



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:55 AM UTC

PDB ID : 6E3B / pdb\_00006e3b  
Title : STRUCTURE OF Siw14 CATALYTIC CORE  
Authors : Florio, T.; Lokareddy, R.; Cingolani, G.  
Deposited on : 2018-07-13  
Resolution : 2.50 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                                                             |

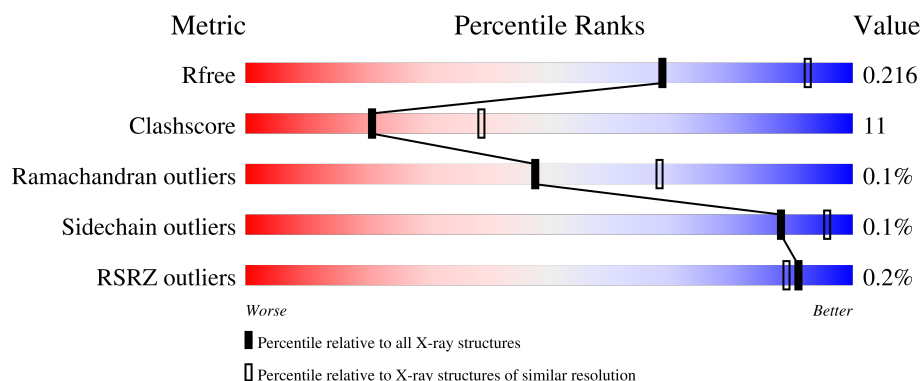
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



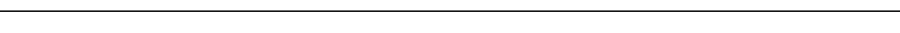
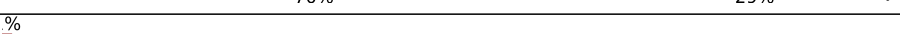
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

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     | 169    | <div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>73%</span> <span>27%</span> </div> </div>   |
| 1   | B     | 169    | <div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between;"> <span>72%</span> <span>28%</span> </div> </div> |
| 1   | C     | 169    | <div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between;"> <span>76%</span> <span>23%</span> </div> </div> |
| 1   | D     | 169    | <div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between;"> <span>85%</span> <span>14%</span> </div> </div> |
| 1   | E     | 169    | <div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between;"> <span>68%</span> <span>29%</span> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | F     | 169    |  75% 24% .    |
| 1   | G     | 169    |  76% 24%      |
| 1   | H     | 169    |  72% 27% ..   |
| 1   | I     | 169    |  74% 26%      |
| 1   | J     | 169    |  74% 26%      |
| 1   | K     | 169    |  71% 29%      |
| 1   | L     | 169    |  72% 27% .    |
| 1   | M     | 169    |  75% 24% .    |
| 1   | N     | 169    |  77% 22% .    |
| 1   | O     | 169    |  74% 26%      |
| 1   | P     | 169    |  73% 25% .    |
| 1   | Q     | 169    |  76% 24% .    |
| 1   | R     | 169    |  74% 25% .  |
| 1   | S     | 169    |  59% 41%    |
| 1   | T     | 169    |  70% 29% .  |
| 1   | V     | 169    |  72% 28%    |
| 1   | W     | 169    |  68% 31% .  |
| 1   | X     | 169    |  70% 29% .  |
| 1   | Y     | 169    |  72% 26% .. |

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   | SO4  | H     | 301 | -         | -        | X       | -                |
| 2   | SO4  | P     | 301 | -         | -        | X       | -                |
| 2   | SO4  | T     | 301 | -         | -        | X       | -                |
| 2   | SO4  | W     | 301 | -         | -        | X       | -                |
| 2   | SO4  | Y     | 301 | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34047 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 Tyrosine-protein phosphatase SIW14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | B     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | C     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | D     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | E     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | F     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1395  | 903 | 242 | 245 | 5 |         |         |       |
| 1   | G     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | H     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1395  | 903 | 242 | 245 | 5 |         |         |       |
| 1   | I     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1395  | 903 | 242 | 245 | 5 |         |         |       |
| 1   | J     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | K     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | L     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1395  | 903 | 242 | 245 | 5 |         |         |       |
| 1   | M     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | N     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | O     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1395  | 903 | 242 | 245 | 5 |         |         |       |
| 1   | P     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | Q     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1395  | 903 | 242 | 245 | 5 |         |         |       |
| 1   | R     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | S     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1377  | 903 | 242 | 227 | 5 |         |         |       |
| 1   | T     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1393  | 900 | 244 | 244 | 5 |         |         |       |
| 1   | V     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | W     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |
| 1   | X     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1387  | 898 | 241 | 243 | 5 |         |         |       |
| 1   | Y     | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 906 | 245 | 245 | 5 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

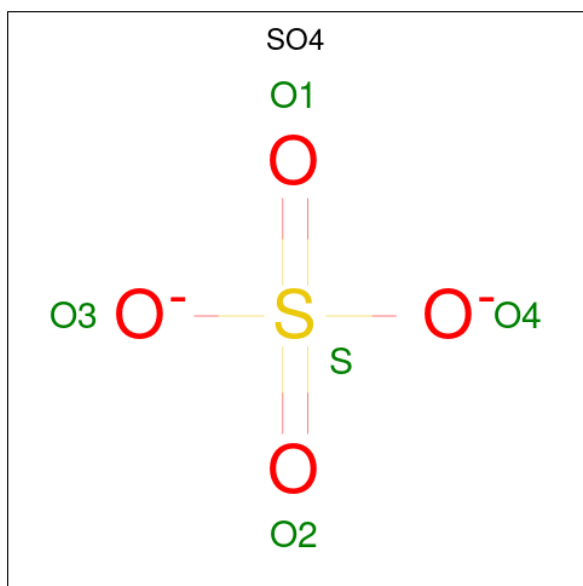
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 214     | SER      | CYS    | conflict | UNP P53965 |
| B     | 214     | SER      | CYS    | conflict | UNP P53965 |
| C     | 214     | SER      | CYS    | conflict | UNP P53965 |
| D     | 214     | SER      | CYS    | conflict | UNP P53965 |
| E     | 214     | SER      | CYS    | conflict | UNP P53965 |
| F     | 214     | SER      | CYS    | conflict | UNP P53965 |
| G     | 214     | SER      | CYS    | conflict | UNP P53965 |
| H     | 214     | SER      | CYS    | conflict | UNP P53965 |
| I     | 214     | SER      | CYS    | conflict | UNP P53965 |
| J     | 214     | SER      | CYS    | conflict | UNP P53965 |
| K     | 214     | SER      | CYS    | conflict | UNP P53965 |
| L     | 214     | SER      | CYS    | conflict | UNP P53965 |
| M     | 214     | SER      | CYS    | conflict | UNP P53965 |
| N     | 214     | SER      | CYS    | conflict | UNP P53965 |
| O     | 214     | SER      | CYS    | conflict | UNP P53965 |
| P     | 214     | SER      | CYS    | conflict | UNP P53965 |
| Q     | 214     | SER      | CYS    | conflict | UNP P53965 |
| R     | 214     | SER      | CYS    | conflict | UNP P53965 |
| S     | 214     | SER      | CYS    | conflict | UNP P53965 |
| T     | 214     | SER      | CYS    | conflict | UNP P53965 |
| V     | 214     | SER      | CYS    | conflict | UNP P53965 |
| W     | 214     | SER      | CYS    | conflict | UNP P53965 |
| X     | 214     | SER      | CYS    | conflict | UNP P53965 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Y     | 214     | SER      | CYS    | conflict | UNP P53965 |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | N     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | P     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | S     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | T     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | W     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | X     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Y     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 3   | B     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 3   | C     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 3   | D     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 3   | E     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 3   | F     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |

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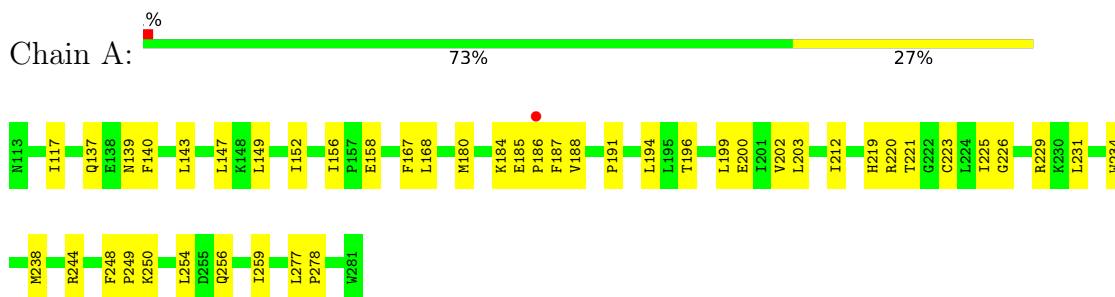
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | G     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | H     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 3   | I     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 3   | J     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | K     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 3   | L     | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 3   | M     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | N     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | O     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | P     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 3   | Q     | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 3   | R     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 3   | S     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 3   | T     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 3   | V     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 3   | W     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | X     | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | Y     | 14       | Total<br>14 | O<br>14 | 0       | 0       |



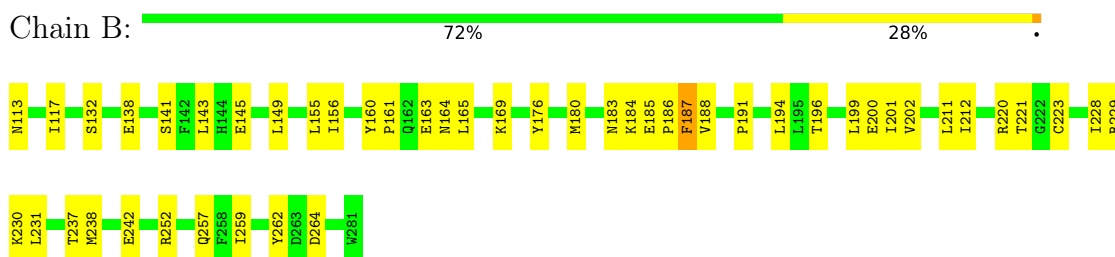
### 3 Residue-property plots

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.

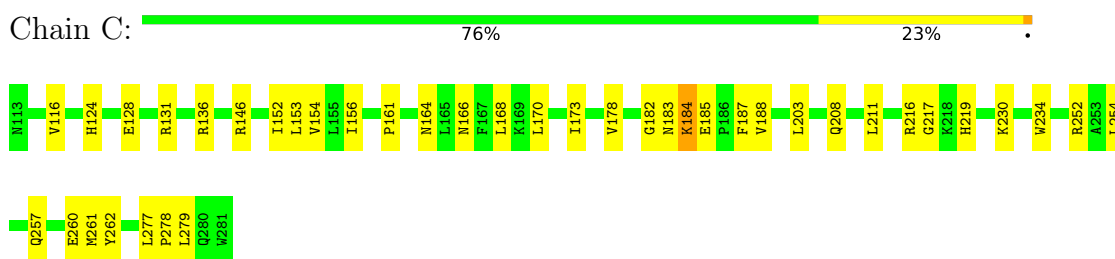
- Molecule 1: Tyrosine-protein phosphatase SIW14



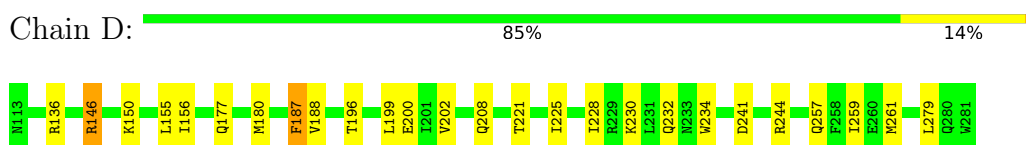
- Molecule 1: Tyrosine-protein phosphatase SIW14



- Molecule 1: Tyrosine-protein phosphatase SIW14

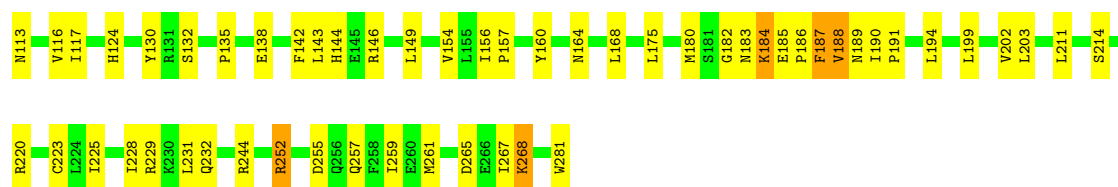


- Molecule 1: Tyrosine-protein phosphatase SIW14



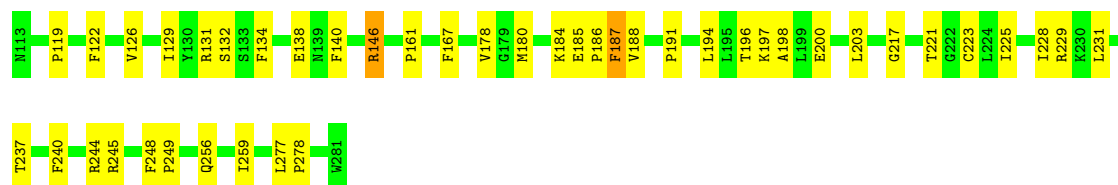
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain E:  68% 29% .



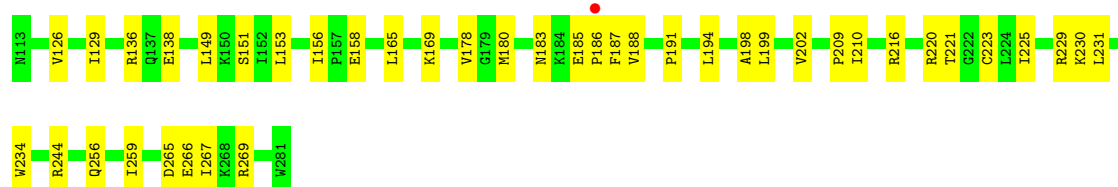
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain F:  75% 24% .



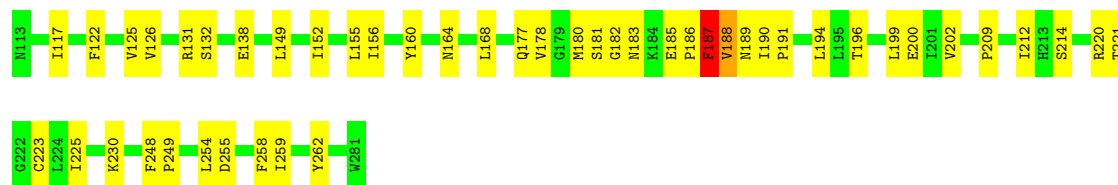
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain G:  % 76% 24%



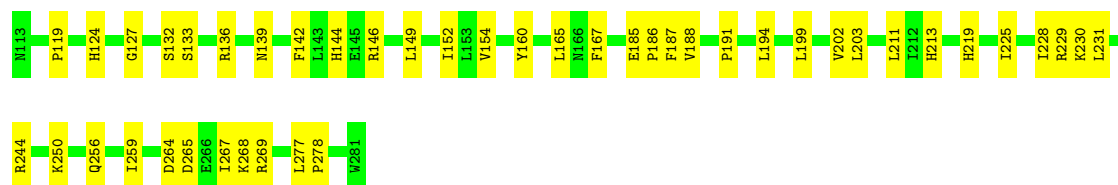
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain H:  72% 27% ..

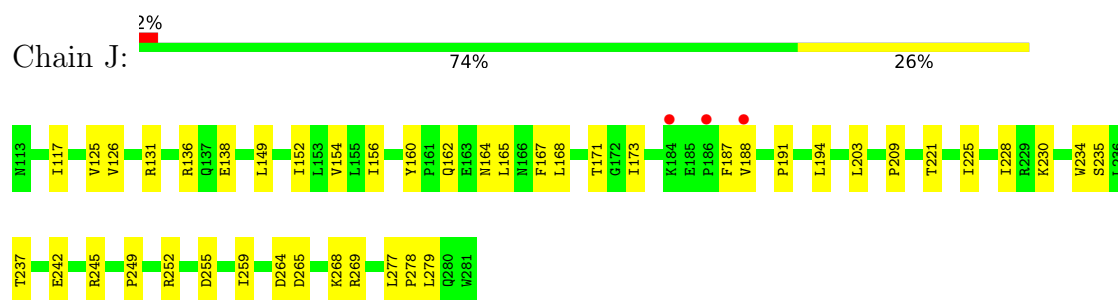


- Molecule 1: Tyrosine-protein phosphatase SIW14

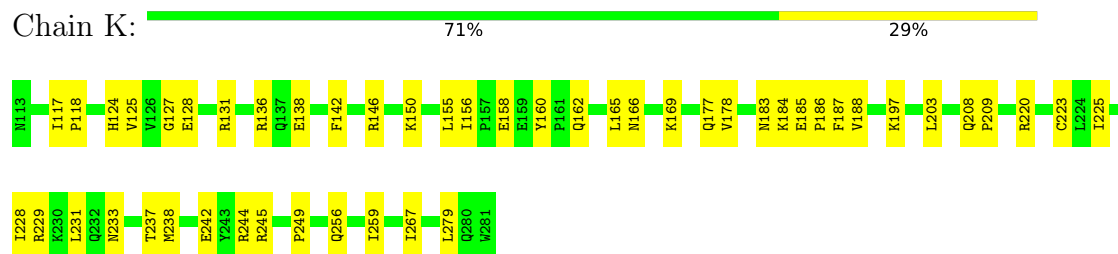
Chain I:  74% 26%



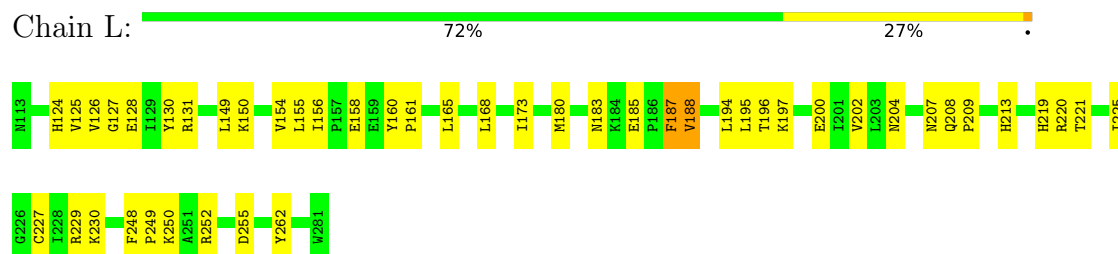
- Molecule 1: Tyrosine-protein phosphatase SIW14



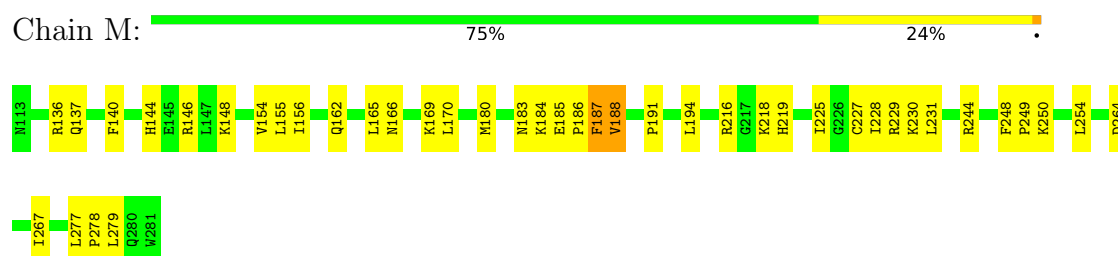
- Molecule 1: Tyrosine-protein phosphatase SIW14



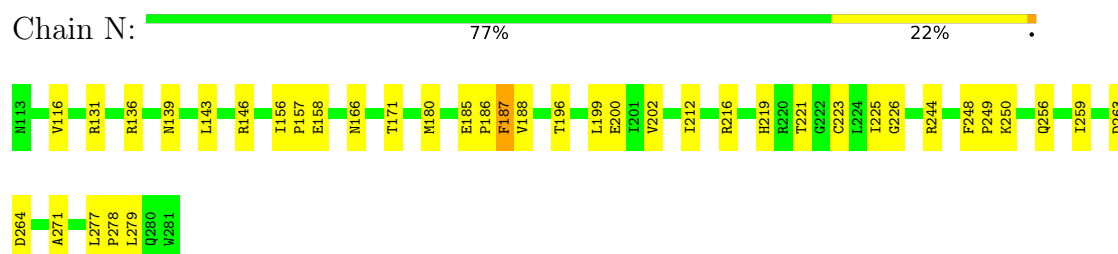
- Molecule 1: Tyrosine-protein phosphatase SIW14



- Molecule 1: Tyrosine-protein phosphatase SIW14



- Molecule 1: Tyrosine-protein phosphatase SIW14



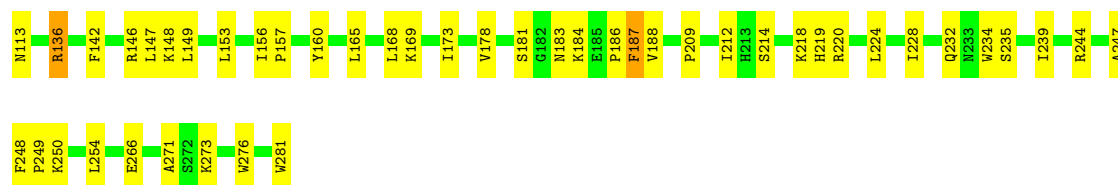
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain O:  74% 26%



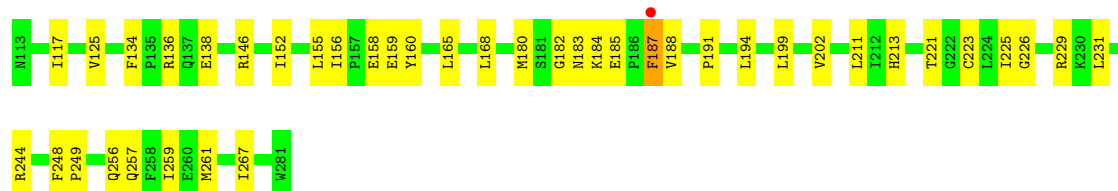
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain P:  73% 25%



- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain Q:  76% 24%



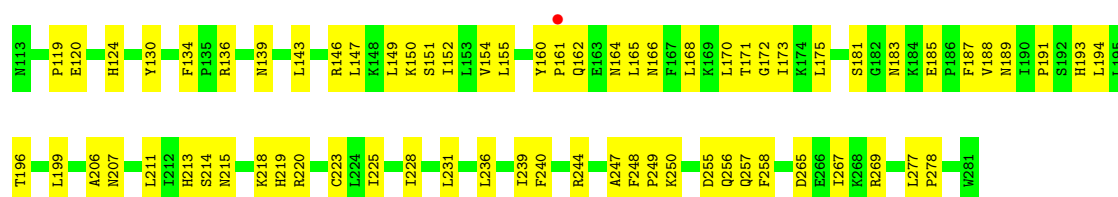
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain R:  74% 25%

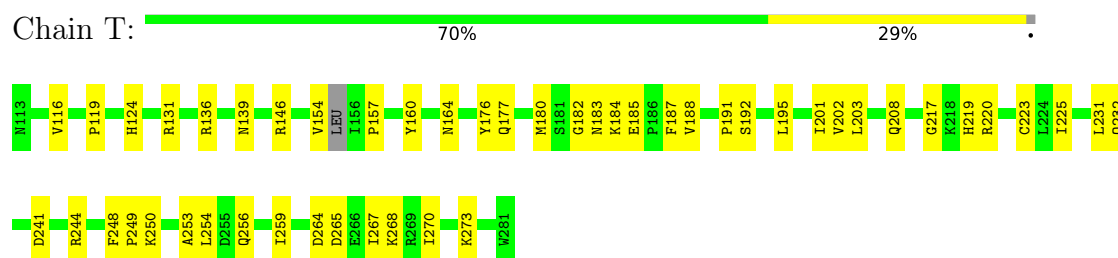


- Molecule 1: Tyrosine-protein phosphatase SIW14

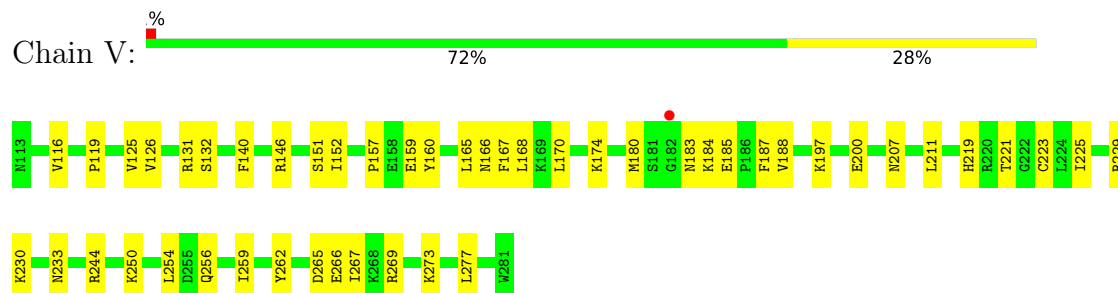
Chain S:  59% 41%



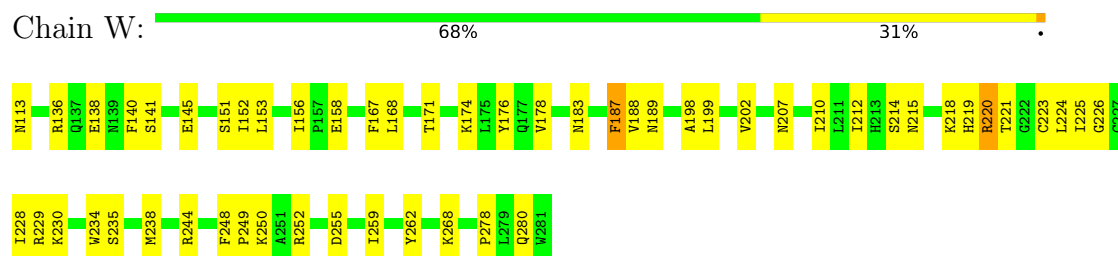
- Molecule 1: Tyrosine-protein phosphatase SIW14



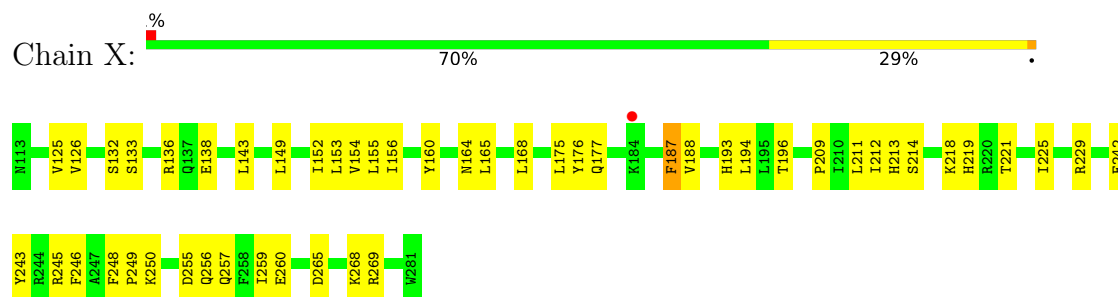
- Molecule 1: Tyrosine-protein phosphatase SIW14



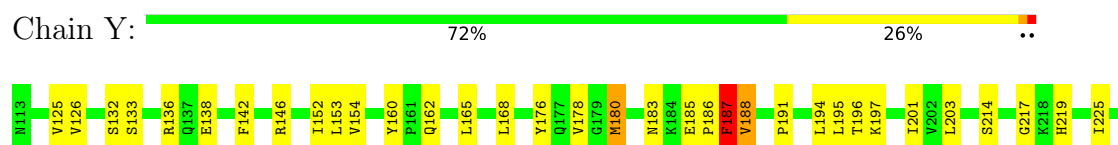
- Molecule 1: Tyrosine-protein phosphatase SIW14



- Molecule 1: Tyrosine-protein phosphatase SIW14



- Molecule 1: Tyrosine-protein phosphatase SIW14



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| R229 | R230 | L231 | F240 | Y243 | F248 | P249 | Q256 | Q257 | M261 | Y262 | E266 | R269 | I270 | W281 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                                                                                                 | Source           |
|-------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                                                                                                                                               | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 92.47Å 160.49Å 360.57Å<br>90.00° 90.32° 90.00°                                                                                                                                        | Depositor        |
| Resolution (Å)                                                          | 14.99 – 2.50<br>14.99 – 2.50                                                                                                                                                          | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.4 (14.99-2.50)<br>83.3 (14.99-2.50)                                                                                                                                                | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                                                                                                                                       | Depositor        |
| $R_{sym}$                                                               | 0.01                                                                                                                                                                                  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.62 (at 2.48Å)                                                                                                                                                                       | Xtriage          |
| Refinement program                                                      | PHENIX 1.14_3260                                                                                                                                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.230 , 0.246<br>0.210 , 0.216                                                                                                                                                        | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2019 reflections (1.21%)                                                                                                                                                              | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 37.4                                                                                                                                                                                  | Xtriage          |
| Anisotropy                                                              | 0.019                                                                                                                                                                                 | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 29.0                                                                                                                                                                           | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$                                                                                                                           | Xtriage          |
| Estimated twinning fraction                                             | 0.336 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l<br>0.357 for -1/2*h+1/2*k,3/2*h+1/2*k,-l<br>0.290 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.340 for 1/2*h+1/2*k,3/2*h-1/2*k,-l<br>0.329 for h,-k,-l | Xtriage          |
| Reported twinning fraction                                              | 0.450 for h,-k,-l                                                                                                                                                                     | Depositor        |
| Outliers                                                                | 1 of 166746 reflections (0.001%)                                                                                                                                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                                                                                                                                                  | EDS              |
| Total number of atoms                                                   | 34047                                                                                                                                                                                 | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 55.0                                                                                                                                                                                  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.20% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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     | 0.17         | 0/1437  | 0.49        | 0/1943          |
| 1   | B     | 0.20         | 0/1437  | 0.57        | 3/1943 (0.2%)   |
| 1   | C     | 0.18         | 0/1437  | 0.49        | 0/1943          |
| 1   | D     | 0.19         | 0/1437  | 0.50        | 2/1943 (0.1%)   |
| 1   | E     | 0.34         | 0/1437  | 0.63        | 3/1943 (0.2%)   |
| 1   | F     | 0.26         | 0/1431  | 0.59        | 3/1936 (0.2%)   |
| 1   | G     | 0.26         | 0/1437  | 0.53        | 0/1943          |
| 1   | H     | 0.22         | 0/1431  | 0.63        | 4/1936 (0.2%)   |
| 1   | I     | 0.27         | 0/1431  | 0.54        | 0/1936          |
| 1   | J     | 0.20         | 0/1437  | 0.50        | 0/1943          |
| 1   | K     | 0.23         | 0/1437  | 0.60        | 0/1943          |
| 1   | L     | 0.24         | 0/1431  | 0.64        | 4/1936 (0.2%)   |
| 1   | M     | 0.22         | 0/1437  | 0.61        | 3/1943 (0.2%)   |
| 1   | N     | 0.17         | 0/1437  | 0.50        | 2/1943 (0.1%)   |
| 1   | O     | 0.17         | 0/1431  | 0.48        | 0/1936          |
| 1   | P     | 0.17         | 0/1437  | 0.52        | 2/1943 (0.1%)   |
| 1   | Q     | 0.19         | 0/1431  | 0.56        | 2/1936 (0.1%)   |
| 1   | R     | 0.23         | 0/1437  | 0.59        | 5/1943 (0.3%)   |
| 1   | S     | 0.20         | 0/1413  | 0.52        | 0/1900          |
| 1   | T     | 0.20         | 0/1428  | 0.56        | 0/1929          |
| 1   | V     | 0.25         | 0/1437  | 0.65        | 3/1943 (0.2%)   |
| 1   | W     | 0.27         | 0/1437  | 0.65        | 3/1943 (0.2%)   |
| 1   | X     | 0.20         | 0/1423  | 0.55        | 2/1927 (0.1%)   |
| 1   | Y     | 0.26         | 0/1437  | 0.63        | 4/1943 (0.2%)   |
| All | All   | 0.22         | 0/34405 | 0.57        | 45/46517 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.



| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 2                   |
| 1   | H     | 0                   | 2                   |
| 1   | K     | 0                   | 1                   |
| 1   | M     | 0                   | 1                   |
| 1   | O     | 0                   | 1                   |
| 1   | P     | 0                   | 2                   |
| 1   | W     | 0                   | 1                   |
| 1   | Y     | 0                   | 2                   |
| All | All   | 0                   | 14                  |

There are no bond length outliers.

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | L     | 187 | PHE  | N-CA-C   | 9.48  | 122.00      | 110.91   |
| 1   | M     | 187 | PHE  | CA-C-N   | 7.68  | 135.53      | 121.70   |
| 1   | M     | 187 | PHE  | C-N-CA   | 7.68  | 135.53      | 121.70   |
| 1   | F     | 187 | PHE  | CA-C-N   | 7.66  | 135.48      | 121.70   |
| 1   | F     | 187 | PHE  | C-N-CA   | 7.66  | 135.48      | 121.70   |
| 1   | B     | 187 | PHE  | CA-C-N   | 7.39  | 135.00      | 121.70   |
| 1   | B     | 187 | PHE  | C-N-CA   | 7.39  | 135.00      | 121.70   |
| 1   | H     | 187 | PHE  | CA-C-N   | 7.25  | 134.75      | 121.70   |
| 1   | H     | 187 | PHE  | C-N-CA   | 7.25  | 134.75      | 121.70   |
| 1   | L     | 187 | PHE  | CA-C-N   | 7.24  | 134.73      | 121.70   |
| 1   | L     | 187 | PHE  | C-N-CA   | 7.24  | 134.73      | 121.70   |
| 1   | F     | 146 | ARG  | CA-CB-CG | -6.76 | 100.58      | 114.10   |
| 1   | R     | 187 | PHE  | CA-C-N   | 6.76  | 133.87      | 121.70   |
| 1   | R     | 187 | PHE  | C-N-CA   | 6.76  | 133.87      | 121.70   |
| 1   | Y     | 187 | PHE  | CA-C-N   | 6.50  | 133.40      | 121.70   |
| 1   | Y     | 187 | PHE  | C-N-CA   | 6.50  | 133.40      | 121.70   |
| 1   | V     | 159 | GLU  | CA-C-N   | 6.31  | 129.45      | 120.49   |
| 1   | V     | 159 | GLU  | C-N-CA   | 6.31  | 129.45      | 120.49   |
| 1   | H     | 188 | VAL  | N-CA-C   | -6.23 | 93.55       | 111.00   |
| 1   | E     | 187 | PHE  | CA-C-N   | 6.09  | 132.67      | 121.70   |
| 1   | E     | 187 | PHE  | C-N-CA   | 6.09  | 132.67      | 121.70   |
| 1   | W     | 187 | PHE  | N-CA-C   | 5.95  | 117.87      | 110.91   |
| 1   | R     | 113 | ASN  | N-CA-C   | -5.89 | 94.51       | 111.00   |
| 1   | H     | 187 | PHE  | N-CA-C   | 5.79  | 123.13      | 110.80   |
| 1   | Q     | 187 | PHE  | CA-C-N   | 5.75  | 132.04      | 121.70   |
| 1   | Q     | 187 | PHE  | C-N-CA   | 5.75  | 132.04      | 121.70   |
| 1   | L     | 188 | VAL  | N-CA-C   | -5.51 | 95.57       | 111.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | Y     | 180 | MET  | CB-CG-SD | 5.47  | 129.11      | 112.70   |
| 1   | R     | 113 | ASN  | CA-C-N   | 5.42  | 132.93      | 122.03   |
| 1   | R     | 113 | ASN  | C-N-CA   | 5.42  | 132.93      | 122.03   |
| 1   | B     | 187 | PHE  | N-CA-C   | 5.37  | 122.24      | 110.80   |
| 1   | V     | 265 | ASP  | N-CA-CB  | -5.36 | 102.22      | 110.20   |
| 1   | X     | 187 | PHE  | CA-C-N   | 5.27  | 131.19      | 121.70   |
| 1   | X     | 187 | PHE  | C-N-CA   | 5.27  | 131.19      | 121.70   |
| 1   | E     | 268 | LYS  | CB-CG-CD | -5.27 | 99.19       | 111.30   |
| 1   | M     | 188 | VAL  | N-CA-C   | -5.18 | 96.50       | 111.00   |
| 1   | Y     | 188 | VAL  | N-CA-C   | -5.14 | 96.59       | 111.00   |
| 1   | D     | 187 | PHE  | CA-C-N   | 5.09  | 130.86      | 121.70   |
| 1   | D     | 187 | PHE  | C-N-CA   | 5.09  | 130.86      | 121.70   |
| 1   | W     | 187 | PHE  | CA-C-N   | 5.06  | 130.80      | 121.70   |
| 1   | W     | 187 | PHE  | C-N-CA   | 5.06  | 130.80      | 121.70   |
| 1   | P     | 187 | PHE  | CA-C-N   | 5.03  | 130.75      | 121.70   |
| 1   | P     | 187 | PHE  | C-N-CA   | 5.03  | 130.75      | 121.70   |
| 1   | N     | 187 | PHE  | CA-C-N   | 5.02  | 130.73      | 121.70   |
| 1   | N     | 187 | PHE  | C-N-CA   | 5.02  | 130.73      | 121.70   |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 186 | PRO  | Peptide   |
| 1   | D     | 146 | ARG  | Sidechain |
| 1   | E     | 186 | PRO  | Peptide   |
| 1   | E     | 252 | ARG  | Sidechain |
| 1   | H     | 186 | PRO  | Peptide   |
| 1   | H     | 187 | PHE  | Peptide   |
| 1   | K     | 186 | PRO  | Peptide   |
| 1   | M     | 186 | PRO  | Peptide   |
| 1   | O     | 186 | PRO  | Peptide   |
| 1   | P     | 136 | ARG  | Sidechain |
| 1   | P     | 186 | PRO  | Peptide   |
| 1   | W     | 220 | ARG  | Sidechain |
| 1   | Y     | 186 | PRO  | Peptide   |
| 1   | Y     | 187 | PHE  | Peptide   |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1401  | 0        | 1416     | 30      | 0            |
| 1   | B     | 1401  | 0        | 1416     | 39      | 0            |
| 1   | C     | 1401  | 0        | 1416     | 28      | 0            |
| 1   | D     | 1401  | 0        | 1416     | 18      | 0            |
| 1   | E     | 1401  | 0        | 1416     | 46      | 0            |
| 1   | F     | 1395  | 0        | 1405     | 30      | 0            |
| 1   | G     | 1401  | 0        | 1416     | 32      | 0            |
| 1   | H     | 1395  | 0        | 1405     | 33      | 0            |
| 1   | I     | 1395  | 0        | 1405     | 26      | 0            |
| 1   | J     | 1401  | 0        | 1416     | 30      | 0            |
| 1   | K     | 1401  | 0        | 1416     | 34      | 0            |
| 1   | L     | 1395  | 0        | 1405     | 31      | 0            |
| 1   | M     | 1401  | 0        | 1416     | 43      | 0            |
| 1   | N     | 1401  | 0        | 1416     | 33      | 0            |
| 1   | O     | 1395  | 0        | 1405     | 33      | 0            |
| 1   | P     | 1401  | 0        | 1416     | 38      | 0            |
| 1   | Q     | 1395  | 0        | 1405     | 32      | 0            |
| 1   | R     | 1401  | 0        | 1416     | 30      | 0            |
| 1   | S     | 1377  | 0        | 1405     | 45      | 0            |
| 1   | T     | 1393  | 0        | 1404     | 37      | 0            |
| 1   | V     | 1401  | 0        | 1416     | 38      | 0            |
| 1   | W     | 1401  | 0        | 1416     | 48      | 0            |
| 1   | X     | 1387  | 0        | 1390     | 31      | 0            |
| 1   | Y     | 1401  | 0        | 1416     | 32      | 0            |
| 2   | A     | 5     | 0        | 0        | 1       | 0            |
| 2   | B     | 5     | 0        | 0        | 0       | 0            |
| 2   | C     | 5     | 0        | 0        | 0       | 0            |
| 2   | D     | 5     | 0        | 0        | 0       | 0            |
| 2   | E     | 5     | 0        | 0        | 0       | 0            |
| 2   | F     | 5     | 0        | 0        | 0       | 0            |
| 2   | G     | 5     | 0        | 0        | 1       | 0            |
| 2   | H     | 5     | 0        | 0        | 2       | 0            |
| 2   | I     | 5     | 0        | 0        | 0       | 0            |
| 2   | J     | 5     | 0        | 0        | 0       | 0            |
| 2   | K     | 5     | 0        | 0        | 0       | 0            |
| 2   | L     | 5     | 0        | 0        | 1       | 0            |
| 2   | M     | 5     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | N     | 5     | 0        | 0        | 0       | 0            |
| 2   | O     | 5     | 0        | 0        | 0       | 0            |
| 2   | P     | 5     | 0        | 0        | 3       | 0            |
| 2   | Q     | 5     | 0        | 0        | 0       | 0            |
| 2   | R     | 5     | 0        | 0        | 0       | 0            |
| 2   | S     | 5     | 0        | 0        | 0       | 0            |
| 2   | T     | 5     | 0        | 0        | 2       | 0            |
| 2   | V     | 5     | 0        | 0        | 0       | 0            |
| 2   | W     | 5     | 0        | 0        | 5       | 0            |
| 2   | X     | 5     | 0        | 0        | 0       | 0            |
| 2   | Y     | 5     | 0        | 0        | 2       | 0            |
| 3   | A     | 14    | 0        | 0        | 0       | 0            |
| 3   | B     | 17    | 0        | 0        | 0       | 0            |
| 3   | C     | 17    | 0        | 0        | 0       | 0            |
| 3   | D     | 17    | 0        | 0        | 0       | 0            |
| 3   | E     | 13    | 0        | 0        | 1       | 0            |
| 3   | F     | 23    | 0        | 0        | 3       | 0            |
| 3   | G     | 15    | 0        | 0        | 0       | 0            |
| 3   | H     | 6     | 0        | 0        | 0       | 0            |
| 3   | I     | 12    | 0        | 0        | 0       | 0            |
| 3   | J     | 18    | 0        | 0        | 2       | 0            |
| 3   | K     | 17    | 0        | 0        | 1       | 0            |
| 3   | L     | 21    | 0        | 0        | 2       | 0            |
| 3   | M     | 18    | 0        | 0        | 2       | 0            |
| 3   | N     | 15    | 0        | 0        | 2       | 0            |
| 3   | O     | 18    | 0        | 0        | 0       | 0            |
| 3   | P     | 16    | 0        | 0        | 3       | 0            |
| 3   | Q     | 23    | 0        | 0        | 1       | 0            |
| 3   | R     | 13    | 0        | 0        | 1       | 0            |
| 3   | S     | 12    | 0        | 0        | 0       | 0            |
| 3   | T     | 17    | 0        | 0        | 2       | 0            |
| 3   | V     | 9     | 0        | 0        | 1       | 0            |
| 3   | W     | 15    | 0        | 0        | 2       | 0            |
| 3   | X     | 25    | 0        | 0        | 0       | 0            |
| 3   | Y     | 14    | 0        | 0        | 0       | 0            |
| All | All   | 34047 | 0        | 33869    | 751     | 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 11.

All (751) 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:V:166:ASN:O    | 1:V:170:LEU:HD12 | 1.44                     | 1.16              |
| 1:E:244:ARG:HD3  | 1:M:244:ARG:HE   | 1.24                     | 1.02              |
| 1:M:230:LYS:HE3  | 1:M:264:ASP:CG   | 1.85                     | 1.02              |
| 1:M:230:LYS:HE3  | 1:M:264:ASP:OD2  | 1.60                     | 1.02              |
| 1:M:187:PHE:HA   | 1:M:188:VAL:HG13 | 1.49                     | 0.93              |
| 1:M:230:LYS:HE3  | 1:M:264:ASP:CB   | 1.99                     | 0.93              |
| 1:R:187:PHE:HA   | 1:R:188:VAL:HG23 | 1.54                     | 0.90              |
| 1:L:187:PHE:HA   | 1:L:188:VAL:HG23 | 1.54                     | 0.90              |
| 1:V:166:ASN:O    | 1:V:170:LEU:CD1  | 2.21                     | 0.86              |
| 1:W:153:LEU:HB3  | 1:W:212:ILE:HG13 | 1.58                     | 0.85              |
| 1:Y:180:MET:SD   | 1:Y:194:LEU:HD13 | 2.18                     | 0.84              |
| 1:J:265:ASP:HA   | 1:J:268:LYS:HD3  | 1.60                     | 0.83              |
| 1:M:216:ARG:HH22 | 1:M:250:LYS:CD   | 1.92                     | 0.82              |
| 1:M:227:CYS:SG   | 3:M:408:HOH:O    | 2.36                     | 0.82              |
| 1:M:216:ARG:HH22 | 1:M:250:LYS:HD2  | 1.45                     | 0.81              |
| 1:I:142:PHE:HE1  | 1:I:146:ARG:HH21 | 1.23                     | 0.80              |
| 1:Q:187:PHE:HA   | 1:Q:188:VAL:HG22 | 1.66                     | 0.77              |
| 1:H:117:ILE:HD13 | 1:H:138:GLU:HB2  | 1.67                     | 0.77              |
| 1:R:187:PHE:HA   | 1:R:188:VAL:CG2  | 2.15                     | 0.76              |
| 1:A:244:ARG:HE   | 1:A:256:GLN:HE22 | 1.31                     | 0.76              |
| 1:W:219:HIS:NE2  | 1:W:250:LYS:O    | 2.20                     | 0.75              |
| 1:M:230:LYS:CE   | 1:M:264:ASP:OD2  | 2.34                     | 0.74              |
| 1:H:220:ARG:NE   | 2:H:301:SO4:O3   | 2.21                     | 0.74              |
| 1:I:230:LYS:NZ   | 1:I:259:ILE:O    | 2.21                     | 0.73              |
| 1:V:165:LEU:HA   | 1:V:168:LEU:HD12 | 1.70                     | 0.73              |
| 1:S:219:HIS:NE2  | 1:S:250:LYS:O    | 2.22                     | 0.72              |
| 1:B:141:SER:HA   | 1:B:145:GLU:OE2  | 1.89                     | 0.72              |
| 1:J:268:LYS:HG2  | 1:J:269:ARG:N    | 2.03                     | 0.72              |
| 1:K:136:ARG:NH2  | 1:K:138:GLU:OE2  | 2.23                     | 0.72              |
| 1:I:244:ARG:HE   | 1:I:256:GLN:HE22 | 1.37                     | 0.72              |
| 1:R:156:ILE:HG22 | 1:R:158:GLU:H    | 1.54                     | 0.71              |
| 1:C:146:ARG:NH2  | 1:T:232:GLN:OE1  | 2.23                     | 0.71              |
| 1:X:136:ARG:NH1  | 1:X:138:GLU:OE2  | 2.24                     | 0.70              |
| 1:F:187:PHE:HA   | 1:F:188:VAL:HG13 | 1.74                     | 0.70              |
| 1:I:244:ARG:NE   | 1:I:256:GLN:HE22 | 1.89                     | 0.70              |
| 1:M:219:HIS:NE2  | 1:M:250:LYS:O    | 2.22                     | 0.70              |
| 1:F:178:VAL:HG12 | 1:F:197:LYS:HE3  | 1.72                     | 0.70              |
| 1:M:162:GLN:HA   | 1:M:165:LEU:HB2  | 1.74                     | 0.70              |
| 1:K:279:LEU:O    | 1:P:146:ARG:NH1  | 2.24                     | 0.70              |
| 1:N:250:LYS:NZ   | 3:N:402:HOH:O    | 2.25                     | 0.69              |
| 1:E:187:PHE:HA   | 1:E:188:VAL:HB   | 1.75                     | 0.69              |
| 1:H:178:VAL:HG13 | 1:H:194:LEU:HD22 | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:223:CYS:HA   | 1:W:259:ILE:HD11 | 1.74                     | 0.69              |
| 1:C:128:GLU:HB2  | 1:C:208:GLN:HB3  | 1.75                     | 0.69              |
| 1:P:244:ARG:NH1  | 3:P:401:HOH:O    | 2.26                     | 0.68              |
| 1:K:155:LEU:O    | 1:K:220:ARG:NH1  | 2.27                     | 0.68              |
| 1:X:152:ILE:HG12 | 1:X:211:LEU:HB3  | 1.76                     | 0.67              |
| 1:P:136:ARG:NH1  | 1:Q:188:VAL:O    | 2.24                     | 0.67              |
| 1:W:215:ASN:HB2  | 1:W:220:ARG:HH22 | 1.59                     | 0.67              |
| 1:V:244:ARG:HE   | 1:V:256:GLN:HE22 | 1.41                     | 0.67              |
| 1:H:156:ILE:O    | 1:H:177:GLN:NE2  | 2.27                     | 0.66              |
| 1:Q:156:ILE:HG22 | 1:Q:158:GLU:H    | 1.60                     | 0.66              |
| 1:F:146:ARG:HH12 | 1:N:278:PRO:HB2  | 1.60                     | 0.66              |
| 1:Y:266:GLU:O    | 1:Y:269:ARG:HG2  | 1.96                     | 0.66              |
| 1:B:187:PHE:HA   | 1:B:188:VAL:CG2  | 2.26                     | 0.65              |
| 1:L:155:LEU:HD22 | 1:L:180:MET:HE2  | 1.78                     | 0.65              |
| 1:V:223:CYS:HA   | 1:V:259:ILE:HD11 | 1.79                     | 0.65              |
| 1:B:223:CYS:HA   | 1:B:259:ILE:HD11 | 1.79                     | 0.65              |
| 1:L:219:HIS:NE2  | 1:L:250:LYS:O    | 2.24                     | 0.65              |
| 1:R:181:SER:HB2  | 1:R:184:LYS:HB2  | 1.79                     | 0.65              |
| 1:F:244:ARG:HE   | 1:F:256:GLN:HE22 | 1.44                     | 0.65              |
| 1:F:196:THR:O    | 1:F:200:GLU:HG3  | 1.97                     | 0.65              |
| 1:W:214:SER:OG   | 1:W:220:ARG:NH2  | 2.30                     | 0.65              |
| 1:R:196:THR:O    | 1:R:200:GLU:HG3  | 1.96                     | 0.65              |
| 1:E:252:ARG:NE   | 1:E:255:ASP:OD1  | 2.29                     | 0.64              |
| 1:K:128:GLU:HG3  | 1:K:208:GLN:HB3  | 1.78                     | 0.64              |
| 1:E:113:ASN:HD21 | 1:O:277:LEU:HD13 | 1.63                     | 0.64              |
| 1:W:219:HIS:N    | 2:W:301:SO4:O4   | 2.31                     | 0.64              |
| 1:X:132:SER:HB3  | 1:X:211:LEU:HD11 | 1.79                     | 0.64              |
| 1:C:131:ARG:NH2  | 1:C:217:GLY:O    | 2.29                     | 0.64              |
| 1:K:178:VAL:HG22 | 1:K:197:LYS:HE3  | 1.79                     | 0.64              |
| 1:C:230:LYS:NZ   | 1:C:262:TYR:O    | 2.31                     | 0.64              |
| 1:E:252:ARG:NH2  | 1:E:255:ASP:OD1  | 2.30                     | 0.64              |
| 1:B:155:LEU:HD22 | 1:B:180:MET:HE2  | 1.78                     | 0.64              |
| 1:B:228:ILE:HA   | 1:B:231:LEU:HD12 | 1.79                     | 0.63              |
| 1:Q:223:CYS:HA   | 1:Q:259:ILE:HD11 | 1.78                     | 0.63              |
| 1:D:146:ARG:NH2  | 1:M:279:LEU:O    | 2.32                     | 0.63              |
| 1:K:244:ARG:NH2  | 1:K:256:GLN:HE22 | 1.96                     | 0.63              |
| 1:G:136:ARG:NH2  | 1:G:138:GLU:OE2  | 2.30                     | 0.62              |
| 1:G:136:ARG:HH21 | 1:G:138:GLU:CD   | 2.07                     | 0.62              |
| 1:L:230:LYS:NZ   | 1:L:262:TYR:O    | 2.33                     | 0.62              |
| 1:N:156:ILE:HG22 | 1:N:158:GLU:H    | 1.62                     | 0.62              |
| 1:S:265:ASP:O    | 1:S:269:ARG:HG3  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:231:LEU:HD21 | 1:G:267:ILE:HG23 | 1.81                     | 0.62              |
| 1:M:191:PRO:HD2  | 1:M:194:LEU:HD12 | 1.81                     | 0.62              |
| 1:P:149:LEU:HA   | 1:P:209:PRO:HB2  | 1.82                     | 0.62              |
| 1:A:156:ILE:HG22 | 1:A:158:GLU:H    | 1.65                     | 0.62              |
| 1:A:277:LEU:HG   | 1:A:278:PRO:HA   | 1.82                     | 0.61              |
| 1:N:219:HIS:NE2  | 1:N:250:LYS:O    | 2.33                     | 0.61              |
| 1:T:187:PHE:HA   | 1:T:188:VAL:HG22 | 1.82                     | 0.61              |
| 1:H:223:CYS:HA   | 1:H:259:ILE:HD11 | 1.81                     | 0.61              |
| 1:P:234:TRP:HB2  | 1:P:239:ILE:HD11 | 1.82                     | 0.61              |
| 1:A:244:ARG:NE   | 1:A:256:GLN:HE22 | 1.98                     | 0.61              |
| 1:B:187:PHE:HA   | 1:B:188:VAL:HG22 | 1.82                     | 0.61              |
| 1:W:252:ARG:NH2  | 1:W:255:ASP:OD2  | 2.25                     | 0.61              |
| 1:Y:266:GLU:O    | 1:Y:270:ILE:HG12 | 2.01                     | 0.61              |
| 1:M:136:ARG:NH2  | 1:N:188:VAL:O    | 2.33                     | 0.61              |
| 1:S:191:PRO:HD2  | 1:S:194:LEU:HD12 | 1.83                     | 0.60              |
| 1:V:152:ILE:HG12 | 1:V:211:LEU:HB3  | 1.82                     | 0.60              |
| 1:S:152:ILE:HD11 | 1:S:175:LEU:HD12 | 1.83                     | 0.60              |
| 1:T:136:ARG:NH1  | 1:V:188:VAL:O    | 2.31                     | 0.60              |
| 1:V:166:ASN:C    | 1:V:170:LEU:HD12 | 2.23                     | 0.60              |
| 1:I:277:LEU:HD12 | 1:I:278:PRO:HA   | 1.81                     | 0.60              |
| 1:G:187:PHE:HA   | 1:G:188:VAL:HB   | 1.84                     | 0.60              |
| 1:K:162:GLN:O    | 1:K:166:ASN:ND2  | 2.34                     | 0.60              |
| 1:G:156:ILE:HD12 | 1:G:158:GLU:HB2  | 1.83                     | 0.60              |
| 1:G:180:MET:HB2  | 1:G:220:ARG:HD2  | 1.82                     | 0.60              |
| 1:G:221:THR:O    | 1:G:225:ILE:HG12 | 2.01                     | 0.60              |
| 1:M:228:ILE:HA   | 1:M:231:LEU:HD12 | 1.82                     | 0.60              |
| 1:W:152:ILE:HG21 | 1:W:168:LEU:HD13 | 1.84                     | 0.60              |
| 1:Y:178:VAL:HG12 | 1:Y:180:MET:HE2  | 1.83                     | 0.60              |
| 1:G:191:PRO:HD2  | 1:G:194:LEU:HD12 | 1.84                     | 0.60              |
| 1:M:216:ARG:HH22 | 1:M:250:LYS:HD3  | 1.66                     | 0.60              |
| 1:K:233:ASN:ND2  | 1:P:113:ASN:O    | 2.31                     | 0.59              |
| 1:A:254:LEU:HD22 | 1:C:136:ARG:HH11 | 1.66                     | 0.59              |
| 1:L:160:TYR:HD2  | 1:L:165:LEU:HG   | 1.67                     | 0.59              |
| 1:Q:244:ARG:HE   | 1:Q:256:GLN:HE22 | 1.50                     | 0.59              |
| 1:R:219:HIS:NE2  | 1:R:250:LYS:O    | 2.34                     | 0.59              |
| 1:Y:178:VAL:CG1  | 1:Y:180:MET:HE2  | 2.33                     | 0.59              |
| 1:C:116:VAL:HG21 | 1:C:146:ARG:HD3  | 1.85                     | 0.59              |
| 1:Y:178:VAL:HG22 | 1:Y:197:LYS:HE2  | 1.83                     | 0.59              |
| 1:J:230:LYS:NZ   | 1:J:259:ILE:O    | 2.33                     | 0.58              |
| 1:B:141:SER:HB2  | 1:B:145:GLU:OE1  | 2.03                     | 0.58              |
| 1:Y:217:GLY:N    | 2:Y:301:SO4:O4   | 2.37                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:183:ASN:O    | 1:E:184:LYS:HG2  | 2.04                     | 0.58              |
| 1:E:244:ARG:HD2  | 3:E:407:HOH:O    | 2.02                     | 0.58              |
| 1:K:156:ILE:HG22 | 1:K:158:GLU:H    | 1.68                     | 0.58              |
| 1:B:187:PHE:HE1  | 1:B:252:ARG:HD2  | 1.69                     | 0.58              |
| 1:W:141:SER:O    | 1:W:145:GLU:HB2  | 2.03                     | 0.58              |
| 1:R:152:ILE:HD12 | 1:R:168:LEU:HD21 | 1.85                     | 0.57              |
| 1:E:252:ARG:HH21 | 1:E:255:ASP:CG   | 2.11                     | 0.57              |
| 1:H:182:GLY:HA2  | 1:H:220:ARG:NH1  | 2.19                     | 0.57              |
| 1:K:117:ILE:HG12 | 1:P:235:SER:HB2  | 1.87                     | 0.57              |
| 1:B:113:ASN:HD21 | 1:V:277:LEU:HD11 | 1.70                     | 0.57              |
| 1:E:146:ARG:HH12 | 1:O:234:TRP:HE1  | 1.51                     | 0.57              |
| 1:N:196:THR:O    | 1:N:200:GLU:HG3  | 2.04                     | 0.57              |
| 1:M:277:LEU:HD12 | 1:M:278:PRO:HA   | 1.85                     | 0.57              |
| 1:P:235:SER:O    | 1:P:239:ILE:HG12 | 2.04                     | 0.57              |
| 1:W:198:ALA:O    | 1:W:202:VAL:HG13 | 2.05                     | 0.57              |
| 1:M:230:LYS:HE3  | 1:M:264:ASP:HB3  | 1.84                     | 0.56              |
| 1:S:277:LEU:HG   | 1:S:278:PRO:HA   | 1.86                     | 0.56              |
| 1:I:185:GLU:HG2  | 1:I:186:PRO:HD2  | 1.87                     | 0.56              |
| 1:D:257:GLN:NE2  | 1:F:138:GLU:OE1  | 2.37                     | 0.56              |
| 1:F:203:LEU:HD11 | 1:F:231:LEU:HD13 | 1.88                     | 0.56              |
| 1:K:187:PHE:HA   | 1:K:188:VAL:HG22 | 1.87                     | 0.56              |
| 1:V:187:PHE:HA   | 1:V:188:VAL:HB   | 1.86                     | 0.56              |
| 1:Y:240:PHE:CD1  | 1:Y:256:GLN:HG2  | 2.41                     | 0.56              |
| 1:C:183:ASN:C    | 1:C:185:GLU:H    | 2.14                     | 0.56              |
| 1:C:188:VAL:HG12 | 1:C:254:LEU:HD13 | 1.88                     | 0.56              |
| 1:J:152:ILE:HD12 | 1:J:168:LEU:HD21 | 1.86                     | 0.56              |
| 1:T:202:VAL:O    | 1:T:208:GLN:NE2  | 2.35                     | 0.56              |
| 1:Y:196:THR:OG1  | 1:Y:262:TYR:OH   | 2.24                     | 0.56              |
| 1:A:244:ARG:NH2  | 1:T:241:ASP:OD1  | 2.36                     | 0.56              |
| 1:Y:191:PRO:HD2  | 1:Y:194:LEU:HD21 | 1.86                     | 0.56              |
| 1:J:187:PHE:HA   | 1:J:188:VAL:HB   | 1.88                     | 0.56              |
| 1:S:214:SER:OG   | 1:S:215:ASN:N    | 2.37                     | 0.56              |
| 1:B:230:LYS:NZ   | 1:B:262:TYR:O    | 2.39                     | 0.56              |
| 1:Q:199:LEU:HA   | 1:Q:202:VAL:HG22 | 1.87                     | 0.56              |
| 1:C:166:ASN:O    | 1:C:170:LEU:HD23 | 2.06                     | 0.56              |
| 1:D:261:MET:HE1  | 3:F:406:HOH:O    | 2.05                     | 0.56              |
| 1:H:183:ASN:C    | 1:H:185:GLU:H    | 2.13                     | 0.56              |
| 1:A:187:PHE:HA   | 1:A:188:VAL:HB   | 1.88                     | 0.55              |
| 1:K:223:CYS:HA   | 1:K:259:ILE:HD11 | 1.89                     | 0.55              |
| 1:N:271:ALA:CB   | 1:N:277:LEU:CD2  | 2.84                     | 0.55              |
| 1:T:184:LYS:NZ   | 3:T:401:HOH:O    | 2.22                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:265:ASP:OD2  | 1:X:269:ARG:NH2  | 2.40                     | 0.55              |
| 1:N:187:PHE:HA   | 1:N:188:VAL:HB   | 1.88                     | 0.55              |
| 1:I:225:ILE:HD13 | 1:I:228:ILE:HD12 | 1.88                     | 0.55              |
| 1:T:219:HIS:NE2  | 1:T:250:LYS:O    | 2.40                     | 0.55              |
| 1:E:214:SER:HB2  | 1:E:220:ARG:HH11 | 1.71                     | 0.55              |
| 1:G:153:LEU:HD11 | 1:G:178:VAL:HG23 | 1.87                     | 0.55              |
| 1:B:191:PRO:HD2  | 1:B:194:LEU:HD12 | 1.88                     | 0.55              |
| 1:G:199:LEU:HA   | 1:G:202:VAL:HG22 | 1.89                     | 0.55              |
| 1:A:152:ILE:HD11 | 1:A:168:LEU:HD11 | 1.89                     | 0.55              |
| 1:Y:152:ILE:HD12 | 1:Y:168:LEU:HD21 | 1.89                     | 0.55              |
| 1:H:181:SER:H    | 1:H:190:ILE:HD11 | 1.72                     | 0.54              |
| 1:N:185:GLU:HG2  | 1:N:186:PRO:HD2  | 1.88                     | 0.54              |
| 1:W:234:TRP:NE1  | 3:W:402:HOH:O    | 2.33                     | 0.54              |
| 1:H:200:GLU:OE2  | 1:L:197:LYS:NZ   | 2.40                     | 0.54              |
| 1:L:131:ARG:HD2  | 1:L:225:ILE:HD13 | 1.90                     | 0.54              |
| 1:K:150:LYS:HG2  | 1:K:209:PRO:HD2  | 1.90                     | 0.54              |
| 1:R:114:LYS:NZ   | 1:R:145:GLU:OE1  | 2.35                     | 0.54              |
| 1:E:117:ILE:HD12 | 1:E:138:GLU:HB2  | 1.89                     | 0.54              |
| 1:E:252:ARG:CZ   | 1:E:255:ASP:OD1  | 2.56                     | 0.54              |
| 1:I:152:ILE:HD13 | 1:I:211:LEU:HB3  | 1.89                     | 0.54              |
| 1:A:219:HIS:N    | 2:A:301:SO4:O4   | 2.34                     | 0.54              |
| 1:E:257:GLN:HG2  | 1:E:261:MET:HE2  | 1.89                     | 0.54              |
| 1:O:152:ILE:HD13 | 1:O:211:LEU:HB3  | 1.88                     | 0.54              |
| 1:S:151:SER:OG   | 1:S:207:ASN:O    | 2.25                     | 0.54              |
| 1:E:231:LEU:HD21 | 1:E:267:ILE:HG23 | 1.89                     | 0.54              |
| 1:L:149:LEU:HA   | 1:L:209:PRO:HB2  | 1.90                     | 0.54              |
| 1:T:253:ALA:HA   | 1:T:256:GLN:OE1  | 2.08                     | 0.54              |
| 1:N:166:ASN:OD1  | 1:R:114:LYS:NZ   | 2.41                     | 0.54              |
| 1:O:187:PHE:HA   | 1:O:188:VAL:HB   | 1.90                     | 0.54              |
| 1:D:156:ILE:O    | 1:D:177:GLN:NE2  | 2.40                     | 0.54              |
| 1:L:202:VAL:O    | 1:L:208:GLN:NE2  | 2.38                     | 0.53              |
| 1:P:188:VAL:O    | 1:R:136:ARG:NH1  | 2.34                     | 0.53              |
| 1:R:180:MET:HG3  | 1:R:194:LEU:HD23 | 1.90                     | 0.53              |
| 1:S:183:ASN:C    | 1:S:185:GLU:H    | 2.16                     | 0.53              |
| 1:F:277:LEU:HD12 | 1:F:278:PRO:HA   | 1.90                     | 0.53              |
| 1:L:127:GLY:HA3  | 3:L:401:HOH:O    | 2.09                     | 0.53              |
| 1:X:194:LEU:HD12 | 1:X:194:LEU:H    | 1.73                     | 0.53              |
| 1:I:219:HIS:NE2  | 1:I:250:LYS:O    | 2.41                     | 0.53              |
| 1:K:242:GLU:HG3  | 1:K:245:ARG:NH2  | 2.24                     | 0.53              |
| 1:M:188:VAL:O    | 1:O:136:ARG:NH1  | 2.39                     | 0.53              |
| 1:R:160:TYR:CE2  | 1:R:164:ASN:HB3  | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:136:ARG:NH1  | 1:Y:138:GLU:OE2  | 2.40                     | 0.53              |
| 1:L:180:MET:HG2  | 1:L:194:LEU:HD13 | 1.90                     | 0.53              |
| 1:T:157:PRO:HD3  | 1:T:180:MET:O    | 2.08                     | 0.53              |
| 1:J:191:PRO:HD2  | 1:J:194:LEU:HD12 | 1.91                     | 0.53              |
| 1:G:156:ILE:HG22 | 1:G:220:ARG:HH21 | 1.73                     | 0.53              |
| 1:H:156:ILE:HD11 | 1:H:220:ARG:CZ   | 2.38                     | 0.53              |
| 1:L:125:VAL:HG12 | 1:L:126:VAL:HG12 | 1.90                     | 0.53              |
| 1:H:230:LYS:NZ   | 1:H:262:TYR:O    | 2.29                     | 0.53              |
| 1:Q:134:PHE:HD1  | 1:Q:213:HIS:CE1  | 2.27                     | 0.53              |
| 1:S:248:PHE:CG   | 1:S:249:PRO:HA   | 2.44                     | 0.53              |
| 1:D:232:GLN:HG2  | 1:D:279:LEU:HD12 | 1.91                     | 0.53              |
| 1:O:159:GLU:OE1  | 1:P:273:LYS:HE2  | 2.08                     | 0.53              |
| 1:S:134:PHE:CZ   | 1:S:161:PRO:HG2  | 2.44                     | 0.53              |
| 1:E:160:TYR:CE2  | 1:E:164:ASN:HB3  | 2.44                     | 0.53              |
| 1:H:212:ILE:HG22 | 1:H:221:THR:HG23 | 1.90                     | 0.53              |
| 1:I:119:PRO:HG3  | 1:I:139:ASN:HB3  | 1.90                     | 0.53              |
| 1:F:178:VAL:HG21 | 1:F:198:ALA:HB2  | 1.91                     | 0.53              |
| 1:Q:136:ARG:HB2  | 1:Q:138:GLU:OE1  | 2.09                     | 0.53              |
| 1:A:234:TRP:HE1  | 1:S:146:ARG:HH12 | 1.55                     | 0.52              |
| 1:Q:187:PHE:HA   | 1:Q:188:VAL:CG2  | 2.39                     | 0.52              |
| 1:V:166:ASN:C    | 1:V:170:LEU:CD1  | 2.82                     | 0.52              |
| 1:A:219:HIS:NE2  | 1:A:250:LYS:O    | 2.36                     | 0.52              |
| 1:G:266:GLU:HA   | 1:G:269:ARG:HE   | 1.75                     | 0.52              |
| 1:N:271:ALA:HB1  | 1:N:277:LEU:HD22 | 1.91                     | 0.52              |
| 1:B:264:ASP:OD1  | 1:B:264:ASP:N    | 2.38                     | 0.52              |
| 1:L:168:LEU:HD22 | 1:L:173:ILE:HB   | 1.91                     | 0.52              |
| 1:J:149:LEU:HA   | 1:J:209:PRO:HB2  | 1.90                     | 0.52              |
| 1:M:154:VAL:HG22 | 1:M:156:ILE:HG12 | 1.92                     | 0.52              |
| 1:M:216:ARG:HH21 | 1:M:219:HIS:CE1  | 2.28                     | 0.52              |
| 1:P:187:PHE:HA   | 1:P:188:VAL:HB   | 1.91                     | 0.52              |
| 1:T:270:ILE:HA   | 1:T:273:LYS:HG2  | 1.92                     | 0.52              |
| 1:B:187:PHE:CE1  | 1:B:252:ARG:HD2  | 2.44                     | 0.52              |
| 1:B:113:ASN:O    | 1:V:233:ASN:ND2  | 2.40                     | 0.52              |
| 1:A:117:ILE:HG21 | 1:B:257:GLN:HE22 | 1.73                     | 0.52              |
| 1:Y:142:PHE:HE1  | 1:Y:146:ARG:HH21 | 1.57                     | 0.52              |
| 1:L:248:PHE:CD1  | 1:L:249:PRO:HA   | 2.44                     | 0.51              |
| 1:O:243:TYR:OH   | 1:O:255:ASP:OD2  | 2.22                     | 0.51              |
| 1:S:134:PHE:HZ   | 1:S:161:PRO:HG2  | 1.75                     | 0.51              |
| 1:E:244:ARG:HD3  | 1:M:244:ARG:NE   | 2.07                     | 0.51              |
| 1:J:167:PHE:O    | 1:J:171:THR:HG22 | 2.10                     | 0.51              |
| 1:O:125:VAL:O    | 1:O:229:ARG:NH2  | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:181:SER:OG   | 1:S:189:ASN:O    | 2.27                     | 0.51              |
| 1:T:264:ASP:OD1  | 1:T:264:ASP:N    | 2.39                     | 0.51              |
| 1:V:131:ARG:HG2  | 1:V:132:SER:N    | 2.24                     | 0.51              |
| 1:W:268:LYS:HB2  | 1:W:268:LYS:NZ   | 2.25                     | 0.51              |
| 1:D:228:ILE:HG22 | 1:D:232:GLN:HE21 | 1.75                     | 0.51              |
| 1:F:180:MET:HG2  | 1:F:194:LEU:HD13 | 1.91                     | 0.51              |
| 1:J:131:ARG:HD2  | 1:J:225:ILE:HD13 | 1.91                     | 0.51              |
| 1:J:171:THR:HG23 | 1:J:173:ILE:H    | 1.74                     | 0.51              |
| 1:O:183:ASN:C    | 1:O:185:GLU:H    | 2.18                     | 0.51              |
| 1:S:165:LEU:HA   | 1:S:168:LEU:HD12 | 1.92                     | 0.51              |
| 1:W:187:PHE:HA   | 1:W:188:VAL:HB   | 1.92                     | 0.51              |
| 1:B:141:SER:O    | 1:B:145:GLU:OE2  | 2.28                     | 0.51              |
| 1:E:244:ARG:CD   | 1:M:244:ARG:HE   | 2.08                     | 0.51              |
| 1:S:255:ASP:HA   | 1:S:258:PHE:CD2  | 2.46                     | 0.51              |
| 1:T:154:VAL:HG23 | 1:T:177:GLN:HG3  | 1.93                     | 0.51              |
| 1:E:183:ASN:C    | 1:E:185:GLU:H    | 2.18                     | 0.51              |
| 1:F:146:ARG:NH2  | 1:N:279:LEU:O    | 2.44                     | 0.51              |
| 1:M:166:ASN:O    | 1:M:170:LEU:HG   | 2.10                     | 0.51              |
| 1:T:231:LEU:HD21 | 1:T:267:ILE:HG23 | 1.92                     | 0.51              |
| 1:Y:180:MET:HG3  | 1:Y:194:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:212:ILE:HG22 | 1:A:221:THR:HG23 | 1.93                     | 0.51              |
| 1:B:176:TYR:HB3  | 1:B:201:ILE:HD13 | 1.93                     | 0.51              |
| 1:W:214:SER:OG   | 1:W:215:ASN:N    | 2.44                     | 0.51              |
| 1:W:252:ARG:HH21 | 1:W:255:ASP:CG   | 2.17                     | 0.51              |
| 1:E:146:ARG:NH2  | 1:O:232:GLN:OE1  | 2.44                     | 0.51              |
| 1:S:136:ARG:NH1  | 1:T:188:VAL:H    | 2.08                     | 0.51              |
| 1:X:168:LEU:HD12 | 1:X:175:LEU:HD12 | 1.92                     | 0.51              |
| 1:J:221:THR:HG22 | 1:J:225:ILE:HD12 | 1.93                     | 0.51              |
| 1:R:156:ILE:HD11 | 1:R:214:SER:HA   | 1.92                     | 0.51              |
| 1:S:162:GLN:O    | 1:S:165:LEU:HG   | 2.09                     | 0.51              |
| 1:W:215:ASN:HB2  | 1:W:220:ARG:NH2  | 2.25                     | 0.51              |
| 1:W:225:ILE:O    | 1:W:229:ARG:HG2  | 2.11                     | 0.51              |
| 1:W:235:SER:HB3  | 1:W:238:MET:HG2  | 1.93                     | 0.51              |
| 1:E:223:CYS:HA   | 1:E:259:ILE:HD11 | 1.93                     | 0.50              |
| 1:L:128:GLU:N    | 3:L:401:HOH:O    | 2.22                     | 0.50              |
| 1:V:131:ARG:HG3  | 1:V:221:THR:HG21 | 1.92                     | 0.50              |
| 1:V:160:TYR:HD2  | 1:V:165:LEU:HG   | 1.75                     | 0.50              |
| 1:E:168:LEU:HD13 | 1:E:175:LEU:HB2  | 1.93                     | 0.50              |
| 1:F:131:ARG:NH2  | 1:F:217:GLY:O    | 2.34                     | 0.50              |
| 1:G:188:VAL:O    | 1:I:136:ARG:NH1  | 2.44                     | 0.50              |
| 1:W:219:HIS:HB3  | 1:W:252:ARG:NH2  | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:228:ILE:HA   | 1:E:231:LEU:HD12 | 1.93                     | 0.50              |
| 1:K:183:ASN:C    | 1:K:185:GLU:H    | 2.18                     | 0.50              |
| 1:N:248:PHE:CD1  | 1:N:249:PRO:HA   | 2.46                     | 0.50              |
| 1:V:225:ILE:O    | 1:V:229:ARG:HG2  | 2.11                     | 0.50              |
| 1:C:152:ILE:HD12 | 1:C:168:LEU:HD21 | 1.93                     | 0.50              |
| 1:N:271:ALA:HB3  | 1:N:277:LEU:CD2  | 2.41                     | 0.50              |
| 1:P:248:PHE:CD1  | 1:P:249:PRO:HA   | 2.46                     | 0.50              |
| 1:S:187:PHE:HA   | 1:S:188:VAL:HG22 | 1.92                     | 0.50              |
| 1:T:191:PRO:HA   | 3:T:403:HOH:O    | 2.11                     | 0.50              |
| 1:A:244:ARG:HD3  | 1:T:244:ARG:CZ   | 2.42                     | 0.50              |
| 1:J:136:ARG:NH1  | 1:K:188:VAL:O    | 2.45                     | 0.50              |
| 1:V:269:ARG:O    | 1:V:273:LYS:HG2  | 2.12                     | 0.50              |
| 1:L:124:HIS:HD2  | 1:L:130:TYR:CZ   | 2.29                     | 0.50              |
| 1:V:165:LEU:HD23 | 1:V:168:LEU:HD12 | 1.93                     | 0.50              |
| 1:Y:214:SER:OG   | 2:Y:301:SO4:O4   | 2.22                     | 0.50              |
| 1:E:191:PRO:HD2  | 1:E:194:LEU:HD12 | 1.93                     | 0.50              |
| 1:H:189:ASN:OD1  | 1:H:258:PHE:HZ   | 1.95                     | 0.50              |
| 1:K:184:LYS:O    | 1:K:185:GLU:HG2  | 2.12                     | 0.50              |
| 1:T:160:TYR:CE2  | 1:T:164:ASN:HB3  | 2.47                     | 0.50              |
| 1:W:229:ARG:HD2  | 1:W:234:TRP:CE3  | 2.47                     | 0.50              |
| 1:S:244:ARG:HE   | 1:S:256:GLN:HE22 | 1.59                     | 0.49              |
| 1:V:174:LYS:HE2  | 1:V:174:LYS:HA   | 1.93                     | 0.49              |
| 1:B:184:LYS:O    | 1:B:185:GLU:HG3  | 2.11                     | 0.49              |
| 1:N:271:ALA:HB1  | 1:N:277:LEU:CD2  | 2.42                     | 0.49              |
| 1:S:240:PHE:CD1  | 1:S:256:GLN:HG2  | 2.47                     | 0.49              |
| 1:P:266:GLU:HB3  | 3:P:410:HOH:O    | 2.11                     | 0.49              |
| 1:E:228:ILE:HG22 | 1:E:232:GLN:HE21 | 1.78                     | 0.49              |
| 1:W:156:ILE:HG22 | 1:W:158:GLU:H    | 1.78                     | 0.49              |
| 1:Y:125:VAL:HG12 | 1:Y:126:VAL:HG12 | 1.94                     | 0.49              |
| 1:B:196:THR:O    | 1:B:200:GLU:HG3  | 2.12                     | 0.49              |
| 1:C:188:VAL:HG21 | 1:C:252:ARG:HH12 | 1.78                     | 0.49              |
| 1:M:144:HIS:O    | 1:M:148:LYS:HA   | 2.13                     | 0.49              |
| 1:R:188:VAL:HG12 | 1:R:189:ASN:N    | 2.27                     | 0.49              |
| 1:R:191:PRO:HD2  | 1:R:194:LEU:HD22 | 1.93                     | 0.49              |
| 1:K:146:ARG:NH1  | 1:P:234:TRP:HE1  | 2.10                     | 0.49              |
| 1:L:220:ARG:NE   | 2:L:301:SO4:O2   | 2.33                     | 0.49              |
| 1:W:249:PRO:HG3  | 1:X:249:PRO:HB2  | 1.94                     | 0.49              |
| 1:P:156:ILE:HG13 | 1:P:157:PRO:HD2  | 1.95                     | 0.49              |
| 1:T:192:SER:HA   | 1:T:195:LEU:HD12 | 1.94                     | 0.49              |
| 1:X:187:PHE:HA   | 1:X:188:VAL:CG1  | 2.42                     | 0.49              |
| 1:P:160:TYR:HD2  | 1:P:165:LEU:HG   | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:156:ILE:HG22 | 1:B:220:ARG:NH2  | 2.28                     | 0.49              |
| 1:I:187:PHE:HA   | 1:I:188:VAL:HB   | 1.95                     | 0.49              |
| 1:K:146:ARG:HH22 | 1:P:232:GLN:CD   | 2.20                     | 0.49              |
| 1:M:166:ASN:ND2  | 3:M:403:HOH:O    | 2.46                     | 0.49              |
| 1:R:245:ARG:NH2  | 3:R:402:HOH:O    | 2.44                     | 0.49              |
| 1:S:119:PRO:HD3  | 1:S:139:ASN:HB3  | 1.95                     | 0.49              |
| 1:E:116:VAL:HG22 | 1:E:142:PHE:HB2  | 1.95                     | 0.48              |
| 1:H:155:LEU:C    | 1:H:156:ILE:HG12 | 2.37                     | 0.48              |
| 1:A:196:THR:O    | 1:A:200:GLU:HG3  | 2.14                     | 0.48              |
| 1:G:244:ARG:CZ   | 1:G:256:GLN:HE22 | 2.26                     | 0.48              |
| 1:H:125:VAL:HG12 | 1:H:126:VAL:HG12 | 1.95                     | 0.48              |
| 1:N:223:CYS:HA   | 1:N:259:ILE:HD11 | 1.94                     | 0.48              |
| 1:X:125:VAL:HG12 | 1:X:126:VAL:HG12 | 1.94                     | 0.48              |
| 1:C:203:LEU:HD22 | 1:C:279:LEU:HD21 | 1.94                     | 0.48              |
| 1:J:154:VAL:HG22 | 1:J:156:ILE:HG12 | 1.95                     | 0.48              |
| 1:O:212:ILE:HG22 | 1:O:221:THR:HG23 | 1.95                     | 0.48              |
| 1:B:160:TYR:CE2  | 1:B:164:ASN:HB3  | 2.48                     | 0.48              |
| 1:D:221:THR:HG22 | 1:D:225:ILE:HD12 | 1.95                     | 0.48              |
| 1:G:229:ARG:HD2  | 1:G:234:TRP:CZ3  | 2.47                     | 0.48              |
| 1:W:199:LEU:HA   | 1:W:202:VAL:HG22 | 1.94                     | 0.48              |
| 1:A:184:LYS:O    | 1:A:185:GLU:HG2  | 2.13                     | 0.48              |
| 1:D:136:ARG:NH1  | 1:E:188:VAL:O    | 2.46                     | 0.48              |
| 1:Q:134:PHE:CD1  | 1:Q:213:HIS:CE1  | 3.02                     | 0.48              |
| 1:S:248:PHE:CD1  | 1:S:249:PRO:HA   | 2.49                     | 0.48              |
| 1:T:116:VAL:HG21 | 1:T:146:ARG:HH11 | 1.79                     | 0.48              |
| 1:I:144:HIS:HB2  | 1:I:167:PHE:HZ   | 1.79                     | 0.48              |
| 1:K:131:ARG:HD2  | 1:K:225:ILE:HG13 | 1.95                     | 0.48              |
| 1:O:219:HIS:NE2  | 1:O:250:LYS:O    | 2.45                     | 0.48              |
| 1:Q:191:PRO:HD2  | 1:Q:194:LEU:HD12 | 1.95                     | 0.48              |
| 1:V:183:ASN:O    | 1:V:185:GLU:N    | 2.47                     | 0.48              |
| 1:M:218:LYS:NZ   | 1:M:248:PHE:O    | 2.43                     | 0.48              |
| 1:Q:231:LEU:HD21 | 1:Q:267:ILE:HG23 | 1.95                     | 0.48              |
| 1:W:278:PRO:O    | 1:W:280:GLN:NE2  | 2.47                     | 0.48              |
| 1:X:143:LEU:HB3  | 1:X:149:LEU:HD12 | 1.96                     | 0.48              |
| 1:C:277:LEU:HD12 | 1:C:279:LEU:HD12 | 1.96                     | 0.48              |
| 1:H:122:PHE:HD1  | 1:H:132:SER:HB3  | 1.79                     | 0.48              |
| 1:N:216:ARG:HH22 | 1:N:250:LYS:NZ   | 2.12                     | 0.48              |
| 1:P:153:LEU:HD11 | 1:P:178:VAL:HG23 | 1.96                     | 0.48              |
| 1:P:214:SER:OG   | 2:P:301:SO4:S    | 2.66                     | 0.48              |
| 1:Q:183:ASN:C    | 1:Q:185:GLU:H    | 2.22                     | 0.48              |
| 1:D:244:ARG:NE   | 1:N:244:ARG:HD3  | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:160:TYR:CE2  | 1:H:164:ASN:HB3  | 2.49                     | 0.47              |
| 1:P:248:PHE:CG   | 1:P:249:PRO:HA   | 2.49                     | 0.47              |
| 1:R:230:LYS:NZ   | 1:R:262:TYR:O    | 2.39                     | 0.47              |
| 1:V:230:LYS:NZ   | 1:V:259:ILE:O    | 2.47                     | 0.47              |
| 1:V:244:ARG:HE   | 1:V:256:GLN:NE2  | 2.11                     | 0.47              |
| 1:A:199:LEU:HA   | 1:A:202:VAL:HG22 | 1.96                     | 0.47              |
| 1:C:187:PHE:HA   | 1:C:188:VAL:HB   | 1.96                     | 0.47              |
| 1:L:195:LEU:HD13 | 1:L:227:CYS:SG   | 2.54                     | 0.47              |
| 1:W:244:ARG:HB3  | 1:W:248:PHE:CZ   | 2.49                     | 0.47              |
| 1:J:203:LEU:HD22 | 1:J:279:LEU:HD21 | 1.96                     | 0.47              |
| 1:W:174:LYS:HD3  | 1:W:176:TYR:CZ   | 2.49                     | 0.47              |
| 1:W:221:THR:O    | 1:W:225:ILE:HG12 | 2.13                     | 0.47              |
| 1:X:132:SER:OG   | 1:X:133:SER:N    | 2.46                     | 0.47              |
| 1:B:132:SER:HB3  | 1:B:211:LEU:HD11 | 1.97                     | 0.47              |
| 1:C:153:LEU:HD11 | 1:C:178:VAL:HG23 | 1.97                     | 0.47              |
| 1:N:116:VAL:HG11 | 1:N:146:ARG:HD3  | 1.95                     | 0.47              |
| 1:P:214:SER:OG   | 2:P:301:SO4:O1   | 2.32                     | 0.47              |
| 1:V:174:LYS:HA   | 1:V:174:LYS:CE   | 2.44                     | 0.47              |
| 1:J:162:GLN:HA   | 1:J:165:LEU:HB2  | 1.96                     | 0.47              |
| 1:K:160:TYR:HD2  | 1:K:165:LEU:HB2  | 1.79                     | 0.47              |
| 1:O:136:ARG:NE   | 1:O:138:GLU:OE2  | 2.48                     | 0.47              |
| 1:V:160:TYR:CE2  | 1:V:168:LEU:HD11 | 2.49                     | 0.47              |
| 1:W:167:PHE:O    | 1:W:171:THR:OG1  | 2.20                     | 0.47              |
| 1:G:266:GLU:HG3  | 1:G:269:ARG:HH21 | 1.79                     | 0.47              |
| 1:K:225:ILE:O    | 1:K:229:ARG:HG2  | 2.14                     | 0.47              |
| 1:M:230:LYS:CE   | 1:M:264:ASP:HB3  | 2.45                     | 0.47              |
| 1:O:116:VAL:HG21 | 1:O:146:ARG:HH11 | 1.80                     | 0.47              |
| 1:T:183:ASN:C    | 1:T:185:GLU:H    | 2.22                     | 0.47              |
| 1:T:219:HIS:ND1  | 2:T:301:SO4:O1   | 2.47                     | 0.47              |
| 1:W:225:ILE:HD13 | 1:W:228:ILE:HD12 | 1.97                     | 0.47              |
| 1:G:149:LEU:HA   | 1:G:209:PRO:HB2  | 1.97                     | 0.47              |
| 1:J:252:ARG:HH21 | 1:J:255:ASP:CG   | 2.22                     | 0.47              |
| 1:T:223:CYS:HA   | 1:T:259:ILE:HD11 | 1.97                     | 0.47              |
| 1:V:116:VAL:HG11 | 1:V:146:ARG:HD3  | 1.96                     | 0.47              |
| 1:O:188:VAL:HG12 | 1:O:254:LEU:HD13 | 1.97                     | 0.47              |
| 1:P:271:ALA:HB1  | 1:P:276:TRP:HB2  | 1.96                     | 0.47              |
| 1:T:248:PHE:CD1  | 1:T:249:PRO:HA   | 2.49                     | 0.47              |
| 1:B:141:SER:CB   | 1:B:145:GLU:OE1  | 2.63                     | 0.47              |
| 1:P:220:ARG:NE   | 2:P:301:SO4:O3   | 2.36                     | 0.47              |
| 1:P:228:ILE:O    | 1:P:232:GLN:HG3  | 2.15                     | 0.47              |
| 1:S:150:LYS:C    | 1:S:173:ILE:HG23 | 2.40                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:155:LEU:HD12 | 1:X:214:SER:HB3  | 1.97                     | 0.47              |
| 1:Y:225:ILE:O    | 1:Y:229:ARG:HG2  | 2.14                     | 0.47              |
| 1:B:237:THR:HG21 | 1:S:257:GLN:HG3  | 1.97                     | 0.46              |
| 1:G:156:ILE:HG22 | 1:G:220:ARG:NH2  | 2.28                     | 0.46              |
| 1:H:196:THR:O    | 1:H:200:GLU:HG3  | 2.14                     | 0.46              |
| 1:K:125:VAL:HG22 | 1:K:131:ARG:HG3  | 1.96                     | 0.46              |
| 1:N:212:ILE:HG22 | 1:N:221:THR:HG23 | 1.96                     | 0.46              |
| 1:P:219:HIS:NE2  | 1:P:250:LYS:O    | 2.47                     | 0.46              |
| 1:F:223:CYS:HA   | 1:F:259:ILE:HD11 | 1.96                     | 0.46              |
| 1:F:228:ILE:HA   | 1:F:231:LEU:HD12 | 1.97                     | 0.46              |
| 1:S:155:LEU:O    | 1:S:220:ARG:NH1  | 2.47                     | 0.46              |
| 1:S:160:TYR:CE2  | 1:S:164:ASN:HB3  | 2.50                     | 0.46              |
| 1:E:143:LEU:HB3  | 1:E:149:LEU:HD12 | 1.97                     | 0.46              |
| 1:I:231:LEU:HD21 | 1:I:267:ILE:HG23 | 1.96                     | 0.46              |
| 1:J:225:ILE:HA   | 1:J:228:ILE:HD12 | 1.96                     | 0.46              |
| 1:X:160:TYR:CE2  | 1:X:164:ASN:HB3  | 2.50                     | 0.46              |
| 1:E:116:VAL:HG11 | 1:E:146:ARG:HH11 | 1.81                     | 0.46              |
| 1:H:131:ARG:HG3  | 1:H:221:THR:HG21 | 1.96                     | 0.46              |
| 1:Q:248:PHE:CD1  | 1:Q:249:PRO:HA   | 2.50                     | 0.46              |
| 1:V:219:HIS:NE2  | 1:V:250:LYS:O    | 2.43                     | 0.46              |
| 1:X:153:LEU:HA   | 1:X:176:TYR:O    | 2.14                     | 0.46              |
| 1:Y:132:SER:OG   | 1:Y:133:SER:N    | 2.48                     | 0.46              |
| 1:B:165:LEU:HB3  | 1:B:169:LYS:NZ   | 2.31                     | 0.46              |
| 1:G:165:LEU:HD23 | 1:G:169:LYS:HE2  | 1.97                     | 0.46              |
| 1:H:223:CYS:HB2  | 1:H:255:ASP:OD2  | 2.15                     | 0.46              |
| 1:L:196:THR:O    | 1:L:200:GLU:HG3  | 2.15                     | 0.46              |
| 1:M:165:LEU:HB3  | 1:M:169:LYS:NZ   | 2.30                     | 0.46              |
| 1:M:225:ILE:O    | 1:M:229:ARG:HG2  | 2.15                     | 0.46              |
| 1:Q:221:THR:O    | 1:Q:225:ILE:HG12 | 2.16                     | 0.46              |
| 1:T:265:ASP:HA   | 1:T:268:LYS:HG2  | 1.97                     | 0.46              |
| 1:Q:184:LYS:O    | 1:Q:185:GLU:CG   | 2.63                     | 0.46              |
| 1:Y:176:TYR:HB3  | 1:Y:201:ILE:HD13 | 1.98                     | 0.46              |
| 1:E:146:ARG:HH12 | 1:O:234:TRP:NE1  | 2.14                     | 0.46              |
| 1:H:221:THR:HG22 | 1:H:225:ILE:HD12 | 1.98                     | 0.46              |
| 1:N:226:GLY:HA3  | 1:N:259:ILE:HD13 | 1.97                     | 0.46              |
| 1:C:152:ILE:HG12 | 1:C:211:LEU:HB3  | 1.98                     | 0.46              |
| 1:E:154:VAL:HG22 | 1:E:156:ILE:HG12 | 1.96                     | 0.46              |
| 1:G:230:LYS:NZ   | 1:G:259:ILE:O    | 2.45                     | 0.46              |
| 1:L:154:VAL:HG12 | 1:L:213:HIS:CE1  | 2.51                     | 0.46              |
| 1:M:254:LEU:HD12 | 1:M:254:LEU:H    | 1.81                     | 0.46              |
| 1:O:221:THR:O    | 1:O:225:ILE:HG12 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:155:LEU:HD22 | 1:Q:180:MET:HE2  | 1.98                     | 0.46              |
| 1:Q:257:GLN:HG2  | 1:Q:261:MET:HE2  | 1.98                     | 0.46              |
| 1:Y:257:GLN:O    | 1:Y:261:MET:HG2  | 2.16                     | 0.46              |
| 1:N:171:THR:HG22 | 1:R:170:LEU:HG   | 1.98                     | 0.46              |
| 1:P:136:ARG:NH1  | 1:Q:188:VAL:H    | 2.14                     | 0.46              |
| 1:T:131:ARG:HD2  | 1:T:225:ILE:HD13 | 1.98                     | 0.46              |
| 1:B:199:LEU:HA   | 1:B:202:VAL:HG22 | 1.98                     | 0.45              |
| 1:Q:152:ILE:HG12 | 1:Q:211:LEU:HB3  | 1.98                     | 0.45              |
| 1:S:207:ASN:HD22 | 1:S:207:ASN:N    | 2.13                     | 0.45              |
| 1:T:217:GLY:N    | 2:T:301:SO4:O2   | 2.49                     | 0.45              |
| 1:W:188:VAL:HG22 | 1:W:189:ASN:N    | 2.31                     | 0.45              |
| 1:G:151:SER:O    | 1:G:210:ILE:HA   | 2.16                     | 0.45              |
| 1:H:199:LEU:HA   | 1:H:202:VAL:HG22 | 1.99                     | 0.45              |
| 1:I:185:GLU:HG2  | 1:I:186:PRO:CD   | 2.47                     | 0.45              |
| 1:I:199:LEU:HA   | 1:I:202:VAL:HG22 | 1.98                     | 0.45              |
| 1:M:137:GLN:HA   | 1:M:140:PHE:CE2  | 2.51                     | 0.45              |
| 1:Q:160:TYR:HD2  | 1:Q:165:LEU:HG   | 1.81                     | 0.45              |
| 1:S:193:HIS:O    | 1:S:196:THR:HG22 | 2.16                     | 0.45              |
| 1:S:244:ARG:NE   | 1:S:256:GLN:HE22 | 2.13                     | 0.45              |
| 1:W:153:LEU:HD11 | 1:W:178:VAL:HG22 | 1.97                     | 0.45              |
| 1:A:180:MET:O    | 1:A:220:ARG:NH1  | 2.49                     | 0.45              |
| 1:R:183:ASN:O    | 1:R:185:GLU:N    | 2.50                     | 0.45              |
| 1:X:160:TYR:HB3  | 1:X:165:LEU:HD21 | 1.99                     | 0.45              |
| 1:Y:219:HIS:HA   | 1:Y:243:TYR:OH   | 2.15                     | 0.45              |
| 1:I:203:LEU:HD11 | 1:I:231:LEU:HD13 | 1.99                     | 0.45              |
| 1:F:140:PHE:HB3  | 1:F:167:PHE:CZ   | 2.51                     | 0.45              |
| 1:I:160:TYR:HD2  | 1:I:165:LEU:HG   | 1.81                     | 0.45              |
| 1:J:234:TRP:HE1  | 1:Q:146:ARG:HH12 | 1.63                     | 0.45              |
| 1:P:165:LEU:O    | 1:P:169:LYS:HG3  | 2.17                     | 0.45              |
| 1:Y:194:LEU:HD12 | 1:Y:195:LEU:N    | 2.31                     | 0.45              |
| 1:D:241:ASP:OD1  | 1:N:244:ARG:NH2  | 2.50                     | 0.45              |
| 1:F:184:LYS:NZ   | 3:F:404:HOH:O    | 2.49                     | 0.45              |
| 1:J:237:THR:HG21 | 1:R:257:GLN:HA   | 1.97                     | 0.45              |
| 1:O:226:GLY:HA3  | 1:O:259:ILE:HD13 | 1.99                     | 0.45              |
| 1:V:140:PHE:HB3  | 1:V:167:PHE:CZ   | 2.52                     | 0.45              |
| 1:H:187:PHE:HA   | 1:H:188:VAL:HB   | 1.99                     | 0.45              |
| 1:S:124:HIS:HD2  | 1:S:130:TYR:CE1  | 2.34                     | 0.45              |
| 1:M:216:ARG:NH2  | 1:M:250:LYS:HD2  | 2.23                     | 0.45              |
| 1:M:230:LYS:HD2  | 1:M:264:ASP:HB3  | 1.99                     | 0.45              |
| 1:N:136:ARG:NH1  | 1:O:188:VAL:O    | 2.40                     | 0.45              |
| 1:T:202:VAL:HG23 | 1:T:203:LEU:HD12 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:230:LYS:NZ   | 1:W:262:TYR:O    | 2.36                     | 0.45              |
| 1:Y:162:GLN:NE2  | 1:Y:165:LEU:HD23 | 2.32                     | 0.45              |
| 1:F:237:THR:HG23 | 1:O:256:GLN:HB2  | 1.98                     | 0.45              |
| 1:H:152:ILE:HD12 | 1:H:168:LEU:HD21 | 1.99                     | 0.45              |
| 1:J:235:SER:HB3  | 1:Q:117:ILE:HG12 | 1.99                     | 0.45              |
| 1:N:157:PRO:HD3  | 1:N:180:MET:O    | 2.17                     | 0.45              |
| 1:X:212:ILE:HG22 | 1:X:221:THR:HG23 | 1.98                     | 0.45              |
| 1:Y:248:PHE:CD1  | 1:Y:249:PRO:HA   | 2.52                     | 0.45              |
| 1:D:150:LYS:HD3  | 1:D:208:GLN:O    | 2.16                     | 0.45              |
| 1:F:126:VAL:HG13 | 1:F:129:ILE:HD12 | 1.99                     | 0.45              |
| 1:G:136:ARG:NH1  | 1:H:254:LEU:HD11 | 2.32                     | 0.45              |
| 1:K:237:THR:HG22 | 1:K:238:MET:HE2  | 1.99                     | 0.45              |
| 1:N:221:THR:HG22 | 1:N:225:ILE:HD12 | 1.98                     | 0.45              |
| 1:J:160:TYR:CE2  | 1:J:164:ASN:HB3  | 2.52                     | 0.44              |
| 1:L:219:HIS:CD2  | 1:L:252:ARG:HD3  | 2.52                     | 0.44              |
| 1:P:147:LEU:HB3  | 1:P:149:LEU:HG   | 1.98                     | 0.44              |
| 1:T:182:GLY:HA2  | 1:T:220:ARG:NH1  | 2.31                     | 0.44              |
| 1:V:197:LYS:HA   | 1:V:200:GLU:HG2  | 2.00                     | 0.44              |
| 1:W:140:PHE:HB3  | 1:W:167:PHE:CE1  | 2.52                     | 0.44              |
| 1:G:136:ARG:NH1  | 1:H:189:ASN:OD1  | 2.43                     | 0.44              |
| 1:J:162:GLN:NE2  | 1:J:165:LEU:HD22 | 2.31                     | 0.44              |
| 1:B:169:LYS:O    | 1:E:144:HIS:HE1  | 2.01                     | 0.44              |
| 1:L:156:ILE:HG22 | 1:L:158:GLU:H    | 1.82                     | 0.44              |
| 1:V:185:GLU:OE1  | 1:V:188:VAL:HA   | 2.18                     | 0.44              |
| 1:X:248:PHE:CD1  | 1:X:249:PRO:HA   | 2.53                     | 0.44              |
| 1:B:183:ASN:C    | 1:B:185:GLU:H    | 2.26                     | 0.44              |
| 1:E:132:SER:HB3  | 1:E:211:LEU:HD11 | 1.99                     | 0.44              |
| 1:F:184:LYS:HE2  | 1:F:184:LYS:HB2  | 1.87                     | 0.44              |
| 1:H:131:ARG:HE   | 1:H:225:ILE:HD13 | 1.81                     | 0.44              |
| 1:L:221:THR:HG22 | 1:L:225:ILE:HD12 | 1.99                     | 0.44              |
| 1:S:225:ILE:HA   | 1:S:228:ILE:HD12 | 1.99                     | 0.44              |
| 1:V:151:SER:OG   | 1:V:207:ASN:O    | 2.27                     | 0.44              |
| 1:X:256:GLN:HA   | 1:X:259:ILE:HD12 | 2.00                     | 0.44              |
| 1:C:146:ARG:HH12 | 1:T:232:GLN:HB3  | 1.82                     | 0.44              |
| 1:D:196:THR:O    | 1:D:200:GLU:HG3  | 2.17                     | 0.44              |
| 1:D:199:LEU:HA   | 1:D:202:VAL:HG22 | 2.00                     | 0.44              |
| 1:G:153:LEU:HD21 | 1:G:198:ALA:HB1  | 1.99                     | 0.44              |
| 1:J:265:ASP:OD2  | 3:J:401:HOH:O    | 2.21                     | 0.44              |
| 1:O:125:VAL:HG12 | 1:O:126:VAL:HG12 | 2.00                     | 0.44              |
| 1:O:225:ILE:HD13 | 1:O:228:ILE:HD12 | 1.99                     | 0.44              |
| 1:S:199:LEU:HD12 | 1:S:231:LEU:HD11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:229:ARG:HH11 | 1:E:232:GLN:HE22 | 1.66                     | 0.44              |
| 1:J:125:VAL:HG23 | 1:J:126:VAL:H    | 1.82                     | 0.44              |
| 1:M:184:LYS:O    | 1:M:185:GLU:HG3  | 2.17                     | 0.44              |
| 1:O:121:ASN:OD1  | 1:O:218:LYS:NZ   | 2.43                     | 0.44              |
| 1:P:148:LYS:HD3  | 3:P:405:HOH:O    | 2.18                     | 0.44              |
| 1:P:212:ILE:HG21 | 1:P:224:LEU:HD23 | 2.00                     | 0.44              |
| 1:C:182:GLY:H    | 1:C:184:LYS:HZ2  | 1.66                     | 0.44              |
| 1:C:277:LEU:HD12 | 1:C:278:PRO:HA   | 2.00                     | 0.44              |
| 1:F:185:GLU:HG3  | 1:F:186:PRO:HD2  | 1.98                     | 0.44              |
| 1:M:183:ASN:C    | 1:M:185:GLU:H    | 2.25                     | 0.44              |
| 1:I:124:HIS:NE2  | 1:I:127:GLY:O    | 2.48                     | 0.44              |
| 1:Q:182:GLY:HA2  | 3:Q:408:HOH:O    | 2.18                     | 0.44              |
| 1:R:119:PRO:HB2  | 1:R:132:SER:HB2  | 2.00                     | 0.44              |
| 1:W:183:ASN:HA   | 1:W:188:VAL:CG2  | 2.47                     | 0.44              |
| 1:X:218:LYS:NZ   | 1:X:246:PHE:O    | 2.50                     | 0.44              |
| 1:F:221:THR:HG22 | 1:F:225:ILE:HD12 | 2.00                     | 0.44              |
| 1:F:248:PHE:CG   | 1:F:249:PRO:HA   | 2.53                     | 0.44              |
| 1:J:249:PRO:HG3  | 1:K:249:PRO:HB2  | 2.00                     | 0.44              |
| 1:K:231:LEU:HD21 | 1:K:267:ILE:HG23 | 1.99                     | 0.44              |
| 1:Q:248:PHE:CG   | 1:Q:249:PRO:HA   | 2.52                     | 0.44              |
| 1:A:238:MET:HE1  | 1:S:120:GLU:HA   | 2.00                     | 0.43              |
| 1:D:187:PHE:HA   | 1:D:188:VAL:HB   | 2.00                     | 0.43              |
| 1:E:135:PRO:HB3  | 1:E:143:LEU:HD11 | 2.00                     | 0.43              |
| 1:H:248:PHE:CD1  | 1:H:249:PRO:HA   | 2.53                     | 0.43              |
| 1:I:132:SER:OG   | 1:I:133:SER:N    | 2.51                     | 0.43              |
| 1:K:118:PRO:HB3  | 1:K:142:PHE:CE2  | 2.53                     | 0.43              |
| 1:W:183:ASN:HA   | 1:W:188:VAL:HG21 | 2.00                     | 0.43              |
| 1:W:188:VAL:O    | 1:Y:136:ARG:NH2  | 2.51                     | 0.43              |
| 1:Y:154:VAL:HG21 | 1:Y:160:TYR:CE1  | 2.53                     | 0.43              |
| 1:A:139:ASN:O    | 1:A:143:LEU:HG   | 2.17                     | 0.43              |
| 1:E:265:ASP:HA   | 1:E:268:LYS:HG2  | 2.01                     | 0.43              |
| 1:M:248:PHE:CG   | 1:M:249:PRO:HA   | 2.53                     | 0.43              |
| 1:X:154:VAL:HG22 | 1:X:213:HIS:NE2  | 2.33                     | 0.43              |
| 1:Y:257:GLN:HG2  | 1:Y:261:MET:HE3  | 2.00                     | 0.43              |
| 1:C:154:VAL:HG22 | 1:C:156:ILE:HG12 | 1.99                     | 0.43              |
| 1:D:155:LEU:HD22 | 1:D:180:MET:HE2  | 2.00                     | 0.43              |
| 1:E:225:ILE:O    | 1:E:229:ARG:HG2  | 2.18                     | 0.43              |
| 1:N:199:LEU:HA   | 1:N:202:VAL:HG22 | 2.00                     | 0.43              |
| 1:P:146:ARG:HE   | 1:P:146:ARG:HA   | 1.83                     | 0.43              |
| 1:R:119:PRO:HG3  | 1:R:139:ASN:HB3  | 2.00                     | 0.43              |
| 1:D:230:LYS:NZ   | 1:D:259:ILE:O    | 2.38                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:134:PHE:HZ   | 1:F:161:PRO:HG2  | 1.83                     | 0.43              |
| 1:Q:136:ARG:NH1  | 1:R:188:VAL:O    | 2.52                     | 0.43              |
| 1:R:195:LEU:O    | 1:R:199:LEU:HG   | 2.18                     | 0.43              |
| 1:V:266:GLU:HG2  | 1:V:267:ILE:N    | 2.33                     | 0.43              |
| 1:B:143:LEU:HB3  | 1:B:149:LEU:HD12 | 1.99                     | 0.43              |
| 1:N:264:ASP:OD1  | 1:N:264:ASP:N    | 2.42                     | 0.43              |
| 1:Y:183:ASN:C    | 1:Y:185:GLU:H    | 2.26                     | 0.43              |
| 1:R:204:ASN:HB3  | 1:R:207:ASN:HD22 | 1.83                     | 0.43              |
| 1:R:231:LEU:HD21 | 1:R:267:ILE:HG23 | 2.00                     | 0.43              |
| 1:S:154:VAL:HG22 | 1:S:213:HIS:CE1  | 2.54                     | 0.43              |
| 1:T:187:PHE:HA   | 1:T:188:VAL:CG2  | 2.48                     | 0.43              |
| 1:B:163:GLU:H    | 1:B:163:GLU:CD   | 2.26                     | 0.43              |
| 1:E:199:LEU:HA   | 1:E:202:VAL:HG22 | 2.01                     | 0.43              |
| 1:E:265:ASP:HA   | 1:E:268:LYS:HE2  | 2.01                     | 0.43              |
| 1:S:154:VAL:HG22 | 1:S:213:HIS:NE2  | 2.34                     | 0.43              |
| 1:E:182:GLY:HA2  | 1:E:220:ARG:HH21 | 1.83                     | 0.43              |
| 1:F:119:PRO:HB2  | 1:F:132:SER:HB2  | 2.00                     | 0.43              |
| 1:S:218:LYS:HB3  | 1:S:247:ALA:HA   | 2.00                     | 0.43              |
| 1:W:136:ARG:NH1  | 1:W:138:GLU:OE2  | 2.51                     | 0.43              |
| 1:X:149:LEU:HA   | 1:X:209:PRO:HB2  | 1.99                     | 0.43              |
| 1:X:193:HIS:O    | 1:X:196:THR:HG22 | 2.18                     | 0.43              |
| 1:B:237:THR:HG22 | 1:B:238:MET:HE2  | 2.01                     | 0.43              |
| 1:C:257:GLN:HG2  | 1:C:261:MET:HE2  | 2.01                     | 0.43              |
| 1:G:225:ILE:O    | 1:G:229:ARG:HG2  | 2.19                     | 0.43              |
| 1:G:244:ARG:NE   | 1:G:256:GLN:HE22 | 2.17                     | 0.43              |
| 1:Q:125:VAL:HG11 | 1:Q:225:ILE:HD12 | 2.01                     | 0.43              |
| 1:B:229:ARG:NH2  | 1:B:242:GLU:OE2  | 2.49                     | 0.43              |
| 1:C:257:GLN:HA   | 1:C:260:GLU:HG2  | 2.00                     | 0.43              |
| 1:G:126:VAL:HG13 | 1:G:129:ILE:HD12 | 2.00                     | 0.43              |
| 1:G:185:GLU:CD   | 1:G:186:PRO:HD2  | 2.43                     | 0.43              |
| 1:I:264:ASP:O    | 1:I:268:LYS:HG3  | 2.19                     | 0.43              |
| 1:P:218:LYS:HG2  | 1:P:247:ALA:HA   | 2.01                     | 0.43              |
| 1:Q:158:GLU:HG2  | 1:Q:159:GLU:N    | 2.33                     | 0.43              |
| 1:F:245:ARG:HD3  | 3:F:405:HOH:O    | 2.17                     | 0.42              |
| 1:G:265:ASP:O    | 1:G:269:ARG:HG3  | 2.19                     | 0.42              |
| 1:I:265:ASP:O    | 1:I:269:ARG:HG3  | 2.19                     | 0.42              |
| 1:J:264:ASP:O    | 1:J:268:LYS:HB3  | 2.19                     | 0.42              |
| 1:A:147:LEU:HD23 | 1:A:149:LEU:HD21 | 2.00                     | 0.42              |
| 1:I:154:VAL:HG13 | 1:I:213:HIS:CE1  | 2.53                     | 0.42              |
| 1:W:219:HIS:N    | 2:W:301:SO4:S    | 2.92                     | 0.42              |
| 1:B:160:TYR:HA   | 1:B:161:PRO:HD3  | 1.93                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:225:ILE:O    | 1:L:229:ARG:HG2  | 2.20                     | 0.42              |
| 1:O:137:GLN:HA   | 1:O:140:PHE:CD2  | 2.54                     | 0.42              |
| 1:R:180:MET:HE2  | 1:R:220:ARG:HB3  | 2.00                     | 0.42              |
| 1:T:188:VAL:HG23 | 1:T:254:LEU:HD12 | 2.02                     | 0.42              |
| 1:V:157:PRO:HD3  | 1:V:180:MET:O    | 2.19                     | 0.42              |
| 1:C:161:PRO:HB2  | 1:C:164:ASN:HD22 | 1.84                     | 0.42              |
| 1:H:255:ASP:O    | 1:H:259:ILE:HG12 | 2.20                     | 0.42              |
| 1:K:203:LEU:HD11 | 1:K:231:LEU:HD13 | 2.01                     | 0.42              |
| 1:L:183:ASN:O    | 1:L:185:GLU:N    | 2.52                     | 0.42              |
| 1:N:244:ARG:NE   | 1:N:256:GLN:HE22 | 2.17                     | 0.42              |
| 1:A:185:GLU:OE1  | 1:A:186:PRO:HD2  | 2.19                     | 0.42              |
| 1:E:146:ARG:HE   | 1:O:281:TRP:HE1  | 1.67                     | 0.42              |
| 1:F:191:PRO:HD2  | 1:F:194:LEU:HD12 | 2.01                     | 0.42              |
| 1:J:125:VAL:HG12 | 3:J:413:HOH:O    | 2.19                     | 0.42              |
| 1:O:168:LEU:HD22 | 1:O:173:ILE:HB   | 2.01                     | 0.42              |
| 1:R:181:SER:CB   | 1:R:184:LYS:HB2  | 2.48                     | 0.42              |
| 1:B:141:SER:CA   | 1:B:145:GLU:OE2  | 2.63                     | 0.42              |
| 1:X:242:GLU:HG3  | 1:X:245:ARG:NH2  | 2.34                     | 0.42              |
| 1:E:157:PRO:HD3  | 1:E:180:MET:O    | 2.19                     | 0.42              |
| 1:G:216:ARG:NH2  | 2:G:301:SO4:O3   | 2.48                     | 0.42              |
| 1:I:225:ILE:O    | 1:I:229:ARG:HG2  | 2.19                     | 0.42              |
| 1:K:225:ILE:HD13 | 1:K:228:ILE:HD12 | 2.02                     | 0.42              |
| 1:W:215:ASN:H    | 1:W:220:ARG:HH21 | 1.67                     | 0.42              |
| 1:W:218:LYS:N    | 2:W:301:SO4:S    | 2.93                     | 0.42              |
| 1:A:137:GLN:HA   | 1:A:140:PHE:CE2  | 2.55                     | 0.42              |
| 1:B:185:GLU:O    | 1:B:187:PHE:N    | 2.53                     | 0.42              |
| 1:J:242:GLU:HG3  | 1:J:245:ARG:NH2  | 2.34                     | 0.42              |
| 1:L:252:ARG:HE   | 1:L:255:ASP:CG   | 2.27                     | 0.42              |
| 1:M:165:LEU:O    | 1:M:169:LYS:HG3  | 2.20                     | 0.42              |
| 1:M:183:ASN:HA   | 1:M:188:VAL:HG12 | 2.02                     | 0.42              |
| 1:N:139:ASN:O    | 1:N:143:LEU:HG   | 2.20                     | 0.42              |
| 1:S:168:LEU:O    | 1:S:172:GLY:N    | 2.49                     | 0.42              |
| 1:F:225:ILE:HA   | 1:F:228:ILE:HD12 | 2.02                     | 0.42              |
| 1:W:214:SER:HB3  | 2:W:301:SO4:O2   | 2.19                     | 0.42              |
| 1:X:156:ILE:O    | 1:X:177:GLN:NE2  | 2.53                     | 0.42              |
| 1:X:243:TYR:OH   | 1:X:255:ASP:OD2  | 2.36                     | 0.42              |
| 1:B:212:ILE:HG22 | 1:B:221:THR:HG23 | 2.02                     | 0.42              |
| 1:C:182:GLY:H    | 1:C:184:LYS:NZ   | 2.18                     | 0.42              |
| 1:G:183:ASN:C    | 1:G:185:GLU:H    | 2.26                     | 0.42              |
| 1:L:160:TYR:HA   | 1:L:161:PRO:HD3  | 1.96                     | 0.42              |
| 1:O:248:PHE:CG   | 1:O:249:PRO:HA   | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:254:LEU:HD13 | 1:P:254:LEU:HA   | 1.87                     | 0.42              |
| 1:A:223:CYS:HA   | 1:A:259:ILE:HD11 | 2.02                     | 0.41              |
| 1:Q:152:ILE:HD12 | 1:Q:168:LEU:HD21 | 2.02                     | 0.41              |
| 1:V:119:PRO:HB2  | 1:V:132:SER:HB2  | 2.02                     | 0.41              |
| 1:W:113:ASN:N    | 3:W:404:HOH:O    | 2.52                     | 0.41              |
| 1:W:212:ILE:HG21 | 1:W:224:LEU:HD23 | 2.01                     | 0.41              |
| 1:C:216:ARG:HH11 | 1:C:219:HIS:HE1  | 1.68                     | 0.41              |
| 1:I:191:PRO:HD2  | 1:I:194:LEU:HD12 | 2.02                     | 0.41              |
| 1:K:169:LYS:HA   | 1:K:169:LYS:HD3  | 1.86                     | 0.41              |
| 1:M:231:LEU:HD21 | 1:M:267:ILE:HG23 | 2.01                     | 0.41              |
| 1:S:199:LEU:HB3  | 1:S:267:ILE:HG12 | 2.01                     | 0.41              |
| 1:S:206:ALA:C    | 1:S:207:ASN:HD22 | 2.28                     | 0.41              |
| 1:W:167:PHE:CE1  | 1:W:171:THR:HG21 | 2.55                     | 0.41              |
| 1:X:265:ASP:O    | 1:X:268:LYS:HG3  | 2.19                     | 0.41              |
| 1:D:234:TRP:HE1  | 1:M:146:ARG:HH12 | 1.67                     | 0.41              |
| 1:L:204:ASN:HB3  | 1:L:207:ASN:HD22 | 1.84                     | 0.41              |
| 1:R:131:ARG:HD2  | 1:R:225:ILE:HD13 | 2.01                     | 0.41              |
| 1:S:160:TYR:HA   | 1:S:161:PRO:HD3  | 1.96                     | 0.41              |
| 1:S:236:LEU:HD12 | 1:S:239:ILE:HD12 | 2.02                     | 0.41              |
| 1:T:119:PRO:HG3  | 1:T:139:ASN:HB3  | 2.03                     | 0.41              |
| 1:A:226:GLY:HA3  | 1:A:259:ILE:HD13 | 2.02                     | 0.41              |
| 1:M:155:LEU:HD22 | 1:M:180:MET:HE2  | 2.03                     | 0.41              |
| 1:Q:225:ILE:O    | 1:Q:229:ARG:HG2  | 2.21                     | 0.41              |
| 1:T:154:VAL:HG11 | 1:T:160:TYR:CE1  | 2.55                     | 0.41              |
| 1:W:151:SER:O    | 1:W:210:ILE:HA   | 2.20                     | 0.41              |
| 1:X:219:HIS:NE2  | 1:X:250:LYS:O    | 2.49                     | 0.41              |
| 1:X:257:GLN:O    | 1:X:260:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:203:LEU:HD11 | 1:A:231:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:248:PHE:CD1  | 1:A:249:PRO:HA   | 2.56                     | 0.41              |
| 1:H:155:LEU:HD22 | 1:H:180:MET:HE2  | 2.01                     | 0.41              |
| 1:O:225:ILE:O    | 1:O:229:ARG:HG2  | 2.20                     | 0.41              |
| 1:S:143:LEU:HD23 | 1:S:147:LEU:HD12 | 2.02                     | 0.41              |
| 1:W:220:ARG:N    | 2:W:301:SO4:O1   | 2.41                     | 0.41              |
| 1:D:146:ARG:HD2  | 1:D:146:ARG:HA   | 1.83                     | 0.41              |
| 1:G:223:CYS:HA   | 1:G:259:ILE:HD11 | 2.03                     | 0.41              |
| 1:K:146:ARG:HG2  | 1:P:281:TRP:CD1  | 2.56                     | 0.41              |
| 1:O:223:CYS:HA   | 1:O:259:ILE:HD11 | 2.01                     | 0.41              |
| 1:Q:226:GLY:HA3  | 1:Q:259:ILE:HD13 | 2.02                     | 0.41              |
| 1:X:225:ILE:O    | 1:X:229:ARG:HG2  | 2.20                     | 0.41              |
| 1:Y:203:LEU:HD11 | 1:Y:231:LEU:HD12 | 2.02                     | 0.41              |
| 1:E:189:ASN:OD1  | 1:E:190:ILE:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:149:LEU:HD13 | 1:I:152:ILE:HD11 | 2.02                     | 0.41              |
| 1:N:263:ASP:O    | 3:N:401:HOH:O    | 2.22                     | 0.41              |
| 1:A:225:ILE:O    | 1:A:229:ARG:HG2  | 2.20                     | 0.41              |
| 1:C:124:HIS:HB3  | 1:T:124:HIS:HB3  | 2.02                     | 0.41              |
| 1:C:168:LEU:HD22 | 1:C:173:ILE:HB   | 2.02                     | 0.41              |
| 1:E:124:HIS:HA   | 1:E:130:TYR:HD1  | 1.86                     | 0.41              |
| 1:F:240:PHE:CD1  | 1:F:256:GLN:HG2  | 2.56                     | 0.41              |
| 1:J:277:LEU:HG   | 1:J:278:PRO:HA   | 2.03                     | 0.41              |
| 1:K:124:HIS:HE1  | 1:K:127:GLY:O    | 2.04                     | 0.41              |
| 1:M:230:LYS:CD   | 1:M:264:ASP:HB3  | 2.51                     | 0.41              |
| 1:N:185:GLU:HG2  | 1:N:186:PRO:CD   | 2.51                     | 0.41              |
| 1:P:183:ASN:HA   | 1:P:188:VAL:HG23 | 2.03                     | 0.41              |
| 1:S:255:ASP:HA   | 1:S:258:PHE:HD2  | 1.83                     | 0.41              |
| 1:V:125:VAL:HG12 | 1:V:126:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:191:PRO:HD2  | 1:A:194:LEU:HD12 | 2.01                     | 0.41              |
| 1:F:225:ILE:O    | 1:F:229:ARG:HG2  | 2.21                     | 0.41              |
| 1:H:149:LEU:HA   | 1:H:209:PRO:HB2  | 2.02                     | 0.41              |
| 3:K:411:HOH:O    | 1:P:142:PHE:HE1  | 2.03                     | 0.41              |
| 1:S:149:LEU:HD13 | 1:S:211:LEU:HB2  | 2.02                     | 0.41              |
| 1:S:166:ASN:O    | 1:S:170:LEU:HD13 | 2.21                     | 0.41              |
| 1:B:117:ILE:HD12 | 1:B:138:GLU:HB2  | 2.04                     | 0.40              |
| 1:F:122:PHE:HA   | 1:F:131:ARG:O    | 2.21                     | 0.40              |
| 1:H:190:ILE:HA   | 1:H:191:PRO:HD3  | 1.89                     | 0.40              |
| 1:K:244:ARG:CZ   | 1:Q:244:ARG:HD2  | 2.51                     | 0.40              |
| 1:P:168:LEU:HD22 | 1:P:173:ILE:HB   | 2.03                     | 0.40              |
| 1:R:235:SER:OG   | 1:R:238:MET:HG2  | 2.20                     | 0.40              |
| 1:Y:153:LEU:HD11 | 1:Y:178:VAL:HG23 | 2.03                     | 0.40              |
| 1:H:214:SER:OG   | 2:H:301:SO4:O1   | 2.39                     | 0.40              |
| 1:K:156:ILE:O    | 1:K:177:GLN:NE2  | 2.49                     | 0.40              |
| 1:L:150:LYS:HG3  | 1:L:209:PRO:HD2  | 2.03                     | 0.40              |
| 1:L:187:PHE:CA   | 1:L:188:VAL:HG23 | 2.38                     | 0.40              |
| 1:N:131:ARG:HG3  | 1:N:221:THR:HG21 | 2.03                     | 0.40              |
| 1:T:176:TYR:HB3  | 1:T:201:ILE:HD13 | 2.03                     | 0.40              |
| 1:V:254:LEU:HG   | 3:V:408:HOH:O    | 2.20                     | 0.40              |
| 1:E:281:TRP:HE1  | 1:O:146:ARG:NH2  | 2.19                     | 0.40              |
| 1:J:117:ILE:HD12 | 1:J:138:GLU:HB2  | 2.03                     | 0.40              |
| 1:X:149:LEU:HD23 | 1:X:209:PRO:HB2  | 2.04                     | 0.40              |
| 1:B:113:ASN:ND2  | 1:V:277:LEU:HD11 | 2.34                     | 0.40              |
| 1:C:234:TRP:HA   | 1:T:116:VAL:O    | 2.21                     | 0.40              |
| 1:L:124:HIS:HD2  | 1:L:130:TYR:CE1  | 2.39                     | 0.40              |
| 1:O:119:PRO:HG3  | 1:O:139:ASN:HB3  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:136:ARG:NH1  | 1:V:188:VAL:H    | 2.19                     | 0.40              |
| 1:W:207:ASN:O    | 1:W:210:ILE:HB   | 2.22                     | 0.40              |
| 1:W:226:GLY:HA3  | 1:W:259:ILE:HD13 | 2.03                     | 0.40              |
| 1:X:138:GLU:CD   | 1:Y:257:GLN:HE22 | 2.29                     | 0.40              |
| 1:A:140:PHE:HB3  | 1:A:167:PHE:CZ   | 2.57                     | 0.40              |
| 1:B:199:LEU:HA   | 1:B:199:LEU:HD23 | 1.88                     | 0.40              |
| 1:E:146:ARG:HH21 | 1:O:281:TRP:HE1  | 1.70                     | 0.40              |
| 1:E:203:LEU:HD11 | 1:E:231:LEU:HD13 | 2.02                     | 0.40              |
| 1:O:160:TYR:HD2  | 1:O:165:LEU:HG   | 1.86                     | 0.40              |
| 1:P:181:SER:OG   | 1:P:184:LYS:HB2  | 2.21                     | 0.40              |
| 1:V:230:LYS:NZ   | 1:V:262:TYR:HB3  | 2.37                     | 0.40              |
| 1:Y:187:PHE:HA   | 1:Y:188:VAL:HB   | 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     | 167/169 (99%) | 158 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 1   | B     | 167/169 (99%) | 156 (93%) | 11 (7%) | 0        | 100         | 100 |
| 1   | C     | 167/169 (99%) | 156 (93%) | 10 (6%) | 1 (1%)   | 21          | 38  |
| 1   | D     | 167/169 (99%) | 157 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | E     | 167/169 (99%) | 155 (93%) | 10 (6%) | 2 (1%)   | 10          | 20  |
| 1   | F     | 167/169 (99%) | 159 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | G     | 167/169 (99%) | 157 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | H     | 167/169 (99%) | 158 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 1   | I     | 167/169 (99%) | 157 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | J     | 167/169 (99%) | 158 (95%) | 9 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | K     | 167/169 (99%)   | 157 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 1   | L     | 167/169 (99%)   | 155 (93%)  | 12 (7%)  | 0        | 100         | 100 |
| 1   | M     | 167/169 (99%)   | 156 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 1   | N     | 167/169 (99%)   | 157 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 1   | O     | 167/169 (99%)   | 157 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 1   | P     | 167/169 (99%)   | 155 (93%)  | 12 (7%)  | 0        | 100         | 100 |
| 1   | Q     | 167/169 (99%)   | 157 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 1   | R     | 167/169 (99%)   | 158 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 1   | S     | 167/169 (99%)   | 157 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 1   | T     | 164/169 (97%)   | 153 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 1   | V     | 167/169 (99%)   | 157 (94%)  | 9 (5%)   | 1 (1%)   | 21          | 38  |
| 1   | W     | 167/169 (99%)   | 156 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 1   | X     | 167/169 (99%)   | 156 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 1   | Y     | 167/169 (99%)   | 156 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| All | All   | 4005/4056 (99%) | 3758 (94%) | 243 (6%) | 4 (0%)   | 48          | 68  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 184 | LYS  |
| 1   | C     | 184 | LYS  |
| 1   | E     | 184 | LYS  |
| 1   | E     | 188 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 156/156 (100%) | 156 (100%) | 0        | 100         | 100 |
| 1   | B     | 156/156 (100%) | 156 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | C     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | D     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | E     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | F     | 155/156 (99%)    | 155 (100%)  | 0        | 100         | 100 |
| 1   | G     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | H     | 155/156 (99%)    | 155 (100%)  | 0        | 100         | 100 |
| 1   | I     | 155/156 (99%)    | 155 (100%)  | 0        | 100         | 100 |
| 1   | J     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | K     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | L     | 155/156 (99%)    | 155 (100%)  | 0        | 100         | 100 |
| 1   | M     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | N     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | O     | 155/156 (99%)    | 155 (100%)  | 0        | 100         | 100 |
| 1   | P     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 155/156 (99%)    | 155 (100%)  | 0        | 100         | 100 |
| 1   | R     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | S     | 155/156 (99%)    | 153 (99%)   | 2 (1%)   | 61          | 82  |
| 1   | T     | 155/156 (99%)    | 155 (100%)  | 0        | 100         | 100 |
| 1   | V     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | W     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | X     | 153/156 (98%)    | 153 (100%)  | 0        | 100         | 100 |
| 1   | Y     | 156/156 (100%)   | 156 (100%)  | 0        | 100         | 100 |
| All | All   | 3733/3744 (100%) | 3731 (100%) | 2 (0%)   | 88          | 96  |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 171 | THR  |
| 1   | S     | 223 | CYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 144 | HIS  |
| 1   | A     | 193 | HIS  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 274 | ASN  |
| 1   | B     | 121 | ASN  |
| 1   | B     | 189 | ASN  |
| 1   | B     | 257 | GLN  |
| 1   | B     | 280 | GLN  |
| 1   | C     | 121 | ASN  |
| 1   | C     | 162 | GLN  |
| 1   | C     | 275 | ASN  |
| 1   | D     | 144 | HIS  |
| 1   | D     | 193 | HIS  |
| 1   | E     | 144 | HIS  |
| 1   | E     | 164 | ASN  |
| 1   | E     | 215 | ASN  |
| 1   | F     | 183 | ASN  |
| 1   | F     | 256 | GLN  |
| 1   | G     | 124 | HIS  |
| 1   | G     | 144 | HIS  |
| 1   | H     | 144 | HIS  |
| 1   | H     | 162 | GLN  |
| 1   | H     | 166 | ASN  |
| 1   | I     | 256 | GLN  |
| 1   | K     | 166 | ASN  |
| 1   | K     | 256 | GLN  |
| 1   | L     | 233 | ASN  |
| 1   | L     | 274 | ASN  |
| 1   | M     | 189 | ASN  |
| 1   | N     | 113 | ASN  |
| 1   | N     | 121 | ASN  |
| 1   | N     | 193 | HIS  |
| 1   | N     | 256 | GLN  |
| 1   | O     | 162 | GLN  |
| 1   | O     | 166 | ASN  |
| 1   | O     | 177 | GLN  |
| 1   | O     | 213 | HIS  |
| 1   | O     | 233 | ASN  |
| 1   | Q     | 213 | HIS  |
| 1   | Q     | 233 | ASN  |
| 1   | R     | 113 | ASN  |
| 1   | R     | 144 | HIS  |
| 1   | R     | 193 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 256 | GLN  |
| 1   | T     | 193 | HIS  |
| 1   | X     | 144 | HIS  |
| 1   | Y     | 162 | GLN  |

### 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](#)

24 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | SO4  | Y     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | D     | 301 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | T     | 301 | -    | 4,4,4        | 0.22 | 0           | 6,6,6       | 0.11 | 0           |
| 2   | SO4  | P     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.21 | 0           |
| 2   | SO4  | L     | 301 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.11 | 0           |
| 2   | SO4  | V     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.14 | 0           |
| 2   | SO4  | H     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.14 | 0           |
| 2   | SO4  | J     | 301 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.13 | 0           |
| 2   | SO4  | X     | 301 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.08 | 0           |
| 2   | SO4  | E     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.17 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | SO4  | S     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.19 | 0           |
| 2   | SO4  | B     | 301 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | I     | 301 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | R     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | A     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.17 | 0           |
| 2   | SO4  | N     | 301 | -    | 4,4,4        | 0.22 | 0           | 6,6,6       | 0.08 | 0           |
| 2   | SO4  | C     | 301 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.06 | 0           |
| 2   | SO4  | F     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.15 | 0           |
| 2   | SO4  | G     | 301 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | M     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.16 | 0           |
| 2   | SO4  | K     | 301 | -    | 4,4,4        | 0.22 | 0           | 6,6,6       | 0.07 | 0           |
| 2   | SO4  | Q     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.14 | 0           |
| 2   | SO4  | W     | 301 | -    | 4,4,4        | 0.20 | 0           | 6,6,6       | 0.37 | 0           |
| 2   | SO4  | O     | 301 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.09 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | Y     | 301 | SO4  | 2       | 0            |
| 2   | T     | 301 | SO4  | 2       | 0            |
| 2   | P     | 301 | SO4  | 3       | 0            |
| 2   | L     | 301 | SO4  | 1       | 0            |
| 2   | H     | 301 | SO4  | 2       | 0            |
| 2   | A     | 301 | SO4  | 1       | 0            |
| 2   | G     | 301 | SO4  | 1       | 0            |
| 2   | W     | 301 | SO4  | 5       | 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     | 169/169 (100%) | -0.45  | 1 (0%) 85 83 | 34, 52, 69, 84        | 0     |
| 1   | B     | 169/169 (100%) | -0.48  | 0 100 100    | 32, 47, 70, 92        | 0     |
| 1   | C     | 169/169 (100%) | -0.40  | 0 100 100    | 27, 46, 77, 107       | 0     |
| 1   | D     | 169/169 (100%) | -0.50  | 0 100 100    | 29, 48, 70, 100       | 0     |
| 1   | E     | 169/169 (100%) | -0.46  | 0 100 100    | 34, 45, 75, 103       | 0     |
| 1   | F     | 169/169 (100%) | -0.41  | 0 100 100    | 36, 48, 70, 99        | 0     |
| 1   | G     | 169/169 (100%) | -0.47  | 1 (0%) 85 83 | 35, 53, 75, 97        | 0     |
| 1   | H     | 169/169 (100%) | -0.42  | 0 100 100    | 44, 55, 76, 99        | 0     |
| 1   | I     | 169/169 (100%) | -0.42  | 0 100 100    | 42, 54, 80, 94        | 0     |
| 1   | J     | 169/169 (100%) | -0.36  | 3 (1%) 67 64 | 35, 50, 81, 108       | 0     |
| 1   | K     | 169/169 (100%) | -0.39  | 0 100 100    | 40, 53, 79, 110       | 0     |
| 1   | L     | 169/169 (100%) | -0.49  | 0 100 100    | 39, 53, 67, 81        | 0     |
| 1   | M     | 169/169 (100%) | -0.46  | 0 100 100    | 38, 50, 74, 87        | 0     |
| 1   | N     | 169/169 (100%) | -0.47  | 0 100 100    | 35, 48, 66, 102       | 0     |
| 1   | O     | 169/169 (100%) | -0.44  | 0 100 100    | 35, 48, 70, 83        | 0     |
| 1   | P     | 169/169 (100%) | -0.42  | 0 100 100    | 37, 52, 72, 106       | 0     |
| 1   | Q     | 169/169 (100%) | -0.34  | 1 (0%) 85 83 | 33, 47, 78, 124       | 0     |
| 1   | R     | 169/169 (100%) | -0.37  | 0 100 100    | 32, 47, 72, 110       | 0     |
| 1   | S     | 169/169 (100%) | -0.05  | 1 (0%) 85 83 | 42, 69, 92, 100       | 0     |
| 1   | T     | 168/169 (99%)  | -0.20  | 0 100 100    | 34, 57, 86, 102       | 0     |
| 1   | V     | 169/169 (100%) | -0.27  | 1 (0%) 85 83 | 33, 57, 95, 126       | 0     |
| 1   | W     | 169/169 (100%) | 0.10   | 0 100 100    | 50, 72, 112, 131      | 0     |
| 1   | X     | 169/169 (100%) | -0.17  | 1 (0%) 85 83 | 36, 63, 115, 154      | 0     |
| 1   | Y     | 169/169 (100%) | -0.18  | 0 100 100    | 33, 63, 84, 92        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| All | All   | 4055/4056 (99%) | -0.36  | 9 (0%) 91 89 | 27, 52, 84, 154       | 0     |

All (9) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | X     | 184 | LYS  | 3.0  |
| 1   | J     | 186 | PRO  | 2.7  |
| 1   | V     | 182 | GLY  | 2.6  |
| 1   | Q     | 187 | PHE  | 2.3  |
| 1   | J     | 188 | VAL  | 2.3  |
| 1   | G     | 186 | PRO  | 2.3  |
| 1   | S     | 161 | PRO  | 2.1  |
| 1   | J     | 184 | LYS  | 2.1  |
| 1   | A     | 186 | PRO  | 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | SO4  | F     | 301 | 5/5   | 0.96 | 0.08 | 42,42,42,43                | 0     |
| 2   | SO4  | V     | 301 | 5/5   | 0.96 | 0.06 | 51,51,51,51                | 0     |
| 2   | SO4  | W     | 301 | 5/5   | 0.96 | 0.07 | 78,80,81,83                | 0     |
| 2   | SO4  | E     | 301 | 5/5   | 0.97 | 0.10 | 32,33,33,33                | 0     |
| 2   | SO4  | X     | 301 | 5/5   | 0.97 | 0.07 | 58,58,58,59                | 0     |
| 2   | SO4  | B     | 301 | 5/5   | 0.98 | 0.05 | 49,50,50,50                | 0     |
| 2   | SO4  | H     | 301 | 5/5   | 0.98 | 0.05 | 55,55,55,56                | 0     |
| 2   | SO4  | I     | 301 | 5/5   | 0.98 | 0.06 | 42,42,43,43                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | SO4  | J     | 301 | 5/5   | 0.98 | 0.10 | 42,42,43,43                 | 0     |
| 2   | SO4  | K     | 301 | 5/5   | 0.98 | 0.07 | 40,41,41,42                 | 0     |
| 2   | SO4  | L     | 301 | 5/5   | 0.98 | 0.06 | 55,55,56,56                 | 0     |
| 2   | SO4  | O     | 301 | 5/5   | 0.98 | 0.05 | 46,46,46,46                 | 0     |
| 2   | SO4  | P     | 301 | 5/5   | 0.98 | 0.09 | 45,45,45,45                 | 0     |
| 2   | SO4  | Q     | 301 | 5/5   | 0.98 | 0.05 | 51,51,51,52                 | 0     |
| 2   | SO4  | R     | 301 | 5/5   | 0.98 | 0.07 | 26,28,28,29                 | 0     |
| 2   | SO4  | S     | 301 | 5/5   | 0.98 | 0.06 | 47,47,47,48                 | 0     |
| 2   | SO4  | T     | 301 | 5/5   | 0.98 | 0.04 | 50,50,50,50                 | 0     |
| 2   | SO4  | C     | 301 | 5/5   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 2   | SO4  | D     | 301 | 5/5   | 0.98 | 0.05 | 39,39,40,40                 | 0     |
| 2   | SO4  | A     | 301 | 5/5   | 0.98 | 0.10 | 30,30,31,31                 | 0     |
| 2   | SO4  | Y     | 301 | 5/5   | 0.98 | 0.05 | 53,55,56,56                 | 0     |
| 2   | SO4  | M     | 301 | 5/5   | 0.99 | 0.04 | 41,42,42,43                 | 0     |
| 2   | SO4  | N     | 301 | 5/5   | 0.99 | 0.04 | 47,47,47,48                 | 0     |
| 2   | SO4  | G     | 301 | 5/5   | 0.99 | 0.04 | 62,62,62,62                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.