 224 | THR  |
| 1   | P     | 237 | VAL  |
| 1   | P     | 255 | VAL  |
| 1   | Q     | 0   | LEU  |
| 1   | Q     | 6   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 13  | LEU  |
| 1   | Q     | 26  | LEU  |
| 1   | Q     | 28  | ASP  |
| 1   | Q     | 47  | GLN  |
| 1   | Q     | 60  | LYS  |
| 1   | Q     | 74  | VAL  |
| 1   | Q     | 103 | ARG  |
| 1   | Q     | 104 | ILE  |
| 1   | Q     | 113 | ASN  |
| 1   | Q     | 114 | ARG  |
| 1   | Q     | 127 | TYR  |
| 1   | Q     | 133 | VAL  |
| 1   | Q     | 134 | LEU  |
| 1   | Q     | 149 | ILE  |
| 1   | Q     | 152 | VAL  |
| 1   | Q     | 154 | THR  |
| 1   | Q     | 160 | SER  |
| 1   | Q     | 165 | VAL  |
| 1   | Q     | 166 | ILE  |
| 1   | Q     | 191 | GLU  |
| 1   | Q     | 214 | LYS  |
| 1   | Q     | 218 | LEU  |
| 1   | Q     | 224 | THR  |
| 1   | Q     | 237 | VAL  |
| 1   | Q     | 255 | VAL  |
| 1   | R     | 0   | LEU  |
| 1   | R     | 1   | MET  |
| 1   | R     | 6   | LEU  |
| 1   | R     | 13  | LEU  |
| 1   | R     | 26  | LEU  |
| 1   | R     | 28  | ASP  |
| 1   | R     | 47  | GLN  |
| 1   | R     | 60  | LYS  |
| 1   | R     | 74  | VAL  |
| 1   | R     | 103 | ARG  |
| 1   | R     | 104 | ILE  |
| 1   | R     | 113 | ASN  |
| 1   | R     | 114 | ARG  |
| 1   | R     | 127 | TYR  |
| 1   | R     | 133 | VAL  |
| 1   | R     | 134 | LEU  |
| 1   | R     | 149 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 152 | VAL  |
| 1   | R     | 154 | THR  |
| 1   | R     | 160 | SER  |
| 1   | R     | 165 | VAL  |
| 1   | R     | 166 | ILE  |
| 1   | R     | 184 | LYS  |
| 1   | R     | 191 | GLU  |
| 1   | R     | 214 | LYS  |
| 1   | R     | 218 | LEU  |
| 1   | R     | 224 | THR  |
| 1   | R     | 237 | VAL  |
| 1   | R     | 255 | VAL  |
| 1   | S     | 0   | LEU  |
| 1   | S     | 1   | MET  |
| 1   | S     | 6   | LEU  |
| 1   | S     | 13  | LEU  |
| 1   | S     | 26  | LEU  |
| 1   | S     | 28  | ASP  |
| 1   | S     | 47  | GLN  |
| 1   | S     | 60  | LYS  |
| 1   | S     | 74  | VAL  |
| 1   | S     | 103 | ARG  |
| 1   | S     | 104 | ILE  |
| 1   | S     | 113 | ASN  |
| 1   | S     | 114 | ARG  |
| 1   | S     | 127 | TYR  |
| 1   | S     | 133 | VAL  |
| 1   | S     | 134 | LEU  |
| 1   | S     | 149 | ILE  |
| 1   | S     | 152 | VAL  |
| 1   | S     | 154 | THR  |
| 1   | S     | 160 | SER  |
| 1   | S     | 165 | VAL  |
| 1   | S     | 166 | ILE  |
| 1   | S     | 184 | LYS  |
| 1   | S     | 191 | GLU  |
| 1   | S     | 214 | LYS  |
| 1   | S     | 218 | LEU  |
| 1   | S     | 224 | THR  |
| 1   | S     | 237 | VAL  |
| 1   | S     | 255 | VAL  |
| 1   | T     | 6   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 13  | LEU  |
| 1   | T     | 26  | LEU  |
| 1   | T     | 28  | ASP  |
| 1   | T     | 47  | GLN  |
| 1   | T     | 60  | LYS  |
| 1   | T     | 74  | VAL  |
| 1   | T     | 103 | ARG  |
| 1   | T     | 104 | ILE  |
| 1   | T     | 113 | ASN  |
| 1   | T     | 114 | ARG  |
| 1   | T     | 127 | TYR  |
| 1   | T     | 133 | VAL  |
| 1   | T     | 134 | LEU  |
| 1   | T     | 149 | ILE  |
| 1   | T     | 152 | VAL  |
| 1   | T     | 154 | THR  |
| 1   | T     | 160 | SER  |
| 1   | T     | 165 | VAL  |
| 1   | T     | 166 | ILE  |
| 1   | T     | 191 | GLU  |
| 1   | T     | 214 | LYS  |
| 1   | T     | 218 | LEU  |
| 1   | T     | 224 | THR  |
| 1   | T     | 237 | VAL  |
| 1   | T     | 255 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | GLN  |
| 1   | A     | 69  | GLN  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 128 | ASN  |
| 1   | A     | 180 | ASN  |
| 1   | B     | 8   | GLN  |
| 1   | B     | 69  | GLN  |
| 1   | B     | 91  | ASN  |
| 1   | B     | 128 | ASN  |
| 1   | B     | 180 | ASN  |
| 1   | C     | 19  | GLN  |
| 1   | C     | 43  | HIS  |
| 1   | C     | 47  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 69  | GLN  |
| 1   | C     | 91  | ASN  |
| 1   | C     | 128 | ASN  |
| 1   | C     | 180 | ASN  |
| 1   | D     | 69  | GLN  |
| 1   | D     | 91  | ASN  |
| 1   | D     | 128 | ASN  |
| 1   | D     | 180 | ASN  |
| 1   | E     | 8   | GLN  |
| 1   | E     | 69  | GLN  |
| 1   | E     | 91  | ASN  |
| 1   | E     | 128 | ASN  |
| 1   | E     | 180 | ASN  |
| 1   | F     | 19  | GLN  |
| 1   | F     | 43  | HIS  |
| 1   | F     | 47  | GLN  |
| 1   | F     | 69  | GLN  |
| 1   | F     | 91  | ASN  |
| 1   | F     | 113 | ASN  |
| 1   | F     | 128 | ASN  |
| 1   | F     | 248 | HIS  |
| 1   | G     | 8   | GLN  |
| 1   | G     | 43  | HIS  |
| 1   | G     | 47  | GLN  |
| 1   | G     | 69  | GLN  |
| 1   | G     | 91  | ASN  |
| 1   | G     | 113 | ASN  |
| 1   | G     | 128 | ASN  |
| 1   | G     | 180 | ASN  |
| 1   | H     | 4   | HIS  |
| 1   | H     | 8   | GLN  |
| 1   | H     | 19  | GLN  |
| 1   | H     | 43  | HIS  |
| 1   | H     | 47  | GLN  |
| 1   | H     | 69  | GLN  |
| 1   | H     | 91  | ASN  |
| 1   | H     | 113 | ASN  |
| 1   | H     | 128 | ASN  |
| 1   | H     | 180 | ASN  |
| 1   | I     | 43  | HIS  |
| 1   | I     | 47  | GLN  |
| 1   | I     | 69  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 91  | ASN  |
| 1   | I     | 113 | ASN  |
| 1   | I     | 128 | ASN  |
| 1   | I     | 180 | ASN  |
| 1   | J     | 8   | GLN  |
| 1   | J     | 19  | GLN  |
| 1   | J     | 69  | GLN  |
| 1   | J     | 91  | ASN  |
| 1   | J     | 128 | ASN  |
| 1   | J     | 180 | ASN  |
| 1   | K     | 8   | GLN  |
| 1   | K     | 43  | HIS  |
| 1   | K     | 47  | GLN  |
| 1   | K     | 69  | GLN  |
| 1   | K     | 91  | ASN  |
| 1   | K     | 113 | ASN  |
| 1   | K     | 128 | ASN  |
| 1   | K     | 150 | GLN  |
| 1   | K     | 180 | ASN  |
| 1   | L     | 8   | GLN  |
| 1   | L     | 69  | GLN  |
| 1   | L     | 91  | ASN  |
| 1   | L     | 113 | ASN  |
| 1   | L     | 128 | ASN  |
| 1   | L     | 180 | ASN  |
| 1   | M     | 8   | GLN  |
| 1   | M     | 19  | GLN  |
| 1   | M     | 43  | HIS  |
| 1   | M     | 47  | GLN  |
| 1   | M     | 69  | GLN  |
| 1   | M     | 91  | ASN  |
| 1   | M     | 113 | ASN  |
| 1   | M     | 128 | ASN  |
| 1   | M     | 180 | ASN  |
| 1   | N     | 8   | GLN  |
| 1   | N     | 43  | HIS  |
| 1   | N     | 47  | GLN  |
| 1   | N     | 69  | GLN  |
| 1   | N     | 91  | ASN  |
| 1   | N     | 113 | ASN  |
| 1   | N     | 128 | ASN  |
| 1   | N     | 180 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 8   | GLN  |
| 1   | O     | 19  | GLN  |
| 1   | O     | 43  | HIS  |
| 1   | O     | 47  | GLN  |
| 1   | O     | 69  | GLN  |
| 1   | O     | 91  | ASN  |
| 1   | O     | 113 | ASN  |
| 1   | O     | 128 | ASN  |
| 1   | O     | 180 | ASN  |
| 1   | P     | 8   | GLN  |
| 1   | P     | 69  | GLN  |
| 1   | P     | 91  | ASN  |
| 1   | P     | 113 | ASN  |
| 1   | P     | 128 | ASN  |
| 1   | P     | 180 | ASN  |
| 1   | Q     | 8   | GLN  |
| 1   | Q     | 43  | HIS  |
| 1   | Q     | 47  | GLN  |
| 1   | Q     | 69  | GLN  |
| 1   | Q     | 91  | ASN  |
| 1   | Q     | 113 | ASN  |
| 1   | Q     | 128 | ASN  |
| 1   | Q     | 180 | ASN  |
| 1   | R     | 8   | GLN  |
| 1   | R     | 43  | HIS  |
| 1   | R     | 47  | GLN  |
| 1   | R     | 69  | GLN  |
| 1   | R     | 91  | ASN  |
| 1   | R     | 113 | ASN  |
| 1   | R     | 128 | ASN  |
| 1   | R     | 180 | ASN  |
| 1   | S     | 8   | GLN  |
| 1   | S     | 19  | GLN  |
| 1   | S     | 69  | GLN  |
| 1   | S     | 91  | ASN  |
| 1   | S     | 113 | ASN  |
| 1   | S     | 128 | ASN  |
| 1   | S     | 180 | ASN  |
| 1   | T     | 43  | HIS  |
| 1   | T     | 47  | GLN  |
| 1   | T     | 69  | GLN  |
| 1   | T     | 91  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 113 | ASN  |
| 1   | T     | 128 | ASN  |
| 1   | T     | 180 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 40 are monoatomic - leaving 38 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  | A     | 1262 | -    | 4,4,4        | 0.93 | 0           | 6,6,6       | 0.64 | 0           |
| 2   | PO4  | P     | 1264 | -    | 4,4,4        | 1.36 | 1 (25%)     | 6,6,6       | 0.44 | 0           |
| 2   | PO4  | I     | 1262 | -    | 4,4,4        | 0.85 | 0           | 6,6,6       | 0.51 | 0           |
| 2   | PO4  | H     | 1263 | -    | 4,4,4        | 0.98 | 0           | 6,6,6       | 0.47 | 0           |
| 2   | PO4  | H     | 1262 | -    | 4,4,4        | 0.91 | 0           | 6,6,6       | 0.65 | 0           |
| 2   | PO4  | S     | 1262 | -    | 4,4,4        | 0.77 | 0           | 6,6,6       | 0.75 | 0           |
| 2   | PO4  | E     | 1262 | -    | 4,4,4        | 0.89 | 0           | 6,6,6       | 0.71 | 0           |
| 2   | PO4  | P     | 1262 | -    | 4,4,4        | 0.93 | 0           | 6,6,6       | 0.45 | 0           |
| 2   | PO4  | B     | 1263 | -    | 4,4,4        | 0.95 | 0           | 6,6,6       | 0.59 | 0           |
| 2   | PO4  | G     | 1263 | -    | 4,4,4        | 1.02 | 0           | 6,6,6       | 0.71 | 0           |
| 2   | PO4  | M     | 1262 | -    | 4,4,4        | 0.96 | 0           | 6,6,6       | 0.50 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PO4  | G     | 1262 | -    | 4,4,4        | 0.87 | 0        | 6,6,6       | 0.61 | 0        |
| 2   | PO4  | B     | 1262 | -    | 4,4,4        | 1.13 | 0        | 6,6,6       | 0.54 | 0        |
| 2   | PO4  | G     | 1264 | -    | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.60 | 0        |
| 2   | PO4  | O     | 1262 | -    | 4,4,4        | 1.04 | 0        | 6,6,6       | 0.66 | 0        |
| 2   | PO4  | Q     | 1264 | -    | 4,4,4        | 0.77 | 0        | 6,6,6       | 0.76 | 0        |
| 2   | PO4  | L     | 1263 | -    | 4,4,4        | 1.09 | 0        | 6,6,6       | 0.53 | 0        |
| 2   | PO4  | C     | 1262 | -    | 4,4,4        | 0.88 | 0        | 6,6,6       | 0.63 | 0        |
| 2   | PO4  | A     | 1264 | -    | 4,4,4        | 0.84 | 0        | 6,6,6       | 0.62 | 0        |
| 2   | PO4  | D     | 1263 | -    | 4,4,4        | 0.89 | 0        | 6,6,6       | 0.59 | 0        |
| 2   | PO4  | J     | 1262 | -    | 4,4,4        | 0.96 | 0        | 6,6,6       | 0.48 | 0        |
| 2   | PO4  | F     | 1263 | -    | 4,4,4        | 1.01 | 0        | 6,6,6       | 0.50 | 0        |
| 2   | PO4  | Q     | 1263 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.46 | 0        |
| 2   | PO4  | K     | 1263 | -    | 4,4,4        | 0.84 | 0        | 6,6,6       | 0.51 | 0        |
| 2   | PO4  | N     | 1262 | -    | 4,4,4        | 0.95 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | L     | 1262 | -    | 4,4,4        | 1.02 | 0        | 6,6,6       | 0.64 | 0        |
| 2   | PO4  | K     | 1264 | -    | 4,4,4        | 0.97 | 0        | 6,6,6       | 0.51 | 0        |
| 2   | PO4  | T     | 1262 | -    | 4,4,4        | 0.89 | 0        | 6,6,6       | 0.49 | 0        |
| 2   | PO4  | K     | 1262 | -    | 4,4,4        | 0.82 | 0        | 6,6,6       | 0.56 | 0        |
| 2   | PO4  | D     | 1264 | -    | 4,4,4        | 0.92 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | P     | 1263 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.64 | 0        |
| 2   | PO4  | D     | 1262 | -    | 4,4,4        | 0.97 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | PO4  | F     | 1262 | -    | 4,4,4        | 0.85 | 0        | 6,6,6       | 0.71 | 0        |
| 2   | PO4  | R     | 1262 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.57 | 0        |
| 2   | PO4  | J     | 1263 | -    | 4,4,4        | 0.86 | 0        | 6,6,6       | 0.63 | 0        |
| 2   | PO4  | F     | 1264 | -    | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.70 | 0        |
| 2   | PO4  | A     | 1263 | -    | 4,4,4        | 1.09 | 0        | 6,6,6       | 0.51 | 0        |
| 2   | PO4  | Q     | 1262 | -    | 4,4,4        | 0.93 | 0        | 6,6,6       | 0.58 | 0        |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | P     | 1264 | PO4  | P-O1  | 2.41 | 1.56        | 1.50     |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 14 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | E     | 1262 | PO4  | 1       | 0            |
| 2   | B     | 1263 | PO4  | 1       | 0            |
| 2   | G     | 1263 | PO4  | 1       | 0            |
| 2   | G     | 1262 | PO4  | 1       | 0            |
| 2   | A     | 1264 | PO4  | 1       | 0            |
| 2   | D     | 1263 | PO4  | 1       | 0            |
| 2   | L     | 1262 | PO4  | 1       | 0            |
| 2   | K     | 1264 | PO4  | 1       | 0            |
| 2   | T     | 1262 | PO4  | 1       | 0            |
| 2   | P     | 1263 | PO4  | 1       | 0            |
| 2   | F     | 1262 | PO4  | 2       | 0            |
| 2   | R     | 1262 | PO4  | 1       | 0            |
| 2   | Q     | 1262 | PO4  | 1       | 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     | 262/270 (97%)   | 0.03   | 7 (2%) 56 46   | 23, 33, 53, 71        | 0     |
| 1   | B     | 262/270 (97%)   | 0.09   | 5 (1%) 66 57   | 23, 33, 53, 71        | 0     |
| 1   | C     | 262/270 (97%)   | 0.05   | 7 (2%) 56 46   | 23, 33, 53, 71        | 0     |
| 1   | D     | 262/270 (97%)   | 0.01   | 7 (2%) 56 46   | 23, 33, 53, 71        | 0     |
| 1   | E     | 262/270 (97%)   | 0.03   | 7 (2%) 56 46   | 23, 33, 53, 71        | 0     |
| 1   | F     | 262/270 (97%)   | 0.16   | 10 (3%) 44 35  | 23, 33, 53, 71        | 0     |
| 1   | G     | 262/270 (97%)   | 0.10   | 7 (2%) 56 46   | 23, 33, 53, 71        | 0     |
| 1   | H     | 262/270 (97%)   | 0.07   | 10 (3%) 44 35  | 23, 33, 53, 71        | 0     |
| 1   | I     | 262/270 (97%)   | 0.13   | 6 (2%) 61 51   | 23, 33, 53, 71        | 0     |
| 1   | J     | 262/270 (97%)   | 0.05   | 6 (2%) 61 51   | 23, 33, 53, 71        | 0     |
| 1   | K     | 262/270 (97%)   | 0.06   | 7 (2%) 56 46   | 23, 33, 53, 71        | 0     |
| 1   | L     | 262/270 (97%)   | 0.16   | 6 (2%) 61 51   | 23, 33, 53, 71        | 0     |
| 1   | M     | 262/270 (97%)   | 0.07   | 7 (2%) 56 46   | 23, 33, 53, 71        | 0     |
| 1   | N     | 262/270 (97%)   | 0.11   | 6 (2%) 61 51   | 23, 33, 53, 71        | 0     |
| 1   | O     | 262/270 (97%)   | 0.03   | 6 (2%) 61 51   | 23, 33, 53, 71        | 0     |
| 1   | P     | 262/270 (97%)   | 0.02   | 6 (2%) 61 51   | 23, 33, 53, 71        | 0     |
| 1   | Q     | 262/270 (97%)   | 0.01   | 4 (1%) 72 63   | 23, 33, 53, 71        | 0     |
| 1   | R     | 262/270 (97%)   | 0.09   | 10 (3%) 44 35  | 23, 33, 53, 71        | 0     |
| 1   | S     | 262/270 (97%)   | 0.05   | 4 (1%) 72 63   | 23, 33, 53, 71        | 0     |
| 1   | T     | 262/270 (97%)   | 0.04   | 10 (3%) 44 35  | 23, 33, 53, 71        | 0     |
| All | All   | 5240/5400 (97%) | 0.07   | 138 (2%) 57 47 | 23, 33, 53, 71        | 0     |

All (138) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 0   | LEU  | 5.4  |
| 1   | N     | 1   | MET  | 5.1  |
| 1   | J     | 0   | LEU  | 4.7  |
| 1   | H     | 0   | LEU  | 4.6  |
| 1   | C     | 1   | MET  | 4.5  |
| 1   | E     | 70  | GLN  | 4.4  |
| 1   | E     | 1   | MET  | 4.4  |
| 1   | M     | 70  | GLN  | 4.4  |
| 1   | P     | 0   | LEU  | 4.3  |
| 1   | O     | 70  | GLN  | 4.2  |
| 1   | P     | 1   | MET  | 4.2  |
| 1   | E     | 0   | LEU  | 4.2  |
| 1   | M     | 0   | LEU  | 4.2  |
| 1   | A     | 1   | MET  | 4.2  |
| 1   | Q     | 1   | MET  | 4.2  |
| 1   | N     | 70  | GLN  | 4.1  |
| 1   | A     | 70  | GLN  | 4.1  |
| 1   | S     | 1   | MET  | 4.0  |
| 1   | J     | 70  | GLN  | 4.0  |
| 1   | L     | 1   | MET  | 4.0  |
| 1   | S     | 0   | LEU  | 3.9  |
| 1   | F     | 0   | LEU  | 3.9  |
| 1   | D     | 0   | LEU  | 3.8  |
| 1   | B     | 0   | LEU  | 3.8  |
| 1   | Q     | 0   | LEU  | 3.8  |
| 1   | I     | 1   | MET  | 3.8  |
| 1   | I     | 70  | GLN  | 3.8  |
| 1   | F     | 1   | MET  | 3.7  |
| 1   | C     | 70  | GLN  | 3.6  |
| 1   | T     | 1   | MET  | 3.6  |
| 1   | A     | 0   | LEU  | 3.5  |
| 1   | H     | 1   | MET  | 3.5  |
| 1   | O     | 1   | MET  | 3.5  |
| 1   | R     | 67  | LYS  | 3.5  |
| 1   | R     | 0   | LEU  | 3.5  |
| 1   | L     | 0   | LEU  | 3.5  |
| 1   | L     | 70  | GLN  | 3.4  |
| 1   | G     | 0   | LEU  | 3.4  |
| 1   | T     | 0   | LEU  | 3.4  |
| 1   | S     | 70  | GLN  | 3.4  |
| 1   | E     | 75  | ASP  | 3.4  |
| 1   | M     | 1   | MET  | 3.4  |
| 1   | B     | 1   | MET  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 70  | GLN  | 3.4  |
| 1   | G     | 1   | MET  | 3.3  |
| 1   | K     | 0   | LEU  | 3.3  |
| 1   | J     | 1   | MET  | 3.3  |
| 1   | Q     | 70  | GLN  | 3.3  |
| 1   | F     | 180 | ASN  | 3.2  |
| 1   | R     | 1   | MET  | 3.2  |
| 1   | I     | 0   | LEU  | 3.2  |
| 1   | A     | 71  | GLN  | 3.2  |
| 1   | C     | 67  | LYS  | 3.2  |
| 1   | H     | 70  | GLN  | 3.1  |
| 1   | M     | 67  | LYS  | 3.1  |
| 1   | G     | 71  | GLN  | 3.1  |
| 1   | N     | 71  | GLN  | 3.1  |
| 1   | R     | 70  | GLN  | 3.0  |
| 1   | T     | 70  | GLN  | 3.0  |
| 1   | F     | 72  | LEU  | 3.0  |
| 1   | D     | 1   | MET  | 3.0  |
| 1   | I     | 71  | GLN  | 3.0  |
| 1   | B     | 2   | THR  | 3.0  |
| 1   | F     | 70  | GLN  | 2.9  |
| 1   | K     | 70  | GLN  | 2.9  |
| 1   | T     | 71  | GLN  | 2.9  |
| 1   | M     | 75  | ASP  | 2.9  |
| 1   | G     | 67  | LYS  | 2.9  |
| 1   | P     | 71  | GLN  | 2.9  |
| 1   | E     | 67  | LYS  | 2.9  |
| 1   | I     | 28  | ASP  | 2.9  |
| 1   | G     | 70  | GLN  | 2.8  |
| 1   | D     | 70  | GLN  | 2.8  |
| 1   | C     | 0   | LEU  | 2.8  |
| 1   | B     | 67  | LYS  | 2.8  |
| 1   | N     | 0   | LEU  | 2.7  |
| 1   | P     | 67  | LYS  | 2.7  |
| 1   | K     | 67  | LYS  | 2.7  |
| 1   | H     | 33  | ASP  | 2.7  |
| 1   | H     | 261 | SER  | 2.7  |
| 1   | H     | 180 | ASN  | 2.7  |
| 1   | A     | 67  | LYS  | 2.6  |
| 1   | I     | 67  | LYS  | 2.6  |
| 1   | K     | 33  | ASP  | 2.6  |
| 1   | T     | 33  | ASP  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 67  | LYS  | 2.6  |
| 1   | K     | 1   | MET  | 2.6  |
| 1   | D     | 67  | LYS  | 2.6  |
| 1   | F     | 223 | ARG  | 2.5  |
| 1   | H     | 28  | ASP  | 2.5  |
| 1   | M     | 33  | ASP  | 2.4  |
| 1   | K     | 71  | GLN  | 2.4  |
| 1   | P     | 70  | GLN  | 2.4  |
| 1   | F     | 179 | LYS  | 2.4  |
| 1   | H     | 67  | LYS  | 2.4  |
| 1   | D     | 78  | ASP  | 2.4  |
| 1   | L     | 67  | LYS  | 2.3  |
| 1   | H     | 68  | VAL  | 2.3  |
| 1   | J     | 33  | ASP  | 2.3  |
| 1   | R     | 28  | ASP  | 2.3  |
| 1   | E     | 71  | GLN  | 2.3  |
| 1   | F     | 71  | GLN  | 2.3  |
| 1   | L     | 113 | ASN  | 2.3  |
| 1   | F     | 67  | LYS  | 2.3  |
| 1   | L     | 196 | ARG  | 2.2  |
| 1   | C     | 76  | GLN  | 2.2  |
| 1   | A     | 36  | GLU  | 2.2  |
| 1   | J     | 146 | ASP  | 2.2  |
| 1   | O     | 146 | ASP  | 2.2  |
| 1   | C     | 68  | VAL  | 2.2  |
| 1   | N     | 67  | LYS  | 2.2  |
| 1   | S     | 67  | LYS  | 2.2  |
| 1   | N     | 76  | GLN  | 2.2  |
| 1   | Q     | 67  | LYS  | 2.2  |
| 1   | T     | 72  | LEU  | 2.2  |
| 1   | T     | 67  | LYS  | 2.1  |
| 1   | E     | 223 | ARG  | 2.1  |
| 1   | O     | 68  | VAL  | 2.1  |
| 1   | G     | 28  | ASP  | 2.1  |
| 1   | D     | 190 | GLU  | 2.1  |
| 1   | M     | 190 | GLU  | 2.1  |
| 1   | R     | 261 | SER  | 2.1  |
| 1   | D     | 113 | ASN  | 2.1  |
| 1   | R     | 180 | ASN  | 2.1  |
| 1   | R     | 29  | LEU  | 2.1  |
| 1   | R     | 71  | GLN  | 2.1  |
| 1   | F     | 33  | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | P     | 223 | ARG  | 2.1  |
| 1   | T     | 28  | ASP  | 2.1  |
| 1   | A     | 76  | GLN  | 2.0  |
| 1   | O     | 74  | VAL  | 2.0  |
| 1   | C     | 189 | ASN  | 2.0  |
| 1   | H     | 113 | ASN  | 2.0  |
| 1   | G     | 20  | GLY  | 2.0  |
| 1   | K     | 223 | ARG  | 2.0  |
| 1   | R     | 73  | GLY  | 2.0  |
| 1   | T     | 75  | ASP  | 2.0  |
| 1   | T     | 180 | ASN  | 2.0  |

## 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 oligosaccharides 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  | B     | 1263 | 5/5   | 0.86 | 0.14 | 73,73,73,73                 | 0     |
| 2   | PO4  | Q     | 1264 | 5/5   | 0.87 | 0.15 | 52,52,52,53                 | 0     |
| 2   | PO4  | D     | 1263 | 5/5   | 0.88 | 0.15 | 62,63,64,64                 | 0     |
| 2   | PO4  | A     | 1264 | 5/5   | 0.88 | 0.14 | 53,53,53,53                 | 0     |
| 3   | NA   | M     | 1307 | 1/1   | 0.88 | 0.28 | 31,31,31,31                 | 0     |
| 2   | PO4  | T     | 1262 | 5/5   | 0.89 | 0.15 | 57,58,58,58                 | 0     |
| 2   | PO4  | P     | 1263 | 5/5   | 0.89 | 0.13 | 65,65,66,66                 | 0     |
| 2   | PO4  | J     | 1263 | 5/5   | 0.90 | 0.11 | 54,55,55,55                 | 0     |
| 2   | PO4  | N     | 1262 | 5/5   | 0.90 | 0.12 | 57,58,59,59                 | 0     |
| 2   | PO4  | I     | 1262 | 5/5   | 0.90 | 0.11 | 55,55,56,56                 | 0     |
| 3   | NA   | N     | 1315 | 1/1   | 0.90 | 0.24 | 24,24,24,24                 | 0     |
| 3   | NA   | I     | 1306 | 1/1   | 0.91 | 0.20 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | S     | 1262 | 5/5   | 0.91 | 0.14 | 53,53,53,54                 | 0     |
| 2   | PO4  | M     | 1262 | 5/5   | 0.91 | 0.13 | 56,56,57,57                 | 0     |
| 2   | PO4  | F     | 1264 | 5/5   | 0.92 | 0.11 | 45,46,46,47                 | 0     |
| 2   | PO4  | P     | 1262 | 5/5   | 0.92 | 0.13 | 51,51,51,51                 | 5     |
| 2   | PO4  | F     | 1262 | 5/5   | 0.92 | 0.10 | 40,41,41,41                 | 0     |
| 3   | NA   | L     | 1314 | 1/1   | 0.93 | 0.24 | 21,21,21,21                 | 0     |
| 3   | NA   | L     | 1319 | 1/1   | 0.93 | 0.19 | 18,18,18,18                 | 0     |
| 3   | NA   | F     | 1312 | 1/1   | 0.93 | 0.23 | 26,26,26,26                 | 0     |
| 2   | PO4  | G     | 1263 | 5/5   | 0.93 | 0.10 | 48,48,50,50                 | 0     |
| 2   | PO4  | O     | 1262 | 5/5   | 0.94 | 0.09 | 53,53,54,54                 | 0     |
| 2   | PO4  | L     | 1262 | 5/5   | 0.94 | 0.08 | 42,43,44,44                 | 0     |
| 2   | PO4  | B     | 1262 | 5/5   | 0.94 | 0.13 | 54,54,55,55                 | 0     |
| 2   | PO4  | K     | 1263 | 5/5   | 0.94 | 0.13 | 65,65,65,65                 | 0     |
| 3   | NA   | O     | 1301 | 1/1   | 0.94 | 0.24 | 26,26,26,26                 | 0     |
| 3   | NA   | R     | 1318 | 1/1   | 0.94 | 0.23 | 15,15,15,15                 | 0     |
| 3   | NA   | S     | 1320 | 1/1   | 0.94 | 0.31 | 27,27,27,27                 | 0     |
| 4   | K    | G     | 1265 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 2   | PO4  | H     | 1263 | 5/5   | 0.95 | 0.08 | 53,53,54,54                 | 0     |
| 2   | PO4  | F     | 1263 | 5/5   | 0.95 | 0.12 | 69,69,69,69                 | 0     |
| 3   | NA   | K     | 1305 | 1/1   | 0.95 | 0.20 | 21,21,21,21                 | 0     |
| 2   | PO4  | C     | 1262 | 5/5   | 0.95 | 0.10 | 52,53,53,53                 | 0     |
| 2   | PO4  | K     | 1262 | 5/5   | 0.95 | 0.08 | 44,45,46,46                 | 0     |
| 2   | PO4  | D     | 1262 | 5/5   | 0.95 | 0.07 | 52,52,52,52                 | 5     |
| 2   | PO4  | Q     | 1262 | 5/5   | 0.95 | 0.10 | 44,45,45,45                 | 0     |
| 2   | PO4  | K     | 1264 | 5/5   | 0.95 | 0.12 | 42,43,44,44                 | 0     |
| 3   | NA   | P     | 1317 | 1/1   | 0.95 | 0.26 | 19,19,19,19                 | 0     |
| 2   | PO4  | R     | 1262 | 5/5   | 0.95 | 0.08 | 61,61,62,62                 | 0     |
| 2   | PO4  | G     | 1264 | 5/5   | 0.95 | 0.14 | 55,55,56,56                 | 0     |
| 4   | K    | C     | 1263 | 1/1   | 0.95 | 0.14 | 42,42,42,42                 | 0     |
| 2   | PO4  | L     | 1263 | 5/5   | 0.95 | 0.10 | 53,54,54,54                 | 0     |
| 4   | K    | G     | 1408 | 1/1   | 0.95 | 0.18 | 39,39,39,39                 | 0     |
| 4   | K    | N     | 1263 | 1/1   | 0.95 | 0.16 | 46,46,46,46                 | 0     |
| 2   | PO4  | P     | 1264 | 5/5   | 0.96 | 0.07 | 57,57,57,57                 | 5     |
| 3   | NA   | A     | 1265 | 1/1   | 0.96 | 0.30 | 22,22,22,22                 | 0     |
| 3   | NA   | C     | 1310 | 1/1   | 0.96 | 0.32 | 24,24,24,24                 | 0     |
| 3   | NA   | D     | 1304 | 1/1   | 0.96 | 0.20 | 18,18,18,18                 | 0     |
| 3   | NA   | Q     | 1302 | 1/1   | 0.96 | 0.15 | 11,11,11,11                 | 0     |
| 2   | PO4  | A     | 1262 | 5/5   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 3   | NA   | G     | 1313 | 1/1   | 0.96 | 0.22 | 18,18,18,18                 | 0     |
| 3   | NA   | T     | 1303 | 1/1   | 0.96 | 0.21 | 29,29,29,29                 | 0     |
| 4   | K    | B     | 1264 | 1/1   | 0.96 | 0.23 | 48,48,48,48                 | 0     |
| 2   | PO4  | Q     | 1263 | 5/5   | 0.96 | 0.11 | 57,57,57,57                 | 0     |

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*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | PO4  | A     | 1263 | 5/5   | 0.96 | 0.10 | 51,51,52,52                 | 0     |
| 2   | PO4  | H     | 1262 | 5/5   | 0.96 | 0.07 | 46,46,46,47                 | 0     |
| 4   | K    | I     | 1263 | 1/1   | 0.96 | 0.18 | 57,57,57,57                 | 0     |
| 4   | K    | L     | 1415 | 1/1   | 0.96 | 0.15 | 41,41,41,41                 | 0     |
| 2   | PO4  | E     | 1262 | 5/5   | 0.96 | 0.11 | 44,44,45,45                 | 0     |
| 4   | K    | T     | 1263 | 1/1   | 0.96 | 0.17 | 42,42,42,42                 | 0     |
| 3   | NA   | E     | 1311 | 1/1   | 0.97 | 0.24 | 17,17,17,17                 | 0     |
| 2   | PO4  | J     | 1262 | 5/5   | 0.97 | 0.06 | 35,35,36,37                 | 0     |
| 2   | PO4  | G     | 1262 | 5/5   | 0.97 | 0.07 | 38,39,39,40                 | 0     |
| 4   | K    | Q     | 1412 | 1/1   | 0.97 | 0.14 | 40,40,40,40                 | 0     |
| 4   | K    | S     | 1413 | 1/1   | 0.97 | 0.16 | 47,47,47,47                 | 0     |
| 4   | K    | A     | 1266 | 1/1   | 0.97 | 0.20 | 49,49,49,49                 | 0     |
| 3   | NA   | O     | 1316 | 1/1   | 0.98 | 0.27 | 21,21,21,21                 | 0     |
| 4   | K    | L     | 1264 | 1/1   | 0.98 | 0.17 | 42,42,42,42                 | 0     |
| 2   | PO4  | D     | 1264 | 5/5   | 0.98 | 0.12 | 47,47,48,48                 | 5     |
| 4   | K    | E     | 1263 | 1/1   | 0.98 | 0.19 | 45,45,45,45                 | 0     |
| 4   | K    | P     | 1265 | 1/1   | 0.98 | 0.16 | 46,46,46,46                 | 0     |
| 4   | K    | F     | 1265 | 1/1   | 0.98 | 0.19 | 47,47,47,47                 | 0     |
| 4   | K    | R     | 1263 | 1/1   | 0.98 | 0.22 | 44,44,44,44                 | 0     |
| 3   | NA   | S     | 1308 | 1/1   | 0.98 | 0.35 | 30,30,30,30                 | 0     |
| 4   | K    | A     | 1401 | 1/1   | 0.98 | 0.12 | 42,42,42,42                 | 0     |
| 4   | K    | K     | 1265 | 1/1   | 0.99 | 0.20 | 46,46,46,46                 | 0     |
| 4   | K    | D     | 1265 | 1/1   | 0.99 | 0.18 | 42,42,42,42                 | 0     |
| 4   | K    | Q     | 1416 | 1/1   | 0.99 | 0.19 | 46,46,46,46                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.