



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 5WJT / pdb\_00005wjt  
EMDB ID : EMD-8847  
Title : Cryo-EM structure of B. subtilis flagellar filaments N226Y  
Authors : Wang, F.; Burrage, A.M.; Kearns, D.B.; Egelman, E.H.  
Deposited on : 2017-07-24  
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

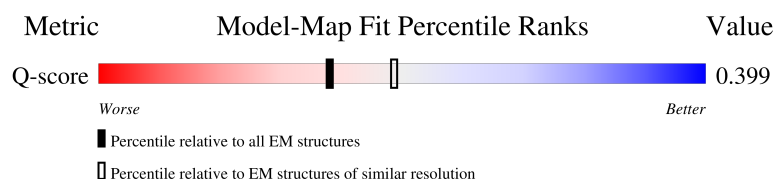
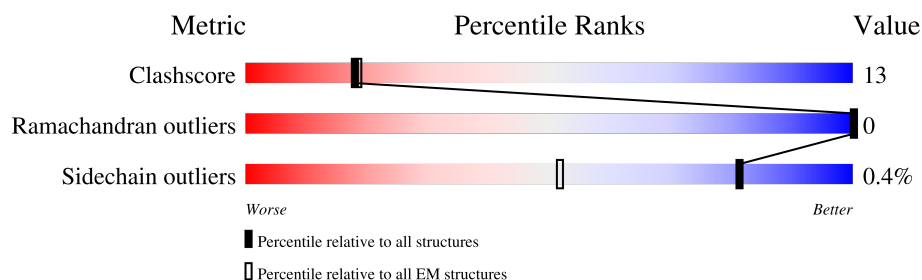
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | A     | 304    |  77% 21% .. |
| 1   | B     | 304    |  78% 20% .. |
| 1   | C     | 304    |  78% 20% .. |
| 1   | D     | 304    |  77% 21% .. |

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| Mol | Chain | Length | Quality of chain                                                                     |            |
|-----|-------|--------|--------------------------------------------------------------------------------------|------------|
| 1   | E     | 304    |    | 78% 20% .. |
| 1   | F     | 304    |    | 77% 21% .. |
| 1   | G     | 304    |    | 78% 20% .. |
| 1   | H     | 304    |    | 78% 20% .. |
| 1   | I     | 304    |    | 78% 20% .. |
| 1   | J     | 304    |    | 79% 19% .. |
| 1   | K     | 304    |    | 79% 19% .. |
| 1   | L     | 304    |    | 79% 19% .. |
| 1   | M     | 304    |    | 78% 20% .. |
| 1   | N     | 304    |    | 79% 19% .. |
| 1   | O     | 304    |    | 78% 20% .. |
| 1   | P     | 304    |    | 79% 19% .. |
| 1   | Q     | 304    |  | 79% 19% .. |
| 1   | R     | 304    |  | 78% 20% .. |
| 1   | S     | 304    |  | 78% 20% .. |
| 1   | T     | 304    |  | 80% 18% .. |
| 1   | U     | 304    |  | 80% 19% .  |
| 1   | V     | 304    |  | 81% 17% .. |
| 1   | W     | 304    |  | 80% 19% .  |
| 1   | X     | 304    |  | 81% 17% .. |
| 1   | Y     | 304    |  | 79% 19% .. |
| 1   | Z     | 304    |  | 81% 17% .. |
| 1   | a     | 304    |  | 80% 18% .. |
| 1   | b     | 304    |  | 81% 17% .. |
| 1   | c     | 304    |  | 81% 17% .. |

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| Mol | Chain | Length | Quality of chain                                                                   |            |
|-----|-------|--------|------------------------------------------------------------------------------------|------------|
| 1   | d     | 304    |  | 81% 17% .. |
| 1   | e     | 304    |  | 79% 19% .. |
| 1   | f     | 304    |  | 81% 17% .. |
| 1   | g     | 304    |  | 81% 18% .  |
| 1   | h     | 304    |  | 82% 16% .. |
| 1   | i     | 304    |  | 79% 19% .. |
| 1   | j     | 304    |  | 81% 17% .. |
| 1   | k     | 304    |  | 80% 18% .. |
| 1   | l     | 304    |  | 83% 15% .. |
| 1   | m     | 304    |  | 81% 17% .. |
| 1   | n     | 304    |  | 81% 17% .. |
| 1   | o     | 304    |  | 81% 18% .. |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 92947 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Flagellin.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | A     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | B     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | C     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | D     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | E     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | F     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | G     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | H     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | I     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | J     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | K     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | L     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | M     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | N     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | O     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | P     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | Q     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | R     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | S     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | T     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | U     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | V     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | W     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | X     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | Y     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | Z     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | a     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | b     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | c     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | d     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | e     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | f     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | g     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | h     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | i     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | j     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | k     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |
| 1   | l     | 302      | Total<br>2267 | C<br>1371 | N<br>414 | O<br>474 | S<br>8 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | m     | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2267  | 1371 | 414 | 474 | 8 |         |       |
| 1   | n     | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2267  | 1371 | 414 | 474 | 8 |         |       |
| 1   | o     | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2267  | 1371 | 414 | 474 | 8 |         |       |

There are 82 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| A     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| A     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| B     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| B     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| C     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| C     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| D     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| D     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| E     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| E     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| F     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| F     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| G     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| G     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| H     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| H     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| I     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| I     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| J     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| J     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| K     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| K     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| L     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| L     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| M     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| M     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| N     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| N     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| O     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| O     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| P     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| P     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| Q     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| Q     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| R     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| R     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| S     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| S     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| T     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| T     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| U     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| U     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| V     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| V     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| W     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| W     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| X     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| X     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| Y     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| Y     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| Z     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| Z     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| a     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| a     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| b     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| b     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| c     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| c     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| d     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| d     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| e     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| e     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| f     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| f     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| g     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| g     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| h     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| h     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| i     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| i     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| j     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| j     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| k     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| k     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |

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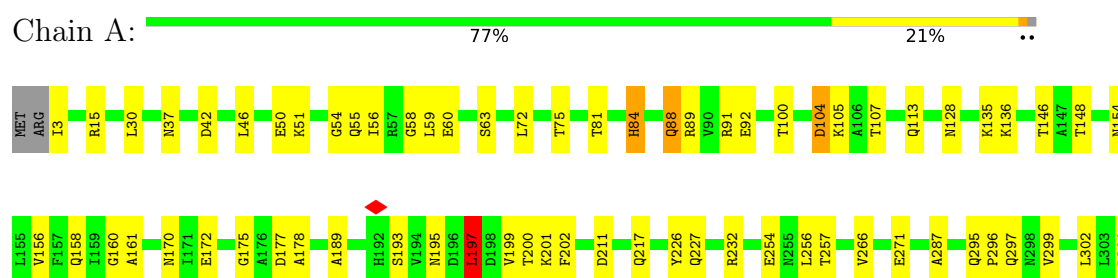
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| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| l     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| l     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| m     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| m     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| n     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| n     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |
| o     | 209     | CYS      | THR    | engineered mutation | UNP A0A162QQD4 |
| o     | 226     | TYR      | ASN    | engineered mutation | UNP A0A162QQD4 |

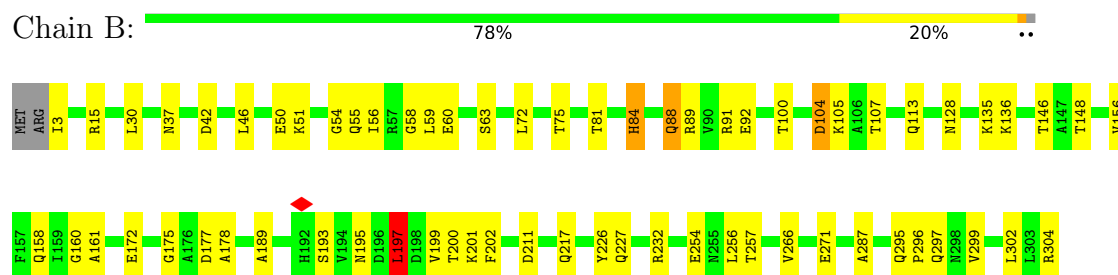
### 3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

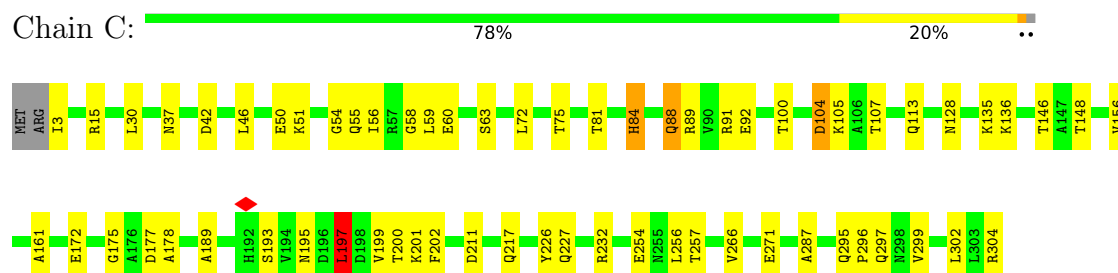
#### • Molecule 1: Flagellin



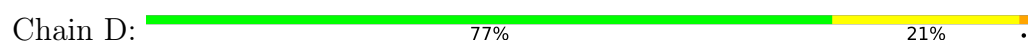
#### • Molecule 1: Flagellin

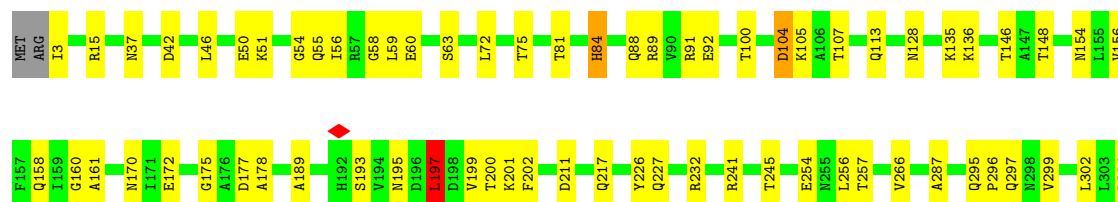


#### • Molecule 1: Flagellin



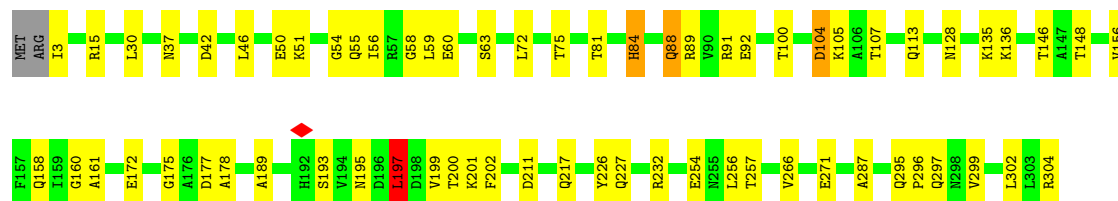
#### • Molecule 1: Flagellin





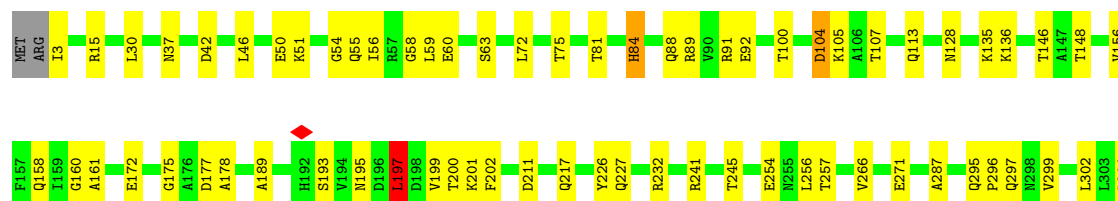
- Molecule 1: Flagellin

Chain E: 78% 20% ..



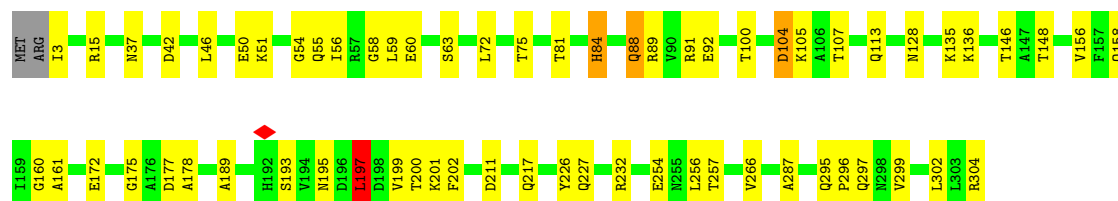
- Molecule 1: Flagellin

Chain F: 77% 21% ..



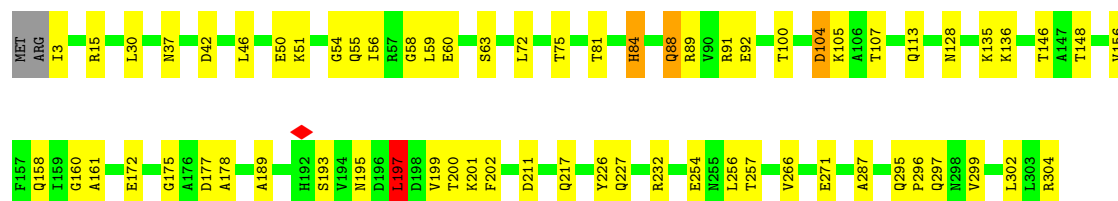
- Molecule 1: Flagellin

Chain G: 78% 20% ..



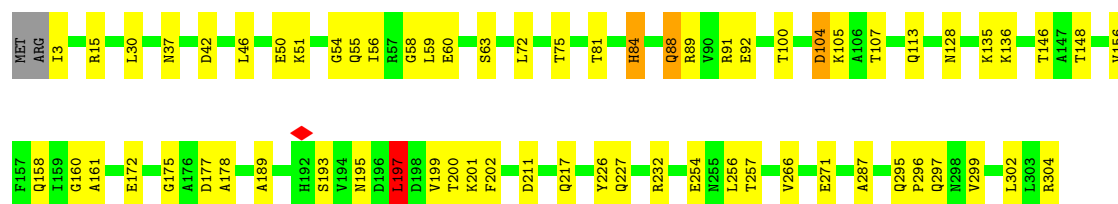
- Molecule 1: Flagellin

Chain H: 78% 20% ..



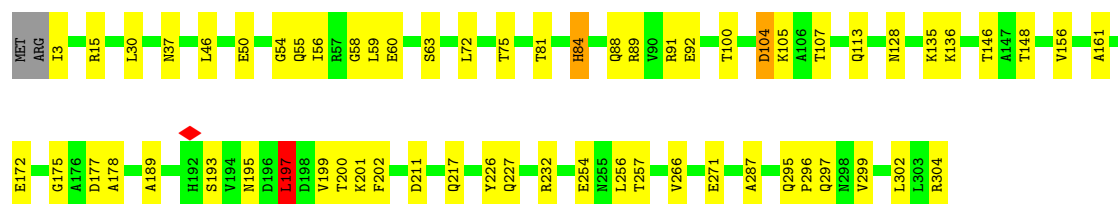
- Molecule 1: Flagellin

Chain I:  78% 20% ..



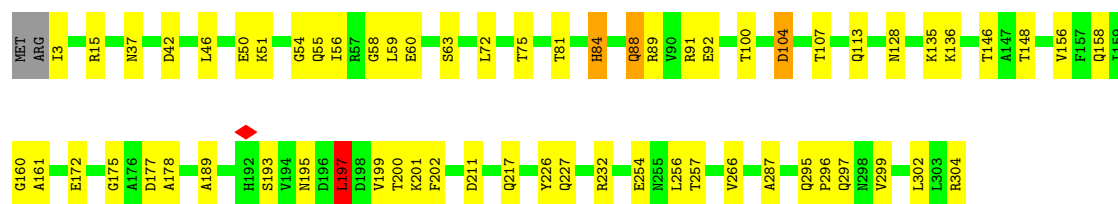
• Molecule 1: Flagellin

Chain J:  79% 19% ..



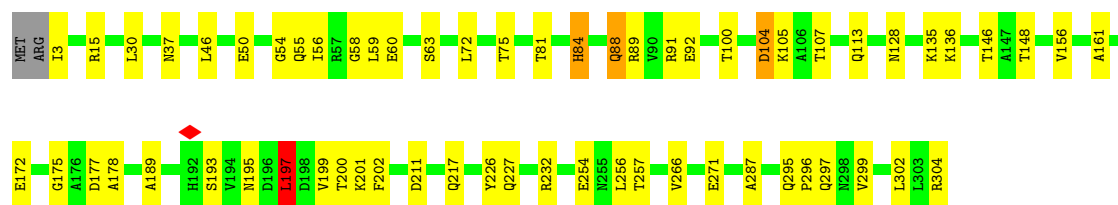
• Molecule 1: Flagellin

Chain K:  79% 19% ..



• Molecule 1: Flagellin

Chain L:  79% 19% ..



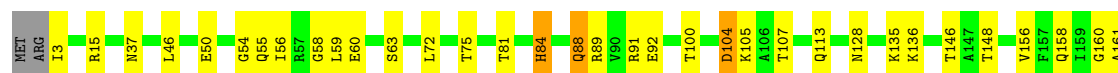
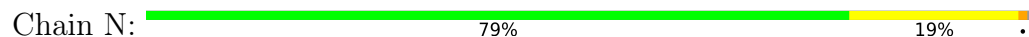
• Molecule 1: Flagellin

Chain M:  78% 20% ..

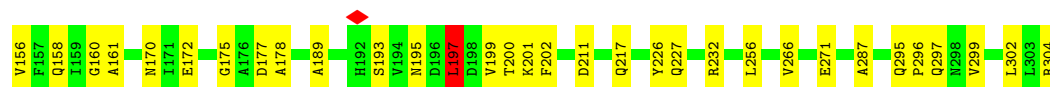
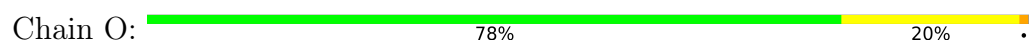




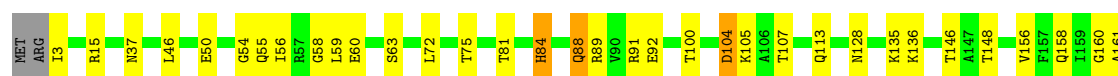
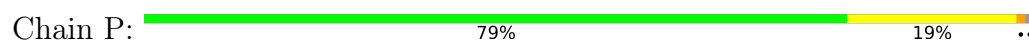
• Molecule 1: Flagellin



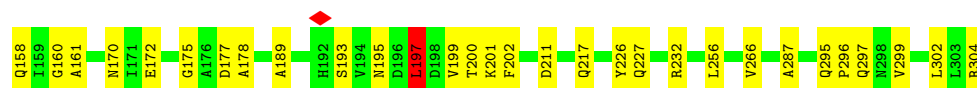
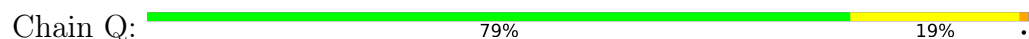
• Molecule 1: Flagellin



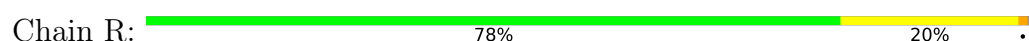
• Molecule 1: Flagellin

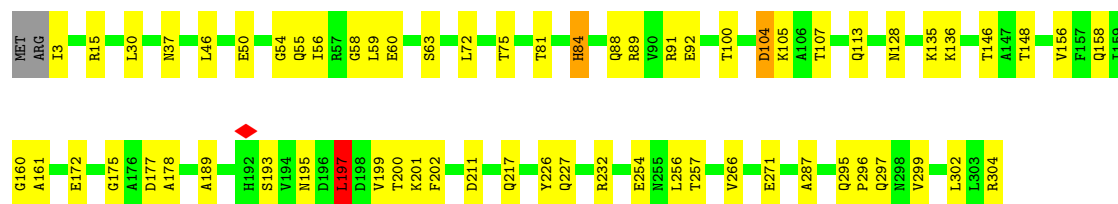


• Molecule 1: Flagellin



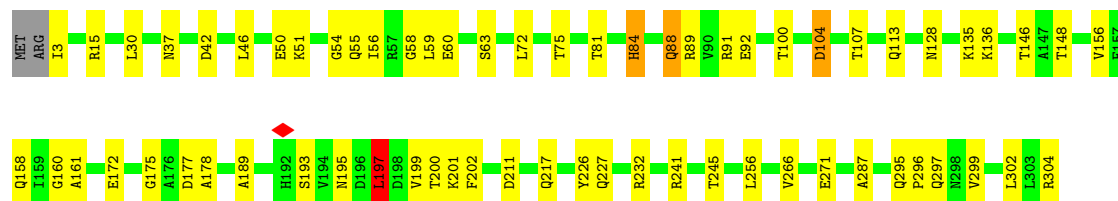
• Molecule 1: Flagellin





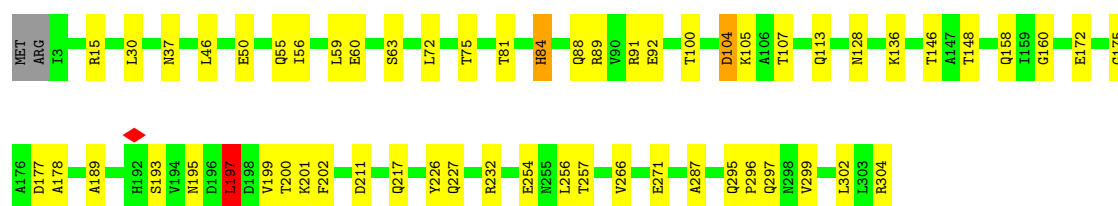
• Molecule 1: Flagellin

Chain S: 78% 20% ..



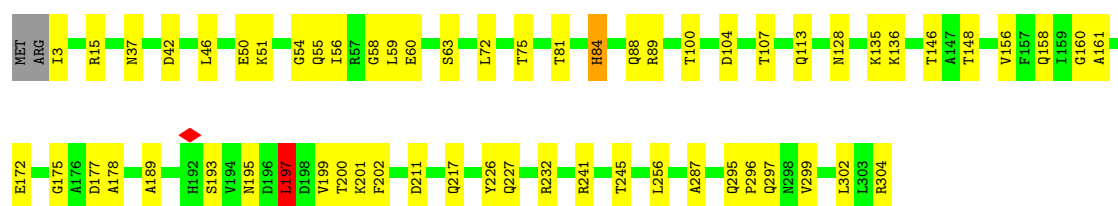
• Molecule 1: Flagellin

Chain T: 80% 18% ..



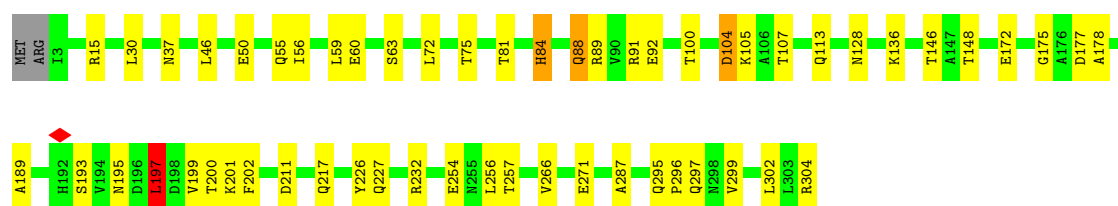
• Molecule 1: Flagellin

Chain U: 80% 19% .



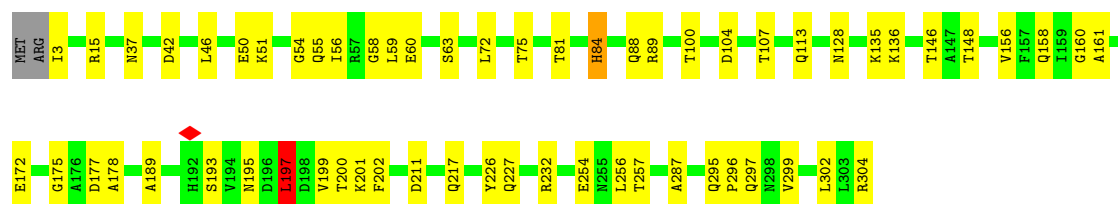
• Molecule 1: Flagellin

Chain V: 81% 17% ..



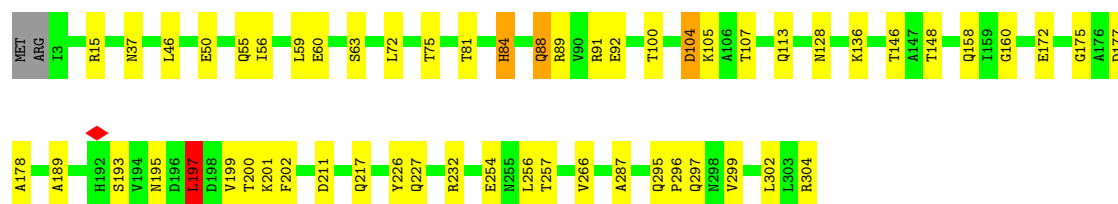
• Molecule 1: Flagellin

Chain W:  80% 19% .



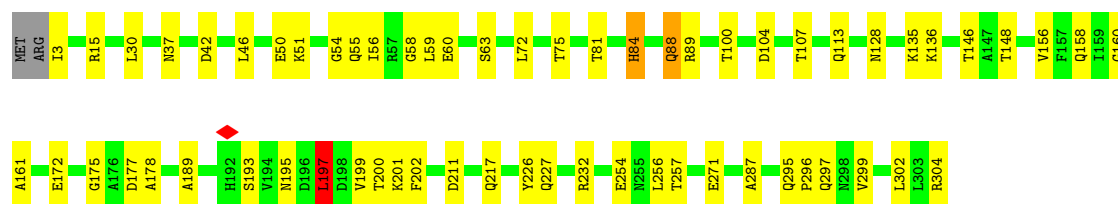
• Molecule 1: Flagellin

Chain X:  81% 17% ..



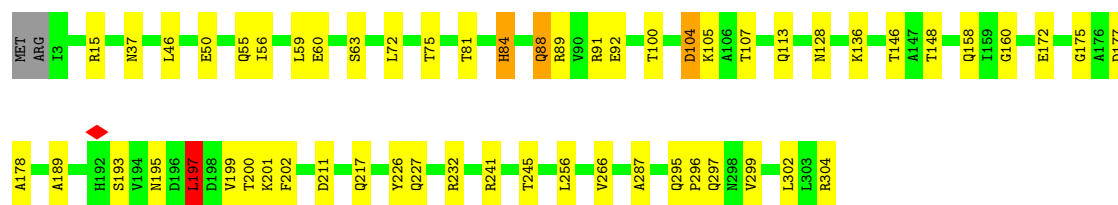
• Molecule 1: Flagellin

Chain Y:  79% 19% ..



• Molecule 1: Flagellin

Chain Z:  81% 17% ..



• Molecule 1: Flagellin

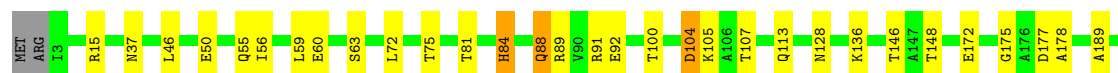
Chain a:  80% 18% ..





• Molecule 1: Flagellin

Chain b: 81% 17% ..



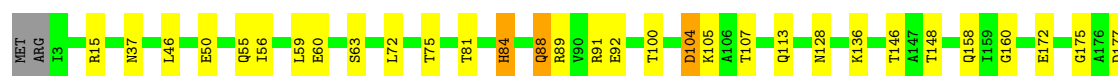
• Molecule 1: Flagellin

Chain c: 81% 17% ..



• Molecule 1: Flagellin

Chain d: 81% 17% ..



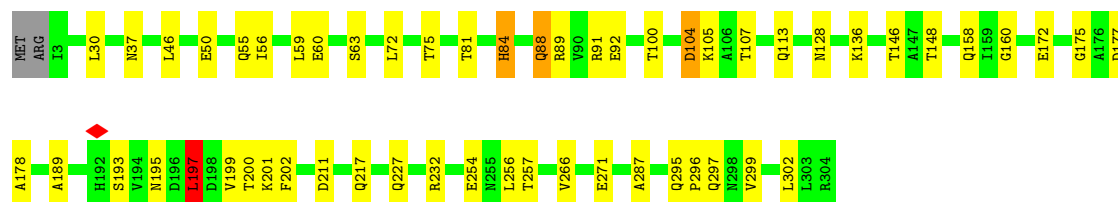
• Molecule 1: Flagellin

Chain e: 79% 19% ..



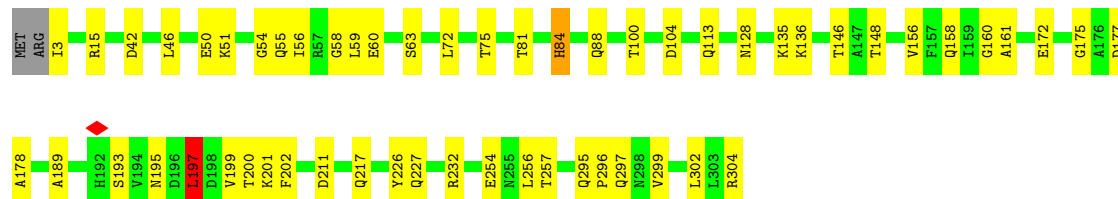
• Molecule 1: Flagellin

Chain f: 81% 17% ..



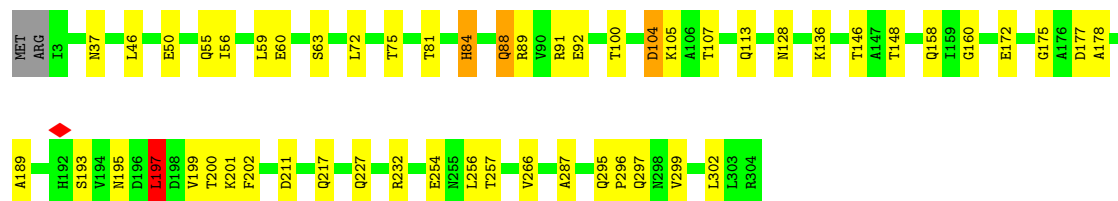
• Molecule 1: Flagellin

Chain g: 81% 18%



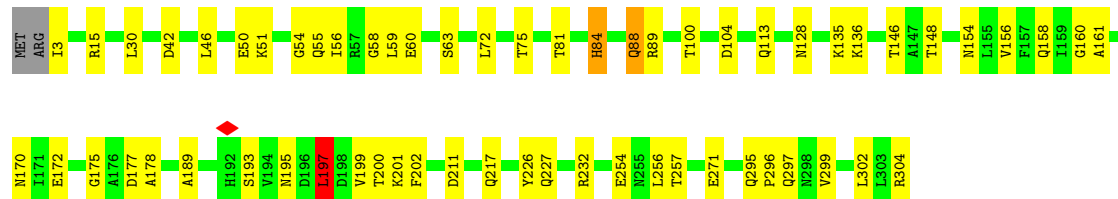
• Molecule 1: Flagellin

Chain h: 82% 16%



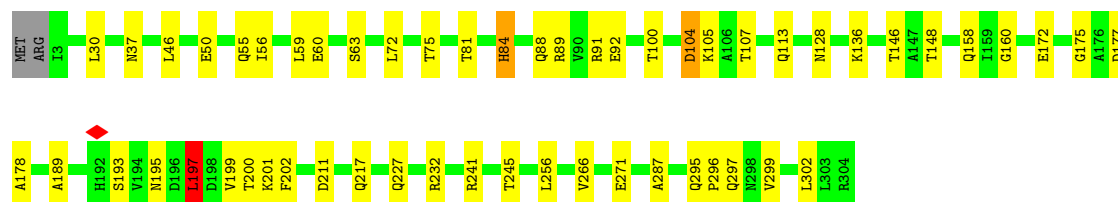
• Molecule 1: Flagellin

Chain i: 79% 19%

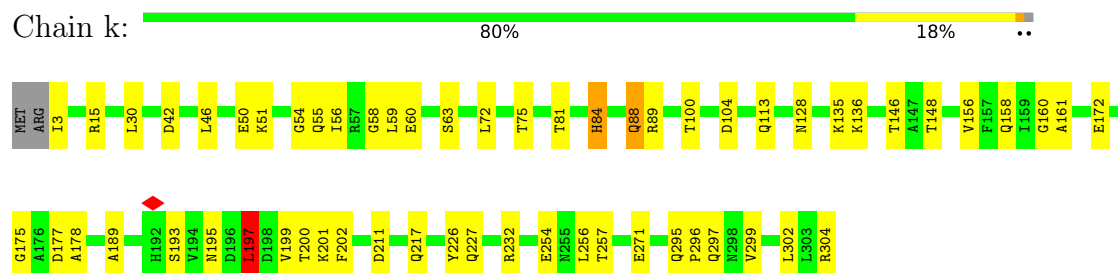


• Molecule 1: Flagellin

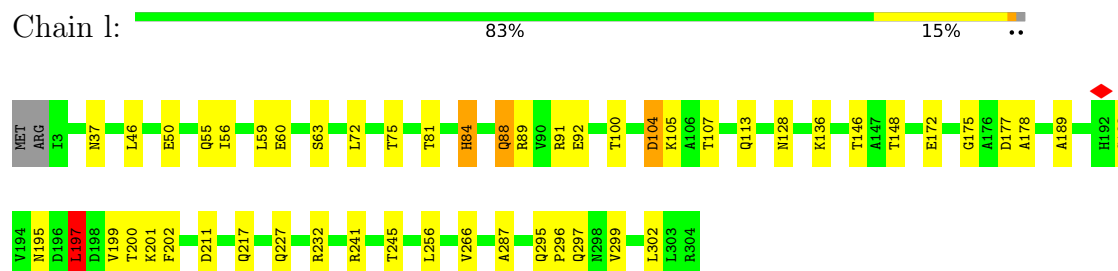
Chain j: 81% 17%



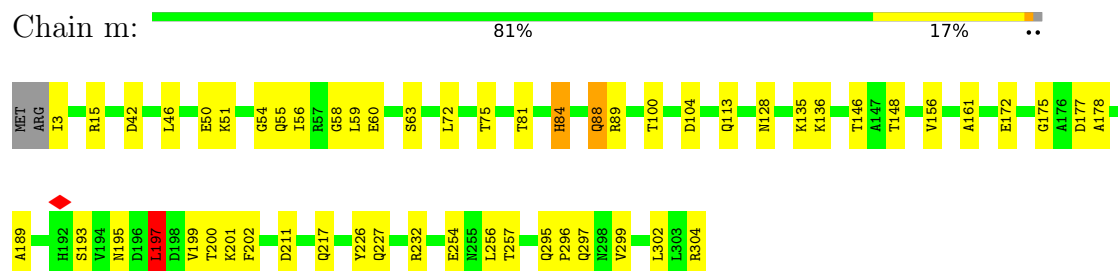
## • Molecule 1: Flagellin



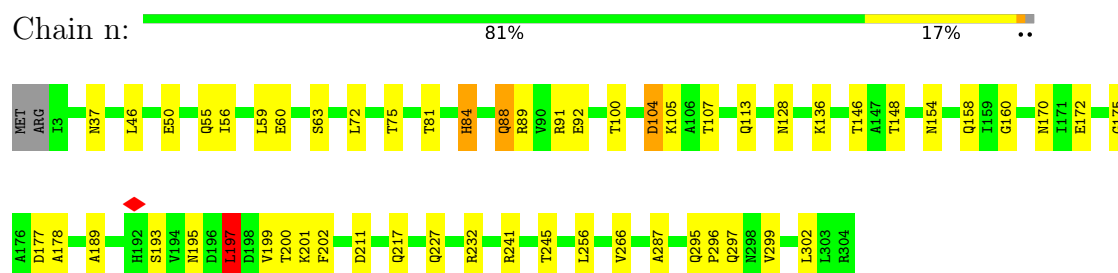
## • Molecule 1: Flagellin



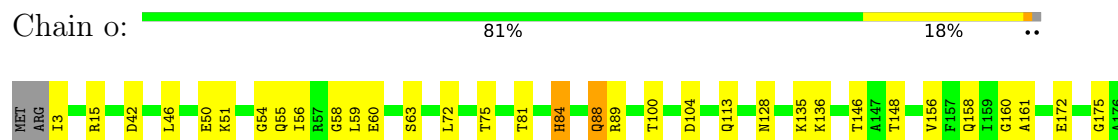
## • Molecule 1: Flagellin

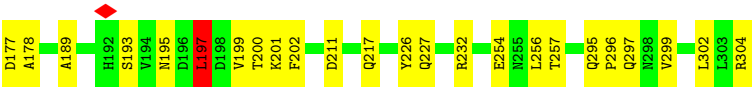


## • Molecule 1: Flagellin



## • Molecule 1: Flagellin





## 4 Experimental information

| Property                           | Value                                            | Source    |
|------------------------------------|--------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                          | Depositor |
| Imposed symmetry                   | HELICAL, twist=65.83°, rise=4.64 Å, axial sym=C1 | Depositor |
| Number of segments used            | 72005                                            | Depositor |
| Resolution determination method    | OTHER                                            | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION          | Depositor |
| Microscope                         | FEI TITAN KRIOS                                  | Depositor |
| Voltage (kV)                       | 300                                              | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 20                                               | Depositor |
| Minimum defocus (nm)               | Not provided                                     |           |
| Maximum defocus (nm)               | Not provided                                     |           |
| Magnification                      | Not provided                                     |           |
| Image detector                     | FEI FALCON II (4k x 4k)                          | Depositor |
| Maximum map value                  | 0.218                                            | Depositor |
| Minimum map value                  | -0.092                                           | Depositor |
| Average map value                  | 0.003                                            | Depositor |
| Map value standard deviation       | 0.017                                            | Depositor |
| Recommended contour level          | 0.02                                             | Depositor |
| Map size (Å)                       | 268.8, 268.8, 1050.0                             | wwPDB     |
| Map dimensions                     | 256, 256, 1000                                   | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                 | wwPDB     |
| Pixel spacing (Å)                  | 1.05, 1.05, 1.05                                 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | B     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | C     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | D     | 0.47         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | E     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | F     | 0.47         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | G     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | H     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | I     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | J     | 0.47         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | K     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | L     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | M     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | N     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | O     | 0.48         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | P     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | Q     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | R     | 0.47         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | S     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | T     | 0.47         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | U     | 0.48         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | V     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | W     | 0.47         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | X     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | Y     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | Z     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | a     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | b     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | c     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | d     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | e     | 0.47         | 0/2279      | 0.68        | 2/3073 (0.1%) |
| 1   | f     | 0.48         | 0/2279      | 0.69        | 2/3073 (0.1%) |
| 1   | g     | 0.47         | 0/2279      | 0.69        | 1/3073 (0.0%) |
| 1   | h     | 0.47         | 0/2279      | 0.69        | 2/3073 (0.1%) |

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | i     | 0.47         | 0/2279  | 0.69        | 2/3073 (0.1%)    |
| 1   | j     | 0.47         | 0/2279  | 0.69        | 1/3073 (0.0%)    |
| 1   | k     | 0.47         | 0/2279  | 0.69        | 2/3073 (0.1%)    |
| 1   | l     | 0.48         | 0/2279  | 0.69        | 2/3073 (0.1%)    |
| 1   | m     | 0.47         | 0/2279  | 0.69        | 2/3073 (0.1%)    |
| 1   | n     | 0.48         | 0/2279  | 0.69        | 2/3073 (0.1%)    |
| 1   | o     | 0.47         | 0/2279  | 0.69        | 2/3073 (0.1%)    |
| All | All   | 0.47         | 0/93439 | 0.69        | 72/125993 (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   | A     | 0                   | 3                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 3                   |
| 1   | D     | 0                   | 3                   |
| 1   | E     | 0                   | 3                   |
| 1   | F     | 0                   | 3                   |
| 1   | G     | 0                   | 3                   |
| 1   | H     | 0                   | 3                   |
| 1   | I     | 0                   | 3                   |
| 1   | J     | 0                   | 3                   |
| 1   | K     | 0                   | 3                   |
| 1   | L     | 0                   | 3                   |
| 1   | M     | 0                   | 3                   |
| 1   | N     | 0                   | 3                   |
| 1   | O     | 0                   | 3                   |
| 1   | P     | 0                   | 3                   |
| 1   | Q     | 0                   | 3                   |
| 1   | R     | 0                   | 3                   |
| 1   | S     | 0                   | 3                   |
| 1   | T     | 0                   | 3                   |
| 1   | U     | 0                   | 3                   |
| 1   | V     | 0                   | 3                   |
| 1   | W     | 0                   | 3                   |
| 1   | X     | 0                   | 3                   |
| 1   | Y     | 0                   | 3                   |
| 1   | Z     | 0                   | 3                   |
| 1   | a     | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | b     | 0                   | 3                   |
| 1   | c     | 0                   | 3                   |
| 1   | d     | 0                   | 3                   |
| 1   | e     | 0                   | 3                   |
| 1   | f     | 0                   | 3                   |
| 1   | g     | 0                   | 3                   |
| 1   | h     | 0                   | 3                   |
| 1   | i     | 0                   | 3                   |
| 1   | j     | 0                   | 3                   |
| 1   | k     | 0                   | 3                   |
| 1   | l     | 0                   | 3                   |
| 1   | m     | 0                   | 3                   |
| 1   | n     | 0                   | 3                   |
| 1   | o     | 0                   | 3                   |
| All | All   | 0                   | 123                 |

There are no bond length outliers.

All (72) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | E     | 197 | LEU  | N-CA-C | 5.17 | 121.80      | 110.80   |
| 1   | C     | 197 | LEU  | N-CA-C | 5.16 | 121.80      | 110.80   |
| 1   | R     | 197 | LEU  | N-CA-C | 5.16 | 121.80      | 110.80   |
| 1   | W     | 197 | LEU  | N-CA-C | 5.16 | 121.79      | 110.80   |
| 1   | m     | 197 | LEU  | N-CA-C | 5.16 | 121.79      | 110.80   |
| 1   | i     | 197 | LEU  | N-CA-C | 5.16 | 121.79      | 110.80   |
| 1   | D     | 197 | LEU  | N-CA-C | 5.16 | 121.78      | 110.80   |
| 1   | b     | 197 | LEU  | N-CA-C | 5.16 | 121.78      | 110.80   |
| 1   | G     | 197 | LEU  | N-CA-C | 5.15 | 121.77      | 110.80   |
| 1   | U     | 197 | LEU  | N-CA-C | 5.15 | 121.78      | 110.80   |
| 1   | N     | 197 | LEU  | N-CA-C | 5.15 | 121.77      | 110.80   |
| 1   | I     | 197 | LEU  | N-CA-C | 5.15 | 121.76      | 110.80   |
| 1   | S     | 197 | LEU  | N-CA-C | 5.15 | 121.76      | 110.80   |
| 1   | h     | 197 | LEU  | N-CA-C | 5.15 | 121.76      | 110.80   |
| 1   | K     | 197 | LEU  | N-CA-C | 5.14 | 121.76      | 110.80   |
| 1   | j     | 197 | LEU  | N-CA-C | 5.14 | 121.76      | 110.80   |
| 1   | A     | 197 | LEU  | N-CA-C | 5.14 | 121.75      | 110.80   |
| 1   | J     | 197 | LEU  | N-CA-C | 5.14 | 121.75      | 110.80   |
| 1   | X     | 197 | LEU  | N-CA-C | 5.14 | 121.75      | 110.80   |
| 1   | c     | 197 | LEU  | N-CA-C | 5.14 | 121.75      | 110.80   |
| 1   | H     | 197 | LEU  | N-CA-C | 5.14 | 121.75      | 110.80   |
| 1   | d     | 197 | LEU  | N-CA-C | 5.14 | 121.75      | 110.80   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | g     | 197 | LEU  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | n     | 197 | LEU  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | F     | 197 | LEU  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | P     | 197 | LEU  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | T     | 197 | LEU  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | l     | 197 | LEU  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | V     | 197 | LEU  | N-CA-C | 5.14  | 121.74      | 110.80   |
| 1   | f     | 197 | LEU  | N-CA-C | 5.14  | 121.74      | 110.80   |
| 1   | M     | 197 | LEU  | N-CA-C | 5.14  | 121.74      | 110.80   |
| 1   | e     | 197 | LEU  | N-CA-C | 5.14  | 121.74      | 110.80   |
| 1   | B     | 197 | LEU  | N-CA-C | 5.13  | 121.73      | 110.80   |
| 1   | L     | 197 | LEU  | N-CA-C | 5.13  | 121.74      | 110.80   |
| 1   | Q     | 197 | LEU  | N-CA-C | 5.13  | 121.73      | 110.80   |
| 1   | Z     | 197 | LEU  | N-CA-C | 5.13  | 121.73      | 110.80   |
| 1   | k     | 197 | LEU  | N-CA-C | 5.13  | 121.73      | 110.80   |
| 1   | Y     | 197 | LEU  | N-CA-C | 5.13  | 121.72      | 110.80   |
| 1   | o     | 197 | LEU  | N-CA-C | 5.13  | 121.72      | 110.80   |
| 1   | a     | 197 | LEU  | N-CA-C | 5.13  | 121.72      | 110.80   |
| 1   | O     | 197 | LEU  | N-CA-C | 5.12  | 121.71      | 110.80   |
| 1   | Q     | 88  | GLN  | N-CA-C | -5.06 | 105.67      | 111.14   |
| 1   | k     | 88  | GLN  | N-CA-C | -5.04 | 105.69      | 111.14   |
| 1   | e     | 88  | GLN  | N-CA-C | -5.04 | 105.70      | 111.14   |
| 1   | n     | 88  | GLN  | N-CA-C | -5.04 | 105.70      | 111.14   |
| 1   | B     | 88  | GLN  | N-CA-C | -5.04 | 105.70      | 111.14   |
| 1   | h     | 88  | GLN  | N-CA-C | -5.04 | 105.70      | 111.14   |
| 1   | X     | 88  | GLN  | N-CA-C | -5.03 | 105.71      | 111.14   |
| 1   | H     | 88  | GLN  | N-CA-C | -5.03 | 105.71      | 111.14   |
| 1   | Z     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | d     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | f     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | C     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | N     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | V     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | l     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | o     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | G     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | I     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | M     | 88  | GLN  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | E     | 88  | GLN  | N-CA-C | -5.01 | 105.72      | 111.14   |
| 1   | c     | 88  | GLN  | N-CA-C | -5.01 | 105.72      | 111.14   |
| 1   | i     | 88  | GLN  | N-CA-C | -5.01 | 105.72      | 111.14   |
| 1   | A     | 88  | GLN  | N-CA-C | -5.01 | 105.73      | 111.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | b     | 88  | GLN  | N-CA-C | -5.01 | 105.73      | 111.14   |
| 1   | m     | 88  | GLN  | N-CA-C | -5.01 | 105.73      | 111.14   |
| 1   | Y     | 88  | GLN  | N-CA-C | -5.01 | 105.73      | 111.14   |
| 1   | a     | 88  | GLN  | N-CA-C | -5.01 | 105.73      | 111.14   |
| 1   | K     | 88  | GLN  | N-CA-C | -5.01 | 105.73      | 111.14   |
| 1   | P     | 88  | GLN  | N-CA-C | -5.00 | 105.73      | 111.14   |
| 1   | L     | 88  | GLN  | N-CA-C | -5.00 | 105.73      | 111.14   |
| 1   | S     | 88  | GLN  | N-CA-C | -5.00 | 105.74      | 111.14   |

There are no chirality outliers.

All (123) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 104 | ASP  | Peptide |
| 1   | A     | 197 | LEU  | Peptide |
| 1   | A     | 200 | THR  | Peptide |
| 1   | B     | 104 | ASP  | Peptide |
| 1   | B     | 197 | LEU  | Peptide |
| 1   | B     | 200 | THR  | Peptide |
| 1   | C     | 104 | ASP  | Peptide |
| 1   | C     | 197 | LEU  | Peptide |
| 1   | C     | 200 | THR  | Peptide |
| 1   | D     | 104 | ASP  | Peptide |
| 1   | D     | 197 | LEU  | Peptide |
| 1   | D     | 200 | THR  | Peptide |
| 1   | E     | 104 | ASP  | Peptide |
| 1   | E     | 197 | LEU  | Peptide |
| 1   | E     | 200 | THR  | Peptide |
| 1   | F     | 104 | ASP  | Peptide |
| 1   | F     | 197 | LEU  | Peptide |
| 1   | F     | 200 | THR  | Peptide |
| 1   | G     | 104 | ASP  | Peptide |
| 1   | G     | 197 | LEU  | Peptide |
| 1   | G     | 200 | THR  | Peptide |
| 1   | H     | 104 | ASP  | Peptide |
| 1   | H     | 197 | LEU  | Peptide |
| 1   | H     | 200 | THR  | Peptide |
| 1   | I     | 104 | ASP  | Peptide |
| 1   | I     | 197 | LEU  | Peptide |
| 1   | I     | 200 | THR  | Peptide |
| 1   | J     | 104 | ASP  | Peptide |
| 1   | J     | 197 | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | J     | 200 | THR  | Peptide |
| 1   | K     | 104 | ASP  | Peptide |
| 1   | K     | 197 | LEU  | Peptide |
| 1   | K     | 200 | THR  | Peptide |
| 1   | L     | 104 | ASP  | Peptide |
| 1   | L     | 197 | LEU  | Peptide |
| 1   | L     | 200 | THR  | Peptide |
| 1   | M     | 104 | ASP  | Peptide |
| 1   | M     | 197 | LEU  | Peptide |
| 1   | M     | 200 | THR  | Peptide |
| 1   | N     | 104 | ASP  | Peptide |
| 1   | N     | 197 | LEU  | Peptide |
| 1   | N     | 200 | THR  | Peptide |
| 1   | O     | 104 | ASP  | Peptide |
| 1   | O     | 197 | LEU  | Peptide |
| 1   | O     | 200 | THR  | Peptide |
| 1   | P     | 104 | ASP  | Peptide |
| 1   | P     | 197 | LEU  | Peptide |
| 1   | P     | 200 | THR  | Peptide |
| 1   | Q     | 104 | ASP  | Peptide |
| 1   | Q     | 197 | LEU  | Peptide |
| 1   | Q     | 200 | THR  | Peptide |
| 1   | R     | 104 | ASP  | Peptide |
| 1   | R     | 197 | LEU  | Peptide |
| 1   | R     | 200 | THR  | Peptide |
| 1   | S     | 104 | ASP  | Peptide |
| 1   | S     | 197 | LEU  | Peptide |
| 1   | S     | 200 | THR  | Peptide |
| 1   | T     | 104 | ASP  | Peptide |
| 1   | T     | 197 | LEU  | Peptide |
| 1   | T     | 200 | THR  | Peptide |
| 1   | U     | 104 | ASP  | Peptide |
| 1   | U     | 197 | LEU  | Peptide |
| 1   | U     | 200 | THR  | Peptide |
| 1   | V     | 104 | ASP  | Peptide |
| 1   | V     | 197 | LEU  | Peptide |
| 1   | V     | 200 | THR  | Peptide |
| 1   | W     | 104 | ASP  | Peptide |
| 1   | W     | 197 | LEU  | Peptide |
| 1   | W     | 200 | THR  | Peptide |
| 1   | X     | 104 | ASP  | Peptide |
| 1   | X     | 197 | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | X     | 200 | THR  | Peptide |
| 1   | Y     | 104 | ASP  | Peptide |
| 1   | Y     | 197 | LEU  | Peptide |
| 1   | Y     | 200 | THR  | Peptide |
| 1   | Z     | 104 | ASP  | Peptide |
| 1   | Z     | 197 | LEU  | Peptide |
| 1   | Z     | 200 | THR  | Peptide |
| 1   | a     | 104 | ASP  | Peptide |
| 1   | a     | 197 | LEU  | Peptide |
| 1   | a     | 200 | THR  | Peptide |
| 1   | b     | 104 | ASP  | Peptide |
| 1   | b     | 197 | LEU  | Peptide |
| 1   | b     | 200 | THR  | Peptide |
| 1   | c     | 104 | ASP  | Peptide |
| 1   | c     | 197 | LEU  | Peptide |
| 1   | c     | 200 | THR  | Peptide |
| 1   | d     | 104 | ASP  | Peptide |
| 1   | d     | 197 | LEU  | Peptide |
| 1   | d     | 200 | THR  | Peptide |
| 1   | e     | 104 | ASP  | Peptide |
| 1   | e     | 197 | LEU  | Peptide |
| 1   | e     | 200 | THR  | Peptide |
| 1   | f     | 104 | ASP  | Peptide |
| 1   | f     | 197 | LEU  | Peptide |
| 1   | f     | 200 | THR  | Peptide |
| 1   | g     | 104 | ASP  | Peptide |
| 1   | g     | 197 | LEU  | Peptide |
| 1   | g     | 200 | THR  | Peptide |
| 1   | h     | 104 | ASP  | Peptide |
| 1   | h     | 197 | LEU  | Peptide |
| 1   | h     | 200 | THR  | Peptide |
| 1   | i     | 104 | ASP  | Peptide |
| 1   | i     | 197 | LEU  | Peptide |
| 1   | i     | 200 | THR  | Peptide |
| 1   | j     | 104 | ASP  | Peptide |
| 1   | j     | 197 | LEU  | Peptide |
| 1   | j     | 200 | THR  | Peptide |
| 1   | k     | 104 | ASP  | Peptide |
| 1   | k     | 197 | LEU  | Peptide |
| 1   | k     | 200 | THR  | Peptide |
| 1   | l     | 104 | ASP  | Peptide |
| 1   | l     | 197 | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | l     | 200 | THR  | Peptide |
| 1   | m     | 104 | ASP  | Peptide |
| 1   | m     | 197 | LEU  | Peptide |
| 1   | m     | 200 | THR  | Peptide |
| 1   | n     | 104 | ASP  | Peptide |
| 1   | n     | 197 | LEU  | Peptide |
| 1   | n     | 200 | THR  | Peptide |
| 1   | o     | 104 | ASP  | Peptide |
| 1   | o     | 197 | LEU  | Peptide |
| 1   | o     | 200 | THR  | 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     | 2267  | 0        | 2252     | 113     | 0            |
| 1   | B     | 2267  | 0        | 2252     | 112     | 0            |
| 1   | C     | 2267  | 0        | 2252     | 110     | 0            |
| 1   | D     | 2267  | 0        | 2252     | 112     | 0            |
| 1   | E     | 2267  | 0        | 2252     | 111     | 0            |
| 1   | F     | 2267  | 0        | 2252     | 112     | 0            |
| 1   | G     | 2267  | 0        | 2252     | 111     | 0            |
| 1   | H     | 2267  | 0        | 2252     | 109     | 0            |
| 1   | I     | 2267  | 0        | 2252     | 110     | 0            |
| 1   | J     | 2267  | 0        | 2252     | 102     | 0            |
| 1   | K     | 2267  | 0        | 2252     | 101     | 0            |
| 1   | L     | 2267  | 0        | 2252     | 102     | 0            |
| 1   | M     | 2267  | 0        | 2252     | 105     | 0            |
| 1   | N     | 2267  | 0        | 2252     | 102     | 0            |
| 1   | O     | 2267  | 0        | 2252     | 103     | 0            |
| 1   | P     | 2267  | 0        | 2252     | 100     | 0            |
| 1   | Q     | 2267  | 0        | 2252     | 100     | 0            |
| 1   | R     | 2267  | 0        | 2252     | 103     | 0            |
| 1   | S     | 2267  | 0        | 2252     | 101     | 0            |
| 1   | T     | 2267  | 0        | 2252     | 77      | 0            |
| 1   | U     | 2267  | 0        | 2252     | 77      | 0            |
| 1   | V     | 2267  | 0        | 2252     | 76      | 0            |
| 1   | W     | 2267  | 0        | 2252     | 74      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | X     | 2267  | 0        | 2252     | 75      | 0            |
| 1   | Y     | 2267  | 0        | 2252     | 77      | 0            |
| 1   | Z     | 2267  | 0        | 2252     | 76      | 0            |
| 1   | a     | 2267  | 0        | 2252     | 73      | 0            |
| 1   | b     | 2267  | 0        | 2252     | 75      | 0            |
| 1   | c     | 2267  | 0        | 2252     | 72      | 0            |
| 1   | d     | 2267  | 0        | 2252     | 73      | 0            |
| 1   | e     | 2267  | 0        | 2252     | 72      | 0            |
| 1   | f     | 2267  | 0        | 2252     | 71      | 0            |
| 1   | g     | 2267  | 0        | 2252     | 70      | 0            |
| 1   | h     | 2267  | 0        | 2252     | 70      | 0            |
| 1   | i     | 2267  | 0        | 2252     | 73      | 0            |
| 1   | j     | 2267  | 0        | 2252     | 71      | 0            |
| 1   | k     | 2267  | 0        | 2252     | 72      | 0            |
| 1   | l     | 2267  | 0        | 2252     | 70      | 0            |
| 1   | m     | 2267  | 0        | 2252     | 70      | 0            |
| 1   | n     | 2267  | 0        | 2252     | 70      | 0            |
| 1   | o     | 2267  | 0        | 2252     | 71      | 0            |
| All | All   | 92947 | 0        | 92332    | 2456    | 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 13.

All (2456) 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:F:42:ASP:OD1 | 1:l:89:ARG:NH2 | 1.63                     | 1.31              |
| 1:H:42:ASP:OD1 | 1:n:89:ARG:NH2 | 1.63                     | 1.31              |
| 1:E:42:ASP:OD1 | 1:b:89:ARG:NH2 | 1.63                     | 1.30              |
| 1:G:42:ASP:OD1 | 1:Z:89:ARG:NH2 | 1.63                     | 1.30              |
| 1:P:89:ARG:NH2 | 1:Q:42:ASP:OD1 | 1.63                     | 1.30              |
| 1:C:42:ASP:OD1 | 1:d:89:ARG:NH2 | 1.63                     | 1.29              |
| 1:E:89:ARG:NH2 | 1:k:42:ASP:OD1 | 1.63                     | 1.29              |
| 1:O:42:ASP:OD1 | 1:R:89:ARG:NH2 | 1.63                     | 1.29              |
| 1:A:42:ASP:OD1 | 1:f:89:ARG:NH2 | 1.63                     | 1.29              |
| 1:F:89:ARG:NH2 | 1:a:42:ASP:OD1 | 1.63                     | 1.29              |
| 1:M:42:ASP:OD1 | 1:T:89:ARG:NH2 | 1.63                     | 1.29              |
| 1:D:42:ASP:OD1 | 1:j:89:ARG:NH2 | 1.63                     | 1.28              |
| 1:C:89:ARG:NH2 | 1:i:42:ASP:OD1 | 1.63                     | 1.28              |
| 1:G:89:ARG:NH2 | 1:m:42:ASP:OD1 | 1.63                     | 1.28              |
| 1:H:89:ARG:NH2 | 1:Y:42:ASP:OD1 | 1.63                     | 1.28              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:I:89:ARG:NH2 | 1:o:42:ASP:OD1  | 1.63                     | 1.28              |
| 1:K:42:ASP:OD1 | 1:V:89:ARG:NH2  | 1.63                     | 1.28              |
| 1:D:89:ARG:NH2 | 1:c:42:ASP:OD1  | 1.63                     | 1.28              |
| 1:A:89:ARG:NH2 | 1:g:42:ASP:OD1  | 1.63                     | 1.28              |
| 1:J:89:ARG:NH2 | 1:W:42:ASP:OD1  | 1.63                     | 1.28              |
| 1:B:89:ARG:NH2 | 1:e:42:ASP:OD1  | 1.63                     | 1.28              |
| 1:L:89:ARG:NH2 | 1:U:42:ASP:OD1  | 1.63                     | 1.28              |
| 1:B:42:ASP:OD1 | 1:h:89:ARG:NH2  | 1.63                     | 1.27              |
| 1:I:42:ASP:OD1 | 1:X:89:ARG:NH2  | 1.63                     | 1.27              |
| 1:N:89:ARG:NH2 | 1:S:42:ASP:OD1  | 1.63                     | 1.27              |
| 1:F:50:GLU:OE1 | 1:b:84:HIS:ND1  | 1.81                     | 1.14              |
| 1:G:50:GLU:OE1 | 1:P:84:HIS:ND1  | 1.81                     | 1.14              |
| 1:I:50:GLU:OE1 | 1:N:84:HIS:ND1  | 1.81                     | 1.14              |
| 1:D:50:GLU:OE1 | 1:Z:84:HIS:ND1  | 1.81                     | 1.14              |
| 1:E:50:GLU:OE1 | 1:R:84:HIS:ND1  | 1.81                     | 1.14              |
| 1:B:50:GLU:OE1 | 1:X:84:HIS:ND1  | 1.81                     | 1.13              |
| 1:D:84:HIS:ND1 | 1:S:50:GLU:OE1  | 1.81                     | 1.13              |
| 1:H:50:GLU:OE1 | 1:d:84:HIS:ND1  | 1.81                     | 1.13              |
| 1:P:50:GLU:OE1 | 1:l:84:HIS:ND1  | 1.81                     | 1.13              |
| 1:R:50:GLU:OE1 | 1:m:84:HIS:ND1  | 1.81                     | 1.13              |
| 1:B:84:HIS:ND1 | 1:U:50:GLU:OE1  | 1.81                     | 1.13              |
| 1:F:84:HIS:ND1 | 1:Q:50:GLU:OE1  | 1.81                     | 1.13              |
| 1:K:50:GLU:OE1 | 1:L:84:HIS:ND1  | 1.81                     | 1.13              |
| 1:N:50:GLU:OE1 | 1:j:84:HIS:ND1  | 1.81                     | 1.13              |
| 1:Q:84:HIS:ND1 | 1:m:50:GLU:OE1  | 1.81                     | 1.13              |
| 1:C:50:GLU:OE1 | 1:T:84:HIS:ND1  | 1.81                     | 1.13              |
| 1:H:84:HIS:ND1 | 1:O:50:GLU:OE1  | 1.81                     | 1.12              |
| 1:S:84:HIS:ND1 | 1:o:50:GLU:OE1  | 1.81                     | 1.12              |
| 1:A:50:GLU:OE1 | 1:V:84:HIS:ND1  | 1.81                     | 1.12              |
| 1:L:50:GLU:OE1 | 1:h:84:HIS:ND1  | 1.81                     | 1.12              |
| 1:O:84:HIS:ND1 | 1:k:50:GLU:OE1  | 1.81                     | 1.12              |
| 1:I:84:HIS:ND1 | 1:e:50:GLU:OE1  | 1.81                     | 1.12              |
| 1:J:50:GLU:OE1 | 1:f:84:HIS:ND1  | 1.81                     | 1.12              |
| 1:J:84:HIS:ND1 | 1:M:50:GLU:OE1  | 1.81                     | 1.12              |
| 1:G:84:HIS:ND1 | 1:c:50:GLU:OE1  | 1.81                     | 1.11              |
| 1:A:84:HIS:ND1 | 1:W:50:GLU:OE1  | 1.81                     | 1.11              |
| 1:E:84:HIS:ND1 | 1:a:50:GLU:OE1  | 1.81                     | 1.11              |
| 1:C:84:HIS:ND1 | 1:Y:50:GLU:OE1  | 1.81                     | 1.11              |
| 1:K:84:HIS:ND1 | 1:g:50:GLU:OE1  | 1.81                     | 1.11              |
| 1:M:84:HIS:ND1 | 1:i:50:GLU:OE1  | 1.81                     | 1.11              |
| 1:F:51:LYS:NZ  | 1:l:105:LYS:HD3 | 1.77                     | 1.00              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:105:LYS:HD3 | 1:k:51:LYS:NZ   | 1.77                     | 0.99              |
| 1:P:105:LYS:HD3 | 1:Q:51:LYS:NZ   | 1.77                     | 0.99              |
| 1:C:51:LYS:NZ   | 1:d:105:LYS:HD3 | 1.77                     | 0.99              |
| 1:D:105:LYS:HD3 | 1:c:51:LYS:NZ   | 1.77                     | 0.99              |
| 1:H:51:LYS:NZ   | 1:n:105:LYS:HD3 | 1.77                     | 0.99              |
| 1:E:51:LYS:NZ   | 1:b:105:LYS:HD3 | 1.77                     | 0.99              |
| 1:G:105:LYS:HD3 | 1:m:51:LYS:NZ   | 1.77                     | 0.99              |
| 1:O:51:LYS:NZ   | 1:R:105:LYS:HD3 | 1.77                     | 0.99              |
| 1:D:51:LYS:NZ   | 1:j:105:LYS:HD3 | 1.77                     | 0.99              |
| 1:F:105:LYS:HD3 | 1:a:51:LYS:NZ   | 1.78                     | 0.99              |
| 1:H:105:LYS:HD3 | 1:Y:51:LYS:NZ   | 1.77                     | 0.98              |
| 1:C:105:LYS:HD3 | 1:i:51:LYS:NZ   | 1.78                     | 0.98              |
| 1:J:105:LYS:HD3 | 1:W:51:LYS:NZ   | 1.77                     | 0.98              |
| 1:M:51:LYS:NZ   | 1:T:105:LYS:HD3 | 1.77                     | 0.98              |
| 1:I:105:LYS:HD3 | 1:o:51:LYS:NZ   | 1.77                     | 0.98              |
| 1:N:105:LYS:HD3 | 1:S:51:LYS:NZ   | 1.77                     | 0.98              |
| 1:I:51:LYS:NZ   | 1:X:105:LYS:HD3 | 1.78                     | 0.98              |
| 1:B:105:LYS:HD3 | 1:e:51:LYS:NZ   | 1.77                     | 0.98              |
| 1:G:51:LYS:NZ   | 1:Z:105:LYS:HD3 | 1.77                     | 0.97              |
| 1:K:51:LYS:NZ   | 1:V:105:LYS:HD3 | 1.77                     | 0.97              |
| 1:H:81:THR:OG1  | 1:H:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:O:81:THR:OG1  | 1:O:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:R:81:THR:OG1  | 1:R:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:Y:81:THR:OG1  | 1:Y:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:a:81:THR:OG1  | 1:a:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:f:81:THR:OG1  | 1:f:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:i:81:THR:OG1  | 1:i:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:n:81:THR:OG1  | 1:n:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:C:81:THR:OG1  | 1:C:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:Q:81:THR:OG1  | 1:Q:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:d:81:THR:OG1  | 1:d:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:A:51:LYS:NZ   | 1:f:105:LYS:HD3 | 1.77                     | 0.97              |
| 1:M:81:THR:OG1  | 1:M:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:L:105:LYS:HD3 | 1:U:51:LYS:NZ   | 1.77                     | 0.97              |
| 1:W:81:THR:OG1  | 1:W:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:b:81:THR:OG1  | 1:b:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:k:81:THR:OG1  | 1:k:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:A:81:THR:OG1  | 1:A:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:V:81:THR:OG1  | 1:V:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:E:81:THR:OG1  | 1:E:232:ARG:NH2 | 1.98                     | 0.97              |
| 1:K:81:THR:OG1  | 1:K:232:ARG:NH2 | 1.98                     | 0.96              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:T:81:THR:OG1  | 1:T:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:B:51:LYS:NZ   | 1:h:105:LYS:HD3 | 1.78                     | 0.96              |
| 1:G:81:THR:OG1  | 1:G:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:J:81:THR:OG1  | 1:J:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:l:81:THR:OG1  | 1:l:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:g:81:THR:OG1  | 1:g:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:U:81:THR:OG1  | 1:U:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:L:81:THR:OG1  | 1:L:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:h:81:THR:OG1  | 1:h:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:I:81:THR:OG1  | 1:I:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:D:81:THR:OG1  | 1:D:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:o:81:THR:OG1  | 1:o:232:ARG:NH2 | 1.98                     | 0.96              |
| 1:A:105:LYS:HD3 | 1:g:51:LYS:NZ   | 1.77                     | 0.95              |
| 1:c:81:THR:OG1  | 1:c:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:e:81:THR:OG1  | 1:e:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:F:81:THR:OG1  | 1:F:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:P:81:THR:OG1  | 1:P:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:S:81:THR:OG1  | 1:S:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:m:81:THR:OG1  | 1:m:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:B:81:THR:OG1  | 1:B:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:X:81:THR:OG1  | 1:X:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:Z:81:THR:OG1  | 1:Z:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:N:81:THR:OG1  | 1:N:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:j:81:THR:OG1  | 1:j:232:ARG:NH2 | 1.98                     | 0.95              |
| 1:A:50:GLU:CG   | 1:V:84:HIS:HE1  | 1.82                     | 0.93              |
| 1:P:50:GLU:CG   | 1:l:84:HIS:HE1  | 1.82                     | 0.93              |
| 1:K:84:HIS:HE1  | 1:g:50:GLU:CG   | 1.82                     | 0.93              |
| 1:F:50:GLU:CG   | 1:b:84:HIS:HE1  | 1.82                     | 0.93              |
| 1:S:84:HIS:HE1  | 1:o:50:GLU:CG   | 1.82                     | 0.93              |
| 1:I:84:HIS:HE1  | 1:e:50:GLU:CG   | 1.82                     | 0.93              |
| 1:F:84:HIS:HE1  | 1:Q:50:GLU:CG   | 1.82                     | 0.92              |
| 1:E:84:HIS:HE1  | 1:a:50:GLU:CG   | 1.82                     | 0.92              |
| 1:G:50:GLU:CG   | 1:P:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:E:50:GLU:CG   | 1:R:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:L:50:GLU:CG   | 1:h:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:B:84:HIS:HE1  | 1:U:50:GLU:CG   | 1.82                     | 0.92              |
| 1:C:50:GLU:CG   | 1:T:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:D:50:GLU:CG   | 1:Z:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:I:50:GLU:CG   | 1:N:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:B:50:GLU:CG   | 1:X:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:J:84:HIS:HE1  | 1:M:50:GLU:CG   | 1.82                     | 0.92              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:84:HIS:HE1  | 1:S:50:GLU:CG   | 1.82                     | 0.92              |
| 1:J:50:GLU:CG   | 1:f:84:HIS:HE1  | 1.82                     | 0.92              |
| 1:O:84:HIS:HE1  | 1:k:50:GLU:CG   | 1.82                     | 0.92              |
| 1:H:84:HIS:HE1  | 1:O:50:GLU:CG   | 1.82                     | 0.92              |
| 1:M:84:HIS:HE1  | 1:i:50:GLU:CG   | 1.82                     | 0.92              |
| 1:A:84:HIS:HE1  | 1:W:50:GLU:CG   | 1.82                     | 0.91              |
| 1:G:84:HIS:HE1  | 1:c:50:GLU:CG   | 1.82                     | 0.91              |
| 1:K:50:GLU:CG   | 1:L:84:HIS:HE1  | 1.82                     | 0.91              |
| 1:N:50:GLU:CG   | 1:j:84:HIS:HE1  | 1.82                     | 0.91              |
| 1:Q:84:HIS:HE1  | 1:m:50:GLU:CG   | 1.82                     | 0.91              |
| 1:R:50:GLU:CG   | 1:n:84:HIS:HE1  | 1.82                     | 0.91              |
| 1:P:100:THR:OG1 | 1:P:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:a:100:THR:OG1 | 1:a:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:d:100:THR:OG1 | 1:d:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:l:100:THR:OG1 | 1:l:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:m:100:THR:OG1 | 1:m:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:C:84:HIS:HE1  | 1:Y:50:GLU:CG   | 1.82                     | 0.91              |
| 1:R:100:THR:OG1 | 1:R:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:Y:100:THR:OG1 | 1:Y:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:c:100:THR:OG1 | 1:c:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:k:100:THR:OG1 | 1:k:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:D:100:THR:OG1 | 1:D:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:P:135:LYS:CE  | 1:l:104:ASP:HB3 | 2.01                     | 0.91              |
| 1:b:100:THR:OG1 | 1:b:202:PHE:CD2 | 2.24                     | 0.91              |
| 1:A:104:ASP:HB3 | 1:W:135:LYS:CE  | 2.01                     | 0.91              |
| 1:J:104:ASP:HB3 | 1:M:135:LYS:CE  | 2.01                     | 0.91              |
| 1:J:135:LYS:CE  | 1:f:104:ASP:HB3 | 2.01                     | 0.91              |
| 1:F:100:THR:OG1 | 1:F:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:Q:104:ASP:HB3 | 1:m:135:LYS:CE  | 2.01                     | 0.90              |
| 1:n:100:THR:OG1 | 1:n:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:o:100:THR:OG1 | 1:o:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:A:135:LYS:CE  | 1:V:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:C:135:LYS:CE  | 1:T:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:O:100:THR:OG1 | 1:O:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:F:104:ASP:HB3 | 1:Q:135:LYS:CE  | 2.01                     | 0.90              |
| 1:G:104:ASP:HB3 | 1:c:135:LYS:CE  | 2.01                     | 0.90              |
| 1:K:104:ASP:HB3 | 1:g:135:LYS:CE  | 2.01                     | 0.90              |
| 1:Q:100:THR:OG1 | 1:Q:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:Z:100:THR:OG1 | 1:Z:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:K:135:LYS:CE  | 1:L:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:M:104:ASP:HB3 | 1:i:135:LYS:CE  | 2.01                     | 0.90              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:N:100:THR:OG1 | 1:N:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:T:100:THR:OG1 | 1:T:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:E:104:ASP:HB3 | 1:a:135:LYS:CE  | 2.02                     | 0.90              |
| 1:H:50:GLU:CG   | 1:d:84:HIS:HE1  | 1.82                     | 0.90              |
| 1:E:135:LYS:CE  | 1:R:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:G:100:THR:OG1 | 1:G:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:G:135:LYS:CE  | 1:P:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:L:135:LYS:CE  | 1:h:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:i:100:THR:OG1 | 1:i:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:B:104:ASP:HB3 | 1:U:135:LYS:CE  | 2.02                     | 0.90              |
| 1:D:104:ASP:HB3 | 1:S:135:LYS:CE  | 2.01                     | 0.90              |
| 1:H:135:LYS:CE  | 1:d:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:S:104:ASP:HB3 | 1:o:135:LYS:CE  | 2.01                     | 0.90              |
| 1:C:104:ASP:HB3 | 1:Y:135:LYS:CE  | 2.01                     | 0.90              |
| 1:I:104:ASP:HB3 | 1:e:135:LYS:CE  | 2.01                     | 0.90              |
| 1:f:100:THR:OG1 | 1:f:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:B:135:LYS:CE  | 1:X:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:D:135:LYS:CE  | 1:Z:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:F:135:LYS:CE  | 1:b:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:H:100:THR:OG1 | 1:H:202:PHE:CD2 | 2.24                     | 0.90              |
| 1:I:135:LYS:CE  | 1:N:104:ASP:HB3 | 2.01                     | 0.90              |
| 1:O:104:ASP:HB3 | 1:k:135:LYS:CE  | 2.02                     | 0.90              |
| 1:M:100:THR:OG1 | 1:M:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:N:135:LYS:CE  | 1:j:104:ASP:HB3 | 2.01                     | 0.89              |
| 1:W:100:THR:OG1 | 1:W:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:A:100:THR:OG1 | 1:A:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:I:100:THR:OG1 | 1:I:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:R:135:LYS:CE  | 1:n:104:ASP:HB3 | 2.01                     | 0.89              |
| 1:e:100:THR:OG1 | 1:e:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:C:100:THR:OG1 | 1:C:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:H:104:ASP:HB3 | 1:O:135:LYS:CE  | 2.01                     | 0.89              |
| 1:X:100:THR:OG1 | 1:X:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:B:100:THR:OG1 | 1:B:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:V:100:THR:OG1 | 1:V:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:E:100:THR:OG1 | 1:E:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:J:100:THR:OG1 | 1:J:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:S:100:THR:OG1 | 1:S:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:g:100:THR:OG1 | 1:g:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:j:100:THR:OG1 | 1:j:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:L:100:THR:OG1 | 1:L:202:PHE:CD2 | 2.24                     | 0.89              |
| 1:h:100:THR:OG1 | 1:h:202:PHE:CD2 | 2.24                     | 0.89              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:U:100:THR:OG1 | 1:U:202:PHE:CD2 | 2.24                     | 0.88              |
| 1:D:51:LYS:HZ1  | 1:j:105:LYS:HD3 | 1.38                     | 0.88              |
| 1:H:51:LYS:HZ1  | 1:n:105:LYS:HD3 | 1.39                     | 0.88              |
| 1:I:51:LYS:HZ1  | 1:X:105:LYS:HD3 | 1.39                     | 0.88              |
| 1:F:105:LYS:HD3 | 1:a:51:LYS:HZ1  | 1.39                     | 0.88              |
| 1:H:105:LYS:HD3 | 1:Y:51:LYS:HZ1  | 1.38                     | 0.88              |
| 1:F:51:LYS:HZ1  | 1:l:105:LYS:HD3 | 1.39                     | 0.88              |
| 1:P:105:LYS:HD3 | 1:Q:51:LYS:HZ1  | 1.38                     | 0.87              |
| 1:K:100:THR:OG1 | 1:K:202:PHE:CD2 | 2.24                     | 0.87              |
| 1:O:51:LYS:HZ1  | 1:R:105:LYS:HD3 | 1.38                     | 0.87              |
| 1:M:51:LYS:HZ1  | 1:T:105:LYS:HD3 | 1.39                     | 0.87              |
| 1:D:105:LYS:HD3 | 1:c:51:LYS:HZ1  | 1.39                     | 0.87              |
| 1:P:50:GLU:CG   | 1:l:84:HIS:CE1  | 2.59                     | 0.86              |
| 1:D:50:GLU:CG   | 1:Z:84:HIS:CE1  | 2.59                     | 0.86              |
| 1:F:84:HIS:CE1  | 1:Q:50:GLU:CG   | 2.59                     | 0.86              |
| 1:G:84:HIS:CE1  | 1:c:50:GLU:CG   | 2.59                     | 0.86              |
| 1:I:84:HIS:CE1  | 1:e:50:GLU:CG   | 2.59                     | 0.86              |
| 1:B:50:GLU:CG   | 1:X:84:HIS:CE1  | 2.59                     | 0.86              |
| 1:I:50:GLU:CG   | 1:N:84:HIS:CE1  | 2.59                     | 0.86              |
| 1:S:84:HIS:CE1  | 1:o:50:GLU:CG   | 2.59                     | 0.86              |
| 1:C:51:LYS:HZ1  | 1:d:105:LYS:HD3 | 1.39                     | 0.86              |
| 1:D:84:HIS:CE1  | 1:S:50:GLU:CG   | 2.59                     | 0.86              |
| 1:N:50:GLU:CG   | 1:j:84:HIS:CE1  | 2.59                     | 0.86              |
| 1:E:50:GLU:CG   | 1:R:84:HIS:CE1  | 2.59                     | 0.86              |
| 1:M:84:HIS:CE1  | 1:i:50:GLU:CG   | 2.59                     | 0.86              |
| 1:G:50:GLU:CG   | 1:P:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:J:50:GLU:CG   | 1:f:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:C:50:GLU:CG   | 1:T:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:Q:84:HIS:CE1  | 1:m:50:GLU:CG   | 2.59                     | 0.85              |
| 1:A:84:HIS:CE1  | 1:W:50:GLU:CG   | 2.59                     | 0.85              |
| 1:B:51:LYS:HZ1  | 1:h:105:LYS:HD3 | 1.38                     | 0.85              |
| 1:G:51:LYS:HZ1  | 1:Z:105:LYS:HD3 | 1.39                     | 0.85              |
| 1:K:50:GLU:CG   | 1:L:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:B:84:HIS:CE1  | 1:U:50:GLU:CG   | 2.59                     | 0.85              |
| 1:O:84:HIS:CE1  | 1:k:50:GLU:CG   | 2.59                     | 0.85              |
| 1:N:105:LYS:HD3 | 1:S:51:LYS:HZ1  | 1.39                     | 0.85              |
| 1:F:50:GLU:CG   | 1:b:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:H:50:GLU:CG   | 1:d:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:L:105:LYS:HD3 | 1:U:51:LYS:HZ1  | 1.40                     | 0.85              |
| 1:H:84:HIS:CE1  | 1:O:50:GLU:CG   | 2.59                     | 0.85              |
| 1:A:105:LYS:HD3 | 1:g:51:LYS:HZ1  | 1.38                     | 0.85              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:50:GLU:CG   | 1:n:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:A:51:LYS:HZ1  | 1:f:105:LYS:HD3 | 1.38                     | 0.85              |
| 1:E:105:LYS:HD3 | 1:k:51:LYS:HZ1  | 1.39                     | 0.85              |
| 1:L:50:GLU:CG   | 1:h:84:HIS:CE1  | 2.59                     | 0.85              |
| 1:E:84:HIS:CE1  | 1:a:50:GLU:CG   | 2.59                     | 0.84              |
| 1:B:105:LYS:HD3 | 1:e:51:LYS:HZ1  | 1.39                     | 0.84              |
| 1:J:84:HIS:CE1  | 1:M:50:GLU:CG   | 2.59                     | 0.84              |
| 1:E:51:LYS:HZ1  | 1:b:105:LYS:HD3 | 1.39                     | 0.84              |
| 1:A:50:GLU:CG   | 1:V:84:HIS:CE1  | 2.59                     | 0.84              |
| 1:C:84:HIS:CE1  | 1:Y:50:GLU:CG   | 2.59                     | 0.84              |
| 1:m:100:THR:HG1 | 1:m:202:PHE:HD2 | 1.21                     | 0.84              |
| 1:G:105:LYS:HD3 | 1:m:51:LYS:HZ1  | 1.39                     | 0.84              |
| 1:K:84:HIS:CE1  | 1:g:50:GLU:CG   | 2.59                     | 0.84              |
| 1:C:105:LYS:HD3 | 1:i:51:LYS:HZ1  | 1.39                     | 0.83              |
| 1:L:100:THR:HG1 | 1:L:202:PHE:HE2 | 1.26                     | 0.83              |
| 1:I:100:THR:HG1 | 1:I:202:PHE:HE2 | 1.26                     | 0.83              |
| 1:K:51:LYS:HZ1  | 1:V:105:LYS:HD3 | 1.39                     | 0.83              |
| 1:J:105:LYS:HD3 | 1:W:51:LYS:HZ1  | 1.39                     | 0.82              |
| 1:S:100:THR:HG1 | 1:S:202:PHE:HE2 | 1.26                     | 0.82              |
| 1:B:100:THR:HG1 | 1:B:202:PHE:HE2 | 1.28                     | 0.82              |
| 1:I:105:LYS:HD3 | 1:o:51:LYS:HZ1  | 1.39                     | 0.82              |
| 1:P:50:GLU:HG3  | 1:l:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:B:50:GLU:HG3  | 1:X:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:F:84:HIS:CE1  | 1:Q:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:G:84:HIS:CE1  | 1:c:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:I:50:GLU:HG3  | 1:N:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:N:50:GLU:HG3  | 1:j:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:S:84:HIS:CE1  | 1:o:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:B:84:HIS:CE1  | 1:U:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:E:100:THR:OG1 | 1:E:202:PHE:CE2 | 2.34                     | 0.81              |
| 1:I:84:HIS:CE1  | 1:e:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:k:100:THR:OG1 | 1:k:202:PHE:CE2 | 2.34                     | 0.81              |
| 1:n:100:THR:OG1 | 1:n:202:PHE:CE2 | 2.34                     | 0.81              |
| 1:E:84:HIS:CE1  | 1:a:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:F:50:GLU:HG3  | 1:b:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:H:100:THR:OG1 | 1:H:202:PHE:CE2 | 2.34                     | 0.81              |
| 1:G:50:GLU:HG3  | 1:P:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:K:84:HIS:CE1  | 1:g:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:A:84:HIS:CE1  | 1:W:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:D:84:HIS:CE1  | 1:S:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:b:100:THR:OG1 | 1:b:202:PHE:CE2 | 2.34                     | 0.81              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:50:GLU:HG3  | 1:h:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:Y:100:THR:OG1 | 1:Y:202:PHE:CE2 | 2.34                     | 0.81              |
| 1:D:50:GLU:HG3  | 1:Z:84:HIS:CE1  | 2.16                     | 0.81              |
| 1:J:84:HIS:CE1  | 1:M:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:O:84:HIS:CE1  | 1:k:50:GLU:HG3  | 2.16                     | 0.81              |
| 1:m:100:THR:OG1 | 1:m:202:PHE:CE2 | 2.34                     | 0.81              |
| 1:Q:84:HIS:CE1  | 1:m:50:GLU:HG3  | 2.16                     | 0.80              |
| 1:F:100:THR:OG1 | 1:F:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:G:50:GLU:HG3  | 1:P:84:HIS:HE1  | 1.47                     | 0.80              |
| 1:P:50:GLU:HG3  | 1:l:84:HIS:HE1  | 1.47                     | 0.80              |
| 1:S:84:HIS:HE1  | 1:o:50:GLU:HG3  | 1.47                     | 0.80              |
| 1:T:100:THR:OG1 | 1:T:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:J:50:GLU:HG3  | 1:f:84:HIS:CE1  | 2.16                     | 0.80              |
| 1:e:100:THR:OG1 | 1:e:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:B:84:HIS:HE1  | 1:U:50:GLU:HG3  | 1.47                     | 0.80              |
| 1:B:100:THR:OG1 | 1:B:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:E:50:GLU:HG3  | 1:R:84:HIS:CE1  | 2.16                     | 0.80              |
| 1:a:100:THR:OG1 | 1:a:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:A:50:GLU:HG3  | 1:V:84:HIS:CE1  | 2.16                     | 0.80              |
| 1:K:50:GLU:HG3  | 1:L:84:HIS:CE1  | 2.16                     | 0.80              |
| 1:L:100:THR:OG1 | 1:L:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:N:50:GLU:HG3  | 1:j:84:HIS:HE1  | 1.47                     | 0.80              |
| 1:l:100:THR:OG1 | 1:l:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:D:84:HIS:HE1  | 1:S:50:GLU:HG3  | 1.47                     | 0.80              |
| 1:E:84:HIS:HE1  | 1:a:50:GLU:HG3  | 1.47                     | 0.80              |
| 1:N:100:THR:OG1 | 1:N:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:U:100:THR:OG1 | 1:U:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:g:100:THR:OG1 | 1:g:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:Q:84:HIS:HE1  | 1:m:50:GLU:HG3  | 1.47                     | 0.80              |
| 1:R:50:GLU:HG3  | 1:n:84:HIS:CE1  | 2.16                     | 0.80              |
| 1:b:100:THR:HG1 | 1:b:202:PHE:HE2 | 1.26                     | 0.80              |
| 1:M:100:THR:OG1 | 1:M:202:PHE:CE2 | 2.34                     | 0.80              |
| 1:N:100:THR:HG1 | 1:N:202:PHE:HE2 | 1.29                     | 0.80              |
| 1:R:100:THR:OG1 | 1:R:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:G:84:HIS:HE1  | 1:c:50:GLU:HG3  | 1.47                     | 0.79              |
| 1:X:100:THR:OG1 | 1:X:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:Z:100:THR:OG1 | 1:Z:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:j:100:THR:OG1 | 1:j:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:H:50:GLU:HG3  | 1:d:84:HIS:CE1  | 2.16                     | 0.79              |
| 1:o:100:THR:OG1 | 1:o:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:D:100:THR:OG1 | 1:D:202:PHE:CE2 | 2.34                     | 0.79              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:84:HIS:CE1  | 1:O:50:GLU:HG3  | 2.16                     | 0.79              |
| 1:I:50:GLU:HG3  | 1:N:84:HIS:HE1  | 1.47                     | 0.79              |
| 1:h:100:THR:OG1 | 1:h:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:B:50:GLU:OE1  | 1:X:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:J:50:GLU:OE1  | 1:f:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:L:50:GLU:OE1  | 1:h:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:L:50:GLU:HG3  | 1:h:84:HIS:HE1  | 1.47                     | 0.79              |
| 1:N:50:GLU:OE1  | 1:j:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:W:100:THR:OG1 | 1:W:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:H:50:GLU:OE1  | 1:d:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:K:100:THR:HG1 | 1:K:202:PHE:HE2 | 1.28                     | 0.79              |
| 1:M:84:HIS:CE1  | 1:i:50:GLU:HG3  | 2.16                     | 0.79              |
| 1:M:84:HIS:CE1  | 1:i:50:GLU:OE1  | 2.36                     | 0.79              |
| 1:O:100:THR:OG1 | 1:O:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:V:100:THR:OG1 | 1:V:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:f:100:THR:OG1 | 1:f:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:C:50:GLU:HG3  | 1:T:84:HIS:CE1  | 2.16                     | 0.79              |
| 1:D:50:GLU:OE1  | 1:Z:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:F:50:GLU:HG3  | 1:b:84:HIS:HE1  | 1.47                     | 0.79              |
| 1:I:100:THR:OG1 | 1:I:202:PHE:CE2 | 2.34                     | 0.79              |
| 1:O:84:HIS:CE1  | 1:k:50:GLU:OE1  | 2.36                     | 0.79              |
| 1:R:50:GLU:OE1  | 1:n:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:S:84:HIS:CE1  | 1:o:50:GLU:OE1  | 2.36                     | 0.79              |
| 1:D:100:THR:HG1 | 1:D:202:PHE:HE2 | 1.27                     | 0.79              |
| 1:A:50:GLU:OE1  | 1:V:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:H:50:GLU:HG3  | 1:d:84:HIS:HE1  | 1.47                     | 0.79              |
| 1:I:50:GLU:OE1  | 1:N:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:K:84:HIS:CE1  | 1:g:50:GLU:OE1  | 2.36                     | 0.79              |
| 1:P:50:GLU:OE1  | 1:l:84:HIS:CE1  | 2.36                     | 0.79              |
| 1:A:100:THR:OG1 | 1:A:202:PHE:CE2 | 2.34                     | 0.78              |
| 1:C:50:GLU:OE1  | 1:T:84:HIS:CE1  | 2.36                     | 0.78              |
| 1:C:84:HIS:CE1  | 1:Y:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:F:50:GLU:OE1  | 1:b:84:HIS:CE1  | 2.36                     | 0.78              |
| 1:K:100:THR:OG1 | 1:K:202:PHE:CE2 | 2.34                     | 0.78              |
| 1:S:100:THR:OG1 | 1:S:202:PHE:CE2 | 2.34                     | 0.78              |
| 1:C:84:HIS:CE1  | 1:Y:50:GLU:HG3  | 2.16                     | 0.78              |
| 1:I:84:HIS:CE1  | 1:e:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:Q:84:HIS:CE1  | 1:m:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:G:50:GLU:OE1  | 1:P:84:HIS:CE1  | 2.36                     | 0.78              |
| 1:A:84:HIS:CE1  | 1:W:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:C:100:THR:HG1 | 1:C:202:PHE:HE2 | 1.25                     | 0.78              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:50:GLU:OE1  | 1:R:84:HIS:CE1  | 2.36                     | 0.78              |
| 1:E:84:HIS:CE1  | 1:a:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:K:50:GLU:OE1  | 1:L:84:HIS:CE1  | 2.36                     | 0.78              |
| 1:G:84:HIS:CE1  | 1:c:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:J:50:GLU:HG3  | 1:f:84:HIS:HE1  | 1.47                     | 0.78              |
| 1:d:100:THR:OG1 | 1:d:202:PHE:CE2 | 2.34                     | 0.78              |
| 1:J:84:HIS:CE1  | 1:M:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:c:100:THR:OG1 | 1:c:202:PHE:CE2 | 2.34                     | 0.78              |
| 1:J:100:THR:OG1 | 1:J:202:PHE:CE2 | 2.34                     | 0.78              |
| 1:B:84:HIS:CE1  | 1:U:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:D:84:HIS:CE1  | 1:S:50:GLU:OE1  | 2.36                     | 0.78              |
| 1:G:100:THR:OG1 | 1:G:202:PHE:CE2 | 2.34                     | 0.78              |
| 1:H:84:HIS:CE1  | 1:O:50:GLU:OE1  | 2.36                     | 0.77              |
| 1:n:100:THR:HG1 | 1:n:202:PHE:HE2 | 1.26                     | 0.77              |
| 1:I:84:HIS:HE1  | 1:e:50:GLU:HG3  | 1.47                     | 0.77              |
| 1:Q:100:THR:OG1 | 1:Q:202:PHE:CE2 | 2.34                     | 0.77              |
| 1:h:100:THR:HG1 | 1:h:202:PHE:HE2 | 1.26                     | 0.77              |
| 1:F:84:HIS:CE1  | 1:Q:50:GLU:OE1  | 2.36                     | 0.77              |
| 1:K:50:GLU:HG3  | 1:L:84:HIS:HE1  | 1.47                     | 0.77              |
| 1:C:100:THR:OG1 | 1:C:202:PHE:CE2 | 2.34                     | 0.77              |
| 1:J:100:THR:HG1 | 1:J:202:PHE:HE2 | 1.26                     | 0.77              |
| 1:P:100:THR:OG1 | 1:P:202:PHE:CE2 | 2.34                     | 0.77              |
| 1:R:100:THR:HG1 | 1:R:202:PHE:HE2 | 1.26                     | 0.77              |
| 1:d:100:THR:HG1 | 1:d:202:PHE:HE2 | 1.26                     | 0.77              |
| 1:H:84:HIS:HE1  | 1:O:50:GLU:HG3  | 1.47                     | 0.77              |
| 1:i:100:THR:OG1 | 1:i:202:PHE:CE2 | 2.34                     | 0.77              |
| 1:F:84:HIS:HE1  | 1:Q:50:GLU:HG3  | 1.47                     | 0.77              |
| 1:U:100:THR:HG1 | 1:U:202:PHE:HE2 | 1.29                     | 0.77              |
| 1:j:100:THR:HG1 | 1:j:202:PHE:HE2 | 1.29                     | 0.77              |
| 1:D:50:GLU:HG3  | 1:Z:84:HIS:HE1  | 1.47                     | 0.77              |
| 1:J:84:HIS:HE1  | 1:M:50:GLU:HG3  | 1.47                     | 0.76              |
| 1:E:100:THR:HG1 | 1:E:202:PHE:HE2 | 1.26                     | 0.76              |
| 1:i:100:THR:HG1 | 1:i:202:PHE:HE2 | 1.27                     | 0.76              |
| 1:D:84:HIS:HE1  | 1:S:50:GLU:CB   | 1.99                     | 0.76              |
| 1:I:50:GLU:CB   | 1:N:84:HIS:HE1  | 1.99                     | 0.76              |
| 1:A:51:LYS:NZ   | 1:f:105:LYS:CD  | 2.49                     | 0.76              |
| 1:C:105:LYS:CD  | 1:i:51:LYS:NZ   | 2.49                     | 0.76              |
| 1:G:84:HIS:HE1  | 1:c:50:GLU:CB   | 1.99                     | 0.76              |
| 1:G:100:THR:HG1 | 1:G:202:PHE:HE2 | 1.26                     | 0.76              |
| 1:K:51:LYS:NZ   | 1:V:105:LYS:CD  | 2.49                     | 0.76              |
| 1:O:100:THR:HG1 | 1:O:202:PHE:HE2 | 1.26                     | 0.76              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:50:GLU:CB   | 1:X:84:HIS:HE1  | 1.99                     | 0.76              |
| 1:C:50:GLU:HG3  | 1:T:84:HIS:HE1  | 1.47                     | 0.76              |
| 1:Q:84:HIS:HE1  | 1:m:50:GLU:CB   | 1.99                     | 0.76              |
| 1:H:105:LYS:CD  | 1:Y:51:LYS:NZ   | 2.49                     | 0.76              |
| 1:L:105:LYS:CD  | 1:U:51:LYS:NZ   | 2.49                     | 0.76              |
| 1:N:105:LYS:CD  | 1:S:51:LYS:NZ   | 2.49                     | 0.76              |
| 1:D:50:GLU:CB   | 1:Z:84:HIS:HE1  | 1.99                     | 0.76              |
| 1:D:51:LYS:NZ   | 1:j:105:LYS:CD  | 2.49                     | 0.76              |
| 1:D:105:LYS:CD  | 1:c:51:LYS:NZ   | 2.49                     | 0.76              |
| 1:F:100:THR:HG1 | 1:F:202:PHE:HE2 | 1.26                     | 0.76              |
| 1:H:100:THR:HG1 | 1:H:202:PHE:HE2 | 1.27                     | 0.76              |
| 1:L:50:GLU:CB   | 1:h:84:HIS:HE1  | 1.99                     | 0.76              |
| 1:N:50:GLU:CB   | 1:j:84:HIS:HE1  | 1.99                     | 0.76              |
| 1:R:50:GLU:CB   | 1:n:84:HIS:HE1  | 1.99                     | 0.75              |
| 1:S:84:HIS:HE1  | 1:o:50:GLU:CB   | 1.99                     | 0.75              |
| 1:B:105:LYS:CD  | 1:e:51:LYS:NZ   | 2.49                     | 0.75              |
| 1:I:51:LYS:NZ   | 1:X:105:LYS:CD  | 2.49                     | 0.75              |
| 1:I:84:HIS:HE1  | 1:e:50:GLU:CB   | 1.99                     | 0.75              |
| 1:G:50:GLU:CB   | 1:P:84:HIS:HE1  | 1.99                     | 0.75              |
| 1:G:105:LYS:CD  | 1:m:51:LYS:NZ   | 2.49                     | 0.75              |
| 1:Y:100:THR:HG1 | 1:Y:202:PHE:HE2 | 1.26                     | 0.75              |
| 1:O:51:LYS:NZ   | 1:R:105:LYS:CD  | 2.49                     | 0.75              |
| 1:A:105:LYS:CD  | 1:g:51:LYS:NZ   | 2.49                     | 0.75              |
| 1:B:84:HIS:HE1  | 1:U:50:GLU:CB   | 1.99                     | 0.75              |
| 1:F:84:HIS:HE1  | 1:Q:50:GLU:CB   | 1.99                     | 0.75              |
| 1:G:51:LYS:NZ   | 1:Z:105:LYS:CD  | 2.49                     | 0.75              |
| 1:H:50:GLU:CB   | 1:d:84:HIS:HE1  | 1.99                     | 0.75              |
| 1:K:84:HIS:HE1  | 1:g:50:GLU:HG3  | 1.46                     | 0.75              |
| 1:V:100:THR:HG1 | 1:V:202:PHE:HE2 | 1.27                     | 0.75              |
| 1:C:51:LYS:NZ   | 1:d:105:LYS:CD  | 2.49                     | 0.75              |
| 1:E:51:LYS:NZ   | 1:b:105:LYS:CD  | 2.49                     | 0.75              |
| 1:I:105:LYS:CD  | 1:o:51:LYS:NZ   | 2.49                     | 0.75              |
| 1:B:51:LYS:NZ   | 1:h:105:LYS:CD  | 2.49                     | 0.75              |
| 1:F:51:LYS:NZ   | 1:l:105:LYS:CD  | 2.49                     | 0.75              |
| 1:H:51:LYS:NZ   | 1:n:105:LYS:CD  | 2.49                     | 0.75              |
| 1:N:100:THR:HG1 | 1:N:202:PHE:HD2 | 1.32                     | 0.75              |
| 1:g:100:THR:HG1 | 1:g:202:PHE:HE2 | 1.26                     | 0.75              |
| 1:k:100:THR:HG1 | 1:k:202:PHE:HE2 | 1.27                     | 0.75              |
| 1:C:50:GLU:CB   | 1:T:84:HIS:HE1  | 1.99                     | 0.75              |
| 1:E:50:GLU:CB   | 1:R:84:HIS:HE1  | 1.99                     | 0.75              |
| 1:M:51:LYS:NZ   | 1:T:105:LYS:CD  | 2.49                     | 0.75              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:84:HIS:HE1  | 1:i:50:GLU:CB   | 1.99                     | 0.75              |
| 1:O:84:HIS:HE1  | 1:k:50:GLU:HG3  | 1.47                     | 0.75              |
| 1:P:50:GLU:CB   | 1:l:84:HIS:HE1  | 1.99                     | 0.75              |
| 1:Z:100:THR:HG1 | 1:Z:202:PHE:HE2 | 1.29                     | 0.75              |
| 1:C:84:HIS:HE1  | 1:Y:50:GLU:HG3  | 1.47                     | 0.75              |
| 1:E:84:HIS:HE1  | 1:a:50:GLU:CB   | 1.99                     | 0.75              |
| 1:H:84:HIS:HE1  | 1:O:50:GLU:CB   | 1.99                     | 0.75              |
| 1:J:105:LYS:CD  | 1:W:51:LYS:NZ   | 2.49                     | 0.75              |
| 1:K:84:HIS:HE1  | 1:g:50:GLU:CB   | 1.99                     | 0.75              |
| 1:T:100:THR:HG1 | 1:T:202:PHE:HE2 | 1.26                     | 0.75              |
| 1:A:84:HIS:HE1  | 1:W:50:GLU:CB   | 1.99                     | 0.74              |
| 1:C:84:HIS:HE1  | 1:Y:50:GLU:CB   | 1.99                     | 0.74              |
| 1:F:50:GLU:CB   | 1:b:84:HIS:HE1  | 1.99                     | 0.74              |
| 1:J:84:HIS:HE1  | 1:M:50:GLU:CB   | 1.99                     | 0.74              |
| 1:K:50:GLU:CB   | 1:L:84:HIS:HE1  | 1.99                     | 0.74              |
| 1:P:105:LYS:CD  | 1:Q:51:LYS:NZ   | 2.49                     | 0.74              |
| 1:R:50:GLU:HG3  | 1:n:84:HIS:HE1  | 1.47                     | 0.74              |
| 1:F:105:LYS:CD  | 1:a:51:LYS:NZ   | 2.49                     | 0.74              |
| 1:M:84:HIS:HE1  | 1:i:50:GLU:HG3  | 1.47                     | 0.74              |
| 1:A:50:GLU:CB   | 1:V:84:HIS:HE1  | 1.99                     | 0.74              |
| 1:E:105:LYS:CD  | 1:k:51:LYS:NZ   | 2.49                     | 0.74              |
| 1:O:84:HIS:HE1  | 1:k:50:GLU:CB   | 1.99                     | 0.74              |
| 1:A:50:GLU:HG3  | 1:V:84:HIS:HE1  | 1.47                     | 0.74              |
| 1:e:100:THR:HG1 | 1:e:202:PHE:HE2 | 1.28                     | 0.74              |
| 1:J:50:GLU:CB   | 1:f:84:HIS:HE1  | 1.99                     | 0.73              |
| 1:B:50:GLU:HG3  | 1:X:84:HIS:HE1  | 1.47                     | 0.73              |
| 1:X:100:THR:HG1 | 1:X:202:PHE:HE2 | 1.28                     | 0.73              |
| 1:o:100:THR:HG1 | 1:o:202:PHE:HE2 | 1.31                     | 0.72              |
| 1:M:100:THR:HG1 | 1:M:202:PHE:HE2 | 1.29                     | 0.72              |
| 1:P:175:GLY:O   | 1:P:193:SER:OG  | 2.08                     | 0.72              |
| 1:A:84:HIS:HE1  | 1:W:50:GLU:HG3  | 1.47                     | 0.72              |
| 1:L:100:THR:OG1 | 1:L:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:W:100:THR:OG1 | 1:W:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:f:100:THR:OG1 | 1:f:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:o:100:THR:HG1 | 1:o:202:PHE:HD2 | 1.29                     | 0.71              |
| 1:C:91:ARG:NH2  | 1:Y:161:ALA:O   | 2.24                     | 0.71              |
| 1:R:161:ALA:O   | 1:n:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:Z:175:GLY:O   | 1:Z:193:SER:OG  | 2.08                     | 0.71              |
| 1:J:161:ALA:O   | 1:f:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:O:91:ARG:NH2  | 1:k:161:ALA:O   | 2.24                     | 0.71              |
| 1:A:100:THR:OG1 | 1:A:202:PHE:HD2 | 1.73                     | 0.71              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:91:ARG:NH2  | 1:U:161:ALA:O   | 2.24                     | 0.71              |
| 1:E:50:GLU:HG3  | 1:R:84:HIS:HE1  | 1.47                     | 0.71              |
| 1:F:91:ARG:NH2  | 1:Q:161:ALA:O   | 2.24                     | 0.71              |
| 1:F:161:ALA:O   | 1:b:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:I:91:ARG:NH2  | 1:e:161:ALA:O   | 2.24                     | 0.71              |
| 1:J:100:THR:OG1 | 1:J:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:g:175:GLY:O   | 1:g:193:SER:OG  | 2.07                     | 0.71              |
| 1:C:100:THR:OG1 | 1:C:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:D:91:ARG:NH2  | 1:S:161:ALA:O   | 2.24                     | 0.71              |
| 1:I:161:ALA:O   | 1:N:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:J:91:ARG:NH2  | 1:M:161:ALA:O   | 2.24                     | 0.71              |
| 1:Y:100:THR:OG1 | 1:Y:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:C:161:ALA:O   | 1:T:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:F:135:LYS:NZ  | 1:b:104:ASP:CB  | 2.54                     | 0.71              |
| 1:L:135:LYS:NZ  | 1:h:104:ASP:CB  | 2.54                     | 0.71              |
| 1:h:100:THR:OG1 | 1:h:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:B:104:ASP:CB  | 1:U:135:LYS:NZ  | 2.54                     | 0.71              |
| 1:E:104:ASP:CB  | 1:a:135:LYS:NZ  | 2.54                     | 0.71              |
| 1:E:161:ALA:O   | 1:R:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:G:104:ASP:CB  | 1:c:135:LYS:NZ  | 2.54                     | 0.71              |
| 1:K:91:ARG:NH2  | 1:g:161:ALA:O   | 2.24                     | 0.71              |
| 1:S:91:ARG:NH2  | 1:o:161:ALA:O   | 2.24                     | 0.71              |
| 1:A:104:ASP:CB  | 1:W:135:LYS:NZ  | 2.54                     | 0.71              |
| 1:C:135:LYS:NZ  | 1:T:104:ASP:CB  | 2.54                     | 0.71              |
| 1:G:91:ARG:NH2  | 1:c:161:ALA:O   | 2.24                     | 0.71              |
| 1:H:135:LYS:NZ  | 1:d:104:ASP:CB  | 2.54                     | 0.71              |
| 1:K:135:LYS:NZ  | 1:L:104:ASP:CB  | 2.54                     | 0.71              |
| 1:K:161:ALA:O   | 1:L:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:N:135:LYS:NZ  | 1:j:104:ASP:CB  | 2.54                     | 0.71              |
| 1:S:104:ASP:CB  | 1:o:135:LYS:NZ  | 2.54                     | 0.71              |
| 1:g:100:THR:OG1 | 1:g:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:B:161:ALA:O   | 1:X:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:C:104:ASP:CB  | 1:Y:135:LYS:NZ  | 2.54                     | 0.71              |
| 1:D:135:LYS:NZ  | 1:Z:104:ASP:CB  | 2.54                     | 0.71              |
| 1:J:135:LYS:NZ  | 1:f:104:ASP:CB  | 2.54                     | 0.71              |
| 1:B:135:LYS:NZ  | 1:X:104:ASP:CB  | 2.54                     | 0.71              |
| 1:D:161:ALA:O   | 1:Z:91:ARG:NH2  | 2.24                     | 0.71              |
| 1:E:135:LYS:NZ  | 1:R:104:ASP:CB  | 2.54                     | 0.71              |
| 1:Q:91:ARG:NH2  | 1:m:161:ALA:O   | 2.24                     | 0.71              |
| 1:d:100:THR:OG1 | 1:d:202:PHE:HD2 | 1.73                     | 0.71              |
| 1:A:91:ARG:NH2  | 1:W:161:ALA:O   | 2.24                     | 0.70              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:50:GLU:CD   | 1:X:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:D:104:ASP:CB  | 1:S:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:F:175:GLY:O   | 1:F:193:SER:OG  | 2.08                     | 0.70              |
| 1:G:50:GLU:CD   | 1:P:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:H:91:ARG:NH2  | 1:O:161:ALA:O   | 2.24                     | 0.70              |
| 1:O:104:ASP:CB  | 1:k:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:Q:104:ASP:CB  | 1:m:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:A:84:HIS:CE1  | 1:W:50:GLU:CD   | 2.69                     | 0.70              |
| 1:G:161:ALA:O   | 1:P:91:ARG:NH2  | 2.24                     | 0.70              |
| 1:H:100:THR:OG1 | 1:H:202:PHE:HD2 | 1.73                     | 0.70              |
| 1:H:104:ASP:CB  | 1:O:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:I:104:ASP:CB  | 1:e:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:J:104:ASP:CB  | 1:M:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:K:50:GLU:CD   | 1:L:84:HIS:CE1  | 2.70                     | 0.70              |
| 1:M:91:ARG:NH2  | 1:i:161:ALA:O   | 2.24                     | 0.70              |
| 1:M:104:ASP:CB  | 1:i:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:Q:84:HIS:CE1  | 1:m:50:GLU:CD   | 2.69                     | 0.70              |
| 1:m:175:GLY:O   | 1:m:193:SER:OG  | 2.07                     | 0.70              |
| 1:D:84:HIS:CE1  | 1:S:50:GLU:CD   | 2.69                     | 0.70              |
| 1:F:50:GLU:CD   | 1:b:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:H:50:GLU:CD   | 1:d:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:H:161:ALA:O   | 1:d:91:ARG:NH2  | 2.24                     | 0.70              |
| 1:J:50:GLU:CD   | 1:f:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:M:84:HIS:CE1  | 1:i:50:GLU:CD   | 2.70                     | 0.70              |
| 1:P:135:LYS:NZ  | 1:l:104:ASP:CB  | 2.54                     | 0.70              |
| 1:R:135:LYS:NZ  | 1:n:104:ASP:CB  | 2.54                     | 0.70              |
| 1:C:50:GLU:CD   | 1:T:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:F:104:ASP:CB  | 1:Q:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:G:135:LYS:NZ  | 1:P:104:ASP:CB  | 2.54                     | 0.70              |
| 1:N:161:ALA:O   | 1:j:91:ARG:NH2  | 2.24                     | 0.70              |
| 1:j:175:GLY:O   | 1:j:193:SER:OG  | 2.08                     | 0.70              |
| 1:A:161:ALA:O   | 1:V:91:ARG:NH2  | 2.24                     | 0.70              |
| 1:E:84:HIS:CE1  | 1:a:50:GLU:CD   | 2.69                     | 0.70              |
| 1:I:84:HIS:CE1  | 1:e:50:GLU:CD   | 2.69                     | 0.70              |
| 1:N:50:GLU:CD   | 1:j:84:HIS:CE1  | 2.70                     | 0.70              |
| 1:N:50:GLU:HB3  | 1:j:84:HIS:HE1  | 1.57                     | 0.70              |
| 1:O:84:HIS:CE1  | 1:k:50:GLU:CD   | 2.70                     | 0.70              |
| 1:S:84:HIS:HE1  | 1:o:50:GLU:HB3  | 1.57                     | 0.70              |
| 1:C:84:HIS:CE1  | 1:Y:50:GLU:CD   | 2.70                     | 0.70              |
| 1:E:50:GLU:CD   | 1:R:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:I:135:LYS:NZ  | 1:N:104:ASP:CB  | 2.54                     | 0.70              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:84:HIS:HE1  | 1:S:50:GLU:HB3  | 1.57                     | 0.70              |
| 1:E:91:ARG:NH2  | 1:a:161:ALA:O   | 2.24                     | 0.70              |
| 1:H:84:HIS:CE1  | 1:O:50:GLU:CD   | 2.69                     | 0.70              |
| 1:J:84:HIS:HE1  | 1:M:50:GLU:HB3  | 1.57                     | 0.70              |
| 1:L:161:ALA:O   | 1:h:91:ARG:NH2  | 2.24                     | 0.70              |
| 1:P:50:GLU:HB3  | 1:l:84:HIS:HE1  | 1.57                     | 0.70              |
| 1:R:50:GLU:CD   | 1:n:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:A:135:LYS:NZ  | 1:V:104:ASP:CB  | 2.54                     | 0.70              |
| 1:J:84:HIS:CE1  | 1:M:50:GLU:CD   | 2.69                     | 0.70              |
| 1:K:104:ASP:CB  | 1:g:135:LYS:NZ  | 2.54                     | 0.70              |
| 1:Q:84:HIS:HE1  | 1:m:50:GLU:HB3  | 1.57                     | 0.70              |
| 1:I:50:GLU:CD   | 1:N:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:L:50:GLU:HB3  | 1:h:84:HIS:HE1  | 1.57                     | 0.70              |
| 1:P:161:ALA:O   | 1:l:91:ARG:NH2  | 2.24                     | 0.70              |
| 1:S:84:HIS:CE1  | 1:o:50:GLU:CD   | 2.70                     | 0.70              |
| 1:S:100:THR:OG1 | 1:S:202:PHE:HD2 | 1.73                     | 0.70              |
| 1:a:100:THR:OG1 | 1:a:202:PHE:HD2 | 1.73                     | 0.70              |
| 1:n:100:THR:OG1 | 1:n:202:PHE:HD2 | 1.73                     | 0.70              |
| 1:B:84:HIS:CE1  | 1:U:50:GLU:CD   | 2.69                     | 0.70              |
| 1:D:50:GLU:CD   | 1:Z:84:HIS:CE1  | 2.69                     | 0.70              |
| 1:F:84:HIS:CE1  | 1:Q:50:GLU:CD   | 2.70                     | 0.70              |
| 1:I:50:GLU:HB3  | 1:N:84:HIS:HE1  | 1.57                     | 0.70              |
| 1:M:100:THR:HG1 | 1:M:202:PHE:HD2 | 1.32                     | 0.70              |
| 1:b:175:GLY:O   | 1:b:193:SER:OG  | 2.08                     | 0.70              |
| 1:i:175:GLY:O   | 1:i:193:SER:OG  | 2.08                     | 0.70              |
| 1:B:84:HIS:HE1  | 1:U:50:GLU:HB3  | 1.57                     | 0.69              |
| 1:D:84:HIS:HD1  | 1:S:50:GLU:CD   | 1.99                     | 0.69              |
| 1:F:84:HIS:HE1  | 1:Q:50:GLU:HB3  | 1.57                     | 0.69              |
| 1:G:84:HIS:CE1  | 1:c:50:GLU:CD   | 2.70                     | 0.69              |
| 1:K:100:THR:OG1 | 1:K:202:PHE:HD2 | 1.73                     | 0.69              |
| 1:O:175:GLY:O   | 1:O:193:SER:OG  | 2.08                     | 0.69              |
| 1:P:50:GLU:CD   | 1:l:84:HIS:CE1  | 2.70                     | 0.69              |
| 1:P:135:LYS:HE3 | 1:l:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:A:50:GLU:CD   | 1:V:84:HIS:CE1  | 2.69                     | 0.69              |
| 1:G:50:GLU:HB3  | 1:P:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:I:50:GLU:CD   | 1:N:84:HIS:HD1  | 1.99                     | 0.69              |
| 1:K:84:HIS:CE1  | 1:g:50:GLU:CD   | 2.69                     | 0.69              |
| 1:L:50:GLU:CD   | 1:h:84:HIS:CE1  | 2.69                     | 0.69              |
| 1:R:50:GLU:HB3  | 1:n:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:S:84:HIS:HD1  | 1:o:50:GLU:CD   | 1.99                     | 0.69              |
| 1:E:175:GLY:O   | 1:E:193:SER:OG  | 2.08                     | 0.69              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:l:100:THR:OG1 | 1:l:202:PHE:HD2 | 1.73                     | 0.69              |
| 1:D:50:GLU:HB3  | 1:Z:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:D:135:LYS:HE3 | 1:Z:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:F:100:THR:OG1 | 1:F:202:PHE:HD2 | 1.73                     | 0.69              |
| 1:F:135:LYS:HE3 | 1:b:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:K:50:GLU:HB3  | 1:L:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:R:135:LYS:HE3 | 1:n:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:X:100:THR:OG1 | 1:X:202:PHE:HD2 | 1.73                     | 0.69              |
| 1:i:60:GLU:O    | 1:i:63:SER:OG   | 2.10                     | 0.69              |
| 1:B:50:GLU:CD   | 1:X:84:HIS:HD1  | 1.99                     | 0.69              |
| 1:G:84:HIS:HD1  | 1:c:50:GLU:CD   | 1.99                     | 0.69              |
| 1:I:84:HIS:HD1  | 1:e:50:GLU:CD   | 1.99                     | 0.69              |
| 1:J:50:GLU:HB3  | 1:f:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:c:175:GLY:O   | 1:c:193:SER:OG  | 2.08                     | 0.69              |
| 1:A:84:HIS:HE1  | 1:W:50:GLU:HB3  | 1.57                     | 0.69              |
| 1:C:60:GLU:O    | 1:C:63:SER:OG   | 2.10                     | 0.69              |
| 1:E:50:GLU:HB3  | 1:R:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:G:135:LYS:HE3 | 1:P:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:I:50:GLU:HB3  | 1:N:84:HIS:CE1  | 2.28                     | 0.69              |
| 1:N:135:LYS:HE3 | 1:j:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:P:50:GLU:CD   | 1:l:84:HIS:HD1  | 1.99                     | 0.69              |
| 1:W:60:GLU:O    | 1:W:63:SER:OG   | 2.10                     | 0.69              |
| 1:W:175:GLY:O   | 1:W:193:SER:OG  | 2.08                     | 0.69              |
| 1:k:175:GLY:O   | 1:k:193:SER:OG  | 2.08                     | 0.69              |
| 1:B:50:GLU:HB3  | 1:X:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:D:84:HIS:CE1  | 1:S:50:GLU:HB3  | 2.28                     | 0.69              |
| 1:H:175:GLY:O   | 1:H:193:SER:OG  | 2.08                     | 0.69              |
| 1:I:100:THR:OG1 | 1:I:202:PHE:HD2 | 1.73                     | 0.69              |
| 1:M:100:THR:OG1 | 1:M:202:PHE:HD2 | 1.73                     | 0.69              |
| 1:O:84:HIS:HE1  | 1:k:50:GLU:HB3  | 1.57                     | 0.69              |
| 1:V:100:THR:OG1 | 1:V:202:PHE:HD2 | 1.73                     | 0.69              |
| 1:Y:60:GLU:O    | 1:Y:63:SER:OG   | 2.10                     | 0.69              |
| 1:D:104:ASP:HB3 | 1:S:135:LYS:HE3 | 1.74                     | 0.69              |
| 1:E:135:LYS:HE3 | 1:R:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:F:50:GLU:HB3  | 1:b:84:HIS:HE1  | 1.57                     | 0.69              |
| 1:G:84:HIS:CE1  | 1:c:50:GLU:HB3  | 2.28                     | 0.69              |
| 1:N:50:GLU:CD   | 1:j:84:HIS:HD1  | 1.99                     | 0.69              |
| 1:B:50:GLU:HB3  | 1:X:84:HIS:CE1  | 2.28                     | 0.69              |
| 1:C:84:HIS:HE1  | 1:Y:50:GLU:HB3  | 1.57                     | 0.69              |
| 1:F:50:GLU:CD   | 1:b:84:HIS:HD1  | 1.99                     | 0.69              |
| 1:F:104:ASP:HB3 | 1:Q:135:LYS:HE3 | 1.74                     | 0.69              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:135:LYS:HE3 | 1:d:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:I:135:LYS:HE3 | 1:N:104:ASP:HB3 | 1.74                     | 0.69              |
| 1:N:50:GLU:HB3  | 1:j:84:HIS:CE1  | 2.28                     | 0.69              |
| 1:S:84:HIS:CE1  | 1:o:50:GLU:HB3  | 2.28                     | 0.69              |
| 1:A:50:GLU:HB3  | 1:V:84:HIS:HE1  | 1.57                     | 0.68              |
| 1:C:50:GLU:HB3  | 1:T:84:HIS:HE1  | 1.57                     | 0.68              |
| 1:I:84:HIS:HE1  | 1:e:50:GLU:HB3  | 1.57                     | 0.68              |
| 1:O:107:THR:O   | 1:Y:226:TYR:OH  | 2.11                     | 0.68              |
| 1:Q:84:HIS:HD1  | 1:m:50:GLU:CD   | 1.99                     | 0.68              |
| 1:Y:107:THR:O   | 1:i:226:TYR:OH  | 2.11                     | 0.68              |
| 1:Y:175:GLY:O   | 1:Y:193:SER:OG  | 2.08                     | 0.68              |
| 1:B:84:HIS:HD1  | 1:U:50:GLU:CD   | 1.99                     | 0.68              |
| 1:C:50:GLU:HB3  | 1:T:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:D:50:GLU:CD   | 1:Z:84:HIS:HD1  | 1.99                     | 0.68              |
| 1:G:104:ASP:HB3 | 1:c:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:L:50:GLU:CD   | 1:h:84:HIS:HD1  | 1.99                     | 0.68              |
| 1:V:226:TYR:OH  | 1:f:107:THR:O   | 2.11                     | 0.68              |
| 1:g:60:GLU:O    | 1:g:63:SER:OG   | 2.10                     | 0.68              |
| 1:D:50:GLU:HB3  | 1:Z:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:J:84:HIS:CE1  | 1:M:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:A:50:GLU:CD   | 1:V:84:HIS:ND1  | 2.52                     | 0.68              |
| 1:E:107:THR:O   | 1:O:226:TYR:OH  | 2.11                     | 0.68              |
| 1:F:50:GLU:HB3  | 1:b:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:G:84:HIS:HE1  | 1:c:50:GLU:HB3  | 1.57                     | 0.68              |
| 1:H:84:HIS:HE1  | 1:O:50:GLU:HB3  | 1.57                     | 0.68              |
| 1:H:104:ASP:HB3 | 1:O:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:I:84:HIS:CE1  | 1:e:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:J:50:GLU:CD   | 1:f:84:HIS:ND1  | 2.52                     | 0.68              |
| 1:K:84:HIS:CE1  | 1:g:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:L:60:GLU:O    | 1:L:63:SER:OG   | 2.10                     | 0.68              |
| 1:P:50:GLU:HB3  | 1:l:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:P:100:THR:OG1 | 1:P:202:PHE:HD2 | 1.73                     | 0.68              |
| 1:Q:84:HIS:CE1  | 1:m:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:T:226:TYR:OH  | 1:d:107:THR:O   | 2.11                     | 0.68              |
| 1:d:226:TYR:OH  | 1:n:107:THR:O   | 2.11                     | 0.68              |
| 1:C:84:HIS:ND1  | 1:Y:50:GLU:CD   | 2.52                     | 0.68              |
| 1:E:50:GLU:HB3  | 1:R:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:E:104:ASP:HB3 | 1:a:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:J:60:GLU:O    | 1:J:63:SER:OG   | 2.10                     | 0.68              |
| 1:L:50:GLU:HB3  | 1:h:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:M:84:HIS:ND1  | 1:i:50:GLU:CD   | 2.52                     | 0.68              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:T:60:GLU:O    | 1:T:63:SER:OG   | 2.10                     | 0.68              |
| 1:c:100:THR:OG1 | 1:c:202:PHE:HD2 | 1.73                     | 0.68              |
| 1:l:175:GLY:O   | 1:l:193:SER:OG  | 2.08                     | 0.68              |
| 1:E:84:HIS:HE1  | 1:a:50:GLU:HB3  | 1.57                     | 0.68              |
| 1:G:100:THR:OG1 | 1:G:202:PHE:HD2 | 1.73                     | 0.68              |
| 1:H:50:GLU:CD   | 1:d:84:HIS:ND1  | 2.52                     | 0.68              |
| 1:J:175:GLY:O   | 1:J:193:SER:OG  | 2.08                     | 0.68              |
| 1:K:84:HIS:HE1  | 1:g:50:GLU:HB3  | 1.57                     | 0.68              |
| 1:O:100:THR:OG1 | 1:O:202:PHE:HD2 | 1.73                     | 0.68              |
| 1:Q:100:THR:OG1 | 1:Q:202:PHE:HD2 | 1.73                     | 0.68              |
| 1:S:175:GLY:O   | 1:S:193:SER:OG  | 2.08                     | 0.68              |
| 1:T:100:THR:OG1 | 1:T:202:PHE:HD2 | 1.73                     | 0.68              |
| 1:W:107:THR:O   | 1:g:226:TYR:OH  | 2.11                     | 0.68              |
| 1:A:84:HIS:CE1  | 1:W:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:B:135:LYS:HE3 | 1:X:104:ASP:HB3 | 1.74                     | 0.68              |
| 1:C:135:LYS:HE3 | 1:T:104:ASP:HB3 | 1.74                     | 0.68              |
| 1:D:107:THR:O   | 1:G:226:TYR:OH  | 2.11                     | 0.68              |
| 1:E:50:GLU:CD   | 1:R:84:HIS:HD1  | 1.99                     | 0.68              |
| 1:H:50:GLU:HB3  | 1:d:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:H:84:HIS:CE1  | 1:O:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:M:107:THR:O   | 1:W:226:TYR:OH  | 2.11                     | 0.68              |
| 1:Q:104:ASP:HB3 | 1:m:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:S:104:ASP:HB3 | 1:o:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:C:107:THR:O   | 1:M:226:TYR:OH  | 2.11                     | 0.68              |
| 1:D:226:TYR:OH  | 1:N:107:THR:O   | 2.11                     | 0.68              |
| 1:G:50:GLU:CD   | 1:P:84:HIS:HD1  | 1.99                     | 0.68              |
| 1:G:50:GLU:HB3  | 1:P:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:H:84:HIS:ND1  | 1:O:50:GLU:CD   | 2.52                     | 0.68              |
| 1:I:104:ASP:HB3 | 1:e:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:K:50:GLU:CD   | 1:L:84:HIS:ND1  | 2.52                     | 0.68              |
| 1:K:84:HIS:ND1  | 1:g:50:GLU:CD   | 2.52                     | 0.68              |
| 1:L:226:TYR:OH  | 1:V:107:THR:O   | 2.11                     | 0.68              |
| 1:B:84:HIS:CE1  | 1:U:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:C:84:HIS:CE1  | 1:Y:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:C:104:ASP:HB3 | 1:Y:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:J:104:ASP:HB3 | 1:M:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:J:135:LYS:HE3 | 1:f:104:ASP:HB3 | 1.74                     | 0.68              |
| 1:R:50:GLU:CD   | 1:n:84:HIS:HD1  | 1.99                     | 0.68              |
| 1:R:50:GLU:CD   | 1:n:84:HIS:ND1  | 2.52                     | 0.68              |
| 1:R:50:GLU:HB3  | 1:n:84:HIS:CE1  | 2.28                     | 0.68              |
| 1:o:100:THR:OG1 | 1:o:202:PHE:HD2 | 1.73                     | 0.68              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:50:GLU:CD   | 1:T:84:HIS:ND1  | 2.52                     | 0.68              |
| 1:E:84:HIS:ND1  | 1:a:50:GLU:CD   | 2.52                     | 0.68              |
| 1:M:84:HIS:CE1  | 1:i:50:GLU:HB3  | 2.28                     | 0.68              |
| 1:M:104:ASP:HB3 | 1:i:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:O:104:ASP:HB3 | 1:k:135:LYS:HE3 | 1.74                     | 0.68              |
| 1:a:107:THR:O   | 1:k:226:TYR:OH  | 2.11                     | 0.68              |
| 1:A:84:HIS:ND1  | 1:W:50:GLU:CD   | 2.52                     | 0.67              |
| 1:B:50:GLU:CD   | 1:X:84:HIS:ND1  | 2.52                     | 0.67              |
| 1:E:84:HIS:CE1  | 1:a:50:GLU:HB3  | 2.28                     | 0.67              |
| 1:F:84:HIS:HD1  | 1:Q:50:GLU:CD   | 1.99                     | 0.67              |
| 1:J:50:GLU:HB3  | 1:f:84:HIS:CE1  | 2.28                     | 0.67              |
| 1:M:84:HIS:HE1  | 1:i:50:GLU:HB3  | 1.57                     | 0.67              |
| 1:N:175:GLY:O   | 1:N:193:SER:OG  | 2.08                     | 0.67              |
| 1:N:226:TYR:OH  | 1:X:107:THR:O   | 2.11                     | 0.67              |
| 1:O:84:HIS:CE1  | 1:k:50:GLU:HB3  | 2.28                     | 0.67              |
| 1:R:100:THR:OG1 | 1:R:202:PHE:HD2 | 1.73                     | 0.67              |
| 1:d:60:GLU:O    | 1:d:63:SER:OG   | 2.10                     | 0.67              |
| 1:A:50:GLU:HB3  | 1:V:84:HIS:CE1  | 2.28                     | 0.67              |
| 1:B:107:THR:O   | 1:I:226:TYR:OH  | 2.11                     | 0.67              |
| 1:C:226:TYR:OH  | 1:H:107:THR:O   | 2.11                     | 0.67              |
| 1:E:226:TYR:OH  | 1:F:107:THR:O   | 2.11                     | 0.67              |
| 1:K:50:GLU:CD   | 1:L:84:HIS:HD1  | 1.99                     | 0.67              |
| 1:L:50:GLU:CD   | 1:h:84:HIS:ND1  | 2.52                     | 0.67              |
| 1:O:84:HIS:ND1  | 1:k:50:GLU:CD   | 2.52                     | 0.67              |
| 1:R:60:GLU:O    | 1:R:63:SER:OG   | 2.10                     | 0.67              |
| 1:G:107:THR:O   | 1:Q:226:TYR:OH  | 2.11                     | 0.67              |
| 1:H:84:HIS:HD1  | 1:O:50:GLU:CD   | 1.99                     | 0.67              |
| 1:I:107:THR:O   | 1:S:226:TYR:OH  | 2.11                     | 0.67              |
| 1:Q:107:THR:O   | 1:a:226:TYR:OH  | 2.11                     | 0.67              |
| 1:F:84:HIS:CE1  | 1:Q:50:GLU:HB3  | 2.28                     | 0.67              |
| 1:K:104:ASP:HB3 | 1:g:135:LYS:HE3 | 1.74                     | 0.67              |
| 1:e:107:THR:O   | 1:o:226:TYR:OH  | 2.11                     | 0.67              |
| 1:B:104:ASP:HB3 | 1:U:135:LYS:HE3 | 1.74                     | 0.67              |
| 1:E:84:HIS:HD1  | 1:a:50:GLU:CD   | 1.99                     | 0.67              |
| 1:F:84:HIS:ND1  | 1:Q:50:GLU:CD   | 2.52                     | 0.67              |
| 1:I:50:GLU:CD   | 1:N:84:HIS:ND1  | 2.52                     | 0.67              |
| 1:K:50:GLU:HB3  | 1:L:84:HIS:CE1  | 2.28                     | 0.67              |
| 1:K:84:HIS:HD1  | 1:g:50:GLU:CD   | 1.99                     | 0.67              |
| 1:a:175:GLY:O   | 1:a:193:SER:OG  | 2.08                     | 0.67              |
| 1:G:50:GLU:CD   | 1:P:84:HIS:ND1  | 2.52                     | 0.67              |
| 1:K:60:GLU:O    | 1:K:63:SER:OG   | 2.10                     | 0.67              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:k:128:ASN:O   | 1:k:136:LYS:NZ  | 2.25                     | 0.67              |
| 1:A:104:ASP:HB3 | 1:W:135:LYS:HE3 | 1.74                     | 0.67              |
| 1:B:226:TYR:OH  | 1:L:107:THR:O   | 2.11                     | 0.67              |
| 1:D:50:GLU:CD   | 1:Z:84:HIS:ND1  | 2.52                     | 0.67              |
| 1:E:50:GLU:CD   | 1:R:84:HIS:ND1  | 2.52                     | 0.67              |
| 1:K:135:LYS:HE3 | 1:L:104:ASP:HB3 | 1.74                     | 0.67              |
| 1:L:135:LYS:HE3 | 1:h:104:ASP:HB3 | 1.74                     | 0.67              |
| 1:S:84:HIS:ND1  | 1:o:50:GLU:CD   | 2.52                     | 0.67              |
| 1:E:100:THR:OG1 | 1:E:202:PHE:HD2 | 1.73                     | 0.67              |
| 1:H:50:GLU:CD   | 1:d:84:HIS:HD1  | 1.99                     | 0.67              |
| 1:H:50:GLU:HB3  | 1:d:84:HIS:HE1  | 1.57                     | 0.67              |
| 1:J:84:HIS:ND1  | 1:M:50:GLU:CD   | 2.52                     | 0.67              |
| 1:P:226:TYR:OH  | 1:Z:107:THR:O   | 2.11                     | 0.67              |
| 1:C:84:HIS:HD1  | 1:Y:50:GLU:CD   | 1.99                     | 0.67              |
| 1:F:226:TYR:OH  | 1:P:107:THR:O   | 2.11                     | 0.67              |
| 1:H:226:TYR:OH  | 1:R:107:THR:O   | 2.11                     | 0.67              |
| 1:X:226:TYR:OH  | 1:h:107:THR:O   | 2.11                     | 0.67              |
| 1:b:60:GLU:O    | 1:b:63:SER:OG   | 2.10                     | 0.67              |
| 1:A:84:HIS:HD1  | 1:W:50:GLU:CD   | 1.99                     | 0.67              |
| 1:M:84:HIS:HD1  | 1:i:50:GLU:CD   | 1.99                     | 0.67              |
| 1:Z:100:THR:OG1 | 1:Z:202:PHE:HD2 | 1.73                     | 0.67              |
| 1:I:84:HIS:ND1  | 1:e:50:GLU:CD   | 2.52                     | 0.66              |
| 1:O:84:HIS:HD1  | 1:k:50:GLU:CD   | 1.99                     | 0.66              |
| 1:U:107:THR:O   | 1:e:226:TYR:OH  | 2.11                     | 0.66              |
| 1:b:226:TYR:OH  | 1:l:107:THR:O   | 2.11                     | 0.66              |
| 1:n:60:GLU:O    | 1:n:63:SER:OG   | 2.10                     | 0.66              |
| 1:A:135:LYS:HE3 | 1:V:104:ASP:HB3 | 1.74                     | 0.66              |
| 1:C:50:GLU:CD   | 1:T:84:HIS:HD1  | 1.99                     | 0.66              |
| 1:Z:226:TYR:OH  | 1:j:107:THR:O   | 2.11                     | 0.66              |
| 1:n:175:GLY:O   | 1:n:193:SER:OG  | 2.07                     | 0.66              |
| 1:A:50:GLU:CD   | 1:V:84:HIS:HD1  | 1.99                     | 0.66              |
| 1:N:50:GLU:CD   | 1:j:84:HIS:ND1  | 2.52                     | 0.66              |
| 1:k:100:THR:OG1 | 1:k:202:PHE:HD2 | 1.73                     | 0.66              |
| 1:J:84:HIS:HD1  | 1:M:50:GLU:CD   | 1.99                     | 0.66              |
| 1:K:128:ASN:O   | 1:K:136:LYS:NZ  | 2.25                     | 0.66              |
| 1:U:60:GLU:O    | 1:U:63:SER:OG   | 2.10                     | 0.66              |
| 1:j:60:GLU:O    | 1:j:63:SER:OG   | 2.10                     | 0.66              |
| 1:K:175:GLY:O   | 1:K:193:SER:OG  | 2.08                     | 0.66              |
| 1:P:50:GLU:CD   | 1:l:84:HIS:ND1  | 2.52                     | 0.66              |
| 1:Q:84:HIS:ND1  | 1:m:50:GLU:CD   | 2.52                     | 0.66              |
| 1:f:175:GLY:O   | 1:f:193:SER:OG  | 2.08                     | 0.66              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:100:THR:OG1 | 1:D:202:PHE:HD2 | 1.73                     | 0.66              |
| 1:I:60:GLU:O    | 1:I:63:SER:OG   | 2.10                     | 0.66              |
| 1:A:107:THR:O   | 1:K:226:TYR:OH  | 2.11                     | 0.66              |
| 1:D:84:HIS:ND1  | 1:S:50:GLU:CD   | 2.52                     | 0.66              |
| 1:K:107:THR:O   | 1:U:226:TYR:OH  | 2.11                     | 0.66              |
| 1:f:60:GLU:O    | 1:f:63:SER:OG   | 2.10                     | 0.66              |
| 1:k:60:GLU:O    | 1:k:63:SER:OG   | 2.10                     | 0.66              |
| 1:G:84:HIS:ND1  | 1:c:50:GLU:CD   | 2.52                     | 0.66              |
| 1:f:128:ASN:O   | 1:f:136:LYS:NZ  | 2.25                     | 0.66              |
| 1:m:60:GLU:O    | 1:m:63:SER:OG   | 2.10                     | 0.66              |
| 1:A:226:TYR:OH  | 1:J:107:THR:O   | 2.11                     | 0.66              |
| 1:B:84:HIS:ND1  | 1:U:50:GLU:CD   | 2.52                     | 0.66              |
| 1:J:128:ASN:O   | 1:J:136:LYS:NZ  | 2.25                     | 0.66              |
| 1:Z:60:GLU:O    | 1:Z:63:SER:OG   | 2.10                     | 0.66              |
| 1:e:60:GLU:O    | 1:e:63:SER:OG   | 2.10                     | 0.66              |
| 1:J:50:GLU:CD   | 1:f:84:HIS:HD1  | 1.99                     | 0.66              |
| 1:V:175:GLY:O   | 1:V:193:SER:OG  | 2.08                     | 0.66              |
| 1:b:100:THR:OG1 | 1:b:202:PHE:HD2 | 1.73                     | 0.66              |
| 1:R:226:TYR:OH  | 1:b:107:THR:O   | 2.11                     | 0.65              |
| 1:c:107:THR:O   | 1:m:226:TYR:OH  | 2.11                     | 0.65              |
| 1:B:100:THR:OG1 | 1:B:202:PHE:HD2 | 1.73                     | 0.65              |
| 1:F:50:GLU:CD   | 1:b:84:HIS:ND1  | 2.52                     | 0.65              |
| 1:Q:37:ASN:OD1  | 1:a:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:S:107:THR:O   | 1:c:226:TYR:OH  | 2.11                     | 0.65              |
| 1:V:60:GLU:O    | 1:V:63:SER:OG   | 2.10                     | 0.65              |
| 1:A:15:ARG:NH1  | 1:J:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:G:60:GLU:O    | 1:G:63:SER:OG   | 2.10                     | 0.65              |
| 1:J:226:TYR:OH  | 1:T:107:THR:O   | 2.11                     | 0.65              |
| 1:l:60:GLU:O    | 1:l:63:SER:OG   | 2.10                     | 0.65              |
| 1:A:37:ASN:OD1  | 1:K:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:C:15:ARG:NH1  | 1:H:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:F:15:ARG:NH1  | 1:P:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:V:15:ARG:NH1  | 1:f:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:W:37:ASN:OD1  | 1:g:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:Y:37:ASN:OD1  | 1:i:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:d:15:ARG:NH1  | 1:n:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:H:15:ARG:NH1  | 1:R:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:M:175:GLY:O   | 1:M:193:SER:OG  | 2.08                     | 0.65              |
| 1:T:128:ASN:O   | 1:T:136:LYS:NZ  | 2.25                     | 0.65              |
| 1:a:37:ASN:OD1  | 1:k:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:e:100:THR:OG1 | 1:e:202:PHE:HD2 | 1.73                     | 0.65              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:i:128:ASN:O   | 1:i:136:LYS:NZ  | 2.25                     | 0.65              |
| 1:o:60:GLU:O    | 1:o:63:SER:OG   | 2.10                     | 0.65              |
| 1:E:15:ARG:NH1  | 1:F:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:b:15:ARG:NH1  | 1:l:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:S:37:ASN:OD1  | 1:c:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:T:15:ARG:NH1  | 1:d:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:X:15:ARG:NH1  | 1:h:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:O:37:ASN:OD1  | 1:Y:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:B:15:ARG:NH1  | 1:L:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:C:37:ASN:OD1  | 1:M:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:D:15:ARG:NH1  | 1:N:37:ASN:OD1  | 2.30                     | 0.65              |
| 1:J:135:LYS:NZ  | 1:f:104:ASP:HB2 | 2.13                     | 0.65              |
| 1:M:104:ASP:HB2 | 1:i:135:LYS:HZ3 | 1.61                     | 0.65              |
| 1:U:37:ASN:OD1  | 1:e:15:ARG:NH1  | 2.30                     | 0.65              |
| 1:X:175:GLY:O   | 1:X:193:SER:OG  | 2.08                     | 0.65              |
| 1:A:135:LYS:NZ  | 1:V:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:D:135:LYS:NZ  | 1:Z:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:G:104:ASP:HB2 | 1:c:135:LYS:NZ  | 2.13                     | 0.64              |
| 1:I:104:ASP:HB2 | 1:e:135:LYS:NZ  | 2.13                     | 0.64              |
| 1:a:60:GLU:O    | 1:a:63:SER:OG   | 2.10                     | 0.64              |
| 1:A:104:ASP:HB2 | 1:W:135:LYS:NZ  | 2.13                     | 0.64              |
| 1:B:37:ASN:OD1  | 1:I:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:D:37:ASN:OD1  | 1:G:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:F:135:LYS:NZ  | 1:b:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:G:37:ASN:OD1  | 1:Q:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:H:128:ASN:O   | 1:H:136:LYS:NZ  | 2.26                     | 0.64              |
| 1:Z:15:ARG:NH1  | 1:j:37:ASN:OD1  | 2.30                     | 0.64              |
| 1:c:37:ASN:OD1  | 1:m:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:B:135:LYS:NZ  | 1:X:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:K:104:ASP:HB2 | 1:g:135:LYS:NZ  | 2.13                     | 0.64              |
| 1:e:37:ASN:OD1  | 1:o:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:E:128:ASN:O   | 1:E:136:LYS:NZ  | 2.25                     | 0.64              |
| 1:J:15:ARG:NH1  | 1:T:37:ASN:OD1  | 2.30                     | 0.64              |
| 1:J:104:ASP:HB2 | 1:M:135:LYS:NZ  | 2.13                     | 0.64              |
| 1:K:135:LYS:NZ  | 1:L:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:Q:128:ASN:O   | 1:Q:136:LYS:NZ  | 2.25                     | 0.64              |
| 1:i:100:THR:OG1 | 1:i:202:PHE:HD2 | 1.73                     | 0.64              |
| 1:M:37:ASN:OD1  | 1:W:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:O:104:ASP:HB2 | 1:k:135:LYS:NZ  | 2.13                     | 0.64              |
| 1:Q:175:GLY:O   | 1:Q:193:SER:OG  | 2.08                     | 0.64              |
| 1:F:104:ASP:HB2 | 1:Q:135:LYS:NZ  | 2.13                     | 0.64              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:135:LYS:NZ  | 1:N:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:P:15:ARG:NH1  | 1:Z:37:ASN:OD1  | 2.30                     | 0.64              |
| 1:R:15:ARG:NH1  | 1:b:37:ASN:OD1  | 2.30                     | 0.64              |
| 1:C:135:LYS:NZ  | 1:T:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:D:104:ASP:HB2 | 1:S:135:LYS:NZ  | 2.13                     | 0.64              |
| 1:E:37:ASN:OD1  | 1:O:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:F:104:ASP:HB2 | 1:Q:135:LYS:HZ3 | 1.63                     | 0.64              |
| 1:G:135:LYS:NZ  | 1:P:104:ASP:HB2 | 2.13                     | 0.64              |
| 1:I:175:GLY:O   | 1:I:193:SER:OG  | 2.08                     | 0.64              |
| 1:L:15:ARG:NH1  | 1:V:37:ASN:OD1  | 2.30                     | 0.64              |
| 1:M:104:ASP:HB2 | 1:i:135:LYS:NZ  | 2.12                     | 0.64              |
| 1:P:128:ASN:O   | 1:P:136:LYS:NZ  | 2.25                     | 0.64              |
| 1:T:175:GLY:O   | 1:T:193:SER:OG  | 2.08                     | 0.64              |
| 1:a:113:GLN:NE2 | 1:a:195:ASN:O   | 2.31                     | 0.64              |
| 1:k:113:GLN:NE2 | 1:k:195:ASN:O   | 2.31                     | 0.64              |
| 1:n:113:GLN:NE2 | 1:n:195:ASN:O   | 2.31                     | 0.64              |
| 1:B:60:GLU:O    | 1:B:63:SER:OG   | 2.10                     | 0.64              |
| 1:I:37:ASN:OD1  | 1:S:15:ARG:NH1  | 2.30                     | 0.64              |
| 1:Y:113:GLN:NE2 | 1:Y:195:ASN:O   | 2.31                     | 0.64              |
| 1:c:60:GLU:O    | 1:c:63:SER:OG   | 2.10                     | 0.64              |
| 1:m:113:GLN:NE2 | 1:m:195:ASN:O   | 2.31                     | 0.64              |
| 1:B:104:ASP:HB2 | 1:U:135:LYS:NZ  | 2.12                     | 0.63              |
| 1:K:37:ASN:OD1  | 1:U:15:ARG:NH1  | 2.30                     | 0.63              |
| 1:L:135:LYS:NZ  | 1:h:104:ASP:HB2 | 2.12                     | 0.63              |
| 1:D:128:ASN:O   | 1:D:136:LYS:NZ  | 2.25                     | 0.63              |
| 1:E:104:ASP:HB2 | 1:a:135:LYS:NZ  | 2.13                     | 0.63              |
| 1:O:113:GLN:NE2 | 1:O:195:ASN:O   | 2.31                     | 0.63              |
| 1:R:135:LYS:NZ  | 1:n:104:ASP:HB2 | 2.12                     | 0.63              |
| 1:b:113:GLN:NE2 | 1:b:195:ASN:O   | 2.31                     | 0.63              |
| 1:b:128:ASN:O   | 1:b:136:LYS:NZ  | 2.25                     | 0.63              |
| 1:d:113:GLN:NE2 | 1:d:195:ASN:O   | 2.31                     | 0.63              |
| 1:m:128:ASN:O   | 1:m:136:LYS:NZ  | 2.25                     | 0.63              |
| 1:H:104:ASP:HB2 | 1:O:135:LYS:NZ  | 2.13                     | 0.63              |
| 1:N:15:ARG:NH1  | 1:X:37:ASN:OD1  | 2.30                     | 0.63              |
| 1:O:60:GLU:O    | 1:O:63:SER:OG   | 2.10                     | 0.63              |
| 1:Q:104:ASP:HB2 | 1:m:135:LYS:HZ3 | 1.62                     | 0.63              |
| 1:Q:113:GLN:NE2 | 1:Q:195:ASN:O   | 2.31                     | 0.63              |
| 1:h:128:ASN:O   | 1:h:136:LYS:NZ  | 2.25                     | 0.63              |
| 1:i:113:GLN:NE2 | 1:i:195:ASN:O   | 2.31                     | 0.63              |
| 1:j:100:THR:OG1 | 1:j:202:PHE:HD2 | 1.73                     | 0.63              |
| 1:l:113:GLN:NE2 | 1:l:195:ASN:O   | 2.31                     | 0.63              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:P:135:LYS:HZ3 | 1:l:104:ASP:HB2 | 1.62                     | 0.63              |
| 1:c:113:GLN:NE2 | 1:c:195:ASN:O   | 2.31                     | 0.63              |
| 1:C:104:ASP:HB2 | 1:Y:135:LYS:NZ  | 2.12                     | 0.63              |
| 1:H:135:LYS:NZ  | 1:d:104:ASP:HB2 | 2.13                     | 0.63              |
| 1:Q:104:ASP:HB2 | 1:m:135:LYS:NZ  | 2.13                     | 0.63              |
| 1:S:60:GLU:O    | 1:S:63:SER:OG   | 2.10                     | 0.63              |
| 1:A:104:ASP:HB2 | 1:W:135:LYS:HZ3 | 1.64                     | 0.63              |
| 1:C:105:LYS:CD  | 1:i:51:LYS:HZ1  | 2.10                     | 0.63              |
| 1:E:113:GLN:NE2 | 1:E:195:ASN:O   | 2.31                     | 0.63              |
| 1:N:135:LYS:NZ  | 1:j:104:ASP:HB2 | 2.13                     | 0.63              |
| 1:R:113:GLN:NE2 | 1:R:195:ASN:O   | 2.31                     | 0.63              |
| 1:f:113:GLN:NE2 | 1:f:195:ASN:O   | 2.31                     | 0.63              |
| 1:T:113:GLN:NE2 | 1:T:195:ASN:O   | 2.31                     | 0.63              |
| 1:o:175:GLY:O   | 1:o:193:SER:OG  | 2.08                     | 0.63              |
| 1:G:54:GLY:O    | 1:P:91:ARG:NH1  | 2.32                     | 0.63              |
| 1:K:135:LYS:HZ3 | 1:L:104:ASP:HB2 | 1.63                     | 0.63              |
| 1:L:113:GLN:NE2 | 1:L:195:ASN:O   | 2.31                     | 0.63              |
| 1:Q:60:GLU:O    | 1:Q:63:SER:OG   | 2.10                     | 0.63              |
| 1:R:175:GLY:O   | 1:R:193:SER:OG  | 2.08                     | 0.63              |
| 1:V:128:ASN:O   | 1:V:136:LYS:NZ  | 2.26                     | 0.63              |
| 1:X:113:GLN:NE2 | 1:X:195:ASN:O   | 2.31                     | 0.63              |
| 1:e:113:GLN:NE2 | 1:e:195:ASN:O   | 2.31                     | 0.63              |
| 1:C:113:GLN:NE2 | 1:C:195:ASN:O   | 2.31                     | 0.63              |
| 1:D:54:GLY:O    | 1:Z:91:ARG:NH1  | 2.32                     | 0.63              |
| 1:F:91:ARG:NH1  | 1:Q:54:GLY:O    | 2.32                     | 0.63              |
| 1:G:113:GLN:NE2 | 1:G:195:ASN:O   | 2.31                     | 0.63              |
| 1:M:113:GLN:NE2 | 1:M:195:ASN:O   | 2.31                     | 0.63              |
| 1:P:135:LYS:NZ  | 1:l:104:ASP:HB2 | 2.12                     | 0.63              |
| 1:S:113:GLN:NE2 | 1:S:195:ASN:O   | 2.31                     | 0.63              |
| 1:E:91:ARG:NH1  | 1:a:54:GLY:O    | 2.32                     | 0.62              |
| 1:J:104:ASP:HB2 | 1:M:135:LYS:HZ3 | 1.63                     | 0.62              |
| 1:S:104:ASP:HB2 | 1:o:135:LYS:NZ  | 2.13                     | 0.62              |
| 1:g:128:ASN:O   | 1:g:136:LYS:NZ  | 2.25                     | 0.62              |
| 1:h:113:GLN:NE2 | 1:h:195:ASN:O   | 2.31                     | 0.62              |
| 1:B:128:ASN:O   | 1:B:136:LYS:NZ  | 2.25                     | 0.62              |
| 1:K:113:GLN:NE2 | 1:K:195:ASN:O   | 2.31                     | 0.62              |
| 1:N:54:GLY:O    | 1:j:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:O:128:ASN:O   | 1:O:136:LYS:NZ  | 2.25                     | 0.62              |
| 1:P:113:GLN:NE2 | 1:P:195:ASN:O   | 2.31                     | 0.62              |
| 1:U:128:ASN:O   | 1:U:136:LYS:NZ  | 2.25                     | 0.62              |
| 1:o:113:GLN:NE2 | 1:o:195:ASN:O   | 2.31                     | 0.62              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:54:GLY:O    | 1:R:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:H:113:GLN:NE2 | 1:H:195:ASN:O   | 2.31                     | 0.62              |
| 1:H:135:LYS:NZ  | 1:d:104:ASP:HB3 | 2.14                     | 0.62              |
| 1:J:54:GLY:O    | 1:f:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:L:54:GLY:O    | 1:h:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:S:91:ARG:NH1  | 1:o:54:GLY:O    | 2.32                     | 0.62              |
| 1:V:113:GLN:NE2 | 1:V:195:ASN:O   | 2.31                     | 0.62              |
| 1:A:54:GLY:O    | 1:V:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:C:104:ASP:HB3 | 1:Y:135:LYS:NZ  | 2.14                     | 0.62              |
| 1:F:54:GLY:O    | 1:b:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:F:113:GLN:NE2 | 1:F:195:ASN:O   | 2.31                     | 0.62              |
| 1:I:113:GLN:NE2 | 1:I:195:ASN:O   | 2.31                     | 0.62              |
| 1:J:113:GLN:NE2 | 1:J:195:ASN:O   | 2.31                     | 0.62              |
| 1:n:128:ASN:O   | 1:n:136:LYS:NZ  | 2.25                     | 0.62              |
| 1:D:175:GLY:O   | 1:D:193:SER:OG  | 2.08                     | 0.62              |
| 1:E:135:LYS:NZ  | 1:R:104:ASP:HB2 | 2.13                     | 0.62              |
| 1:G:91:ARG:NH1  | 1:c:54:GLY:O    | 2.32                     | 0.62              |
| 1:H:91:ARG:NH1  | 1:O:54:GLY:O    | 2.32                     | 0.62              |
| 1:O:91:ARG:NH1  | 1:k:54:GLY:O    | 2.32                     | 0.62              |
| 1:W:113:GLN:NE2 | 1:W:195:ASN:O   | 2.31                     | 0.62              |
| 1:D:113:GLN:NE2 | 1:D:195:ASN:O   | 2.31                     | 0.62              |
| 1:K:91:ARG:NH1  | 1:g:54:GLY:O    | 2.32                     | 0.62              |
| 1:P:54:GLY:O    | 1:l:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:U:100:THR:OG1 | 1:U:202:PHE:HD2 | 1.73                     | 0.62              |
| 1:U:175:GLY:O   | 1:U:193:SER:OG  | 2.08                     | 0.62              |
| 1:Z:113:GLN:NE2 | 1:Z:195:ASN:O   | 2.31                     | 0.62              |
| 1:A:113:GLN:NE2 | 1:A:195:ASN:O   | 2.31                     | 0.62              |
| 1:C:54:GLY:O    | 1:T:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:E:60:GLU:O    | 1:E:63:SER:OG   | 2.10                     | 0.62              |
| 1:H:104:ASP:HB3 | 1:O:135:LYS:NZ  | 2.14                     | 0.62              |
| 1:I:128:ASN:O   | 1:I:136:LYS:NZ  | 2.25                     | 0.62              |
| 1:L:128:ASN:O   | 1:L:136:LYS:NZ  | 2.25                     | 0.62              |
| 1:M:104:ASP:HB3 | 1:i:135:LYS:NZ  | 2.14                     | 0.62              |
| 1:C:135:LYS:NZ  | 1:T:104:ASP:HB3 | 2.14                     | 0.62              |
| 1:M:91:ARG:NH1  | 1:i:54:GLY:O    | 2.32                     | 0.62              |
| 1:R:135:LYS:NZ  | 1:n:104:ASP:HB3 | 2.14                     | 0.62              |
| 1:B:54:GLY:O    | 1:X:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:B:113:GLN:NE2 | 1:B:195:ASN:O   | 2.31                     | 0.62              |
| 1:B:175:GLY:O   | 1:B:193:SER:OG  | 2.08                     | 0.62              |
| 1:C:91:ARG:NH1  | 1:Y:54:GLY:O    | 2.32                     | 0.62              |
| 1:I:91:ARG:NH1  | 1:e:54:GLY:O    | 2.32                     | 0.62              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:U:113:GLN:NE2 | 1:U:195:ASN:O   | 2.31                     | 0.62              |
| 1:X:60:GLU:O    | 1:X:63:SER:OG   | 2.10                     | 0.62              |
| 1:E:104:ASP:HB2 | 1:a:135:LYS:HZ3 | 1.64                     | 0.62              |
| 1:J:91:ARG:NH1  | 1:M:54:GLY:O    | 2.32                     | 0.62              |
| 1:J:197:LEU:O   | 1:J:199:VAL:N   | 2.33                     | 0.62              |
| 1:R:54:GLY:O    | 1:n:91:ARG:NH1  | 2.32                     | 0.62              |
| 1:T:197:LEU:O   | 1:T:199:VAL:N   | 2.33                     | 0.62              |
| 1:Z:197:LEU:O   | 1:Z:199:VAL:N   | 2.33                     | 0.62              |
| 1:d:175:GLY:O   | 1:d:193:SER:OG  | 2.08                     | 0.62              |
| 1:e:175:GLY:O   | 1:e:193:SER:OG  | 2.08                     | 0.62              |
| 1:A:175:GLY:O   | 1:A:193:SER:OG  | 2.08                     | 0.61              |
| 1:A:197:LEU:O   | 1:A:199:VAL:N   | 2.33                     | 0.61              |
| 1:D:91:ARG:NH1  | 1:S:54:GLY:O    | 2.32                     | 0.61              |
| 1:D:104:ASP:HB2 | 1:S:135:LYS:HZ3 | 1.65                     | 0.61              |
| 1:F:128:ASN:O   | 1:F:136:LYS:NZ  | 2.25                     | 0.61              |
| 1:N:113:GLN:NE2 | 1:N:195:ASN:O   | 2.31                     | 0.61              |
| 1:P:60:GLU:O    | 1:P:63:SER:OG   | 2.10                     | 0.61              |
| 1:P:197:LEU:O   | 1:P:199:VAL:N   | 2.33                     | 0.61              |
| 1:Q:91:ARG:NH1  | 1:m:54:GLY:O    | 2.32                     | 0.61              |
| 1:b:197:LEU:O   | 1:b:199:VAL:N   | 2.33                     | 0.61              |
| 1:l:197:LEU:O   | 1:l:199:VAL:N   | 2.33                     | 0.61              |
| 1:o:197:LEU:O   | 1:o:199:VAL:N   | 2.33                     | 0.61              |
| 1:K:54:GLY:O    | 1:L:91:ARG:NH1  | 2.32                     | 0.61              |
| 1:R:197:LEU:O   | 1:R:199:VAL:N   | 2.33                     | 0.61              |
| 1:d:197:LEU:O   | 1:d:199:VAL:N   | 2.33                     | 0.61              |
| 1:f:197:LEU:O   | 1:f:199:VAL:N   | 2.33                     | 0.61              |
| 1:g:113:GLN:NE2 | 1:g:195:ASN:O   | 2.31                     | 0.61              |
| 1:j:197:LEU:O   | 1:j:199:VAL:N   | 2.33                     | 0.61              |
| 1:A:91:ARG:NH1  | 1:W:54:GLY:O    | 2.32                     | 0.61              |
| 1:B:135:LYS:NZ  | 1:X:104:ASP:HB3 | 2.14                     | 0.61              |
| 1:H:54:GLY:O    | 1:d:91:ARG:NH1  | 2.32                     | 0.61              |
| 1:I:54:GLY:O    | 1:N:91:ARG:NH1  | 2.32                     | 0.61              |
| 1:K:197:LEU:O   | 1:K:199:VAL:N   | 2.33                     | 0.61              |
| 1:V:197:LEU:O   | 1:V:199:VAL:N   | 2.33                     | 0.61              |
| 1:e:197:LEU:O   | 1:e:199:VAL:N   | 2.33                     | 0.61              |
| 1:j:113:GLN:NE2 | 1:j:195:ASN:O   | 2.31                     | 0.61              |
| 1:A:135:LYS:NZ  | 1:V:104:ASP:HB3 | 2.14                     | 0.61              |
| 1:E:104:ASP:HB3 | 1:a:135:LYS:NZ  | 2.14                     | 0.61              |
| 1:F:197:LEU:O   | 1:F:199:VAL:N   | 2.33                     | 0.61              |
| 1:H:197:LEU:O   | 1:H:199:VAL:N   | 2.33                     | 0.61              |
| 1:J:135:LYS:NZ  | 1:f:104:ASP:HB3 | 2.14                     | 0.61              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:U:197:LEU:O   | 1:U:199:VAL:N   | 2.33                     | 0.61              |
| 1:n:197:LEU:O   | 1:n:199:VAL:N   | 2.33                     | 0.61              |
| 1:B:91:ARG:NH1  | 1:U:54:GLY:O    | 2.32                     | 0.61              |
| 1:C:197:LEU:O   | 1:C:199:VAL:N   | 2.33                     | 0.61              |
| 1:F:104:ASP:HB3 | 1:Q:135:LYS:NZ  | 2.14                     | 0.61              |
| 1:G:128:ASN:O   | 1:G:136:LYS:NZ  | 2.25                     | 0.61              |
| 1:I:104:ASP:HB3 | 1:e:135:LYS:NZ  | 2.14                     | 0.61              |
| 1:R:128:ASN:O   | 1:R:136:LYS:NZ  | 2.25                     | 0.61              |
| 1:R:135:LYS:HZ3 | 1:n:104:ASP:HB2 | 1.65                     | 0.61              |
| 1:D:135:LYS:NZ  | 1:Z:104:ASP:HB3 | 2.14                     | 0.61              |
| 1:L:197:LEU:O   | 1:L:199:VAL:N   | 2.33                     | 0.61              |
| 1:N:100:THR:OG1 | 1:N:202:PHE:HD2 | 1.73                     | 0.61              |
| 1:Q:104:ASP:HB3 | 1:m:135:LYS:NZ  | 2.14                     | 0.61              |
| 1:W:128:ASN:O   | 1:W:136:LYS:NZ  | 2.25                     | 0.61              |
| 1:c:197:LEU:O   | 1:c:199:VAL:N   | 2.33                     | 0.61              |
| 1:m:197:LEU:O   | 1:m:199:VAL:N   | 2.33                     | 0.61              |
| 1:C:104:ASP:HB2 | 1:Y:135:LYS:HZ3 | 1.65                     | 0.61              |
| 1:M:60:GLU:O    | 1:M:63:SER:OG   | 2.10                     | 0.61              |
| 1:M:197:LEU:O   | 1:M:199:VAL:N   | 2.33                     | 0.61              |
| 1:h:60:GLU:O    | 1:h:63:SER:OG   | 2.10                     | 0.61              |
| 1:h:175:GLY:O   | 1:h:193:SER:OG  | 2.08                     | 0.61              |
| 1:C:128:ASN:O   | 1:C:136:LYS:NZ  | 2.25                     | 0.61              |
| 1:D:197:LEU:O   | 1:D:199:VAL:N   | 2.33                     | 0.61              |
| 1:G:197:LEU:O   | 1:G:199:VAL:N   | 2.33                     | 0.61              |
| 1:J:104:ASP:HB3 | 1:M:135:LYS:NZ  | 2.14                     | 0.61              |
| 1:S:197:LEU:O   | 1:S:199:VAL:N   | 2.33                     | 0.61              |
| 1:W:197:LEU:O   | 1:W:199:VAL:N   | 2.33                     | 0.61              |
| 1:k:197:LEU:O   | 1:k:199:VAL:N   | 2.33                     | 0.61              |
| 1:B:197:LEU:O   | 1:B:199:VAL:N   | 2.33                     | 0.61              |
| 1:E:197:LEU:O   | 1:E:199:VAL:N   | 2.33                     | 0.61              |
| 1:I:197:LEU:O   | 1:I:199:VAL:N   | 2.33                     | 0.61              |
| 1:K:135:LYS:NZ  | 1:L:104:ASP:HB3 | 2.14                     | 0.61              |
| 1:P:135:LYS:CE  | 1:l:104:ASP:CB  | 2.79                     | 0.61              |
| 1:g:197:LEU:O   | 1:g:199:VAL:N   | 2.33                     | 0.61              |
| 1:i:197:LEU:O   | 1:i:199:VAL:N   | 2.33                     | 0.61              |
| 1:D:135:LYS:CE  | 1:Z:104:ASP:CB  | 2.79                     | 0.61              |
| 1:E:135:LYS:NZ  | 1:R:104:ASP:HB3 | 2.14                     | 0.61              |
| 1:I:104:ASP:HB2 | 1:e:135:LYS:HZ3 | 1.65                     | 0.61              |
| 1:I:135:LYS:CE  | 1:N:104:ASP:CB  | 2.79                     | 0.61              |
| 1:N:197:LEU:O   | 1:N:199:VAL:N   | 2.33                     | 0.61              |
| 1:O:104:ASP:HB3 | 1:k:135:LYS:NZ  | 2.14                     | 0.61              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:135:LYS:CE  | 1:X:104:ASP:CB  | 2.79                     | 0.60              |
| 1:G:104:ASP:HB3 | 1:c:135:LYS:NZ  | 2.14                     | 0.60              |
| 1:G:104:ASP:HB2 | 1:c:135:LYS:HZ3 | 1.65                     | 0.60              |
| 1:G:135:LYS:NZ  | 1:P:104:ASP:HB3 | 2.14                     | 0.60              |
| 1:G:175:GLY:O   | 1:G:193:SER:OG  | 2.08                     | 0.60              |
| 1:R:135:LYS:CE  | 1:n:104:ASP:CB  | 2.79                     | 0.60              |
| 1:N:135:LYS:CE  | 1:j:104:ASP:CB  | 2.79                     | 0.60              |
| 1:O:197:LEU:O   | 1:O:199:VAL:N   | 2.33                     | 0.60              |
| 1:Y:197:LEU:O   | 1:Y:199:VAL:N   | 2.33                     | 0.60              |
| 1:a:197:LEU:O   | 1:a:199:VAL:N   | 2.33                     | 0.60              |
| 1:D:60:GLU:O    | 1:D:63:SER:OG   | 2.10                     | 0.60              |
| 1:D:135:LYS:HZ3 | 1:Z:104:ASP:HB2 | 1.67                     | 0.60              |
| 1:K:104:ASP:HB3 | 1:g:135:LYS:NZ  | 2.14                     | 0.60              |
| 1:L:175:GLY:O   | 1:L:193:SER:OG  | 2.08                     | 0.60              |
| 1:Q:197:LEU:O   | 1:Q:199:VAL:N   | 2.33                     | 0.60              |
| 1:X:197:LEU:O   | 1:X:199:VAL:N   | 2.33                     | 0.60              |
| 1:A:104:ASP:HB3 | 1:W:135:LYS:NZ  | 2.14                     | 0.60              |
| 1:B:135:LYS:HZ3 | 1:X:104:ASP:HB2 | 1.67                     | 0.60              |
| 1:P:135:LYS:NZ  | 1:l:104:ASP:HB3 | 2.14                     | 0.60              |
| 1:F:135:LYS:NZ  | 1:b:104:ASP:HB3 | 2.14                     | 0.60              |
| 1:K:104:ASP:HB2 | 1:g:135:LYS:HZ3 | 1.65                     | 0.60              |
| 1:L:135:LYS:NZ  | 1:h:104:ASP:HB3 | 2.14                     | 0.60              |
| 1:S:128:ASN:O   | 1:S:136:LYS:NZ  | 2.25                     | 0.60              |
| 1:Y:128:ASN:O   | 1:Y:136:LYS:NZ  | 2.25                     | 0.60              |
| 1:F:60:GLU:O    | 1:F:63:SER:OG   | 2.10                     | 0.60              |
| 1:H:60:GLU:O    | 1:H:63:SER:OG   | 2.10                     | 0.60              |
| 1:N:60:GLU:O    | 1:N:63:SER:OG   | 2.10                     | 0.60              |
| 1:h:197:LEU:O   | 1:h:199:VAL:N   | 2.33                     | 0.60              |
| 1:B:104:ASP:HB3 | 1:U:135:LYS:NZ  | 2.14                     | 0.60              |
| 1:H:135:LYS:CE  | 1:d:104:ASP:CB  | 2.79                     | 0.60              |
| 1:a:128:ASN:O   | 1:a:136:LYS:NZ  | 2.25                     | 0.60              |
| 1:m:100:THR:OG1 | 1:m:202:PHE:HD2 | 1.73                     | 0.60              |
| 1:A:128:ASN:O   | 1:A:136:LYS:NZ  | 2.25                     | 0.60              |
| 1:C:175:GLY:O   | 1:C:193:SER:OG  | 2.08                     | 0.59              |
| 1:j:128:ASN:O   | 1:j:136:LYS:NZ  | 2.25                     | 0.59              |
| 1:C:104:ASP:CB  | 1:Y:135:LYS:CE  | 2.79                     | 0.59              |
| 1:N:135:LYS:HZ3 | 1:j:104:ASP:HB2 | 1.67                     | 0.59              |
| 1:N:135:LYS:NZ  | 1:j:104:ASP:HB3 | 2.14                     | 0.59              |
| 1:J:135:LYS:HZ3 | 1:f:104:ASP:HB2 | 1.67                     | 0.59              |
| 1:J:104:ASP:CB  | 1:M:135:LYS:CE  | 2.79                     | 0.59              |
| 1:J:135:LYS:CE  | 1:f:104:ASP:CB  | 2.79                     | 0.59              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:S:104:ASP:HB3 | 1:o:135:LYS:NZ  | 2.14                     | 0.59              |
| 1:I:135:LYS:NZ  | 1:N:104:ASP:HB3 | 2.14                     | 0.59              |
| 1:C:135:LYS:CE  | 1:T:104:ASP:CB  | 2.79                     | 0.59              |
| 1:D:104:ASP:HB3 | 1:S:135:LYS:NZ  | 2.14                     | 0.59              |
| 1:H:72:LEU:O    | 1:H:75:THR:OG1  | 2.21                     | 0.59              |
| 1:d:128:ASN:O   | 1:d:136:LYS:NZ  | 2.25                     | 0.59              |
| 1:e:72:LEU:O    | 1:e:75:THR:OG1  | 2.21                     | 0.59              |
| 1:m:100:THR:HG1 | 1:m:202:PHE:HE2 | 1.41                     | 0.59              |
| 1:A:135:LYS:HZ3 | 1:V:104:ASP:HB2 | 1.68                     | 0.59              |
| 1:X:72:LEU:O    | 1:X:75:THR:OG1  | 2.21                     | 0.59              |
| 1:j:72:LEU:O    | 1:j:75:THR:OG1  | 2.21                     | 0.59              |
| 1:L:135:LYS:HZ3 | 1:h:104:ASP:HB2 | 1.68                     | 0.58              |
| 1:M:104:ASP:CB  | 1:i:135:LYS:CE  | 2.79                     | 0.58              |
| 1:S:72:LEU:O    | 1:S:75:THR:OG1  | 2.21                     | 0.58              |
| 1:F:104:ASP:CB  | 1:Q:135:LYS:HZ3 | 2.16                     | 0.58              |
| 1:l:100:THR:HG1 | 1:l:202:PHE:HE2 | 1.45                     | 0.58              |
| 1:J:72:LEU:O    | 1:J:75:THR:OG1  | 2.21                     | 0.58              |
| 1:O:72:LEU:O    | 1:O:75:THR:OG1  | 2.21                     | 0.58              |
| 1:T:72:LEU:O    | 1:T:75:THR:OG1  | 2.21                     | 0.58              |
| 1:l:128:ASN:O   | 1:l:136:LYS:NZ  | 2.25                     | 0.58              |
| 1:L:72:LEU:O    | 1:L:75:THR:OG1  | 2.21                     | 0.58              |
| 1:U:72:LEU:O    | 1:U:75:THR:OG1  | 2.21                     | 0.58              |
| 1:X:128:ASN:O   | 1:X:136:LYS:NZ  | 2.25                     | 0.58              |
| 1:F:135:LYS:HZ3 | 1:b:104:ASP:HB2 | 1.68                     | 0.58              |
| 1:N:72:LEU:O    | 1:N:75:THR:OG1  | 2.21                     | 0.58              |
| 1:R:72:LEU:O    | 1:R:75:THR:OG1  | 2.21                     | 0.58              |
| 1:E:135:LYS:HZ3 | 1:R:104:ASP:HB2 | 1.68                     | 0.58              |
| 1:F:72:LEU:O    | 1:F:75:THR:OG1  | 2.21                     | 0.58              |
| 1:I:72:LEU:O    | 1:I:75:THR:OG1  | 2.21                     | 0.58              |
| 1:I:100:THR:O   | 1:e:156:VAL:O   | 2.22                     | 0.58              |
| 1:O:104:ASP:HB2 | 1:k:135:LYS:HZ3 | 1.68                     | 0.58              |
| 1:e:128:ASN:O   | 1:e:136:LYS:NZ  | 2.25                     | 0.58              |
| 1:G:72:LEU:O    | 1:G:75:THR:OG1  | 2.21                     | 0.58              |
| 1:I:156:VAL:O   | 1:N:100:THR:O   | 2.22                     | 0.58              |
| 1:K:100:THR:O   | 1:g:156:VAL:O   | 2.22                     | 0.58              |
| 1:k:72:LEU:O    | 1:k:75:THR:OG1  | 2.21                     | 0.58              |
| 1:B:100:THR:O   | 1:U:156:VAL:O   | 2.22                     | 0.58              |
| 1:B:156:VAL:O   | 1:X:100:THR:O   | 2.22                     | 0.58              |
| 1:G:135:LYS:HZ3 | 1:P:104:ASP:HB2 | 1.67                     | 0.58              |
| 1:K:156:VAL:O   | 1:L:100:THR:O   | 2.22                     | 0.58              |
| 1:N:156:VAL:O   | 1:j:100:THR:O   | 2.22                     | 0.58              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:S:100:THR:O  | 1:o:156:VAL:O   | 2.22                     | 0.58              |
| 1:h:72:LEU:O   | 1:h:75:THR:OG1  | 2.21                     | 0.58              |
| 1:o:72:LEU:O   | 1:o:75:THR:OG1  | 2.21                     | 0.58              |
| 1:A:60:GLU:O   | 1:A:63:SER:OG   | 2.10                     | 0.58              |
| 1:B:72:LEU:O   | 1:B:75:THR:OG1  | 2.21                     | 0.58              |
| 1:D:100:THR:O  | 1:S:156:VAL:O   | 2.22                     | 0.58              |
| 1:L:156:VAL:O  | 1:h:100:THR:O   | 2.22                     | 0.58              |
| 1:A:156:VAL:O  | 1:V:100:THR:O   | 2.22                     | 0.57              |
| 1:D:72:LEU:O   | 1:D:75:THR:OG1  | 2.21                     | 0.57              |
| 1:c:72:LEU:O   | 1:c:75:THR:OG1  | 2.21                     | 0.57              |
| 1:A:72:LEU:O   | 1:A:75:THR:OG1  | 2.21                     | 0.57              |
| 1:d:72:LEU:O   | 1:d:75:THR:OG1  | 2.21                     | 0.57              |
| 1:A:100:THR:O  | 1:W:156:VAL:O   | 2.22                     | 0.57              |
| 1:D:46:LEU:O   | 1:D:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:G:156:VAL:O  | 1:P:100:THR:O   | 2.22                     | 0.57              |
| 1:L:105:LYS:CD | 1:U:51:LYS:HZ2  | 2.17                     | 0.57              |
| 1:e:46:LEU:O   | 1:e:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:g:46:LEU:O   | 1:g:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:j:46:LEU:O   | 1:j:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:m:46:LEU:O   | 1:m:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:D:156:VAL:O  | 1:Z:100:THR:O   | 2.22                     | 0.57              |
| 1:P:46:LEU:O   | 1:P:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:P:156:VAL:O  | 1:l:100:THR:O   | 2.22                     | 0.57              |
| 1:V:46:LEU:O   | 1:V:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:V:72:LEU:O   | 1:V:75:THR:OG1  | 2.21                     | 0.57              |
| 1:f:72:LEU:O   | 1:f:75:THR:OG1  | 2.21                     | 0.57              |
| 1:B:46:LEU:O   | 1:B:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:G:100:THR:O  | 1:c:156:VAL:O   | 2.22                     | 0.57              |
| 1:X:46:LEU:O   | 1:X:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:Y:72:LEU:O   | 1:Y:75:THR:OG1  | 2.21                     | 0.57              |
| 1:b:46:LEU:O   | 1:b:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:c:128:ASN:O  | 1:c:136:LYS:NZ  | 2.25                     | 0.57              |
| 1:h:46:LEU:O   | 1:h:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:o:46:LEU:O   | 1:o:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:H:100:THR:O  | 1:O:156:VAL:O   | 2.22                     | 0.57              |
| 1:K:46:LEU:O   | 1:K:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:K:72:LEU:O   | 1:K:75:THR:OG1  | 2.21                     | 0.57              |
| 1:M:104:ASP:CB | 1:i:135:LYS:HZ3 | 2.15                     | 0.57              |
| 1:Z:46:LEU:O   | 1:Z:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:l:46:LEU:O   | 1:l:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:m:72:LEU:O   | 1:m:75:THR:OG1  | 2.21                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:46:LEU:O    | 1:F:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:J:100:THR:O   | 1:M:156:VAL:O   | 2.22                     | 0.57              |
| 1:L:46:LEU:O    | 1:L:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:M:100:THR:O   | 1:i:156:VAL:O   | 2.22                     | 0.57              |
| 1:Q:46:LEU:O    | 1:Q:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:R:46:LEU:O    | 1:R:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:S:46:LEU:O    | 1:S:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:W:46:LEU:O    | 1:W:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:Z:128:ASN:O   | 1:Z:136:LYS:NZ  | 2.25                     | 0.57              |
| 1:c:46:LEU:O    | 1:c:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:f:46:LEU:O    | 1:f:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:i:46:LEU:O    | 1:i:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:E:100:THR:O   | 1:a:156:VAL:O   | 2.22                     | 0.57              |
| 1:M:128:ASN:O   | 1:M:136:LYS:NZ  | 2.25                     | 0.57              |
| 1:N:46:LEU:O    | 1:N:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:O:100:THR:O   | 1:k:156:VAL:O   | 2.22                     | 0.57              |
| 1:Q:100:THR:O   | 1:m:156:VAL:O   | 2.22                     | 0.57              |
| 1:U:46:LEU:O    | 1:U:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:k:46:LEU:O    | 1:k:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:A:105:LYS:CD  | 1:g:51:LYS:HZ1  | 2.14                     | 0.57              |
| 1:C:100:THR:O   | 1:Y:156:VAL:O   | 2.22                     | 0.57              |
| 1:P:72:LEU:O    | 1:P:75:THR:OG1  | 2.21                     | 0.57              |
| 1:P:135:LYS:HZ3 | 1:l:104:ASP:CB  | 2.16                     | 0.57              |
| 1:T:46:LEU:O    | 1:T:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:a:46:LEU:O    | 1:a:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:E:156:VAL:O   | 1:R:100:THR:O   | 2.22                     | 0.57              |
| 1:I:135:LYS:HZ3 | 1:N:104:ASP:HB2 | 1.68                     | 0.57              |
| 1:J:46:LEU:O    | 1:J:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:Q:72:LEU:O    | 1:Q:75:THR:OG1  | 2.21                     | 0.57              |
| 1:Q:104:ASP:CB  | 1:m:135:LYS:CE  | 2.79                     | 0.57              |
| 1:d:46:LEU:O    | 1:d:50:GLU:HG2  | 2.05                     | 0.57              |
| 1:A:46:LEU:O    | 1:A:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:A:104:ASP:CB  | 1:W:135:LYS:CE  | 2.79                     | 0.56              |
| 1:F:100:THR:O   | 1:Q:156:VAL:O   | 2.22                     | 0.56              |
| 1:I:46:LEU:O    | 1:I:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:J:156:VAL:O   | 1:f:100:THR:O   | 2.22                     | 0.56              |
| 1:M:72:LEU:O    | 1:M:75:THR:OG1  | 2.21                     | 0.56              |
| 1:Y:46:LEU:O    | 1:Y:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:B:84:HIS:CE1  | 1:U:50:GLU:CB   | 2.86                     | 0.56              |
| 1:H:46:LEU:O    | 1:H:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:M:46:LEU:O    | 1:M:50:GLU:HG2  | 2.05                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:a:72:LEU:O    | 1:a:75:THR:OG1  | 2.21                     | 0.56              |
| 1:C:156:VAL:O   | 1:T:100:THR:O   | 2.22                     | 0.56              |
| 1:F:156:VAL:O   | 1:b:100:THR:O   | 2.22                     | 0.56              |
| 1:J:104:ASP:CB  | 1:M:135:LYS:HZ3 | 2.16                     | 0.56              |
| 1:O:46:LEU:O    | 1:O:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:R:156:VAL:O   | 1:n:100:THR:O   | 2.22                     | 0.56              |
| 1:W:72:LEU:O    | 1:W:75:THR:OG1  | 2.21                     | 0.56              |
| 1:D:104:ASP:CB  | 1:S:135:LYS:CE  | 2.79                     | 0.56              |
| 1:n:46:LEU:O    | 1:n:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:E:46:LEU:O    | 1:E:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:G:46:LEU:O    | 1:G:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:H:156:VAL:O   | 1:d:100:THR:O   | 2.22                     | 0.56              |
| 1:K:104:ASP:CB  | 1:g:135:LYS:CE  | 2.79                     | 0.56              |
| 1:E:104:ASP:CB  | 1:a:135:LYS:CE  | 2.79                     | 0.56              |
| 1:b:72:LEU:O    | 1:b:75:THR:OG1  | 2.21                     | 0.56              |
| 1:n:72:LEU:O    | 1:n:75:THR:OG1  | 2.21                     | 0.56              |
| 1:E:72:LEU:O    | 1:E:75:THR:OG1  | 2.21                     | 0.56              |
| 1:G:104:ASP:CB  | 1:c:135:LYS:CE  | 2.79                     | 0.56              |
| 1:S:104:ASP:CB  | 1:o:135:LYS:CE  | 2.79                     | 0.56              |
| 1:C:46:LEU:O    | 1:C:50:GLU:HG2  | 2.05                     | 0.56              |
| 1:H:104:ASP:HB2 | 1:O:135:LYS:HZ3 | 1.71                     | 0.56              |
| 1:o:128:ASN:O   | 1:o:136:LYS:NZ  | 2.25                     | 0.56              |
| 1:F:104:ASP:CB  | 1:Q:135:LYS:CE  | 2.79                     | 0.55              |
| 1:A:135:LYS:CE  | 1:V:104:ASP:CB  | 2.79                     | 0.55              |
| 1:C:72:LEU:O    | 1:C:75:THR:OG1  | 2.21                     | 0.55              |
| 1:Z:72:LEU:O    | 1:Z:75:THR:OG1  | 2.21                     | 0.55              |
| 1:O:104:ASP:CB  | 1:k:135:LYS:CE  | 2.79                     | 0.55              |
| 1:R:178:ALA:HB3 | 1:R:189:ALA:O   | 2.07                     | 0.55              |
| 1:O:178:ALA:HB3 | 1:O:189:ALA:O   | 2.07                     | 0.55              |
| 1:P:178:ALA:HB3 | 1:P:189:ALA:O   | 2.07                     | 0.55              |
| 1:Q:178:ALA:HB3 | 1:Q:189:ALA:O   | 2.07                     | 0.55              |
| 1:R:135:LYS:HZ3 | 1:n:104:ASP:CB  | 2.19                     | 0.55              |
| 1:D:104:ASP:CB  | 1:S:135:LYS:HZ3 | 2.19                     | 0.55              |
| 1:I:104:ASP:CB  | 1:e:135:LYS:HZ3 | 2.19                     | 0.55              |
| 1:N:128:ASN:O   | 1:N:136:LYS:NZ  | 2.25                     | 0.55              |
| 1:T:178:ALA:HB3 | 1:T:189:ALA:O   | 2.07                     | 0.55              |
| 1:B:104:ASP:CB  | 1:U:135:LYS:CE  | 2.79                     | 0.55              |
| 1:E:104:ASP:CB  | 1:a:135:LYS:HZ3 | 2.18                     | 0.55              |
| 1:F:178:ALA:HB3 | 1:F:189:ALA:O   | 2.07                     | 0.55              |
| 1:I:104:ASP:CB  | 1:e:135:LYS:CE  | 2.79                     | 0.55              |
| 1:S:178:ALA:HB3 | 1:S:189:ALA:O   | 2.07                     | 0.55              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:l:72:LEU:O    | 1:l:75:THR:OG1  | 2.21                     | 0.55              |
| 1:D:178:ALA:HB3 | 1:D:189:ALA:O   | 2.07                     | 0.55              |
| 1:K:135:LYS:CE  | 1:L:104:ASP:CB  | 2.79                     | 0.55              |
| 1:K:135:LYS:HZ3 | 1:L:104:ASP:CB  | 2.16                     | 0.55              |
| 1:j:178:ALA:HB3 | 1:j:189:ALA:O   | 2.07                     | 0.55              |
| 1:l:178:ALA:HB3 | 1:l:189:ALA:O   | 2.07                     | 0.55              |
| 1:m:178:ALA:HB3 | 1:m:189:ALA:O   | 2.07                     | 0.55              |
| 1:E:135:LYS:CE  | 1:R:104:ASP:CB  | 2.79                     | 0.54              |
| 1:M:178:ALA:HB3 | 1:M:189:ALA:O   | 2.07                     | 0.54              |
| 1:N:178:ALA:HB3 | 1:N:189:ALA:O   | 2.07                     | 0.54              |
| 1:c:178:ALA:HB3 | 1:c:189:ALA:O   | 2.07                     | 0.54              |
| 1:k:178:ALA:HB3 | 1:k:189:ALA:O   | 2.07                     | 0.54              |
| 1:n:178:ALA:HB3 | 1:n:189:ALA:O   | 2.07                     | 0.54              |
| 1:C:178:ALA:HB3 | 1:C:189:ALA:O   | 2.07                     | 0.54              |
| 1:G:135:LYS:CE  | 1:P:104:ASP:CB  | 2.79                     | 0.54              |
| 1:H:178:ALA:HB3 | 1:H:189:ALA:O   | 2.07                     | 0.54              |
| 1:i:178:ALA:HB3 | 1:i:189:ALA:O   | 2.07                     | 0.54              |
| 1:B:178:ALA:HB3 | 1:B:189:ALA:O   | 2.07                     | 0.54              |
| 1:C:104:ASP:CB  | 1:Y:135:LYS:HZ3 | 2.19                     | 0.54              |
| 1:E:178:ALA:HB3 | 1:E:189:ALA:O   | 2.07                     | 0.54              |
| 1:G:178:ALA:HB3 | 1:G:189:ALA:O   | 2.07                     | 0.54              |
| 1:f:178:ALA:HB3 | 1:f:189:ALA:O   | 2.07                     | 0.54              |
| 1:A:178:ALA:HB3 | 1:A:189:ALA:O   | 2.07                     | 0.54              |
| 1:C:135:LYS:HZ3 | 1:T:104:ASP:HB2 | 1.72                     | 0.54              |
| 1:F:135:LYS:CE  | 1:b:104:ASP:CB  | 2.79                     | 0.54              |
| 1:Q:104:ASP:CB  | 1:m:135:LYS:HZ3 | 2.16                     | 0.54              |
| 1:a:178:ALA:HB3 | 1:a:189:ALA:O   | 2.07                     | 0.54              |
| 1:b:178:ALA:HB3 | 1:b:189:ALA:O   | 2.07                     | 0.54              |
| 1:d:178:ALA:HB3 | 1:d:189:ALA:O   | 2.07                     | 0.54              |
| 1:e:178:ALA:HB3 | 1:e:189:ALA:O   | 2.07                     | 0.54              |
| 1:g:178:ALA:HB3 | 1:g:189:ALA:O   | 2.07                     | 0.54              |
| 1:h:178:ALA:HB3 | 1:h:189:ALA:O   | 2.07                     | 0.54              |
| 1:G:135:LYS:HZ3 | 1:P:104:ASP:CB  | 2.20                     | 0.54              |
| 1:U:178:ALA:HB3 | 1:U:189:ALA:O   | 2.07                     | 0.54              |
| 1:V:178:ALA:HB3 | 1:V:189:ALA:O   | 2.07                     | 0.54              |
| 1:H:104:ASP:CB  | 1:O:135:LYS:CE  | 2.79                     | 0.54              |
| 1:H:135:LYS:HZ3 | 1:d:104:ASP:HB2 | 1.72                     | 0.54              |
| 1:K:104:ASP:CB  | 1:g:135:LYS:HZ3 | 2.19                     | 0.54              |
| 1:K:178:ALA:HB3 | 1:K:189:ALA:O   | 2.07                     | 0.54              |
| 1:o:178:ALA:HB3 | 1:o:189:ALA:O   | 2.07                     | 0.54              |
| 1:A:104:ASP:CB  | 1:W:135:LYS:HZ3 | 2.18                     | 0.54              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:297:GLN:OE1 | 1:B:297:GLN:N   | 2.41                     | 0.54              |
| 1:M:51:LYS:HZ2  | 1:T:105:LYS:CD  | 2.21                     | 0.54              |
| 1:W:178:ALA:HB3 | 1:W:189:ALA:O   | 2.07                     | 0.54              |
| 1:X:297:GLN:OE1 | 1:X:297:GLN:N   | 2.41                     | 0.54              |
| 1:Y:178:ALA:HB3 | 1:Y:189:ALA:O   | 2.07                     | 0.54              |
| 1:K:51:LYS:HZ2  | 1:V:105:LYS:CD  | 2.20                     | 0.54              |
| 1:Z:178:ALA:HB3 | 1:Z:189:ALA:O   | 2.07                     | 0.54              |
| 1:o:297:GLN:N   | 1:o:297:GLN:OE1 | 2.41                     | 0.54              |
| 1:S:297:GLN:OE1 | 1:S:297:GLN:N   | 2.41                     | 0.53              |
| 1:U:297:GLN:OE1 | 1:U:297:GLN:N   | 2.41                     | 0.53              |
| 1:L:178:ALA:HB3 | 1:L:189:ALA:O   | 2.07                     | 0.53              |
| 1:C:51:LYS:HZ2  | 1:d:105:LYS:CD  | 2.19                     | 0.53              |
| 1:D:297:GLN:N   | 1:D:297:GLN:OE1 | 2.41                     | 0.53              |
| 1:I:178:ALA:HB3 | 1:I:189:ALA:O   | 2.07                     | 0.53              |
| 1:J:178:ALA:HB3 | 1:J:189:ALA:O   | 2.07                     | 0.53              |
| 1:X:178:ALA:HB3 | 1:X:189:ALA:O   | 2.07                     | 0.53              |
| 1:I:105:LYS:CD  | 1:o:51:LYS:HZ2  | 2.21                     | 0.53              |
| 1:j:297:GLN:OE1 | 1:j:297:GLN:N   | 2.41                     | 0.53              |
| 1:B:135:LYS:HZ3 | 1:X:104:ASP:CB  | 2.20                     | 0.53              |
| 1:L:135:LYS:CE  | 1:h:104:ASP:CB  | 2.79                     | 0.53              |
| 1:l:297:GLN:N   | 1:l:297:GLN:OE1 | 2.41                     | 0.53              |
| 1:n:177:ASP:O   | 1:n:227:GLN:NE2 | 2.41                     | 0.53              |
| 1:P:297:GLN:OE1 | 1:P:297:GLN:N   | 2.41                     | 0.53              |
| 1:S:104:ASP:HB2 | 1:o:135:LYS:HZ3 | 1.74                     | 0.53              |
| 1:Z:297:GLN:OE1 | 1:Z:297:GLN:N   | 2.41                     | 0.53              |
| 1:G:297:GLN:OE1 | 1:G:297:GLN:N   | 2.41                     | 0.53              |
| 1:N:297:GLN:OE1 | 1:N:297:GLN:N   | 2.41                     | 0.53              |
| 1:c:177:ASP:O   | 1:c:227:GLN:NE2 | 2.41                     | 0.53              |
| 1:g:297:GLN:N   | 1:g:297:GLN:OE1 | 2.41                     | 0.53              |
| 1:I:51:LYS:HZ1  | 1:X:105:LYS:CD  | 2.14                     | 0.53              |
| 1:F:135:LYS:HZ3 | 1:b:104:ASP:CB  | 2.22                     | 0.52              |
| 1:W:177:ASP:O   | 1:W:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:c:297:GLN:OE1 | 1:c:297:GLN:N   | 2.41                     | 0.52              |
| 1:n:84:HIS:O    | 1:n:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:D:135:LYS:HZ3 | 1:Z:104:ASP:CB  | 2.20                     | 0.52              |
| 1:J:105:LYS:CD  | 1:W:51:LYS:HZ2  | 2.21                     | 0.52              |
| 1:K:297:GLN:OE1 | 1:K:297:GLN:N   | 2.41                     | 0.52              |
| 1:V:297:GLN:OE1 | 1:V:297:GLN:N   | 2.41                     | 0.52              |
| 1:a:177:ASP:O   | 1:a:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:F:84:HIS:O    | 1:F:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:H:84:HIS:O    | 1:H:88:GLN:HG2  | 2.10                     | 0.52              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:84:HIS:O    | 1:K:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:N:84:HIS:O    | 1:N:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:P:84:HIS:O    | 1:P:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:Q:84:HIS:O    | 1:Q:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:S:84:HIS:O    | 1:S:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:V:84:HIS:O    | 1:V:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:X:84:HIS:O    | 1:X:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:Z:177:ASP:O   | 1:Z:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:a:84:HIS:O    | 1:a:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:b:177:ASP:O   | 1:b:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:h:177:ASP:O   | 1:h:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:I:297:GLN:N   | 1:I:297:GLN:OE1 | 2.41                     | 0.52              |
| 1:J:84:HIS:O    | 1:J:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:T:84:HIS:O    | 1:T:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:Y:177:ASP:O   | 1:Y:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:f:84:HIS:O    | 1:f:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:f:177:ASP:O   | 1:f:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:A:297:GLN:N   | 1:A:297:GLN:OE1 | 2.41                     | 0.52              |
| 1:I:84:HIS:O    | 1:I:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:L:84:HIS:O    | 1:L:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:L:297:GLN:N   | 1:L:297:GLN:OE1 | 2.41                     | 0.52              |
| 1:R:84:HIS:O    | 1:R:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:U:84:HIS:O    | 1:U:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:e:297:GLN:OE1 | 1:e:297:GLN:N   | 2.41                     | 0.52              |
| 1:l:84:HIS:O    | 1:l:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:m:297:GLN:OE1 | 1:m:297:GLN:N   | 2.41                     | 0.52              |
| 1:A:84:HIS:O    | 1:A:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:B:104:ASP:HB2 | 1:U:135:LYS:HZ3 | 1.75                     | 0.52              |
| 1:O:84:HIS:O    | 1:O:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:d:84:HIS:O    | 1:d:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:e:177:ASP:O   | 1:e:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:o:84:HIS:O    | 1:o:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:I:135:LYS:HZ3 | 1:N:104:ASP:CB  | 2.22                     | 0.52              |
| 1:M:84:HIS:O    | 1:M:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:Y:84:HIS:O    | 1:Y:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:d:177:ASP:O   | 1:d:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:B:105:LYS:CD  | 1:e:51:LYS:HZ2  | 2.22                     | 0.52              |
| 1:W:84:HIS:O    | 1:W:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:W:297:GLN:N   | 1:W:297:GLN:OE1 | 2.41                     | 0.52              |
| 1:h:297:GLN:OE1 | 1:h:297:GLN:N   | 2.41                     | 0.52              |
| 1:k:84:HIS:O    | 1:k:88:GLN:HG2  | 2.10                     | 0.52              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:135:LYS:HZ3 | 1:R:104:ASP:CB  | 2.22                     | 0.52              |
| 1:Q:297:GLN:N   | 1:Q:297:GLN:OE1 | 2.41                     | 0.52              |
| 1:c:84:HIS:O    | 1:c:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:g:177:ASP:O   | 1:g:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:h:84:HIS:O    | 1:h:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:i:84:HIS:O    | 1:i:88:GLN:HG2  | 2.10                     | 0.52              |
| 1:m:177:ASP:O   | 1:m:227:GLN:NE2 | 2.41                     | 0.52              |
| 1:Z:84:HIS:O    | 1:Z:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:D:84:HIS:O    | 1:D:88:GLN:HG2  | 2.09                     | 0.51              |
| 1:F:51:LYS:HZ2  | 1:l:105:LYS:CD  | 2.22                     | 0.51              |
| 1:L:135:LYS:HZ3 | 1:h:104:ASP:CB  | 2.22                     | 0.51              |
| 1:R:297:GLN:OE1 | 1:R:297:GLN:N   | 2.41                     | 0.51              |
| 1:X:177:ASP:O   | 1:X:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:n:297:GLN:OE1 | 1:n:297:GLN:N   | 2.41                     | 0.51              |
| 1:o:55:GLN:O    | 1:o:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:B:51:LYS:HZ1  | 1:h:105:LYS:CD  | 2.14                     | 0.51              |
| 1:C:84:HIS:O    | 1:C:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:E:297:GLN:OE1 | 1:E:297:GLN:N   | 2.41                     | 0.51              |
| 1:G:84:HIS:O    | 1:G:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:G:105:LYS:CD  | 1:m:51:LYS:HZ2  | 2.22                     | 0.51              |
| 1:c:55:GLN:O    | 1:c:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:g:84:HIS:O    | 1:g:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:i:177:ASP:O   | 1:i:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:i:297:GLN:OE1 | 1:i:297:GLN:N   | 2.41                     | 0.51              |
| 1:m:55:GLN:O    | 1:m:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:o:177:ASP:O   | 1:o:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:P:177:ASP:O   | 1:P:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:k:177:ASP:O   | 1:k:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:B:84:HIS:O    | 1:B:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:E:84:HIS:O    | 1:E:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:F:297:GLN:OE1 | 1:F:297:GLN:N   | 2.41                     | 0.51              |
| 1:M:297:GLN:OE1 | 1:M:297:GLN:N   | 2.41                     | 0.51              |
| 1:V:177:ASP:O   | 1:V:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:a:297:GLN:OE1 | 1:a:297:GLN:N   | 2.41                     | 0.51              |
| 1:b:84:HIS:O    | 1:b:88:GLN:HG2  | 2.09                     | 0.51              |
| 1:e:55:GLN:O    | 1:e:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:m:84:HIS:O    | 1:m:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:G:104:ASP:CB  | 1:c:135:LYS:HZ3 | 2.19                     | 0.51              |
| 1:T:297:GLN:OE1 | 1:T:297:GLN:N   | 2.41                     | 0.51              |
| 1:g:55:GLN:O    | 1:g:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:j:84:HIS:O    | 1:j:88:GLN:HG2  | 2.10                     | 0.51              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:297:GLN:OE1 | 1:J:297:GLN:N   | 2.41                     | 0.51              |
| 1:R:177:ASP:O   | 1:R:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:S:55:GLN:O    | 1:S:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:U:55:GLN:O    | 1:U:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:G:55:GLN:O    | 1:G:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:O:104:ASP:CB  | 1:k:135:LYS:HZ3 | 2.22                     | 0.51              |
| 1:Q:55:GLN:O    | 1:Q:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:T:177:ASP:O   | 1:T:227:GLN:NE2 | 2.41                     | 0.51              |
| 1:C:297:GLN:OE1 | 1:C:297:GLN:N   | 2.41                     | 0.51              |
| 1:e:84:HIS:O    | 1:e:88:GLN:HG2  | 2.10                     | 0.51              |
| 1:k:297:GLN:OE1 | 1:k:297:GLN:N   | 2.41                     | 0.51              |
| 1:E:51:LYS:HZ2  | 1:b:105:LYS:CD  | 2.22                     | 0.51              |
| 1:F:105:LYS:CD  | 1:a:51:LYS:HZ2  | 2.23                     | 0.51              |
| 1:I:55:GLN:O    | 1:I:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:K:55:GLN:O    | 1:K:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:M:55:GLN:O    | 1:M:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:W:55:GLN:O    | 1:W:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:b:297:GLN:OE1 | 1:b:297:GLN:N   | 2.41                     | 0.51              |
| 1:i:55:GLN:O    | 1:i:59:LEU:HB2  | 2.11                     | 0.51              |
| 1:J:55:GLN:O    | 1:J:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:V:56:ILE:HG12 | 1:V:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:a:55:GLN:O    | 1:a:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:b:56:ILE:HG12 | 1:b:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:d:55:GLN:O    | 1:d:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:f:297:GLN:OE1 | 1:f:297:GLN:N   | 2.41                     | 0.50              |
| 1:l:100:THR:CB  | 1:l:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:D:55:GLN:O    | 1:D:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:E:56:ILE:HG12 | 1:E:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:N:177:ASP:O   | 1:N:227:GLN:NE2 | 2.41                     | 0.50              |
| 1:Q:100:THR:CB  | 1:Q:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:R:56:ILE:HG12 | 1:R:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:T:100:THR:CB  | 1:T:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:Y:297:GLN:OE1 | 1:Y:297:GLN:N   | 2.41                     | 0.50              |
| 1:f:56:ILE:HG12 | 1:f:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:i:56:ILE:HG12 | 1:i:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:i:100:THR:CB  | 1:i:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:j:55:GLN:O    | 1:j:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:m:56:ILE:HG12 | 1:m:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:A:55:GLN:O    | 1:A:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:F:56:ILE:HG12 | 1:F:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:H:56:ILE:HG12 | 1:H:256:LEU:HB3 | 1.94                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:100:THR:CB  | 1:H:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:M:56:ILE:HG12 | 1:M:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:N:135:LYS:HZ3 | 1:j:104:ASP:CB  | 2.20                     | 0.50              |
| 1:O:51:LYS:HZ1  | 1:R:105:LYS:CD  | 2.15                     | 0.50              |
| 1:O:56:ILE:HG12 | 1:O:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:O:297:GLN:OE1 | 1:O:297:GLN:N   | 2.41                     | 0.50              |
| 1:Y:56:ILE:HG12 | 1:Y:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:c:100:THR:CB  | 1:c:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:h:55:GLN:O    | 1:h:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:l:56:ILE:HG12 | 1:l:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:n:55:GLN:O    | 1:n:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:A:56:ILE:HG12 | 1:A:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:B:55:GLN:O    | 1:B:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:C:56:ILE:HG12 | 1:C:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:F:55:GLN:O    | 1:F:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:H:55:GLN:O    | 1:H:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:J:56:ILE:HG12 | 1:J:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:L:56:ILE:HG12 | 1:L:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:X:55:GLN:O    | 1:X:59:LEU:HB2  | 2.10                     | 0.50              |
| 1:c:56:ILE:HG12 | 1:c:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:f:55:GLN:O    | 1:f:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:E:100:THR:CB  | 1:E:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:O:100:THR:CB  | 1:O:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:P:55:GLN:O    | 1:P:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:P:56:ILE:HG12 | 1:P:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:T:56:ILE:HG12 | 1:T:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:W:56:ILE:HG12 | 1:W:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:a:56:ILE:HG12 | 1:a:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:a:100:THR:CB  | 1:a:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:d:56:ILE:HG12 | 1:d:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:f:100:THR:CB  | 1:f:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:l:55:GLN:O    | 1:l:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:B:56:ILE:HG12 | 1:B:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:C:55:GLN:O    | 1:C:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:G:56:ILE:HG12 | 1:G:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:K:56:ILE:HG12 | 1:K:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:Q:56:ILE:HG12 | 1:Q:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:T:55:GLN:O    | 1:T:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:Z:56:ILE:HG12 | 1:Z:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:Z:100:THR:CB  | 1:Z:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:g:56:ILE:HG12 | 1:g:256:LEU:HB3 | 1.94                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:k:56:ILE:HG12 | 1:k:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:m:100:THR:CB  | 1:m:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:n:56:ILE:HG12 | 1:n:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:H:104:ASP:CB  | 1:O:135:LYS:HZ3 | 2.24                     | 0.50              |
| 1:H:105:LYS:CD  | 1:Y:51:LYS:HZ1  | 2.16                     | 0.50              |
| 1:H:297:GLN:OE1 | 1:H:297:GLN:N   | 2.41                     | 0.50              |
| 1:I:56:ILE:HG12 | 1:I:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:J:100:THR:CB  | 1:J:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:L:55:GLN:O    | 1:L:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:N:55:GLN:O    | 1:N:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:S:56:ILE:HG12 | 1:S:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:U:56:ILE:HG12 | 1:U:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:Z:55:GLN:O    | 1:Z:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:b:55:GLN:O    | 1:b:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:h:56:ILE:HG12 | 1:h:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:o:56:ILE:HG12 | 1:o:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:C:100:THR:CB  | 1:C:202:PHE:HE2 | 2.25                     | 0.50              |
| 1:O:55:GLN:O    | 1:O:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:R:55:GLN:O    | 1:R:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:E:55:GLN:O    | 1:E:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:E:105:LYS:CD  | 1:k:51:LYS:HZ2  | 2.23                     | 0.50              |
| 1:V:55:GLN:O    | 1:V:59:LEU:HB2  | 2.11                     | 0.50              |
| 1:e:56:ILE:HG12 | 1:e:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:j:56:ILE:HG12 | 1:j:256:LEU:HB3 | 1.94                     | 0.50              |
| 1:D:56:ILE:HG12 | 1:D:256:LEU:HB3 | 1.94                     | 0.49              |
| 1:F:177:ASP:O   | 1:F:227:GLN:NE2 | 2.41                     | 0.49              |
| 1:L:177:ASP:O   | 1:L:227:GLN:NE2 | 2.41                     | 0.49              |
| 1:N:56:ILE:HG12 | 1:N:256:LEU:HB3 | 1.94                     | 0.49              |
| 1:S:177:ASP:O   | 1:S:227:GLN:NE2 | 2.41                     | 0.49              |
| 1:W:100:THR:CB  | 1:W:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:X:56:ILE:HG12 | 1:X:256:LEU:HB3 | 1.94                     | 0.49              |
| 1:Y:55:GLN:O    | 1:Y:59:LEU:HB2  | 2.11                     | 0.49              |
| 1:d:100:THR:CB  | 1:d:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:k:55:GLN:O    | 1:k:59:LEU:HB2  | 2.11                     | 0.49              |
| 1:o:100:THR:CB  | 1:o:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:G:100:THR:CB  | 1:G:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:P:100:THR:CB  | 1:P:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:S:100:THR:CB  | 1:S:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:V:100:THR:CB  | 1:V:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:Y:100:THR:CB  | 1:Y:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:d:297:GLN:N   | 1:d:297:GLN:OE1 | 2.41                     | 0.49              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:k:100:THR:CB  | 1:k:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:R:100:THR:CB  | 1:R:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:D:177:ASP:O   | 1:D:227:GLN:NE2 | 2.41                     | 0.49              |
| 1:F:100:THR:CB  | 1:F:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:H:51:LYS:HZ2  | 1:n:105:LYS:CD  | 2.23                     | 0.49              |
| 1:L:100:THR:CB  | 1:L:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:A:51:LYS:HZ1  | 1:f:105:LYS:CD  | 2.13                     | 0.49              |
| 1:I:100:THR:CB  | 1:I:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:J:177:ASP:O   | 1:J:227:GLN:NE2 | 2.41                     | 0.49              |
| 1:K:100:THR:CB  | 1:K:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:O:51:LYS:HZ2  | 1:R:105:LYS:CD  | 2.24                     | 0.49              |
| 1:b:100:THR:CB  | 1:b:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:e:100:THR:CB  | 1:e:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:g:72:LEU:O    | 1:g:75:THR:OG1  | 2.21                     | 0.49              |
| 1:g:100:THR:CB  | 1:g:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:j:100:THR:CB  | 1:j:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:n:100:THR:CB  | 1:n:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:B:177:ASP:O   | 1:B:227:GLN:NE2 | 2.41                     | 0.49              |
| 1:E:51:LYS:HZ1  | 1:b:105:LYS:CD  | 2.17                     | 0.49              |
| 1:G:51:LYS:HZ2  | 1:Z:105:LYS:CD  | 2.24                     | 0.49              |
| 1:H:177:ASP:O   | 1:H:227:GLN:NE2 | 2.41                     | 0.49              |
| 1:M:100:THR:CB  | 1:M:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:N:105:LYS:CD  | 1:S:51:LYS:HZ2  | 2.23                     | 0.49              |
| 1:h:100:THR:CB  | 1:h:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:N:100:THR:CB  | 1:N:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:X:100:THR:CB  | 1:X:202:PHE:HE2 | 2.25                     | 0.49              |
| 1:F:51:LYS:HZ1  | 1:l:105:LYS:CD  | 2.17                     | 0.49              |
| 1:J:135:LYS:HZ3 | 1:f:104:ASP:CB  | 2.20                     | 0.49              |
| 1:D:105:LYS:CD  | 1:c:51:LYS:HZ2  | 2.22                     | 0.49              |
| 1:A:100:THR:CB  | 1:A:202:PHE:HE2 | 2.25                     | 0.48              |
| 1:U:100:THR:CB  | 1:U:202:PHE:HE2 | 2.25                     | 0.48              |
| 1:i:72:LEU:O    | 1:i:75:THR:OG1  | 2.21                     | 0.48              |
| 1:i:254:GLU:O   | 1:i:257:THR:OG1 | 2.28                     | 0.48              |
| 1:A:105:LYS:CD  | 1:g:51:LYS:HZ2  | 2.26                     | 0.48              |
| 1:D:100:THR:CB  | 1:D:202:PHE:HE2 | 2.25                     | 0.48              |
| 1:G:177:ASP:O   | 1:G:227:GLN:NE2 | 2.41                     | 0.48              |
| 1:L:197:LEU:HB2 | 1:L:201:LYS:CE  | 2.44                     | 0.48              |
| 1:P:105:LYS:CD  | 1:Q:51:LYS:HZ2  | 2.24                     | 0.48              |
| 1:O:197:LEU:HB2 | 1:O:201:LYS:CE  | 2.44                     | 0.48              |
| 1:o:197:LEU:HB2 | 1:o:201:LYS:CE  | 2.44                     | 0.48              |
| 1:C:197:LEU:HB2 | 1:C:201:LYS:CE  | 2.44                     | 0.48              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:197:LEU:HB2 | 1:I:201:LYS:CE  | 2.44                     | 0.48              |
| 1:X:197:LEU:HB2 | 1:X:201:LYS:CE  | 2.44                     | 0.48              |
| 1:b:254:GLU:O   | 1:b:257:THR:OG1 | 2.28                     | 0.48              |
| 1:f:197:LEU:HB2 | 1:f:201:LYS:CE  | 2.44                     | 0.48              |
| 1:i:197:LEU:HB2 | 1:i:201:LYS:CE  | 2.44                     | 0.48              |
| 1:B:100:THR:CB  | 1:B:202:PHE:HE2 | 2.25                     | 0.48              |
| 1:D:197:LEU:HB2 | 1:D:201:LYS:CE  | 2.44                     | 0.48              |
| 1:E:197:LEU:HB2 | 1:E:201:LYS:CE  | 2.44                     | 0.48              |
| 1:K:177:ASP:O   | 1:K:227:GLN:NE2 | 2.41                     | 0.48              |
| 1:Q:197:LEU:HB2 | 1:Q:201:LYS:CE  | 2.44                     | 0.48              |
| 1:U:197:LEU:HB2 | 1:U:201:LYS:CE  | 2.44                     | 0.48              |
| 1:c:197:LEU:HB2 | 1:c:201:LYS:CE  | 2.44                     | 0.48              |
| 1:k:197:LEU:HB2 | 1:k:201:LYS:CE  | 2.44                     | 0.48              |
| 1:A:177:ASP:O   | 1:A:227:GLN:NE2 | 2.41                     | 0.48              |
| 1:A:197:LEU:HB2 | 1:A:201:LYS:CE  | 2.44                     | 0.48              |
| 1:F:197:LEU:HB2 | 1:F:201:LYS:CE  | 2.44                     | 0.48              |
| 1:F:295:GLN:HB2 | 1:F:296:PRO:HD3 | 1.96                     | 0.48              |
| 1:H:50:GLU:CB   | 1:d:84:HIS:CE1  | 2.86                     | 0.48              |
| 1:H:105:LYS:CD  | 1:Y:51:LYS:HZ2  | 2.24                     | 0.48              |
| 1:H:197:LEU:HB2 | 1:H:201:LYS:CE  | 2.44                     | 0.48              |
| 1:R:197:LEU:HB2 | 1:R:201:LYS:CE  | 2.44                     | 0.48              |
| 1:T:197:LEU:HB2 | 1:T:201:LYS:CE  | 2.44                     | 0.48              |
| 1:W:197:LEU:HB2 | 1:W:201:LYS:CE  | 2.44                     | 0.48              |
| 1:Z:197:LEU:HB2 | 1:Z:201:LYS:CE  | 2.44                     | 0.48              |
| 1:j:197:LEU:HB2 | 1:j:201:LYS:CE  | 2.44                     | 0.48              |
| 1:l:197:LEU:HB2 | 1:l:201:LYS:CE  | 2.44                     | 0.48              |
| 1:G:50:GLU:CB   | 1:P:84:HIS:CE1  | 2.86                     | 0.48              |
| 1:P:197:LEU:HB2 | 1:P:201:LYS:CE  | 2.44                     | 0.48              |
| 1:Y:197:LEU:HB2 | 1:Y:201:LYS:CE  | 2.44                     | 0.48              |
| 1:b:197:LEU:HB2 | 1:b:201:LYS:CE  | 2.44                     | 0.48              |
| 1:c:295:GLN:HB2 | 1:c:296:PRO:HD3 | 1.96                     | 0.48              |
| 1:n:197:LEU:HB2 | 1:n:201:LYS:CE  | 2.44                     | 0.48              |
| 1:a:197:LEU:HB2 | 1:a:201:LYS:CE  | 2.44                     | 0.48              |
| 1:d:197:LEU:HB2 | 1:d:201:LYS:CE  | 2.44                     | 0.48              |
| 1:l:295:GLN:HB2 | 1:l:296:PRO:HD3 | 1.96                     | 0.48              |
| 1:B:295:GLN:HB2 | 1:B:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:D:295:GLN:HB2 | 1:D:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:K:197:LEU:HB2 | 1:K:201:LYS:CE  | 2.44                     | 0.47              |
| 1:N:197:LEU:HB2 | 1:N:201:LYS:CE  | 2.44                     | 0.47              |
| 1:V:295:GLN:HB2 | 1:V:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:X:295:GLN:HB2 | 1:X:296:PRO:HD3 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:a:295:GLN:HB2  | 1:a:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:e:295:GLN:HB2  | 1:e:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:g:295:GLN:HB2  | 1:g:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:h:295:GLN:HB2  | 1:h:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:j:295:GLN:HB2  | 1:j:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:A:256:LEU:HD23 | 1:A:256:LEU:HA  | 1.78                     | 0.47              |
| 1:E:177:ASP:O    | 1:E:227:GLN:NE2 | 2.41                     | 0.47              |
| 1:G:197:LEU:HB2  | 1:G:201:LYS:CE  | 2.44                     | 0.47              |
| 1:J:89:ARG:HD2   | 1:J:89:ARG:HA   | 1.72                     | 0.47              |
| 1:J:197:LEU:HB2  | 1:J:201:LYS:CE  | 2.44                     | 0.47              |
| 1:K:295:GLN:HB2  | 1:K:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:M:197:LEU:HB2  | 1:M:201:LYS:CE  | 2.44                     | 0.47              |
| 1:Q:89:ARG:HD2   | 1:Q:89:ARG:HA   | 1.72                     | 0.47              |
| 1:T:254:GLU:O    | 1:T:257:THR:OG1 | 2.28                     | 0.47              |
| 1:h:197:LEU:HB2  | 1:h:201:LYS:CE  | 2.44                     | 0.47              |
| 1:n:295:GLN:HB2  | 1:n:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:C:177:ASP:O    | 1:C:227:GLN:NE2 | 2.41                     | 0.47              |
| 1:I:295:GLN:HB2  | 1:I:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:J:50:GLU:CB    | 1:f:84:HIS:CE1  | 2.86                     | 0.47              |
| 1:e:197:LEU:HB2  | 1:e:201:LYS:CE  | 2.44                     | 0.47              |
| 1:g:197:LEU:HB2  | 1:g:201:LYS:CE  | 2.44                     | 0.47              |
| 1:k:254:GLU:O    | 1:k:257:THR:OG1 | 2.28                     | 0.47              |
| 1:l:177:ASP:O    | 1:l:227:GLN:NE2 | 2.41                     | 0.47              |
| 1:H:295:GLN:HB2  | 1:H:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:Z:295:GLN:HB2  | 1:Z:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:A:295:GLN:HB2  | 1:A:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:C:178:ALA:HB3  | 1:C:189:ALA:C   | 2.40                     | 0.47              |
| 1:G:295:GLN:HB2  | 1:G:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:I:178:ALA:HB3  | 1:I:189:ALA:C   | 2.40                     | 0.47              |
| 1:K:178:ALA:HB3  | 1:K:189:ALA:C   | 2.40                     | 0.47              |
| 1:M:295:GLN:HB2  | 1:M:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:O:295:GLN:HB2  | 1:O:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:b:295:GLN:HB2  | 1:b:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:I:177:ASP:O    | 1:I:227:GLN:NE2 | 2.41                     | 0.47              |
| 1:J:84:HIS:CE1   | 1:M:50:GLU:CB   | 2.86                     | 0.47              |
| 1:S:197:LEU:HB2  | 1:S:201:LYS:CE  | 2.44                     | 0.47              |
| 1:U:178:ALA:HB3  | 1:U:189:ALA:C   | 2.40                     | 0.47              |
| 1:m:295:GLN:HB2  | 1:m:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:o:295:GLN:HB2  | 1:o:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:A:135:LYS:HZ3  | 1:V:104:ASP:CB  | 2.22                     | 0.47              |
| 1:B:197:LEU:HB2  | 1:B:201:LYS:CE  | 2.44                     | 0.47              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:178:ALA:HB3 | 1:J:189:ALA:C   | 2.40                     | 0.47              |
| 1:L:178:ALA:HB3 | 1:L:189:ALA:C   | 2.40                     | 0.47              |
| 1:O:178:ALA:HB3 | 1:O:189:ALA:C   | 2.40                     | 0.47              |
| 1:Q:295:GLN:HB2 | 1:Q:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:R:295:GLN:HB2 | 1:R:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:T:295:GLN:HB2 | 1:T:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:W:178:ALA:HB3 | 1:W:189:ALA:C   | 2.40                     | 0.47              |
| 1:X:178:ALA:HB3 | 1:X:189:ALA:C   | 2.40                     | 0.47              |
| 1:Y:295:GLN:HB2 | 1:Y:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:d:178:ALA:HB3 | 1:d:189:ALA:C   | 2.40                     | 0.47              |
| 1:i:178:ALA:HB3 | 1:i:189:ALA:C   | 2.40                     | 0.47              |
| 1:j:178:ALA:HB3 | 1:j:189:ALA:C   | 2.40                     | 0.47              |
| 1:m:197:LEU:HB2 | 1:m:201:LYS:CE  | 2.44                     | 0.47              |
| 1:m:254:GLU:O   | 1:m:257:THR:OG1 | 2.28                     | 0.47              |
| 1:o:178:ALA:HB3 | 1:o:189:ALA:C   | 2.40                     | 0.47              |
| 1:D:178:ALA:HB3 | 1:D:189:ALA:C   | 2.40                     | 0.47              |
| 1:R:178:ALA:HB3 | 1:R:189:ALA:C   | 2.40                     | 0.47              |
| 1:V:178:ALA:HB3 | 1:V:189:ALA:C   | 2.40                     | 0.47              |
| 1:o:254:GLU:O   | 1:o:257:THR:OG1 | 2.28                     | 0.47              |
| 1:E:211:ASP:O   | 1:E:217:GLN:NE2 | 2.48                     | 0.47              |
| 1:F:211:ASP:O   | 1:F:217:GLN:NE2 | 2.48                     | 0.47              |
| 1:Z:211:ASP:O   | 1:Z:217:GLN:NE2 | 2.48                     | 0.47              |
| 1:g:178:ALA:HB3 | 1:g:189:ALA:C   | 2.40                     | 0.47              |
| 1:o:211:ASP:O   | 1:o:217:GLN:NE2 | 2.48                     | 0.47              |
| 1:A:178:ALA:HB3 | 1:A:189:ALA:C   | 2.40                     | 0.47              |
| 1:B:178:ALA:HB3 | 1:B:189:ALA:C   | 2.40                     | 0.47              |
| 1:J:295:GLN:HB2 | 1:J:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:L:254:GLU:O   | 1:L:257:THR:OG1 | 2.28                     | 0.47              |
| 1:O:211:ASP:O   | 1:O:217:GLN:NE2 | 2.48                     | 0.47              |
| 1:P:211:ASP:O   | 1:P:217:GLN:NE2 | 2.48                     | 0.47              |
| 1:P:295:GLN:HB2 | 1:P:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:U:177:ASP:O   | 1:U:227:GLN:NE2 | 2.41                     | 0.47              |
| 1:V:197:LEU:HB2 | 1:V:201:LYS:CE  | 2.44                     | 0.47              |
| 1:Y:178:ALA:HB3 | 1:Y:189:ALA:C   | 2.40                     | 0.47              |
| 1:Z:178:ALA:HB3 | 1:Z:189:ALA:C   | 2.40                     | 0.47              |
| 1:e:178:ALA:HB3 | 1:e:189:ALA:C   | 2.40                     | 0.47              |
| 1:e:211:ASP:O   | 1:e:217:GLN:NE2 | 2.48                     | 0.47              |
| 1:f:178:ALA:HB3 | 1:f:189:ALA:C   | 2.40                     | 0.47              |
| 1:i:295:GLN:HB2 | 1:i:296:PRO:HD3 | 1.96                     | 0.47              |
| 1:o:89:ARG:HA   | 1:o:89:ARG:HD2  | 1.72                     | 0.47              |
| 1:E:295:GLN:HB2 | 1:E:296:PRO:HD3 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:254:GLU:O    | 1:R:257:THR:OG1  | 2.28                     | 0.46              |
| 1:S:295:GLN:HB2  | 1:S:296:PRO:HD3  | 1.96                     | 0.46              |
| 1:a:178:ALA:HB3  | 1:a:189:ALA:C    | 2.40                     | 0.46              |
| 1:b:211:ASP:O    | 1:b:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:c:178:ALA:HB3  | 1:c:189:ALA:C    | 2.40                     | 0.46              |
| 1:i:256:LEU:HA   | 1:i:256:LEU:HD23 | 1.78                     | 0.46              |
| 1:m:211:ASP:O    | 1:m:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:n:211:ASP:O    | 1:n:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:C:89:ARG:HD2   | 1:C:89:ARG:HA    | 1.72                     | 0.46              |
| 1:N:211:ASP:O    | 1:N:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:a:211:ASP:O    | 1:a:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:f:295:GLN:HB2  | 1:f:296:PRO:HD3  | 1.96                     | 0.46              |
| 1:j:211:ASP:O    | 1:j:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:l:178:ALA:HB3  | 1:l:189:ALA:C    | 2.40                     | 0.46              |
| 1:A:51:LYS:HZ2   | 1:f:105:LYS:CG   | 2.29                     | 0.46              |
| 1:D:211:ASP:O    | 1:D:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:F:178:ALA:HB3  | 1:F:189:ALA:C    | 2.40                     | 0.46              |
| 1:G:178:ALA:HB3  | 1:G:189:ALA:C    | 2.40                     | 0.46              |
| 1:G:256:LEU:HD23 | 1:G:256:LEU:HA   | 1.78                     | 0.46              |
| 1:J:254:GLU:O    | 1:J:257:THR:OG1  | 2.28                     | 0.46              |
| 1:M:177:ASP:O    | 1:M:227:GLN:NE2  | 2.41                     | 0.46              |
| 1:N:178:ALA:HB3  | 1:N:189:ALA:C    | 2.40                     | 0.46              |
| 1:N:295:GLN:HB2  | 1:N:296:PRO:HD3  | 1.96                     | 0.46              |
| 1:S:178:ALA:HB3  | 1:S:189:ALA:C    | 2.40                     | 0.46              |
| 1:U:295:GLN:HB2  | 1:U:296:PRO:HD3  | 1.96                     | 0.46              |
| 1:W:295:GLN:HB2  | 1:W:296:PRO:HD3  | 1.96                     | 0.46              |
| 1:X:211:ASP:O    | 1:X:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:e:254:GLU:O    | 1:e:257:THR:OG1  | 2.28                     | 0.46              |
| 1:k:178:ALA:HB3  | 1:k:189:ALA:C    | 2.40                     | 0.46              |
| 1:G:211:ASP:O    | 1:G:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:I:51:LYS:HZ2   | 1:X:105:LYS:CG   | 2.29                     | 0.46              |
| 1:L:295:GLN:HB2  | 1:L:296:PRO:HD3  | 1.96                     | 0.46              |
| 1:M:178:ALA:HB3  | 1:M:189:ALA:C    | 2.40                     | 0.46              |
| 1:N:254:GLU:O    | 1:N:257:THR:OG1  | 2.28                     | 0.46              |
| 1:P:105:LYS:CD   | 1:Q:51:LYS:HZ1   | 2.16                     | 0.46              |
| 1:P:254:GLU:O    | 1:P:257:THR:OG1  | 2.28                     | 0.46              |
| 1:Q:177:ASP:O    | 1:Q:227:GLN:NE2  | 2.41                     | 0.46              |
| 1:R:89:ARG:HD2   | 1:R:89:ARG:HA    | 1.72                     | 0.46              |
| 1:T:178:ALA:HB3  | 1:T:189:ALA:C    | 2.40                     | 0.46              |
| 1:Y:211:ASP:O    | 1:Y:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:D:51:LYS:HZ1   | 1:j:105:LYS:CD   | 2.14                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:105:LYS:CD   | 1:a:51:LYS:HZ1  | 2.16                     | 0.46              |
| 1:L:89:ARG:HD2   | 1:L:89:ARG:HA   | 1.72                     | 0.46              |
| 1:P:178:ALA:HB3  | 1:P:189:ALA:C   | 2.40                     | 0.46              |
| 1:Q:211:ASP:O    | 1:Q:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:U:211:ASP:O    | 1:U:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:c:211:ASP:O    | 1:c:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:d:211:ASP:O    | 1:d:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:d:295:GLN:HB2  | 1:d:296:PRO:HD3 | 1.96                     | 0.46              |
| 1:m:178:ALA:HB3  | 1:m:189:ALA:C   | 2.40                     | 0.46              |
| 1:A:211:ASP:O    | 1:A:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:B:89:ARG:HD2   | 1:B:89:ARG:HA   | 1.72                     | 0.46              |
| 1:C:295:GLN:HB2  | 1:C:296:PRO:HD3 | 1.96                     | 0.46              |
| 1:E:105:LYS:CD   | 1:k:51:LYS:HZ1  | 2.17                     | 0.46              |
| 1:K:211:ASP:O    | 1:K:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:M:84:HIS:CE1   | 1:i:50:GLU:CB   | 2.86                     | 0.46              |
| 1:Q:178:ALA:HB3  | 1:Q:189:ALA:C   | 2.40                     | 0.46              |
| 1:S:211:ASP:O    | 1:S:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:h:178:ALA:HB3  | 1:h:189:ALA:C   | 2.40                     | 0.46              |
| 1:B:105:LYS:CG   | 1:e:51:LYS:HZ2  | 2.29                     | 0.46              |
| 1:C:211:ASP:O    | 1:C:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:E:178:ALA:HB3  | 1:E:189:ALA:C   | 2.40                     | 0.46              |
| 1:H:211:ASP:O    | 1:H:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:M:211:ASP:O    | 1:M:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:R:211:ASP:O    | 1:R:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:W:211:ASP:O    | 1:W:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:Y:256:LEU:HD23 | 1:Y:256:LEU:HA  | 1.78                     | 0.46              |
| 1:h:211:ASP:O    | 1:h:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:l:211:ASP:O    | 1:l:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:B:51:LYS:HZ2   | 1:h:105:LYS:CG  | 2.29                     | 0.46              |
| 1:D:304:ARG:CZ   | 1:P:287:ALA:HB1 | 2.46                     | 0.46              |
| 1:H:178:ALA:HB3  | 1:H:189:ALA:C   | 2.40                     | 0.46              |
| 1:I:105:LYS:CG   | 1:o:51:LYS:HZ2  | 2.29                     | 0.46              |
| 1:I:211:ASP:O    | 1:I:217:GLN:NE2 | 2.48                     | 0.46              |
| 1:R:304:ARG:CZ   | 1:d:287:ALA:HB1 | 2.46                     | 0.46              |
| 1:Y:287:ALA:HB1  | 1:k:304:ARG:CZ  | 2.46                     | 0.46              |
| 1:c:89:ARG:HA    | 1:c:89:ARG:HD2  | 1.72                     | 0.46              |
| 1:k:295:GLN:HB2  | 1:k:296:PRO:HD3 | 1.96                     | 0.46              |
| 1:D:51:LYS:HZ2   | 1:j:105:LYS:CD  | 2.26                     | 0.46              |
| 1:F:287:ALA:HB1  | 1:G:304:ARG:CZ  | 2.46                     | 0.46              |
| 1:F:304:ARG:CZ   | 1:R:287:ALA:HB1 | 2.46                     | 0.46              |
| 1:P:304:ARG:CZ   | 1:b:287:ALA:HB1 | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:256:LEU:HA   | 1:U:256:LEU:HD23 | 1.77                     | 0.46              |
| 1:f:211:ASP:O    | 1:f:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:B:304:ARG:CZ   | 1:N:287:ALA:HB1  | 2.46                     | 0.46              |
| 1:E:50:GLU:CB    | 1:R:84:HIS:CE1   | 2.86                     | 0.46              |
| 1:E:287:ALA:HB1  | 1:Q:304:ARG:CZ   | 2.46                     | 0.46              |
| 1:E:304:ARG:CZ   | 1:H:287:ALA:HB1  | 2.46                     | 0.46              |
| 1:J:105:LYS:CG   | 1:W:51:LYS:HZ2   | 2.29                     | 0.46              |
| 1:L:304:ARG:CZ   | 1:X:287:ALA:HB1  | 2.46                     | 0.46              |
| 1:M:287:ALA:HB1  | 1:Y:304:ARG:CZ   | 2.46                     | 0.46              |
| 1:N:304:ARG:CZ   | 1:Z:287:ALA:HB1  | 2.46                     | 0.46              |
| 1:Z:304:ARG:CZ   | 1:l:287:ALA:HB1  | 2.46                     | 0.46              |
| 1:f:256:LEU:HD23 | 1:f:256:LEU:HA   | 1.78                     | 0.46              |
| 1:g:211:ASP:O    | 1:g:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:h:89:ARG:HA    | 1:h:89:ARG:HD2   | 1.72                     | 0.46              |
| 1:k:211:ASP:O    | 1:k:217:GLN:NE2  | 2.48                     | 0.46              |
| 1:F:105:LYS:CG   | 1:a:51:LYS:HZ2   | 2.29                     | 0.45              |
| 1:L:211:ASP:O    | 1:L:217:GLN:NE2  | 2.48                     | 0.45              |
| 1:S:287:ALA:HB1  | 1:e:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:X:254:GLU:O    | 1:X:257:THR:OG1  | 2.28                     | 0.45              |
| 1:X:304:ARG:CZ   | 1:j:287:ALA:HB1  | 2.46                     | 0.45              |
| 1:a:287:ALA:HB1  | 1:m:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:b:178:ALA:HB3  | 1:b:189:ALA:C    | 2.40                     | 0.45              |
| 1:c:287:ALA:HB1  | 1:o:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:i:211:ASP:O    | 1:i:217:GLN:NE2  | 2.48                     | 0.45              |
| 1:A:105:LYS:CG   | 1:g:51:LYS:HZ2   | 2.29                     | 0.45              |
| 1:B:211:ASP:O    | 1:B:217:GLN:NE2  | 2.48                     | 0.45              |
| 1:E:105:LYS:CG   | 1:k:51:LYS:HZ2   | 2.29                     | 0.45              |
| 1:H:135:LYS:HZ3  | 1:d:104:ASP:CB   | 2.26                     | 0.45              |
| 1:H:304:ARG:CZ   | 1:T:287:ALA:HB1  | 2.46                     | 0.45              |
| 1:M:51:LYS:HZ2   | 1:T:105:LYS:CG   | 2.29                     | 0.45              |
| 1:N:105:LYS:CG   | 1:S:51:LYS:HZ2   | 2.29                     | 0.45              |
| 1:O:51:LYS:HZ2   | 1:R:105:LYS:CG   | 2.29                     | 0.45              |
| 1:P:105:LYS:CG   | 1:Q:51:LYS:HZ2   | 2.29                     | 0.45              |
| 1:T:211:ASP:O    | 1:T:217:GLN:NE2  | 2.48                     | 0.45              |
| 1:h:254:GLU:O    | 1:h:257:THR:OG1  | 2.28                     | 0.45              |
| 1:n:178:ALA:HB3  | 1:n:189:ALA:C    | 2.40                     | 0.45              |
| 1:A:304:ARG:CZ   | 1:L:287:ALA:HB1  | 2.46                     | 0.45              |
| 1:B:287:ALA:HB1  | 1:K:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:D:51:LYS:HZ2   | 1:j:105:LYS:CG   | 2.29                     | 0.45              |
| 1:D:287:ALA:HB1  | 1:I:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:G:51:LYS:HZ1   | 1:Z:105:LYS:CD   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:287:ALA:HB1  | 1:S:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:H:256:LEU:HA   | 1:H:256:LEU:HD23 | 1.78                     | 0.45              |
| 1:J:197:LEU:HB2  | 1:J:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:M:89:ARG:HA    | 1:M:89:ARG:HD2   | 1.72                     | 0.45              |
| 1:M:197:LEU:HB2  | 1:M:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:O:287:ALA:HB1  | 1:a:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:V:211:ASP:O    | 1:V:217:GLN:NE2  | 2.48                     | 0.45              |
| 1:Z:89:ARG:HA    | 1:Z:89:ARG:HD2   | 1.72                     | 0.45              |
| 1:b:304:ARG:CZ   | 1:n:287:ALA:HB1  | 2.46                     | 0.45              |
| 1:j:89:ARG:HD2   | 1:j:89:ARG:HA    | 1.72                     | 0.45              |
| 1:A:197:LEU:HB2  | 1:A:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:A:287:ALA:HB1  | 1:M:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:B:51:LYS:HZ2   | 1:h:105:LYS:HG2  | 1.82                     | 0.45              |
| 1:C:287:ALA:HB1  | 1:O:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:D:84:HIS:CE1   | 1:S:50:GLU:CB    | 2.86                     | 0.45              |
| 1:J:211:ASP:O    | 1:J:217:GLN:NE2  | 2.48                     | 0.45              |
| 1:O:177:ASP:O    | 1:O:227:GLN:NE2  | 2.41                     | 0.45              |
| 1:W:197:LEU:HB2  | 1:W:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:g:158:GLN:NE2  | 1:g:160:GLY:O    | 2.43                     | 0.45              |
| 1:D:105:LYS:CG   | 1:c:51:LYS:HZ2   | 2.29                     | 0.45              |
| 1:E:51:LYS:HZ2   | 1:b:105:LYS:CG   | 2.29                     | 0.45              |
| 1:E:89:ARG:HA    | 1:E:89:ARG:HD2   | 1.72                     | 0.45              |
| 1:F:51:LYS:HZ2   | 1:l:105:LYS:CG   | 2.29                     | 0.45              |
| 1:G:51:LYS:HZ2   | 1:Z:105:LYS:CG   | 2.29                     | 0.45              |
| 1:H:105:LYS:CG   | 1:Y:51:LYS:HZ2   | 2.29                     | 0.45              |
| 1:Q:287:ALA:HB1  | 1:c:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:T:197:LEU:HB2  | 1:T:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:T:304:ARG:CZ   | 1:f:287:ALA:HB1  | 2.46                     | 0.45              |
| 1:a:256:LEU:HA   | 1:a:256:LEU:HD23 | 1.78                     | 0.45              |
| 1:i:197:LEU:HB2  | 1:i:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:A:105:LYS:HG2  | 1:g:51:LYS:HZ2   | 1.82                     | 0.45              |
| 1:C:197:LEU:HB2  | 1:C:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:G:197:LEU:HB2  | 1:G:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:K:256:LEU:HD23 | 1:K:256:LEU:HA   | 1.78                     | 0.45              |
| 1:f:197:LEU:HB2  | 1:f:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:C:256:LEU:HD23 | 1:C:256:LEU:HA   | 1.78                     | 0.45              |
| 1:H:254:GLU:O    | 1:H:257:THR:OG1  | 2.28                     | 0.45              |
| 1:K:197:LEU:HB2  | 1:K:201:LYS:HE2  | 1.98                     | 0.45              |
| 1:K:287:ALA:HB1  | 1:W:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:W:287:ALA:HB1  | 1:i:304:ARG:CZ   | 2.46                     | 0.45              |
| 1:a:89:ARG:HA    | 1:a:89:ARG:HD2   | 1.72                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:d:197:LEU:HB2  | 1:d:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:h:197:LEU:HB2  | 1:h:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:i:89:ARG:HD2   | 1:i:89:ARG:HA   | 1.72                     | 0.45              |
| 1:D:197:LEU:HB2  | 1:D:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:Q:197:LEU:HB2  | 1:Q:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:g:197:LEU:HB2  | 1:g:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:k:256:LEU:HD23 | 1:k:256:LEU:HA  | 1.78                     | 0.45              |
| 1:C:304:ARG:CZ   | 1:J:287:ALA:HB1 | 2.46                     | 0.45              |
| 1:G:51:LYS:HZ2   | 1:Z:105:LYS:HG2 | 1.82                     | 0.45              |
| 1:G:105:LYS:CG   | 1:m:51:LYS:HZ2  | 2.29                     | 0.45              |
| 1:K:51:LYS:HZ2   | 1:V:105:LYS:CG  | 2.30                     | 0.45              |
| 1:Y:197:LEU:HB2  | 1:Y:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:Z:197:LEU:HB2  | 1:Z:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:l:197:LEU:HB2  | 1:l:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:o:197:LEU:HB2  | 1:o:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:A:254:GLU:O    | 1:A:257:THR:OG1 | 2.28                     | 0.45              |
| 1:B:256:LEU:HD23 | 1:B:256:LEU:HA  | 1.78                     | 0.45              |
| 1:H:197:LEU:HB2  | 1:H:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:L:197:LEU:HB2  | 1:L:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:O:197:LEU:HB2  | 1:O:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:P:197:LEU:HB2  | 1:P:201:LYS:HE2 | 1.99                     | 0.45              |
| 1:U:287:ALA:HB1  | 1:g:304:ARG:CZ  | 2.46                     | 0.45              |
| 1:V:197:LEU:HB2  | 1:V:201:LYS:HE2 | 1.99                     | 0.45              |
| 1:c:197:LEU:HB2  | 1:c:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:i:158:GLN:NE2  | 1:i:160:GLY:O   | 2.43                     | 0.45              |
| 1:m:197:LEU:HB2  | 1:m:201:LYS:HE2 | 1.98                     | 0.45              |
| 1:E:105:LYS:HG2  | 1:k:51:LYS:HZ2  | 1.82                     | 0.44              |
| 1:F:105:LYS:HG2  | 1:a:51:LYS:HZ2  | 1.82                     | 0.44              |
| 1:F:197:LEU:HB2  | 1:F:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:I:51:LYS:HZ2   | 1:X:105:LYS:HG2 | 1.82                     | 0.44              |
| 1:J:304:ARG:CZ   | 1:V:287:ALA:HB1 | 2.46                     | 0.44              |
| 1:N:50:GLU:CB    | 1:j:84:HIS:CE1  | 2.86                     | 0.44              |
| 1:N:197:LEU:HB2  | 1:N:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:N:256:LEU:HD23 | 1:N:256:LEU:HA  | 1.78                     | 0.44              |
| 1:S:197:LEU:HB2  | 1:S:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:V:304:ARG:CZ   | 1:h:287:ALA:HB1 | 2.46                     | 0.44              |
| 1:C:51:LYS:HZ2   | 1:d:105:LYS:CG  | 2.30                     | 0.44              |
| 1:D:51:LYS:HZ2   | 1:j:105:LYS:HG2 | 1.82                     | 0.44              |
| 1:H:51:LYS:HZ2   | 1:n:105:LYS:CG  | 2.29                     | 0.44              |
| 1:H:105:LYS:HG2  | 1:Y:51:LYS:HZ2  | 1.82                     | 0.44              |
| 1:I:287:ALA:HB1  | 1:U:304:ARG:CZ  | 2.46                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:j:177:ASP:O    | 1:j:227:GLN:NE2 | 2.41                     | 0.44              |
| 1:j:197:LEU:HB2  | 1:j:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:k:146:THR:OG1  | 1:k:148:THR:O   | 2.36                     | 0.44              |
| 1:k:197:LEU:HB2  | 1:k:201:LYS:HE2 | 1.99                     | 0.44              |
| 1:m:146:THR:OG1  | 1:m:148:THR:O   | 2.36                     | 0.44              |
| 1:n:256:LEU:HD23 | 1:n:256:LEU:HA  | 1.78                     | 0.44              |
| 1:A:51:LYS:HZ2   | 1:f:105:LYS:HG2 | 1.82                     | 0.44              |
| 1:B:254:GLU:O    | 1:B:257:THR:OG1 | 2.28                     | 0.44              |
| 1:K:89:ARG:HD2   | 1:K:89:ARG:HA   | 1.72                     | 0.44              |
| 1:O:89:ARG:HD2   | 1:O:89:ARG:HA   | 1.72                     | 0.44              |
| 1:Y:89:ARG:HA    | 1:Y:89:ARG:HD2  | 1.72                     | 0.44              |
| 1:Y:146:THR:OG1  | 1:Y:148:THR:O   | 2.36                     | 0.44              |
| 1:a:146:THR:OG1  | 1:a:148:THR:O   | 2.36                     | 0.44              |
| 1:b:197:LEU:HB2  | 1:b:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:c:146:THR:OG1  | 1:c:148:THR:O   | 2.36                     | 0.44              |
| 1:d:89:ARG:HA    | 1:d:89:ARG:HD2  | 1.72                     | 0.44              |
| 1:h:158:GLN:NE2  | 1:h:160:GLY:O   | 2.43                     | 0.44              |
| 1:n:197:LEU:HB2  | 1:n:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:B:105:LYS:HG2  | 1:e:51:LYS:HZ2  | 1.83                     | 0.44              |
| 1:C:105:LYS:CG   | 1:i:51:LYS:HZ2  | 2.29                     | 0.44              |
| 1:E:51:LYS:HZ2   | 1:b:105:LYS:HG2 | 1.83                     | 0.44              |
| 1:I:51:LYS:HZ2   | 1:X:105:LYS:CD  | 2.26                     | 0.44              |
| 1:O:146:THR:OG1  | 1:O:148:THR:O   | 2.36                     | 0.44              |
| 1:U:197:LEU:HB2  | 1:U:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:W:158:GLN:NE2  | 1:W:160:GLY:O   | 2.43                     | 0.44              |
| 1:X:89:ARG:HA    | 1:X:89:ARG:HD2  | 1.72                     | 0.44              |
| 1:a:197:LEU:HB2  | 1:a:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:e:89:ARG:HD2   | 1:e:89:ARG:HA   | 1.72                     | 0.44              |
| 1:e:197:LEU:HB2  | 1:e:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:f:158:GLN:NE2  | 1:f:160:GLY:O   | 2.43                     | 0.44              |
| 1:o:146:THR:OG1  | 1:o:148:THR:O   | 2.36                     | 0.44              |
| 1:F:254:GLU:O    | 1:F:257:THR:OG1 | 2.28                     | 0.44              |
| 1:N:105:LYS:HG2  | 1:S:51:LYS:HZ2  | 1.82                     | 0.44              |
| 1:Q:146:THR:OG1  | 1:Q:148:THR:O   | 2.36                     | 0.44              |
| 1:S:146:THR:OG1  | 1:S:148:THR:O   | 2.36                     | 0.44              |
| 1:X:197:LEU:HB2  | 1:X:201:LYS:HE2 | 1.98                     | 0.44              |
| 1:i:146:THR:OG1  | 1:i:148:THR:O   | 2.36                     | 0.44              |
| 1:A:50:GLU:CB    | 1:V:84:HIS:CE1  | 2.86                     | 0.44              |
| 1:C:146:THR:OG1  | 1:C:148:THR:O   | 2.36                     | 0.44              |
| 1:D:232:ARG:HD3  | 1:S:46:LEU:HD21 | 2.00                     | 0.44              |
| 1:E:146:THR:OG1  | 1:E:148:THR:O   | 2.36                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:197:LEU:HB2  | 1:E:201:LYS:HE2  | 1.98                     | 0.44              |
| 1:G:105:LYS:HG2  | 1:m:51:LYS:HZ2   | 1.83                     | 0.44              |
| 1:G:146:THR:OG1  | 1:G:148:THR:O    | 2.36                     | 0.44              |
| 1:I:197:LEU:HB2  | 1:I:201:LYS:HE2  | 1.98                     | 0.44              |
| 1:T:158:GLN:NE2  | 1:T:160:GLY:O    | 2.43                     | 0.44              |
| 1:X:158:GLN:NE2  | 1:X:160:GLY:O    | 2.43                     | 0.44              |
| 1:g:254:GLU:O    | 1:g:257:THR:OG1  | 2.28                     | 0.44              |
| 1:B:232:ARG:HD3  | 1:U:46:LEU:HD21  | 2.00                     | 0.44              |
| 1:D:146:THR:OG1  | 1:D:148:THR:O    | 2.36                     | 0.44              |
| 1:D:254:GLU:O    | 1:D:257:THR:OG1  | 2.28                     | 0.44              |
| 1:H:146:THR:OG1  | 1:H:148:THR:O    | 2.36                     | 0.44              |
| 1:I:46:LEU:HD21  | 1:N:232:ARG:HD3  | 2.00                     | 0.44              |
| 1:I:146:THR:OG1  | 1:I:148:THR:O    | 2.36                     | 0.44              |
| 1:R:197:LEU:HB2  | 1:R:201:LYS:HE2  | 1.98                     | 0.44              |
| 1:e:146:THR:OG1  | 1:e:148:THR:O    | 2.36                     | 0.44              |
| 1:B:46:LEU:HD21  | 1:X:232:ARG:HD3  | 2.00                     | 0.44              |
| 1:B:197:LEU:HB2  | 1:B:201:LYS:HE2  | 1.98                     | 0.44              |
| 1:C:50:GLU:CB    | 1:T:84:HIS:CE1   | 2.86                     | 0.44              |
| 1:G:46:LEU:HD21  | 1:P:232:ARG:HD3  | 2.00                     | 0.44              |
| 1:I:232:ARG:HD3  | 1:e:46:LEU:HD21  | 2.00                     | 0.44              |
| 1:M:146:THR:OG1  | 1:M:148:THR:O    | 2.36                     | 0.44              |
| 1:m:256:LEU:HA   | 1:m:256:LEU:HD23 | 1.78                     | 0.44              |
| 1:D:46:LEU:HD21  | 1:Z:232:ARG:HD3  | 2.00                     | 0.44              |
| 1:F:146:THR:OG1  | 1:F:148:THR:O    | 2.36                     | 0.44              |
| 1:G:232:ARG:HD3  | 1:c:46:LEU:HD21  | 2.00                     | 0.44              |
| 1:J:304:ARG:NH2  | 1:V:287:ALA:O    | 2.51                     | 0.44              |
| 1:K:46:LEU:HD21  | 1:L:232:ARG:HD3  | 2.00                     | 0.44              |
| 1:N:146:THR:OG1  | 1:N:148:THR:O    | 2.36                     | 0.44              |
| 1:S:232:ARG:HD3  | 1:o:46:LEU:HD21  | 2.00                     | 0.44              |
| 1:U:89:ARG:HA    | 1:U:89:ARG:HD2   | 1.72                     | 0.44              |
| 1:f:89:ARG:HA    | 1:f:89:ARG:HD2   | 1.72                     | 0.44              |
| 1:B:51:LYS:HZ2   | 1:h:105:LYS:CD   | 2.26                     | 0.43              |
| 1:B:146:THR:OG1  | 1:B:148:THR:O    | 2.36                     | 0.43              |
| 1:C:287:ALA:O    | 1:O:304:ARG:NH2  | 2.51                     | 0.43              |
| 1:D:89:ARG:HD2   | 1:D:89:ARG:HA    | 1.72                     | 0.43              |
| 1:E:256:LEU:HD23 | 1:E:256:LEU:HA   | 1.78                     | 0.43              |
| 1:M:287:ALA:O    | 1:Y:304:ARG:NH2  | 2.51                     | 0.43              |
| 1:O:51:LYS:HZ2   | 1:R:105:LYS:HG2  | 1.82                     | 0.43              |
| 1:P:105:LYS:HG2  | 1:Q:51:LYS:HZ2   | 1.82                     | 0.43              |
| 1:T:304:ARG:NH2  | 1:f:287:ALA:O    | 2.51                     | 0.43              |
| 1:X:146:THR:OG1  | 1:X:148:THR:O    | 2.36                     | 0.43              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:d:256:LEU:HD23 | 1:d:256:LEU:HA  | 1.78                     | 0.43              |
| 1:A:304:ARG:NH2  | 1:L:287:ALA:O   | 2.51                     | 0.43              |
| 1:C:105:LYS:HG2  | 1:i:51:LYS:HZ2  | 1.83                     | 0.43              |
| 1:C:304:ARG:NH2  | 1:J:287:ALA:O   | 2.51                     | 0.43              |
| 1:D:105:LYS:HG2  | 1:c:51:LYS:HZ2  | 1.83                     | 0.43              |
| 1:F:51:LYS:HZ2   | 1:l:105:LYS:HG2 | 1.83                     | 0.43              |
| 1:F:232:ARG:HD3  | 1:Q:46:LEU:HD21 | 2.00                     | 0.43              |
| 1:H:51:LYS:HZ2   | 1:n:105:LYS:HG2 | 1.82                     | 0.43              |
| 1:I:105:LYS:HG2  | 1:o:51:LYS:HZ2  | 1.83                     | 0.43              |
| 1:J:105:LYS:HG2  | 1:W:51:LYS:HZ2  | 1.83                     | 0.43              |
| 1:N:46:LEU:HD21  | 1:j:232:ARG:HD3 | 2.00                     | 0.43              |
| 1:O:84:HIS:CE1   | 1:k:50:GLU:CB   | 2.86                     | 0.43              |
| 1:P:46:LEU:HD21  | 1:l:232:ARG:HD3 | 2.00                     | 0.43              |
| 1:P:146:THR:OG1  | 1:P:148:THR:O   | 2.36                     | 0.43              |
| 1:R:146:THR:OG1  | 1:R:148:THR:O   | 2.36                     | 0.43              |
| 1:S:104:ASP:CB   | 1:o:135:LYS:HZ3 | 2.27                     | 0.43              |
| 1:T:146:THR:OG1  | 1:T:148:THR:O   | 2.36                     | 0.43              |
| 1:U:146:THR:OG1  | 1:U:148:THR:O   | 2.36                     | 0.43              |
| 1:W:89:ARG:HD2   | 1:W:89:ARG:HA   | 1.72                     | 0.43              |
| 1:h:146:THR:OG1  | 1:h:148:THR:O   | 2.36                     | 0.43              |
| 1:A:51:LYS:HZ2   | 1:f:105:LYS:CD  | 2.27                     | 0.43              |
| 1:A:287:ALA:O    | 1:M:304:ARG:NH2 | 2.51                     | 0.43              |
| 1:C:135:LYS:HZ3  | 1:T:104:ASP:CB  | 2.26                     | 0.43              |
| 1:L:46:LEU:HD21  | 1:h:232:ARG:HD3 | 2.00                     | 0.43              |
| 1:L:146:THR:OG1  | 1:L:148:THR:O   | 2.36                     | 0.43              |
| 1:R:58:GLY:N     | 1:n:92:GLU:OE2  | 2.52                     | 0.43              |
| 1:U:287:ALA:O    | 1:g:304:ARG:NH2 | 2.51                     | 0.43              |
| 1:W:287:ALA:O    | 1:i:304:ARG:NH2 | 2.51                     | 0.43              |
| 1:Z:256:LEU:HD23 | 1:Z:256:LEU:HA  | 1.78                     | 0.43              |
| 1:d:146:THR:OG1  | 1:d:148:THR:O   | 2.36                     | 0.43              |
| 1:A:58:GLY:N     | 1:V:92:GLU:OE2  | 2.52                     | 0.43              |
| 1:C:92:GLU:OE2   | 1:Y:58:GLY:N    | 2.52                     | 0.43              |
| 1:E:304:ARG:NH2  | 1:H:287:ALA:O   | 2.51                     | 0.43              |
| 1:F:256:LEU:HD23 | 1:F:256:LEU:HA  | 1.78                     | 0.43              |
| 1:H:304:ARG:NH2  | 1:T:287:ALA:O   | 2.51                     | 0.43              |
| 1:I:92:GLU:OE2   | 1:e:58:GLY:N    | 2.52                     | 0.43              |
| 1:J:92:GLU:OE2   | 1:M:58:GLY:N    | 2.52                     | 0.43              |
| 1:K:92:GLU:OE2   | 1:g:58:GLY:N    | 2.52                     | 0.43              |
| 1:K:232:ARG:HD3  | 1:g:46:LEU:HD21 | 2.00                     | 0.43              |
| 1:K:287:ALA:O    | 1:W:304:ARG:NH2 | 2.51                     | 0.43              |
| 1:O:92:GLU:OE2   | 1:k:58:GLY:N    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:158:GLN:NE2  | 1:O:160:GLY:O   | 2.43                     | 0.43              |
| 1:P:58:GLY:N     | 1:l:92:GLU:OE2  | 2.52                     | 0.43              |
| 1:Q:92:GLU:OE2   | 1:m:58:GLY:N    | 2.52                     | 0.43              |
| 1:S:92:GLU:OE2   | 1:o:58:GLY:N    | 2.52                     | 0.43              |
| 1:Z:146:THR:OG1  | 1:Z:148:THR:O   | 2.36                     | 0.43              |
| 1:j:146:THR:OG1  | 1:j:148:THR:O   | 2.36                     | 0.43              |
| 1:l:89:ARG:HD2   | 1:l:89:ARG:HA   | 1.72                     | 0.43              |
| 1:C:254:GLU:O    | 1:C:257:THR:OG1 | 2.28                     | 0.43              |
| 1:F:58:GLY:N     | 1:b:92:GLU:OE2  | 2.52                     | 0.43              |
| 1:J:146:THR:OG1  | 1:J:148:THR:O   | 2.36                     | 0.43              |
| 1:N:58:GLY:N     | 1:j:92:GLU:OE2  | 2.52                     | 0.43              |
| 1:U:158:GLN:NE2  | 1:U:160:GLY:O   | 2.43                     | 0.43              |
| 1:V:146:THR:OG1  | 1:V:148:THR:O   | 2.36                     | 0.43              |
| 1:W:146:THR:OG1  | 1:W:148:THR:O   | 2.36                     | 0.43              |
| 1:A:46:LEU:HD21  | 1:V:232:ARG:HD3 | 2.00                     | 0.43              |
| 1:A:92:GLU:OE2   | 1:W:58:GLY:N    | 2.52                     | 0.43              |
| 1:A:232:ARG:HD3  | 1:W:46:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:92:GLU:OE2   | 1:U:58:GLY:N    | 2.52                     | 0.43              |
| 1:B:287:ALA:O    | 1:K:304:ARG:NH2 | 2.51                     | 0.43              |
| 1:C:3:ILE:N      | 1:T:266:VAL:O   | 2.52                     | 0.43              |
| 1:F:46:LEU:HD21  | 1:b:232:ARG:HD3 | 2.00                     | 0.43              |
| 1:G:92:GLU:OE2   | 1:c:58:GLY:N    | 2.52                     | 0.43              |
| 1:H:158:GLN:NE2  | 1:H:160:GLY:O   | 2.43                     | 0.43              |
| 1:I:84:HIS:CE1   | 1:e:50:GLU:CB   | 2.86                     | 0.43              |
| 1:J:3:ILE:N      | 1:f:266:VAL:O   | 2.52                     | 0.43              |
| 1:K:58:GLY:N     | 1:L:92:GLU:OE2  | 2.52                     | 0.43              |
| 1:L:3:ILE:N      | 1:h:266:VAL:O   | 2.52                     | 0.43              |
| 1:L:58:GLY:N     | 1:h:92:GLU:OE2  | 2.52                     | 0.43              |
| 1:S:241:ARG:O    | 1:S:245:THR:OG1 | 2.35                     | 0.43              |
| 1:W:254:GLU:O    | 1:W:257:THR:OG1 | 2.28                     | 0.43              |
| 1:b:146:THR:OG1  | 1:b:148:THR:O   | 2.36                     | 0.43              |
| 1:f:146:THR:OG1  | 1:f:148:THR:O   | 2.36                     | 0.43              |
| 1:l:146:THR:OG1  | 1:l:148:THR:O   | 2.36                     | 0.43              |
| 1:A:3:ILE:N      | 1:V:266:VAL:O   | 2.52                     | 0.43              |
| 1:B:3:ILE:N      | 1:X:266:VAL:O   | 2.52                     | 0.43              |
| 1:E:92:GLU:OE2   | 1:a:58:GLY:N    | 2.52                     | 0.43              |
| 1:I:158:GLN:NE2  | 1:I:160:GLY:O   | 2.43                     | 0.43              |
| 1:J:266:VAL:O    | 1:M:3:ILE:N     | 2.52                     | 0.43              |
| 1:K:51:LYS:HZ2   | 1:V:105:LYS:HG2 | 1.84                     | 0.43              |
| 1:K:146:THR:OG1  | 1:K:148:THR:O   | 2.36                     | 0.43              |
| 1:L:256:LEU:HD23 | 1:L:256:LEU:HA  | 1.78                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:51:LYS:HZ2   | 1:T:105:LYS:HG2  | 1.83                     | 0.43              |
| 1:Q:232:ARG:HD3  | 1:m:46:LEU:HD21  | 2.00                     | 0.43              |
| 1:A:266:VAL:O    | 1:W:3:ILE:N      | 2.52                     | 0.43              |
| 1:B:50:GLU:CB    | 1:X:84:HIS:CE1   | 2.86                     | 0.43              |
| 1:C:266:VAL:O    | 1:Y:3:ILE:N      | 2.52                     | 0.43              |
| 1:H:3:ILE:N      | 1:d:266:VAL:O    | 2.52                     | 0.43              |
| 1:H:92:GLU:OE2   | 1:O:58:GLY:N     | 2.52                     | 0.43              |
| 1:I:3:ILE:N      | 1:N:266:VAL:O    | 2.52                     | 0.43              |
| 1:K:3:ILE:N      | 1:L:266:VAL:O    | 2.52                     | 0.43              |
| 1:K:158:GLN:NE2  | 1:K:160:GLY:O    | 2.43                     | 0.43              |
| 1:L:304:ARG:NH2  | 1:X:287:ALA:O    | 2.51                     | 0.43              |
| 1:N:3:ILE:N      | 1:j:266:VAL:O    | 2.52                     | 0.43              |
| 1:V:256:LEU:HA   | 1:V:256:LEU:HD23 | 1.78                     | 0.43              |
| 1:X:304:ARG:NH2  | 1:j:287:ALA:O    | 2.51                     | 0.43              |
| 1:c:287:ALA:O    | 1:o:304:ARG:NH2  | 2.51                     | 0.43              |
| 1:n:146:THR:OG1  | 1:n:148:THR:O    | 2.36                     | 0.43              |
| 1:o:256:LEU:HD23 | 1:o:256:LEU:HA   | 1.78                     | 0.43              |
| 1:D:58:GLY:N     | 1:Z:92:GLU:OE2   | 2.52                     | 0.43              |
| 1:D:304:ARG:NH2  | 1:P:287:ALA:O    | 2.51                     | 0.43              |
| 1:E:46:LEU:HD21  | 1:R:232:ARG:HD3  | 2.00                     | 0.43              |
| 1:F:84:HIS:CE1   | 1:Q:50:GLU:CB    | 2.86                     | 0.43              |
| 1:G:58:GLY:N     | 1:P:92:GLU:OE2   | 2.52                     | 0.43              |
| 1:M:92:GLU:OE2   | 1:i:58:GLY:N     | 2.52                     | 0.43              |
| 1:N:158:GLN:NE2  | 1:N:160:GLY:O    | 2.43                     | 0.43              |
| 1:P:304:ARG:NH2  | 1:b:287:ALA:O    | 2.51                     | 0.43              |
| 1:R:256:LEU:HA   | 1:R:256:LEU:HD23 | 1.78                     | 0.43              |
| 1:B:58:GLY:N     | 1:X:92:GLU:OE2   | 2.52                     | 0.43              |
| 1:B:266:VAL:O    | 1:U:3:ILE:N      | 2.52                     | 0.43              |
| 1:B:304:ARG:NH2  | 1:N:287:ALA:O    | 2.51                     | 0.43              |
| 1:C:58:GLY:N     | 1:T:92:GLU:OE2   | 2.52                     | 0.43              |
| 1:D:92:GLU:OE2   | 1:S:58:GLY:N     | 2.52                     | 0.43              |
| 1:F:304:ARG:NH2  | 1:R:287:ALA:O    | 2.51                     | 0.43              |
| 1:H:58:GLY:N     | 1:d:92:GLU:OE2   | 2.52                     | 0.43              |
| 1:H:266:VAL:O    | 1:O:3:ILE:N      | 2.52                     | 0.43              |
| 1:L:105:LYS:CG   | 1:U:51:LYS:HZ2   | 2.31                     | 0.43              |
| 1:M:266:VAL:O    | 1:i:3:ILE:N      | 2.52                     | 0.43              |
| 1:N:304:ARG:NH2  | 1:Z:287:ALA:O    | 2.51                     | 0.43              |
| 1:R:304:ARG:NH2  | 1:d:287:ALA:O    | 2.51                     | 0.43              |
| 1:V:299:VAL:HA   | 1:V:302:LEU:CD2  | 2.49                     | 0.43              |
| 1:V:304:ARG:NH2  | 1:h:287:ALA:O    | 2.51                     | 0.43              |
| 1:a:287:ALA:O    | 1:m:304:ARG:NH2  | 2.51                     | 0.43              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:146:THR:OG1  | 1:A:148:THR:O   | 2.36                     | 0.42              |
| 1:A:299:VAL:HA   | 1:A:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:B:299:VAL:HA   | 1:B:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:C:299:VAL:HA   | 1:C:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:D:3:ILE:N      | 1:Z:266:VAL:O   | 2.52                     | 0.42              |
| 1:D:266:VAL:O    | 1:S:3:ILE:N     | 2.52                     | 0.42              |
| 1:E:58:GLY:N     | 1:R:92:GLU:OE2  | 2.52                     | 0.42              |
| 1:E:232:ARG:HD3  | 1:a:46:LEU:HD21 | 2.00                     | 0.42              |
| 1:F:287:ALA:O    | 1:G:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:J:232:ARG:HD3  | 1:M:46:LEU:HD21 | 2.00                     | 0.42              |
| 1:K:266:VAL:O    | 1:g:3:ILE:N     | 2.52                     | 0.42              |
| 1:R:3:ILE:N      | 1:n:266:VAL:O   | 2.52                     | 0.42              |
| 1:Y:287:ALA:O    | 1:k:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:Z:304:ARG:NH2  | 1:l:287:ALA:O   | 2.51                     | 0.42              |
| 1:b:256:LEU:HD23 | 1:b:256:LEU:HA  | 1.78                     | 0.42              |
| 1:b:304:ARG:NH2  | 1:n:287:ALA:O   | 2.51                     | 0.42              |
| 1:e:158:GLN:NE2  | 1:e:160:GLY:O   | 2.43                     | 0.42              |
| 1:g:299:VAL:HA   | 1:g:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:h:299:VAL:HA   | 1:h:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:n:299:VAL:HA   | 1:n:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:C:232:ARG:HD3  | 1:Y:46:LEU:HD21 | 2.00                     | 0.42              |
| 1:E:299:VAL:HA   | 1:E:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:I:266:VAL:O    | 1:e:3:ILE:N     | 2.52                     | 0.42              |
| 1:I:287:ALA:O    | 1:U:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:J:46:LEU:HD21  | 1:f:232:ARG:HD3 | 2.00                     | 0.42              |
| 1:M:232:ARG:HD3  | 1:i:46:LEU:HD21 | 2.00                     | 0.42              |
| 1:S:266:VAL:O    | 1:o:3:ILE:N     | 2.52                     | 0.42              |
| 1:T:299:VAL:HA   | 1:T:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:X:299:VAL:HA   | 1:X:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:Y:299:VAL:HA   | 1:Y:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:i:299:VAL:HA   | 1:i:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:k:299:VAL:HA   | 1:k:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:m:299:VAL:HA   | 1:m:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:D:287:ALA:O    | 1:I:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:I:172:GLU:OE1  | 1:I:172:GLU:N   | 2.53                     | 0.42              |
| 1:J:58:GLY:N     | 1:f:92:GLU:OE2  | 2.52                     | 0.42              |
| 1:N:299:VAL:HA   | 1:N:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:O:232:ARG:HD3  | 1:k:46:LEU:HD21 | 2.00                     | 0.42              |
| 1:Q:299:VAL:HA   | 1:Q:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:R:46:LEU:HD21  | 1:n:232:ARG:HD3 | 2.00                     | 0.42              |
| 1:R:299:VAL:HA   | 1:R:302:LEU:CD2 | 2.50                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:S:287:ALA:O   | 1:e:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:a:299:VAL:HA  | 1:a:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:d:299:VAL:HA  | 1:d:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:g:146:THR:OG1 | 1:g:148:THR:O   | 2.36                     | 0.42              |
| 1:h:172:GLU:OE1 | 1:h:172:GLU:N   | 2.53                     | 0.42              |
| 1:A:172:GLU:OE1 | 1:A:172:GLU:N   | 2.53                     | 0.42              |
| 1:D:299:VAL:HA  | 1:D:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:G:287:ALA:O   | 1:S:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:G:299:VAL:HA  | 1:G:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:H:232:ARG:HD3 | 1:O:46:LEU:HD21 | 2.00                     | 0.42              |
| 1:N:172:GLU:OE1 | 1:N:172:GLU:N   | 2.53                     | 0.42              |
| 1:O:266:VAL:O   | 1:k:3:ILE:N     | 2.52                     | 0.42              |
| 1:U:299:VAL:HA  | 1:U:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:X:172:GLU:OE1 | 1:X:172:GLU:N   | 2.53                     | 0.42              |
| 1:Z:172:GLU:N   | 1:Z:172:GLU:OE1 | 2.53                     | 0.42              |
| 1:g:172:GLU:N   | 1:g:172:GLU:OE1 | 2.53                     | 0.42              |
| 1:j:299:VAL:HA  | 1:j:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:o:172:GLU:N   | 1:o:172:GLU:OE1 | 2.53                     | 0.42              |
| 1:B:104:ASP:CB  | 1:U:135:LYS:HZ3 | 2.29                     | 0.42              |
| 1:B:172:GLU:OE1 | 1:B:172:GLU:N   | 2.53                     | 0.42              |
| 1:C:51:LYS:HZ2  | 1:d:105:LYS:HG2 | 1.84                     | 0.42              |
| 1:F:92:GLU:OE2  | 1:Q:58:GLY:N    | 2.52                     | 0.42              |
| 1:F:241:ARG:O   | 1:F:245:THR:OG1 | 2.35                     | 0.42              |
| 1:G:266:VAL:O   | 1:c:3:ILE:N     | 2.52                     | 0.42              |
| 1:H:46:LEU:HD21 | 1:d:232:ARG:HD3 | 2.00                     | 0.42              |
| 1:P:299:VAL:HA  | 1:P:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:Q:287:ALA:O   | 1:c:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:S:299:VAL:HA  | 1:S:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:U:172:GLU:OE1 | 1:U:172:GLU:N   | 2.53                     | 0.42              |
| 1:W:172:GLU:N   | 1:W:172:GLU:OE1 | 2.53                     | 0.42              |
| 1:W:299:VAL:HA  | 1:W:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:Y:158:GLN:NE2 | 1:Y:160:GLY:O   | 2.43                     | 0.42              |
| 1:e:172:GLU:OE1 | 1:e:172:GLU:N   | 2.53                     | 0.42              |
| 1:f:299:VAL:HA  | 1:f:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:j:172:GLU:N   | 1:j:172:GLU:OE1 | 2.53                     | 0.42              |
| 1:m:89:ARG:HA   | 1:m:89:ARG:HD2  | 1.72                     | 0.42              |
| 1:C:46:LEU:HD21 | 1:T:232:ARG:HD3 | 2.00                     | 0.42              |
| 1:D:172:GLU:N   | 1:D:172:GLU:OE1 | 2.53                     | 0.42              |
| 1:D:241:ARG:O   | 1:D:245:THR:OG1 | 2.35                     | 0.42              |
| 1:E:3:ILE:N     | 1:R:266:VAL:O   | 2.52                     | 0.42              |
| 1:G:3:ILE:N     | 1:P:266:VAL:O   | 2.52                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:58:GLY:N    | 1:N:92:GLU:OE2  | 2.52                     | 0.42              |
| 1:K:172:GLU:OE1 | 1:K:172:GLU:N   | 2.53                     | 0.42              |
| 1:K:254:GLU:O   | 1:K:257:THR:OG1 | 2.28                     | 0.42              |
| 1:K:299:VAL:HA  | 1:K:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:M:158:GLN:NE2 | 1:M:160:GLY:O   | 2.43                     | 0.42              |
| 1:M:254:GLU:O   | 1:M:257:THR:OG1 | 2.28                     | 0.42              |
| 1:S:172:GLU:OE1 | 1:S:172:GLU:N   | 2.53                     | 0.42              |
| 1:b:299:VAL:HA  | 1:b:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:c:299:VAL:HA  | 1:c:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:e:299:VAL:HA  | 1:e:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:l:299:VAL:HA  | 1:l:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:n:158:GLN:NE2 | 1:n:160:GLY:O   | 2.43                     | 0.42              |
| 1:P:3:ILE:N     | 1:l:266:VAL:O   | 2.52                     | 0.42              |
| 1:V:254:GLU:O   | 1:V:257:THR:OG1 | 2.28                     | 0.42              |
| 1:E:287:ALA:O   | 1:Q:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:J:172:GLU:OE1 | 1:J:172:GLU:N   | 2.53                     | 0.42              |
| 1:M:172:GLU:OE1 | 1:M:172:GLU:N   | 2.53                     | 0.42              |
| 1:N:89:ARG:HD2  | 1:N:89:ARG:HA   | 1.72                     | 0.42              |
| 1:P:172:GLU:OE1 | 1:P:172:GLU:N   | 2.53                     | 0.42              |
| 1:Q:266:VAL:O   | 1:m:3:ILE:N     | 2.52                     | 0.42              |
| 1:V:172:GLU:OE1 | 1:V:172:GLU:N   | 2.53                     | 0.42              |
| 1:f:172:GLU:OE1 | 1:f:172:GLU:N   | 2.53                     | 0.42              |
| 1:i:172:GLU:OE1 | 1:i:172:GLU:N   | 2.53                     | 0.42              |
| 1:o:299:VAL:HA  | 1:o:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:A:100:THR:CB  | 1:A:202:PHE:CE2 | 3.03                     | 0.42              |
| 1:A:287:ALA:HB1 | 1:M:304:ARG:NH2 | 2.35                     | 0.42              |
| 1:B:287:ALA:HB1 | 1:K:304:ARG:NH2 | 2.35                     | 0.42              |
| 1:E:254:GLU:O   | 1:E:257:THR:OG1 | 2.28                     | 0.42              |
| 1:F:89:ARG:HD2  | 1:F:89:ARG:HA   | 1.72                     | 0.42              |
| 1:I:287:ALA:HB1 | 1:U:304:ARG:NH2 | 2.35                     | 0.42              |
| 1:I:299:VAL:HA  | 1:I:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:K:287:ALA:HB1 | 1:W:304:ARG:NH2 | 2.35                     | 0.42              |
| 1:M:287:ALA:HB1 | 1:Y:304:ARG:NH2 | 2.35                     | 0.42              |
| 1:M:299:VAL:HA  | 1:M:302:LEU:CD2 | 2.50                     | 0.42              |
| 1:O:287:ALA:O   | 1:a:304:ARG:NH2 | 2.51                     | 0.42              |
| 1:O:299:VAL:HA  | 1:O:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:U:287:ALA:HB1 | 1:g:304:ARG:NH2 | 2.35                     | 0.42              |
| 1:W:287:ALA:HB1 | 1:i:304:ARG:NH2 | 2.35                     | 0.42              |
| 1:Z:299:VAL:HA  | 1:Z:302:LEU:CD2 | 2.49                     | 0.42              |
| 1:A:304:ARG:NH2 | 1:L:287:ALA:HB1 | 2.35                     | 0.42              |
| 1:C:304:ARG:NH2 | 1:J:287:ALA:HB1 | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:256:LEU:HA   | 1:D:256:LEU:HD23 | 1.78                     | 0.42              |
| 1:E:158:GLN:NE2  | 1:E:160:GLY:O    | 2.43                     | 0.42              |
| 1:E:304:ARG:NH2  | 1:H:287:ALA:HB1  | 2.35                     | 0.42              |
| 1:F:3:ILE:N      | 1:b:266:VAL:O    | 2.52                     | 0.42              |
| 1:F:304:ARG:NH2  | 1:R:287:ALA:HB1  | 2.35                     | 0.42              |
| 1:G:172:GLU:N    | 1:G:172:GLU:OE1  | 2.53                     | 0.42              |
| 1:H:299:VAL:HA   | 1:H:302:LEU:CD2  | 2.49                     | 0.42              |
| 1:K:50:GLU:CB    | 1:L:84:HIS:CE1   | 2.86                     | 0.42              |
| 1:L:100:THR:CB   | 1:L:202:PHE:CE2  | 3.03                     | 0.42              |
| 1:L:172:GLU:N    | 1:L:172:GLU:OE1  | 2.53                     | 0.42              |
| 1:L:299:VAL:HA   | 1:L:302:LEU:CD2  | 2.49                     | 0.42              |
| 1:M:256:LEU:HD23 | 1:M:256:LEU:HA   | 1.78                     | 0.42              |
| 1:b:304:ARG:NH2  | 1:n:287:ALA:HB1  | 2.35                     | 0.42              |
| 1:k:158:GLN:NE2  | 1:k:160:GLY:O    | 2.43                     | 0.42              |
| 1:B:304:ARG:NH2  | 1:N:287:ALA:HB1  | 2.35                     | 0.41              |
| 1:C:287:ALA:HB1  | 1:O:304:ARG:NH2  | 2.35                     | 0.41              |
| 1:H:304:ARG:NH2  | 1:T:287:ALA:HB1  | 2.35                     | 0.41              |
| 1:J:304:ARG:NH2  | 1:V:287:ALA:HB1  | 2.35                     | 0.41              |
| 1:L:304:ARG:NH2  | 1:X:287:ALA:HB1  | 2.35                     | 0.41              |
| 1:M:100:THR:CB   | 1:M:202:PHE:CE2  | 3.03                     | 0.41              |
| 1:R:304:ARG:NH2  | 1:d:287:ALA:HB1  | 2.35                     | 0.41              |
| 1:S:287:ALA:HB1  | 1:e:304:ARG:NH2  | 2.35                     | 0.41              |
| 1:c:287:ALA:HB1  | 1:o:304:ARG:NH2  | 2.35                     | 0.41              |
| 1:d:158:GLN:NE2  | 1:d:160:GLY:O    | 2.43                     | 0.41              |
| 1:D:158:GLN:NE2  | 1:D:160:GLY:O    | 2.43                     | 0.41              |
| 1:E:266:VAL:O    | 1:a:3:ILE:N      | 2.52                     | 0.41              |
| 1:G:254:GLU:O    | 1:G:257:THR:OG1  | 2.28                     | 0.41              |
| 1:I:100:THR:CB   | 1:I:202:PHE:CE2  | 3.03                     | 0.41              |
| 1:I:254:GLU:O    | 1:I:257:THR:OG1  | 2.28                     | 0.41              |
| 1:O:287:ALA:HB1  | 1:a:304:ARG:NH2  | 2.35                     | 0.41              |
| 1:P:50:GLU:CB    | 1:l:84:HIS:CE1   | 2.86                     | 0.41              |
| 1:Q:172:GLU:OE1  | 1:Q:172:GLU:N    | 2.53                     | 0.41              |
| 1:V:304:ARG:NH2  | 1:h:287:ALA:HB1  | 2.35                     | 0.41              |
| 1:Y:287:ALA:HB1  | 1:k:304:ARG:NH2  | 2.35                     | 0.41              |
| 1:c:172:GLU:OE1  | 1:c:172:GLU:N    | 2.53                     | 0.41              |
| 1:o:158:GLN:NE2  | 1:o:160:GLY:O    | 2.43                     | 0.41              |
| 1:C:172:GLU:OE1  | 1:C:172:GLU:N    | 2.53                     | 0.41              |
| 1:D:287:ALA:HB1  | 1:I:304:ARG:NH2  | 2.35                     | 0.41              |
| 1:F:172:GLU:OE1  | 1:F:172:GLU:N    | 2.53                     | 0.41              |
| 1:F:266:VAL:O    | 1:Q:3:ILE:N      | 2.52                     | 0.41              |
| 1:F:299:VAL:HA   | 1:F:302:LEU:CD2  | 2.49                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:105:LYS:CD   | 1:m:51:LYS:HZ1  | 2.17                     | 0.41              |
| 1:J:299:VAL:HA   | 1:J:302:LEU:CD2 | 2.49                     | 0.41              |
| 1:T:304:ARG:NH2  | 1:f:287:ALA:HB1 | 2.35                     | 0.41              |
| 1:V:89:ARG:HA    | 1:V:89:ARG:HD2  | 1.72                     | 0.41              |
| 1:Y:172:GLU:OE1  | 1:Y:172:GLU:N   | 2.53                     | 0.41              |
| 1:j:158:GLN:NE2  | 1:j:160:GLY:O   | 2.43                     | 0.41              |
| 1:A:89:ARG:HD2   | 1:A:89:ARG:HA   | 1.72                     | 0.41              |
| 1:G:287:ALA:HB1  | 1:S:304:ARG:NH2 | 2.35                     | 0.41              |
| 1:P:304:ARG:NH2  | 1:b:287:ALA:HB1 | 2.35                     | 0.41              |
| 1:X:304:ARG:NH2  | 1:j:287:ALA:HB1 | 2.35                     | 0.41              |
| 1:m:172:GLU:OE1  | 1:m:172:GLU:N   | 2.53                     | 0.41              |
| 1:A:158:GLN:NE2  | 1:A:160:GLY:O   | 2.43                     | 0.41              |
| 1:E:287:ALA:HB1  | 1:Q:304:ARG:NH2 | 2.35                     | 0.41              |
| 1:W:256:LEU:HD23 | 1:W:256:LEU:HA  | 1.78                     | 0.41              |
| 1:a:158:GLN:NE2  | 1:a:160:GLY:O   | 2.43                     | 0.41              |
| 1:b:172:GLU:N    | 1:b:172:GLU:OE1 | 2.53                     | 0.41              |
| 1:f:254:GLU:O    | 1:f:257:THR:OG1 | 2.28                     | 0.41              |
| 1:h:256:LEU:HD23 | 1:h:256:LEU:HA  | 1.78                     | 0.41              |
| 1:n:89:ARG:HA    | 1:n:89:ARG:HD2  | 1.72                     | 0.41              |
| 1:E:172:GLU:OE1  | 1:E:172:GLU:N   | 2.53                     | 0.41              |
| 1:H:172:GLU:OE1  | 1:H:172:GLU:N   | 2.53                     | 0.41              |
| 1:O:154:ASN:OD1  | 1:O:170:ASN:ND2 | 2.45                     | 0.41              |
| 1:O:172:GLU:N    | 1:O:172:GLU:OE1 | 2.53                     | 0.41              |
| 1:S:158:GLN:NE2  | 1:S:160:GLY:O   | 2.43                     | 0.41              |
| 1:T:172:GLU:OE1  | 1:T:172:GLU:N   | 2.53                     | 0.41              |
| 1:U:100:THR:CB   | 1:U:202:PHE:CE2 | 3.03                     | 0.41              |
| 1:i:154:ASN:OD1  | 1:i:170:ASN:ND2 | 2.45                     | 0.41              |
| 1:k:89:ARG:HA    | 1:k:89:ARG:HD2  | 1.72                     | 0.41              |
| 1:A:154:ASN:OD1  | 1:A:170:ASN:ND2 | 2.45                     | 0.41              |
| 1:N:304:ARG:NH2  | 1:Z:287:ALA:HB1 | 2.35                     | 0.41              |
| 1:R:172:GLU:N    | 1:R:172:GLU:OE1 | 2.53                     | 0.41              |
| 1:a:172:GLU:N    | 1:a:172:GLU:OE1 | 2.53                     | 0.41              |
| 1:b:241:ARG:O    | 1:b:245:THR:OG1 | 2.35                     | 0.41              |
| 1:c:256:LEU:HD23 | 1:c:256:LEU:HA  | 1.78                     | 0.41              |
| 1:g:100:THR:CB   | 1:g:202:PHE:CE2 | 3.03                     | 0.41              |
| 1:g:256:LEU:HD23 | 1:g:256:LEU:HA  | 1.78                     | 0.41              |
| 1:l:172:GLU:OE1  | 1:l:172:GLU:N   | 2.53                     | 0.41              |
| 1:G:89:ARG:HA    | 1:G:89:ARG:HD2  | 1.72                     | 0.41              |
| 1:R:158:GLN:NE2  | 1:R:160:GLY:O   | 2.43                     | 0.41              |
| 1:Z:100:THR:CB   | 1:Z:202:PHE:CE2 | 3.03                     | 0.41              |
| 1:Z:241:ARG:O    | 1:Z:245:THR:OG1 | 2.35                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:d:241:ARG:O    | 1:d:245:THR:OG1 | 2.35                     | 0.41              |
| 1:o:100:THR:CB   | 1:o:202:PHE:CE2 | 3.03                     | 0.41              |
| 1:A:84:HIS:CE1   | 1:W:50:GLU:CB   | 2.86                     | 0.41              |
| 1:C:105:LYS:CD   | 1:i:51:LYS:HZ2  | 2.31                     | 0.41              |
| 1:D:154:ASN:OD1  | 1:D:170:ASN:ND2 | 2.45                     | 0.41              |
| 1:H:30:LEU:N     | 1:H:271:GLU:OE2 | 2.54                     | 0.41              |
| 1:J:30:LEU:N     | 1:J:271:GLU:OE2 | 2.54                     | 0.41              |
| 1:L:105:LYS:HG2  | 1:U:51:LYS:HZ2  | 1.86                     | 0.41              |
| 1:Q:287:ALA:HB1  | 1:c:304:ARG:NH2 | 2.35                     | 0.41              |
| 1:T:256:LEU:HD23 | 1:T:256:LEU:HA  | 1.77                     | 0.41              |
| 1:V:100:THR:CB   | 1:V:202:PHE:CE2 | 3.03                     | 0.41              |
| 1:d:254:GLU:O    | 1:d:257:THR:OG1 | 2.28                     | 0.41              |
| 1:j:241:ARG:O    | 1:j:245:THR:OG1 | 2.35                     | 0.41              |
| 1:k:172:GLU:OE1  | 1:k:172:GLU:N   | 2.53                     | 0.41              |
| 1:l:256:LEU:HD23 | 1:l:256:LEU:HA  | 1.78                     | 0.41              |
| 1:C:30:LEU:N     | 1:C:271:GLU:OE2 | 2.54                     | 0.41              |
| 1:D:105:LYS:CD   | 1:c:51:LYS:HZ1  | 2.17                     | 0.41              |
| 1:D:304:ARG:NH2  | 1:P:287:ALA:HB1 | 2.35                     | 0.41              |
| 1:I:256:LEU:HD23 | 1:I:256:LEU:HA  | 1.78                     | 0.41              |
| 1:Y:100:THR:CB   | 1:Y:202:PHE:CE2 | 3.03                     | 0.41              |
| 1:Z:158:GLN:NE2  | 1:Z:160:GLY:O   | 2.43                     | 0.41              |
| 1:n:172:GLU:OE1  | 1:n:172:GLU:N   | 2.53                     | 0.41              |
| 1:n:241:ARG:O    | 1:n:245:THR:OG1 | 2.35                     | 0.41              |
| 1:A:30:LEU:N     | 1:A:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:E:30:LEU:N     | 1:E:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:F:158:GLN:NE2  | 1:F:160:GLY:O   | 2.43                     | 0.40              |
| 1:F:287:ALA:HB1  | 1:G:304:ARG:NH2 | 2.35                     | 0.40              |
| 1:G:158:GLN:NE2  | 1:G:160:GLY:O   | 2.43                     | 0.40              |
| 1:T:30:LEU:N     | 1:T:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:Z:304:ARG:NH2  | 1:l:287:ALA:HB1 | 2.35                     | 0.40              |
| 1:a:287:ALA:HB1  | 1:m:304:ARG:NH2 | 2.35                     | 0.40              |
| 1:B:158:GLN:NE2  | 1:B:160:GLY:O   | 2.43                     | 0.40              |
| 1:I:30:LEU:N     | 1:I:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:Q:158:GLN:NE2  | 1:Q:160:GLY:O   | 2.43                     | 0.40              |
| 1:U:241:ARG:O    | 1:U:245:THR:OG1 | 2.35                     | 0.40              |
| 1:Y:254:GLU:O    | 1:Y:257:THR:OG1 | 2.28                     | 0.40              |
| 1:e:154:ASN:OD1  | 1:e:170:ASN:ND2 | 2.45                     | 0.40              |
| 1:C:135:LYS:HZ1  | 1:T:104:ASP:CB  | 2.34                     | 0.40              |
| 1:F:30:LEU:N     | 1:F:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:L:30:LEU:N     | 1:L:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:M:30:LEU:N     | 1:M:271:GLU:OE2 | 2.54                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:256:LEU:HD23 | 1:O:256:LEU:HA  | 1.78                     | 0.40              |
| 1:Q:154:ASN:OD1  | 1:Q:170:ASN:ND2 | 2.45                     | 0.40              |
| 1:R:30:LEU:N     | 1:R:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:S:30:LEU:N     | 1:S:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:V:30:LEU:N     | 1:V:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:d:172:GLU:OE1  | 1:d:172:GLU:N   | 2.53                     | 0.40              |
| 1:f:30:LEU:N     | 1:f:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:i:30:LEU:N     | 1:i:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:n:154:ASN:OD1  | 1:n:170:ASN:ND2 | 2.45                     | 0.40              |
| 1:J:100:THR:CB   | 1:J:202:PHE:CE2 | 3.03                     | 0.40              |
| 1:O:30:LEU:N     | 1:O:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:T:89:ARG:HD2   | 1:T:89:ARG:HA   | 1.72                     | 0.40              |
| 1:Y:30:LEU:N     | 1:Y:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:k:30:LEU:N     | 1:k:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:l:241:ARG:O    | 1:l:245:THR:OG1 | 2.35                     | 0.40              |
| 1:B:30:LEU:N     | 1:B:271:GLU:OE2 | 2.54                     | 0.40              |
| 1:B:104:ASP:HB2  | 1:U:135:LYS:HZ1 | 1.86                     | 0.40              |
| 1:G:100:THR:CB   | 1:G:202:PHE:CE2 | 3.03                     | 0.40              |
| 1:P:158:GLN:NE2  | 1:P:160:GLY:O   | 2.43                     | 0.40              |
| 1:S:89:ARG:HD2   | 1:S:89:ARG:HA   | 1.72                     | 0.40              |
| 1:b:89:ARG:HA    | 1:b:89:ARG:HD2  | 1.72                     | 0.40              |
| 1:j:30:LEU:N     | 1:j:271:GLU:OE2 | 2.54                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | B     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | C     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | D     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | E     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | F     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | G     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | H     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | I     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | J     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | K     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | L     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | M     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | N     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | O     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | P     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | Q     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | R     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | S     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | T     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | U     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | V     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | W     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | X     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | Y     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | Z     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | a     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | b     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | c     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | d     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | e     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | f     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | g     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |
| 1   | h     | 300/304 (99%) | 268 (89%) | 32 (11%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 1   | i     | 300/304 (99%)     | 268 (89%)   | 32 (11%)   | 0        | 100         | 100 |
| 1   | j     | 300/304 (99%)     | 268 (89%)   | 32 (11%)   | 0        | 100         | 100 |
| 1   | k     | 300/304 (99%)     | 268 (89%)   | 32 (11%)   | 0        | 100         | 100 |
| 1   | l     | 300/304 (99%)     | 268 (89%)   | 32 (11%)   | 0        | 100         | 100 |
| 1   | m     | 300/304 (99%)     | 268 (89%)   | 32 (11%)   | 0        | 100         | 100 |
| 1   | n     | 300/304 (99%)     | 268 (89%)   | 32 (11%)   | 0        | 100         | 100 |
| 1   | o     | 300/304 (99%)     | 268 (89%)   | 32 (11%)   | 0        | 100         | 100 |
| All | All   | 12300/12464 (99%) | 10988 (89%) | 1312 (11%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | B     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | C     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | D     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | E     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | F     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | G     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | H     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | I     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | J     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | K     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | L     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | M     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |
| 1   | N     | 244/246 (99%) | 243 (100%) | 1 (0%)   | 84          | 83 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 1   | O     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | P     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | Q     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | R     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | S     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | T     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | U     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | V     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | W     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | X     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | Y     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | Z     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | a     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | b     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | c     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | d     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | e     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | f     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | g     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | h     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | i     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | j     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | k     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | l     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | m     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | n     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| 1   | o     | 244/246 (99%)     | 243 (100%)  | 1 (0%)   | 84          | 83 |
| All | All   | 10004/10086 (99%) | 9963 (100%) | 41 (0%)  | 81          | 83 |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 84  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 84  | HIS  |
| 1   | C     | 84  | HIS  |
| 1   | D     | 84  | HIS  |
| 1   | E     | 84  | HIS  |
| 1   | F     | 84  | HIS  |
| 1   | G     | 84  | HIS  |
| 1   | H     | 84  | HIS  |
| 1   | I     | 84  | HIS  |
| 1   | J     | 84  | HIS  |
| 1   | K     | 84  | HIS  |
| 1   | L     | 84  | HIS  |
| 1   | M     | 84  | HIS  |
| 1   | N     | 84  | HIS  |
| 1   | O     | 84  | HIS  |
| 1   | P     | 84  | HIS  |
| 1   | Q     | 84  | HIS  |
| 1   | R     | 84  | HIS  |
| 1   | S     | 84  | HIS  |
| 1   | T     | 84  | HIS  |
| 1   | U     | 84  | HIS  |
| 1   | V     | 84  | HIS  |
| 1   | W     | 84  | HIS  |
| 1   | X     | 84  | HIS  |
| 1   | Y     | 84  | HIS  |
| 1   | Z     | 84  | HIS  |
| 1   | a     | 84  | HIS  |
| 1   | b     | 84  | HIS  |
| 1   | c     | 84  | HIS  |
| 1   | d     | 84  | HIS  |
| 1   | e     | 84  | HIS  |
| 1   | f     | 84  | HIS  |
| 1   | g     | 84  | HIS  |
| 1   | h     | 84  | HIS  |
| 1   | i     | 84  | HIS  |
| 1   | j     | 84  | HIS  |
| 1   | k     | 84  | HIS  |
| 1   | l     | 84  | HIS  |
| 1   | m     | 84  | HIS  |
| 1   | n     | 84  | HIS  |
| 1   | o     | 84  | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 99  | ASN  |
| 1   | A     | 248 | ASN  |
| 1   | A     | 298 | ASN  |
| 1   | B     | 99  | ASN  |
| 1   | B     | 128 | ASN  |
| 1   | B     | 248 | ASN  |
| 1   | B     | 298 | ASN  |
| 1   | C     | 84  | HIS  |
| 1   | C     | 99  | ASN  |
| 1   | C     | 248 | ASN  |
| 1   | C     | 298 | ASN  |
| 1   | D     | 84  | HIS  |
| 1   | D     | 99  | ASN  |
| 1   | D     | 248 | ASN  |
| 1   | D     | 298 | ASN  |
| 1   | E     | 84  | HIS  |
| 1   | E     | 99  | ASN  |
| 1   | E     | 128 | ASN  |
| 1   | E     | 248 | ASN  |
| 1   | E     | 298 | ASN  |
| 1   | F     | 84  | HIS  |
| 1   | F     | 99  | ASN  |
| 1   | F     | 248 | ASN  |
| 1   | F     | 298 | ASN  |
| 1   | G     | 99  | ASN  |
| 1   | G     | 248 | ASN  |
| 1   | G     | 298 | ASN  |
| 1   | H     | 84  | HIS  |
| 1   | H     | 99  | ASN  |
| 1   | H     | 248 | ASN  |
| 1   | H     | 298 | ASN  |
| 1   | I     | 84  | HIS  |
| 1   | I     | 99  | ASN  |
| 1   | I     | 128 | ASN  |
| 1   | I     | 248 | ASN  |
| 1   | I     | 298 | ASN  |
| 1   | J     | 84  | HIS  |
| 1   | J     | 99  | ASN  |
| 1   | J     | 248 | ASN  |
| 1   | J     | 298 | ASN  |
| 1   | K     | 99  | ASN  |
| 1   | K     | 248 | ASN  |
| 1   | K     | 298 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 84  | HIS  |
| 1   | L     | 99  | ASN  |
| 1   | L     | 248 | ASN  |
| 1   | L     | 298 | ASN  |
| 1   | M     | 84  | HIS  |
| 1   | M     | 99  | ASN  |
| 1   | M     | 248 | ASN  |
| 1   | M     | 298 | ASN  |
| 1   | N     | 99  | ASN  |
| 1   | N     | 248 | ASN  |
| 1   | N     | 298 | ASN  |
| 1   | O     | 84  | HIS  |
| 1   | O     | 99  | ASN  |
| 1   | O     | 248 | ASN  |
| 1   | O     | 298 | ASN  |
| 1   | P     | 99  | ASN  |
| 1   | P     | 248 | ASN  |
| 1   | P     | 298 | ASN  |
| 1   | Q     | 99  | ASN  |
| 1   | Q     | 248 | ASN  |
| 1   | Q     | 298 | ASN  |
| 1   | R     | 84  | HIS  |
| 1   | R     | 99  | ASN  |
| 1   | R     | 248 | ASN  |
| 1   | R     | 298 | ASN  |
| 1   | S     | 99  | ASN  |
| 1   | S     | 248 | ASN  |
| 1   | S     | 298 | ASN  |
| 1   | T     | 84  | HIS  |
| 1   | T     | 99  | ASN  |
| 1   | T     | 248 | ASN  |
| 1   | T     | 298 | ASN  |
| 1   | U     | 84  | HIS  |
| 1   | U     | 248 | ASN  |
| 1   | U     | 298 | ASN  |
| 1   | V     | 84  | HIS  |
| 1   | V     | 99  | ASN  |
| 1   | V     | 248 | ASN  |
| 1   | V     | 298 | ASN  |
| 1   | W     | 84  | HIS  |
| 1   | W     | 248 | ASN  |
| 1   | W     | 298 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 84  | HIS  |
| 1   | X     | 99  | ASN  |
| 1   | X     | 248 | ASN  |
| 1   | X     | 298 | ASN  |
| 1   | Y     | 84  | HIS  |
| 1   | Y     | 248 | ASN  |
| 1   | Y     | 298 | ASN  |
| 1   | Z     | 99  | ASN  |
| 1   | Z     | 248 | ASN  |
| 1   | Z     | 298 | ASN  |
| 1   | a     | 84  | HIS  |
| 1   | a     | 248 | ASN  |
| 1   | a     | 298 | ASN  |
| 1   | b     | 84  | HIS  |
| 1   | b     | 99  | ASN  |
| 1   | b     | 248 | ASN  |
| 1   | b     | 298 | ASN  |
| 1   | c     | 84  | HIS  |
| 1   | c     | 248 | ASN  |
| 1   | c     | 298 | ASN  |
| 1   | d     | 84  | HIS  |
| 1   | d     | 99  | ASN  |
| 1   | d     | 248 | ASN  |
| 1   | d     | 298 | ASN  |
| 1   | e     | 84  | HIS  |
| 1   | e     | 248 | ASN  |
| 1   | e     | 283 | GLN  |
| 1   | e     | 298 | ASN  |
| 1   | f     | 84  | HIS  |
| 1   | f     | 99  | ASN  |
| 1   | f     | 248 | ASN  |
| 1   | g     | 84  | HIS  |
| 1   | g     | 248 | ASN  |
| 1   | g     | 298 | ASN  |
| 1   | h     | 84  | HIS  |
| 1   | h     | 99  | ASN  |
| 1   | h     | 248 | ASN  |
| 1   | i     | 84  | HIS  |
| 1   | i     | 248 | ASN  |
| 1   | i     | 298 | ASN  |
| 1   | j     | 99  | ASN  |
| 1   | j     | 248 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | k     | 84  | HIS  |
| 1   | k     | 248 | ASN  |
| 1   | k     | 298 | ASN  |
| 1   | l     | 99  | ASN  |
| 1   | l     | 248 | ASN  |
| 1   | m     | 84  | HIS  |
| 1   | m     | 248 | ASN  |
| 1   | m     | 298 | ASN  |
| 1   | n     | 84  | HIS  |
| 1   | n     | 99  | ASN  |
| 1   | n     | 248 | ASN  |
| 1   | o     | 84  | HIS  |
| 1   | o     | 248 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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.

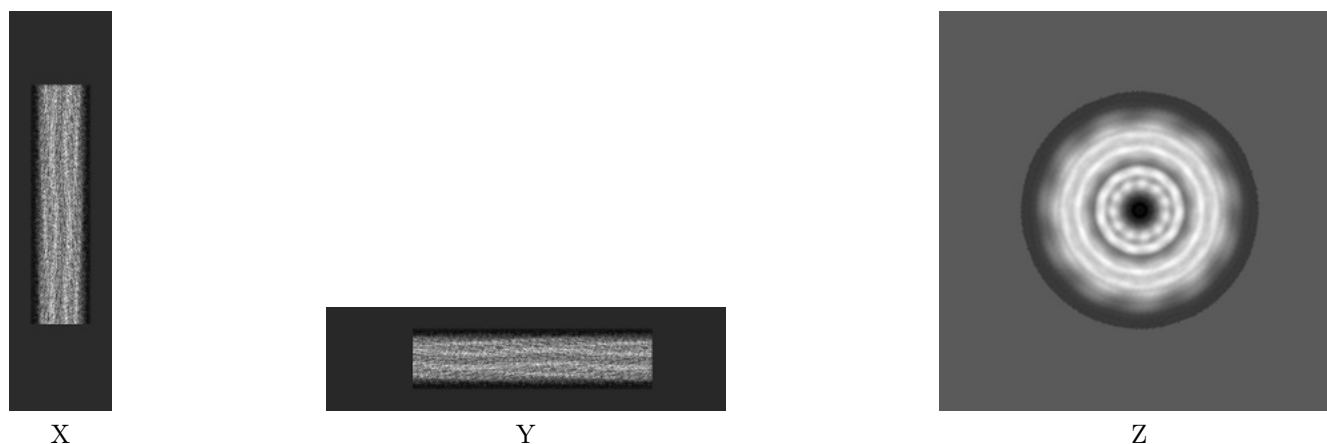
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8847. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

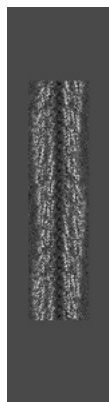
#### 6.1.1 Primary map



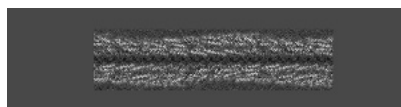
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

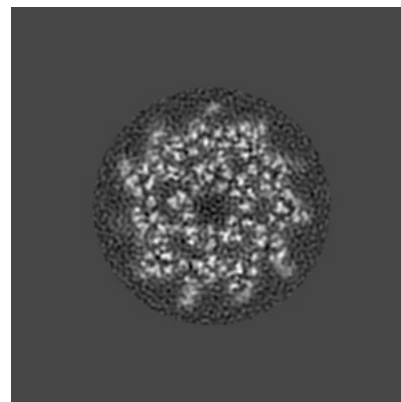
### 6.2.1 Primary map



X Index:  
128



Y Index: 128

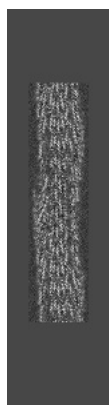


Z Index: 500

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

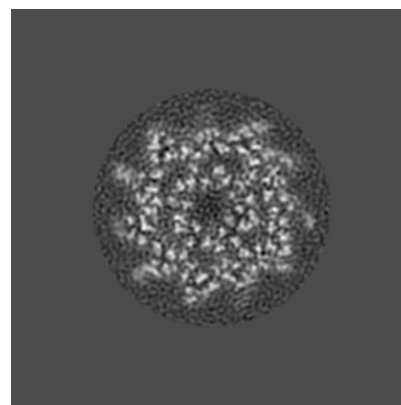
### 6.3.1 Primary map



X Index:  
111



Y Index: 111

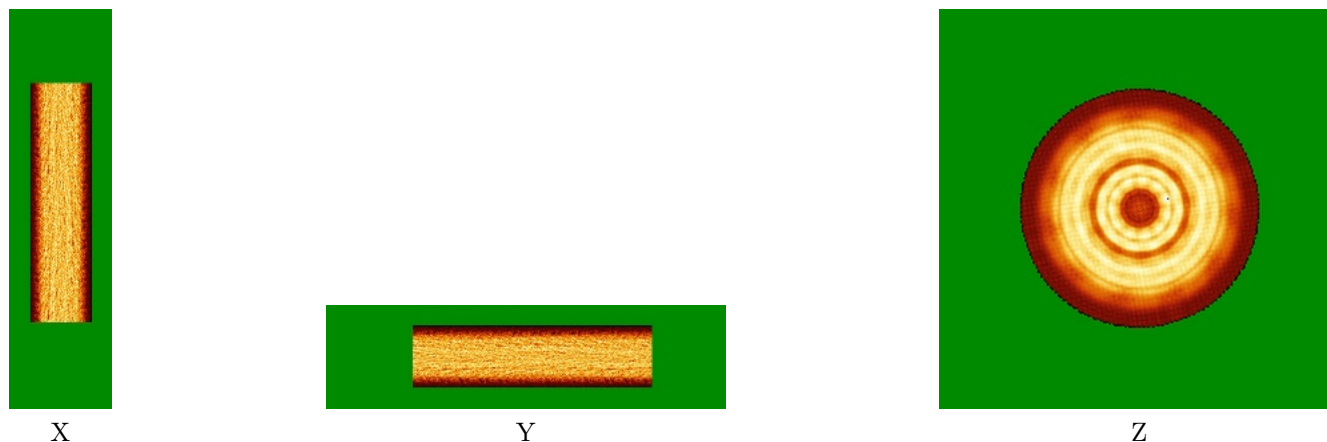


Z Index: 517

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

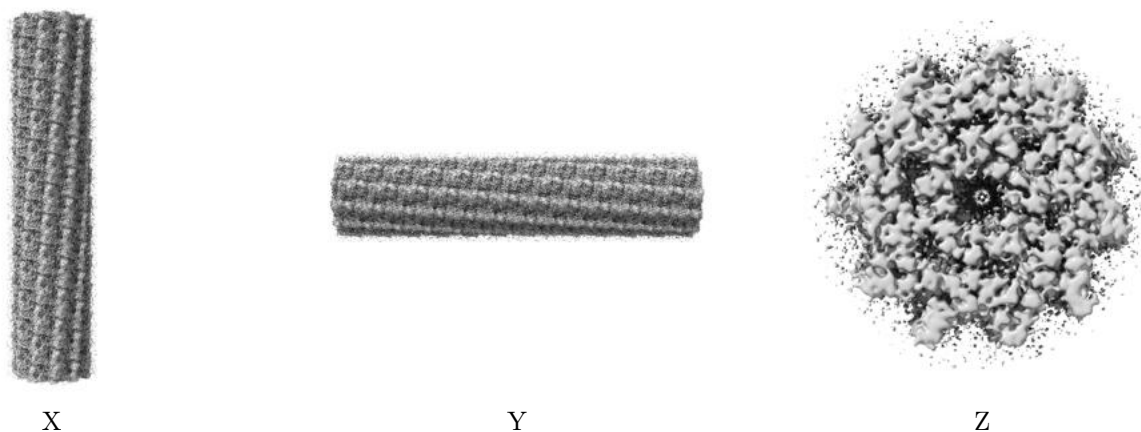
### 6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

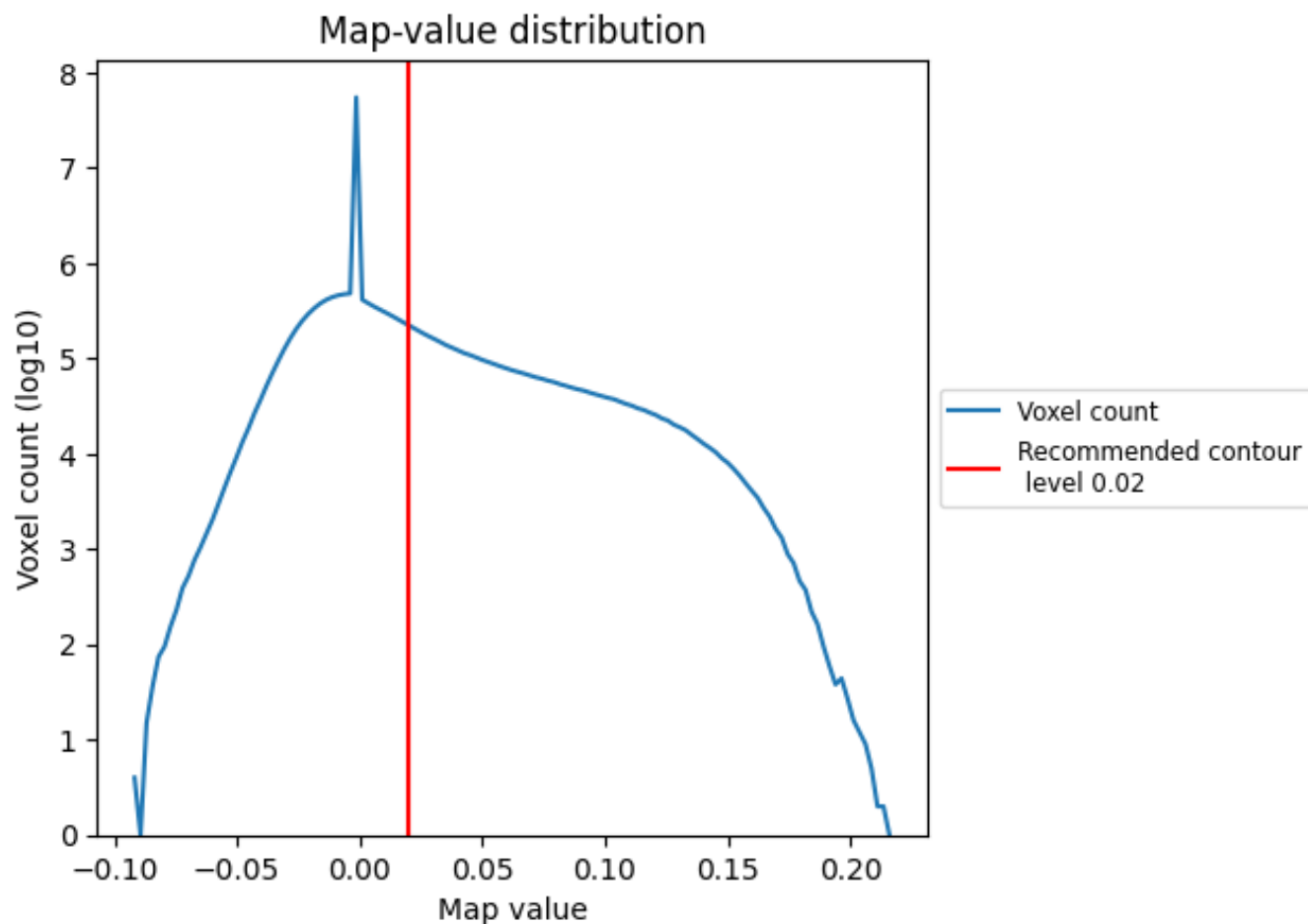
## 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

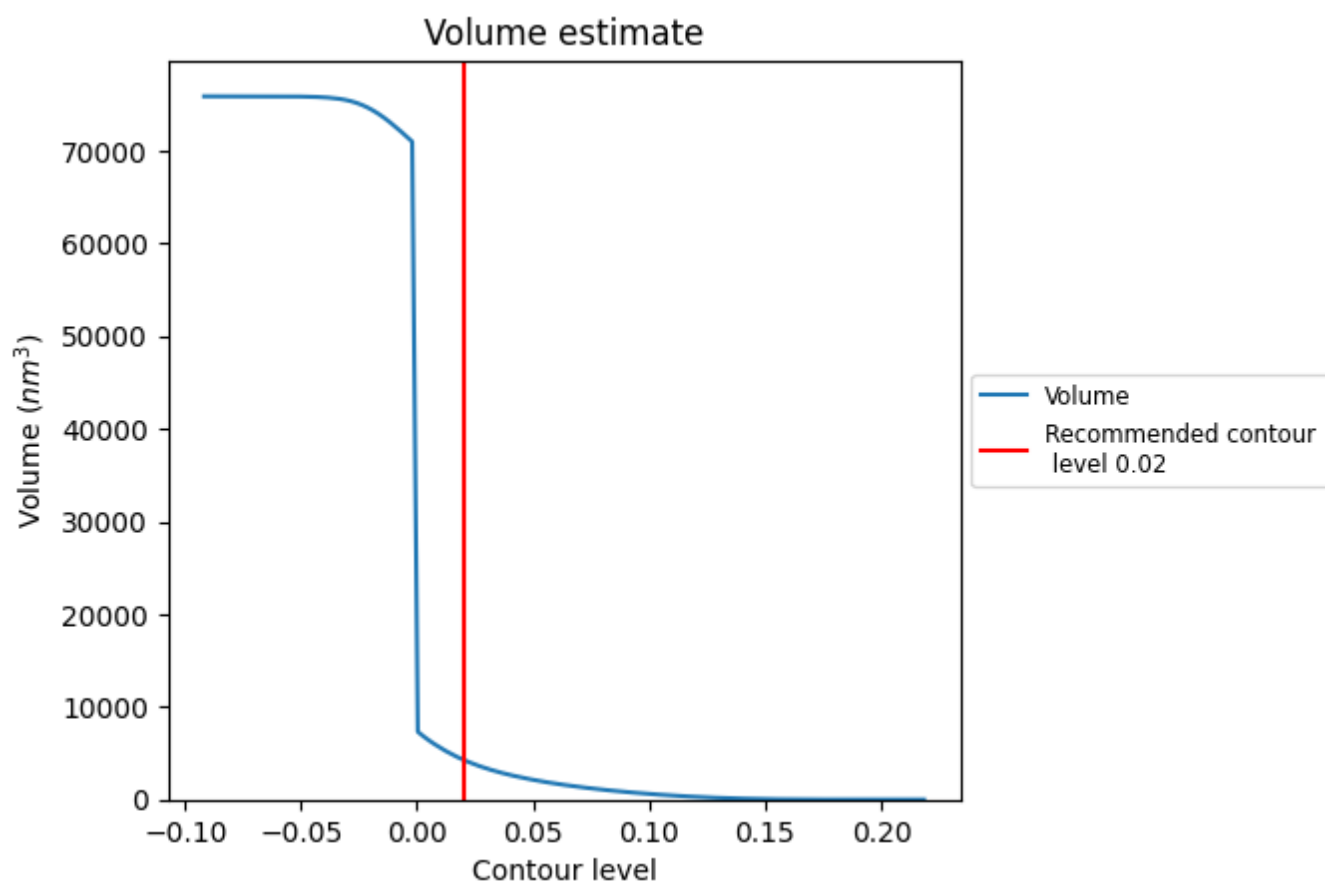
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4287 nm<sup>3</sup>; this corresponds to an approximate mass of 3873 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

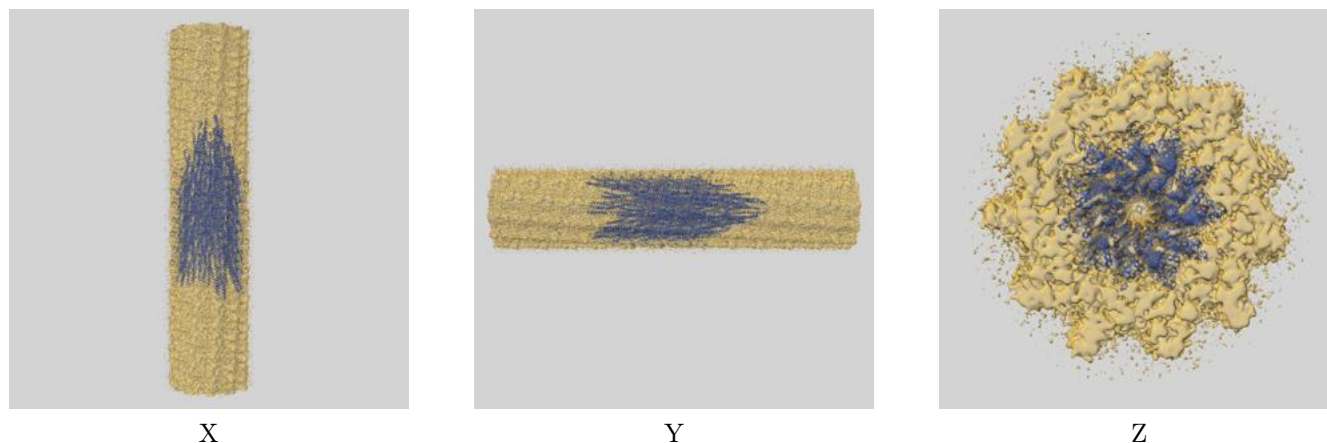
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

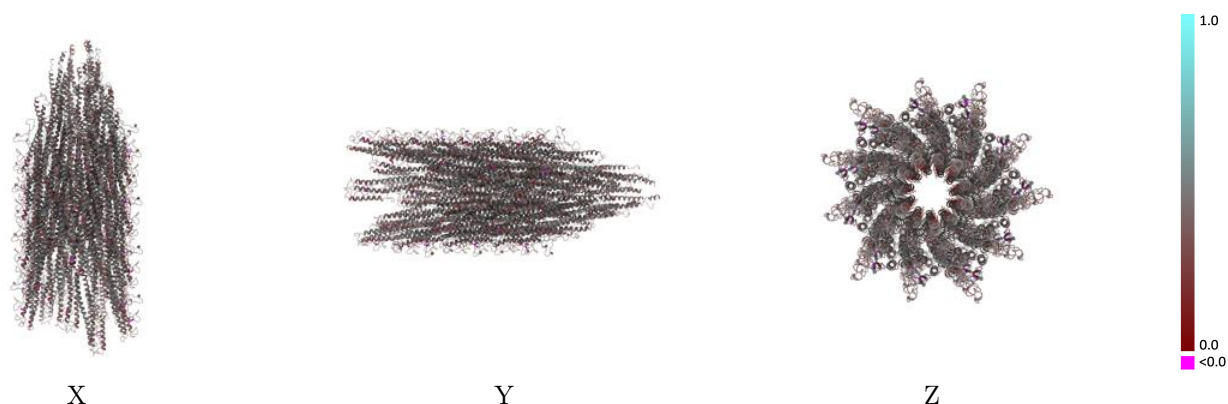
This section contains information regarding the fit between EMDB map EMD-8847 and PDB model 5WJT. Per-residue inclusion information can be found in section [3](#) on page [10](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)

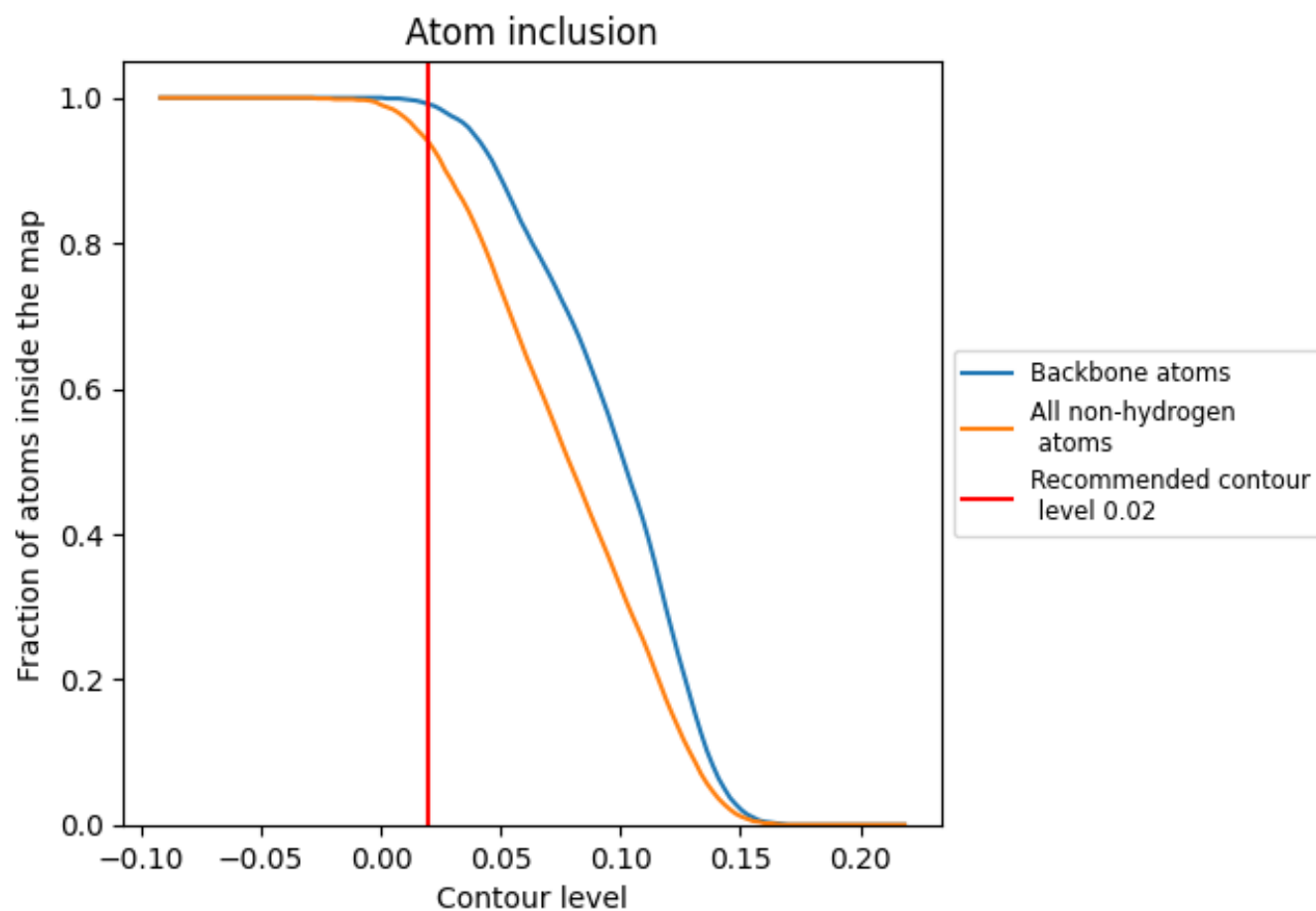


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9390   |  0.3990   |
| A     |  0.9400   |  0.4010   |
| B     |  0.9410   |  0.4020   |
| C     |  0.9390   |  0.3990   |
| D     |  0.9390   |  0.4020   |
| E     |  0.9380   |  0.4010   |
| F     |  0.9380   |  0.4000   |
| G     |  0.9390   |  0.3980   |
| H     |  0.9370   |  0.3990   |
| I     |  0.9400   |  0.4000   |
| J     |  0.9400   |  0.4000   |
| K     |  0.9380   |  0.4010   |
| L     |  0.9380   |  0.4010   |
| M     |  0.9380   |  0.4000   |
| N     |  0.9420   |  0.4000   |
| O     |  0.9390   |  0.3990   |
| P     |  0.9400 |  0.3970 |
| Q     |  0.9380 |  0.3990 |
| R     |  0.9390 |  0.3970 |
| S     |  0.9380 |  0.3990 |
| T     |  0.9380 |  0.4000 |
| U     |  0.9400 |  0.4000 |
| V     |  0.9380 |  0.4000 |
| W     |  0.9410 |  0.3980 |
| X     |  0.9390 |  0.3980 |
| Y     |  0.9400 |  0.3990 |
| Z     |  0.9410 |  0.3990 |
| a     |  0.9370 |  0.4000 |
| b     |  0.9370 |  0.3970 |
| c     |  0.9370 |  0.3980 |
| d     |  0.9410 |  0.3990 |
| e     |  0.9410 |  0.4000 |
| f     |  0.9360 |  0.3970 |
| g     |  0.9390 |  0.4010 |
| h     |  0.9400 |  0.3990 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| i     |  0.9350 |  0.3990 |
| j     |  0.9370 |  0.3990 |
| k     |  0.9380 |  0.3990 |
| l     |  0.9380 |  0.3980 |
| m     |  0.9400 |  0.4010 |
| n     |  0.9390 |  0.4000 |
| o     |  0.9360 |  0.4000 |