



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:44 AM UTC

PDB ID : 6Z0U / pdb\_00006z0u  
EMDB ID : EMD-11023  
Title : CryoEM structure of the Chikungunya virus nsP1 complex  
Authors : Reguera, J.; Jones, R.; Arranz-Avila, R.  
Deposited on : 2020-05-11  
Resolution : 2.90 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

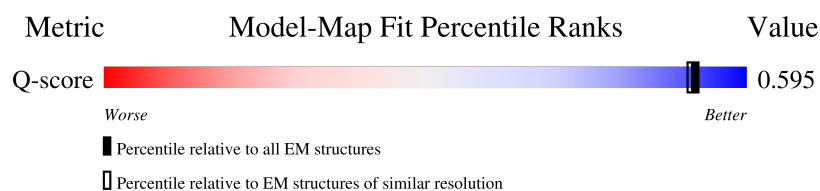
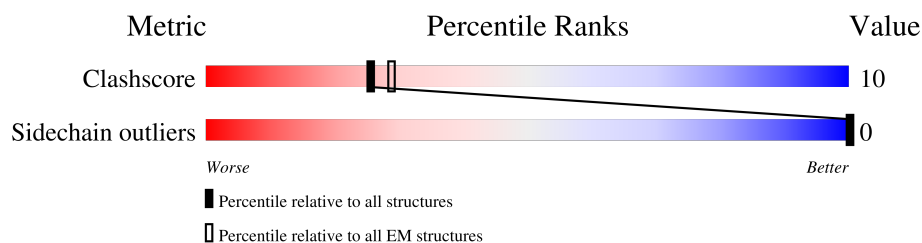
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



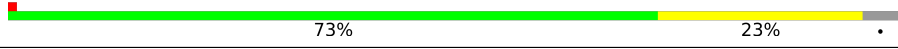
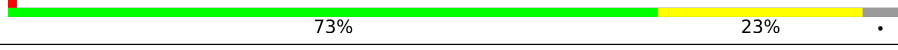
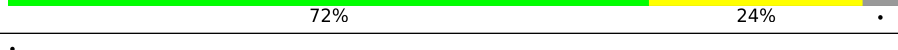
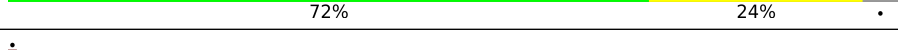
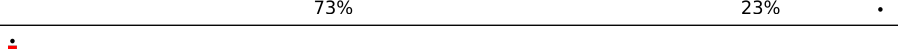
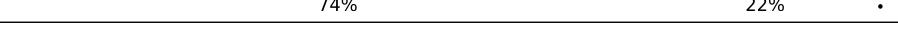
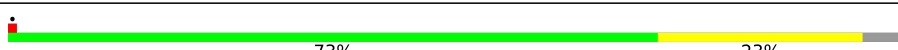
| Metric             | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|--------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore         | 229148                      | 23984                       | -                                                        |
| Sidechain outliers | 223484                      | 23102                       | -                                                        |
| Q-score            | -                           | 25397                       | 13054 ( 2.40 - 3.40 )                                    |

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     | 472    | <br>72% 24% .    |
| 1   | BA    | 472    | <br>74% 22% .    |
| 1   | C     | 472    | <br>73% 23% .    |
| 1   | DA    | 472    | <br>76% 20% .    |
| 1   | E     | 472    | <br>76% 20% .    |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | FA    | 472    |    |
| 1   | G     | 472    |    |
| 1   | HA    | 472    |    |
| 1   | I     | 472    |    |
| 1   | JA    | 472    |    |
| 1   | K     | 472    |    |
| 1   | LA    | 472    |    |
| 1   | M     | 472    |    |
| 1   | NA    | 472    |    |
| 1   | O     | 472    |    |
| 1   | PA    | 472    |    |
| 1   | Q     | 472    |  |
| 1   | RA    | 472    |  |
| 1   | S     | 472    |  |
| 1   | TA    | 472    |  |
| 1   | V     | 472    |  |
| 1   | VA    | 472    |  |
| 1   | X     | 472    |  |
| 1   | Z     | 472    |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 87288 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 Polyprotein P1234.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | C     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | E     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | G     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | I     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | K     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | M     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | O     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | Q     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | S     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | V     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | X     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | Z     | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | BA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | DA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | FA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | HA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | JA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | LA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | NA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | PA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | RA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | TA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |
| 1   | VA    | 454      | Total | C    | N   | O   | S  | 7       | 0     |
|     |       |          | 3578  | 2263 | 621 | 664 | 30 |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 2   | A     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | C     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | E     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | G     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | I     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | K     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | M     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | O     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | Q     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | S     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | V     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 2   | X     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 2   | Z     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | BA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | DA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | FA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | HA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | JA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | LA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | NA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | PA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | RA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | TA    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 2   | VA    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 3   | A     | 59       | Total<br>59 | O<br>59 | 0       |
| 3   | C     | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | E     | 57       | Total<br>57 | O<br>57 | 0       |
| 3   | G     | 59       | Total<br>59 | O<br>59 | 0       |
| 3   | I     | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | K     | 57       | Total<br>57 | O<br>57 | 0       |
| 3   | M     | 59       | Total<br>59 | O<br>59 | 0       |

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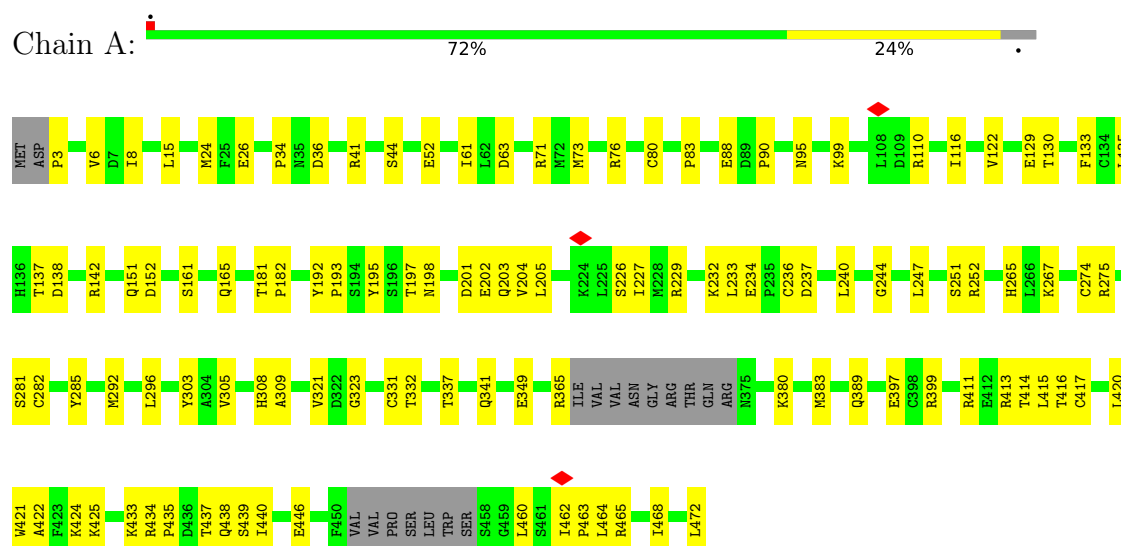
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 3   | O     | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | Q     | 57       | Total<br>57 | O<br>57 | 0       |
| 3   | S     | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | V     | 59       | Total<br>59 | O<br>59 | 0       |
| 3   | X     | 57       | Total<br>57 | O<br>57 | 0       |
| 3   | Z     | 59       | Total<br>59 | O<br>59 | 0       |
| 3   | BA    | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | DA    | 57       | Total<br>57 | O<br>57 | 0       |
| 3   | FA    | 59       | Total<br>59 | O<br>59 | 0       |
| 3   | HA    | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | JA    | 57       | Total<br>57 | O<br>57 | 0       |
| 3   | LA    | 59       | Total<br>59 | O<br>59 | 0       |
| 3   | NA    | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | PA    | 57       | Total<br>57 | O<br>57 | 0       |
| 3   | RA    | 59       | Total<br>59 | O<br>59 | 0       |
| 3   | TA    | 58       | Total<br>58 | O<br>58 | 0       |
| 3   | VA    | 57       | Total<br>57 | O<br>57 | 0       |

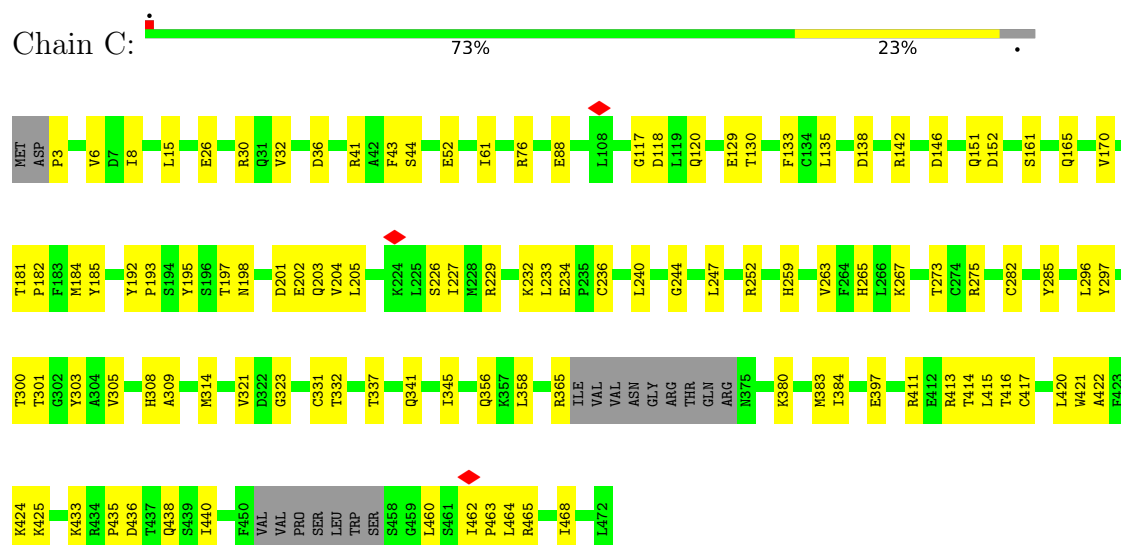
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Polyprotein P1234



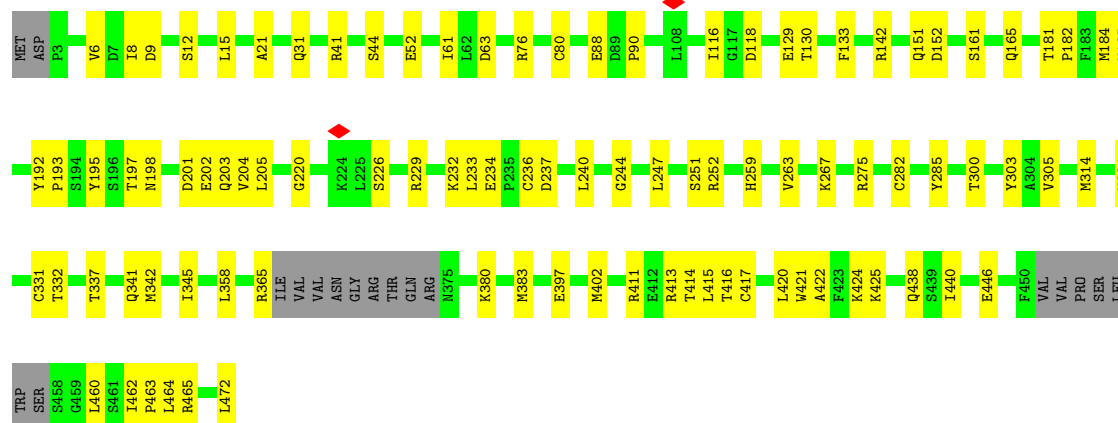
#### • Molecule 1: Polyprotein P1234



#### • Molecule 1: Polyprotein P1234

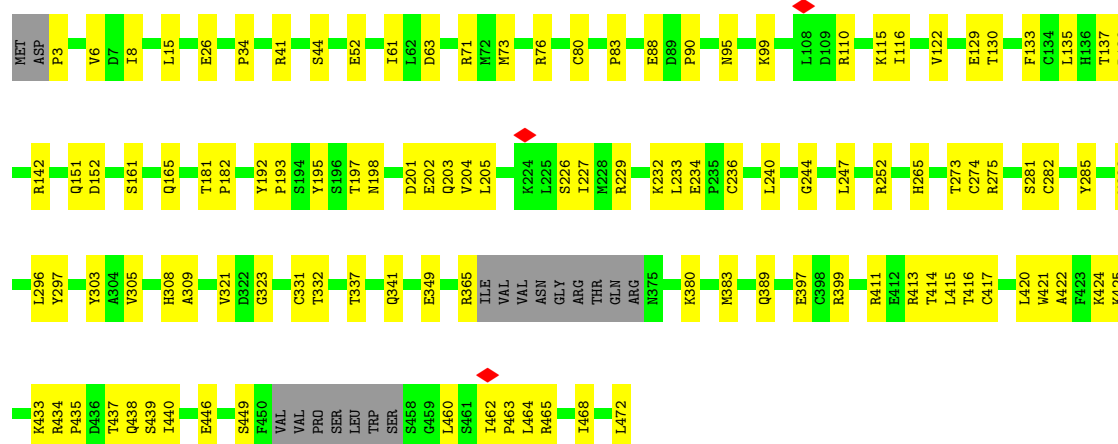


Chain E:  76% 20%



• Molecule 1: Polyprotein P1234

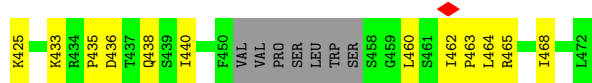
Chain G:  72% 24%



• Molecule 1: Polyprotein P1234

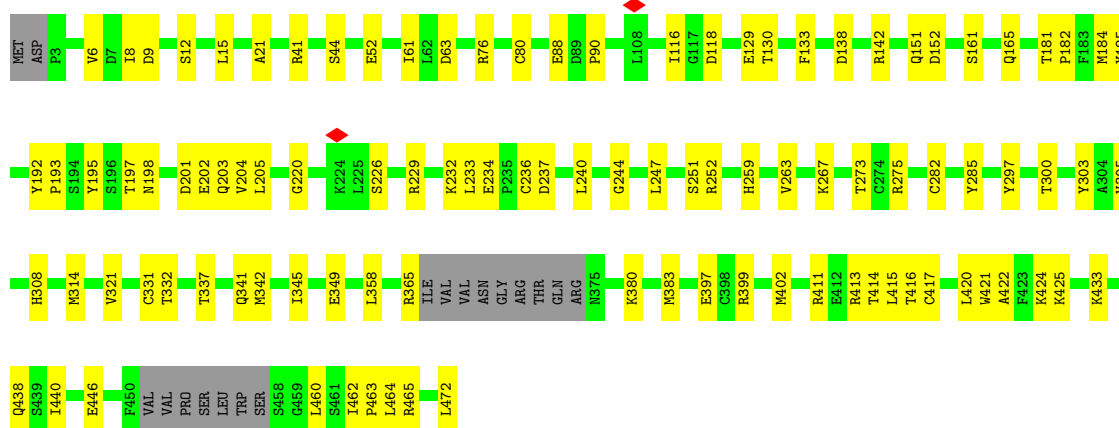
Chain I:  73% 23%





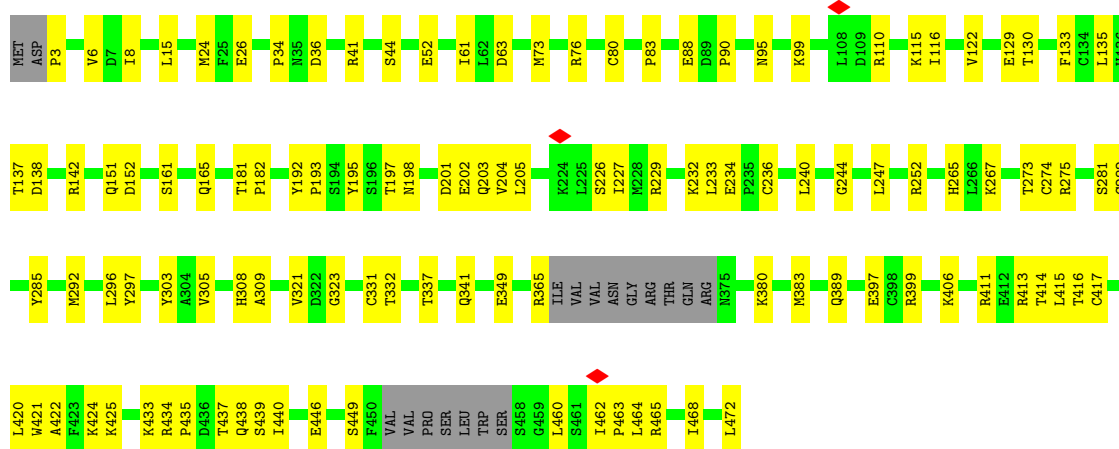
• Molecule 1: Polyprotein P1234

Chain K: 75% 22%



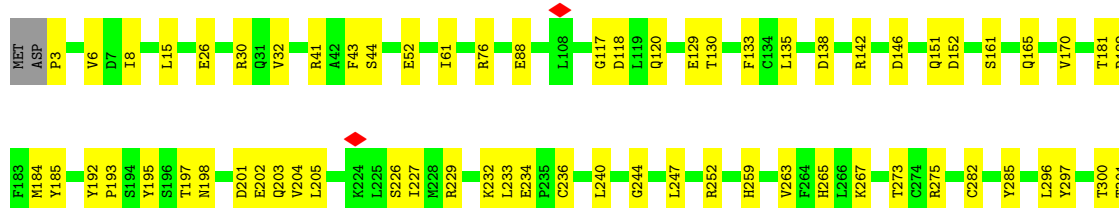
• Molecule 1: Polyprotein P1234

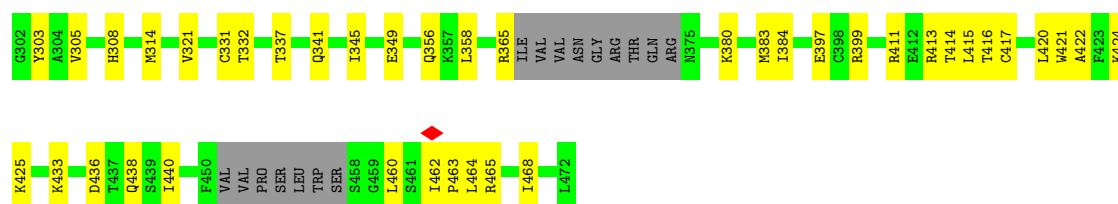
Chain M: 72% 24%



• Molecule 1: Polyprotein P1234

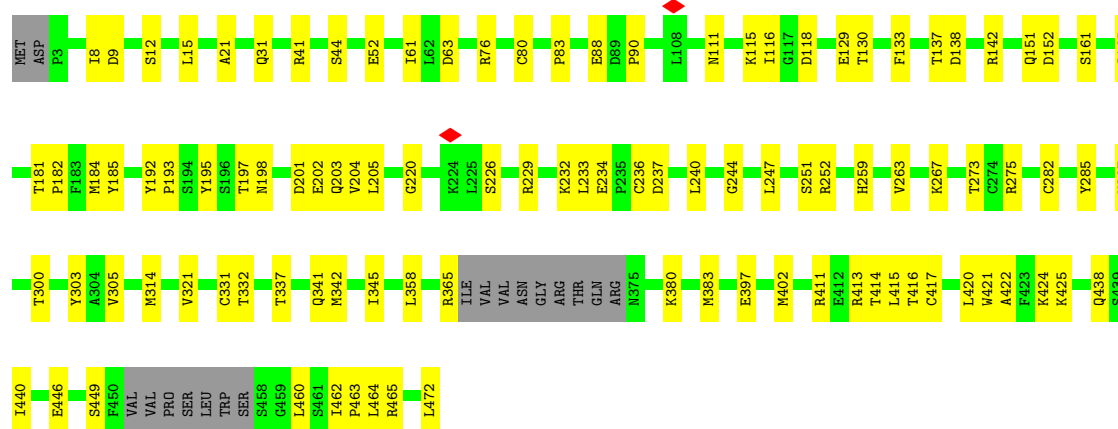
Chain O: 74% 22%





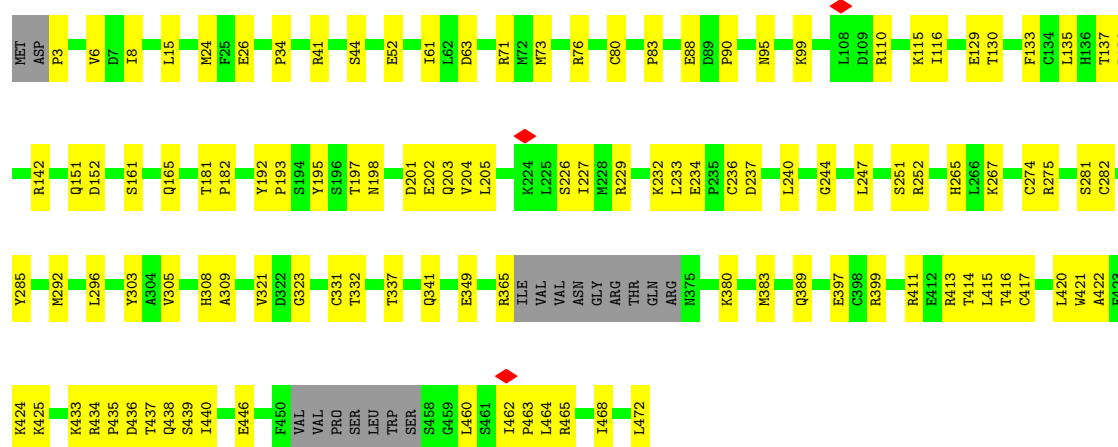
• Molecule 1: Polyprotein P1234

Chain Q: 74% 22% .



• Molecule 1: Polyprotein P1234

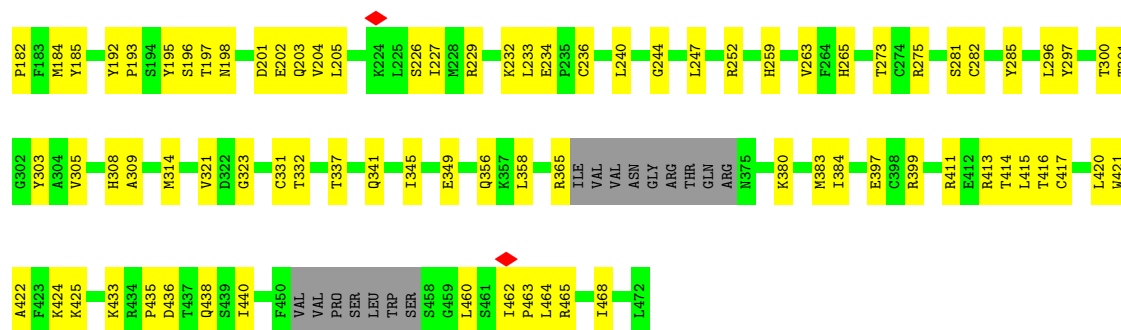
Chain S: 72% 24% .



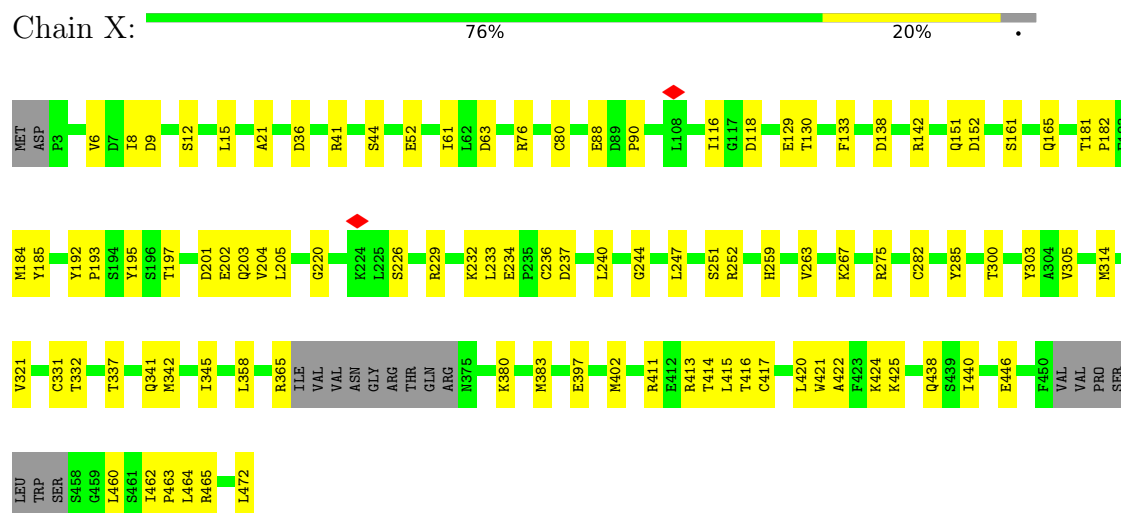
• Molecule 1: Polyprotein P1234

Chain V: 73% 23% .

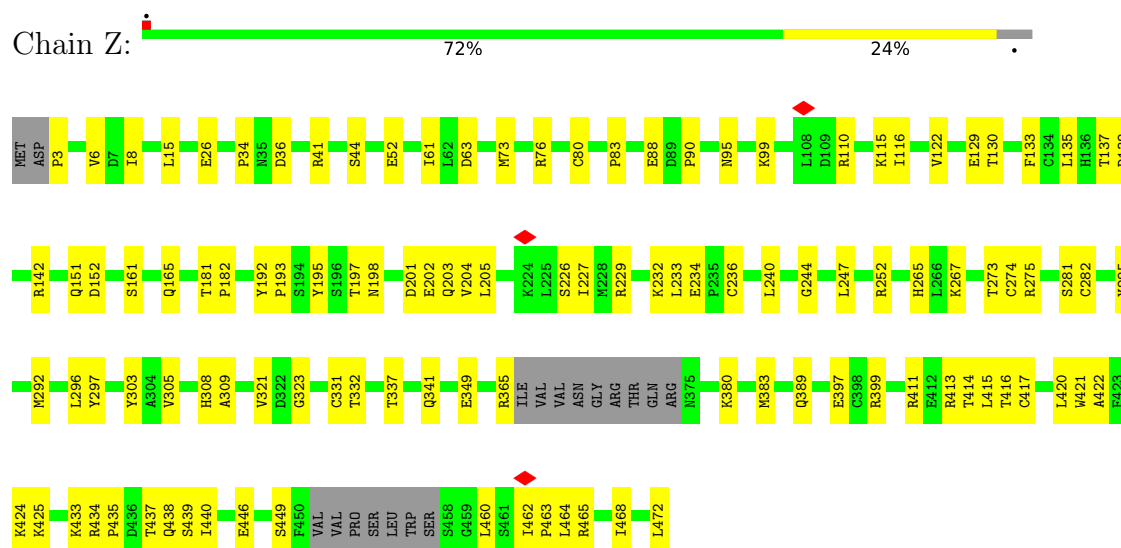




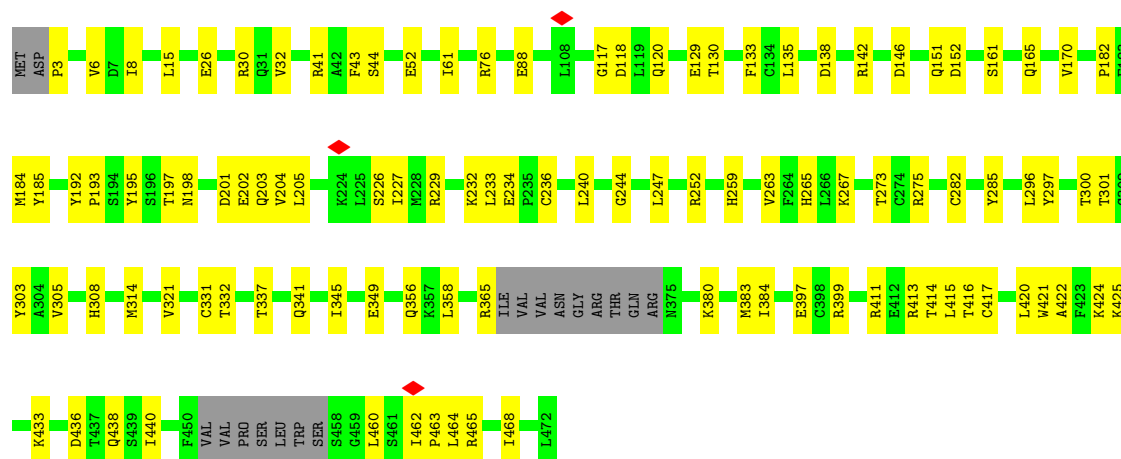
• Molecule 1: Polyprotein P1234



• Molecule 1: Polyprotein P1234

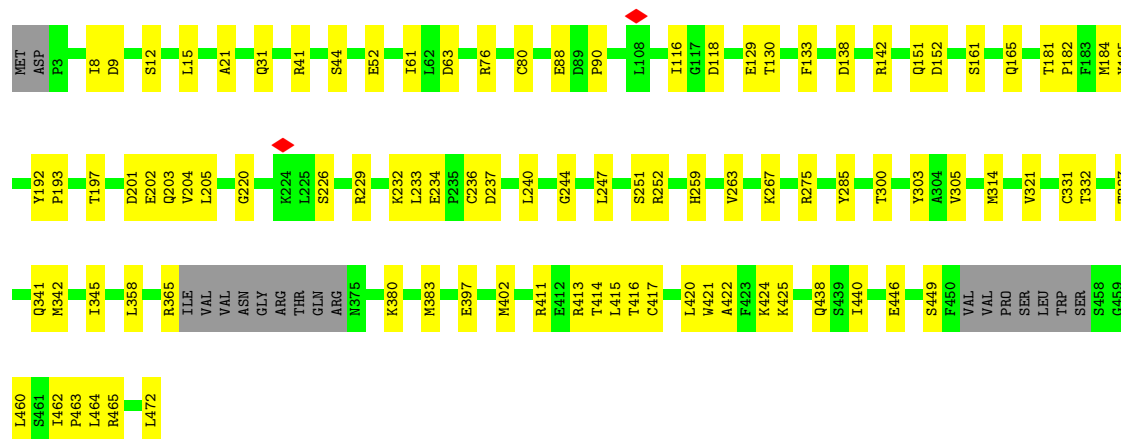


• Molecule 1: Polyprotein P1234



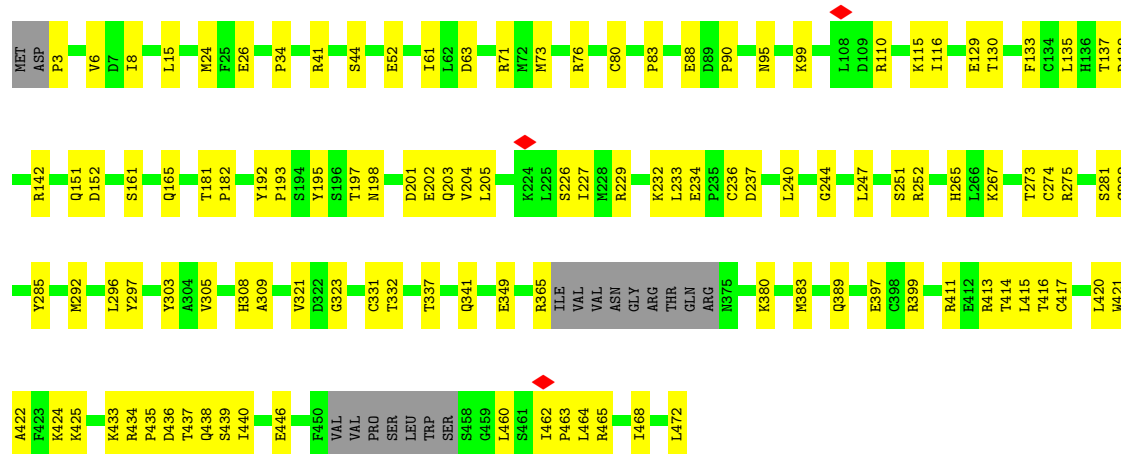
### • Molecule 1: Polyprotein P1234

Chain DA: 76% 20%

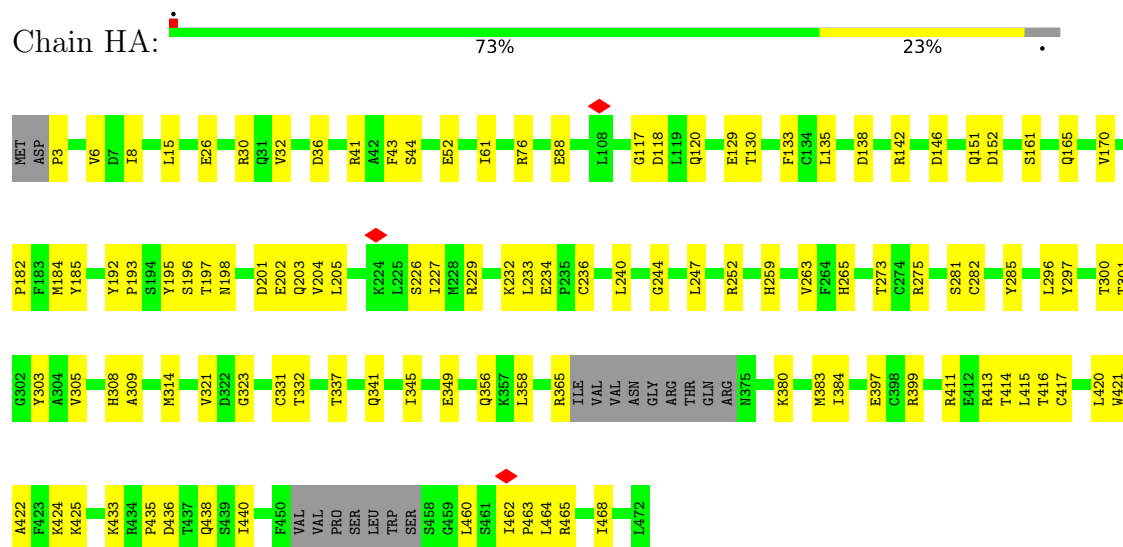


### • Molecule 1: Polyprotein P1234

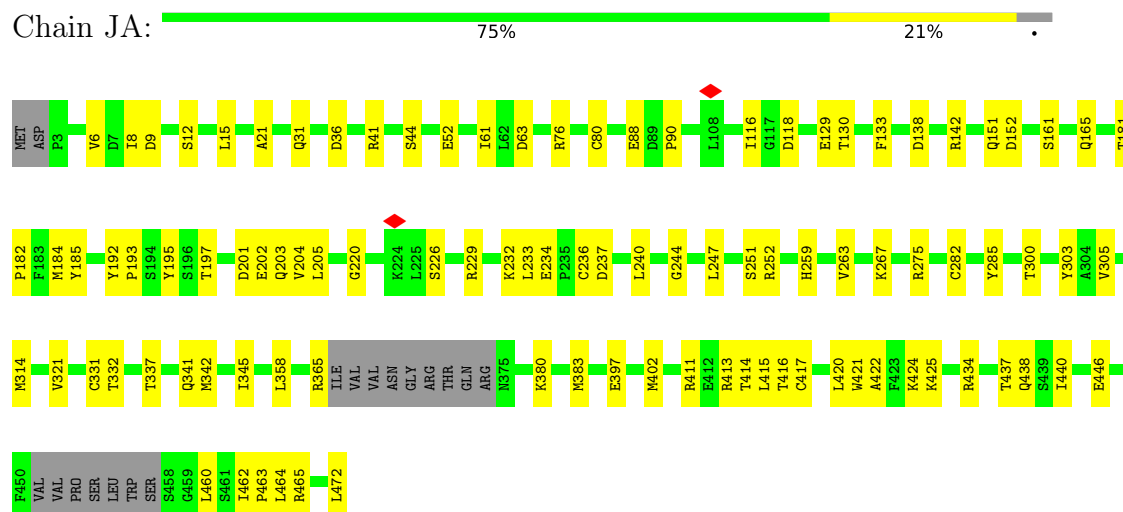
Chain FA: 72% 24%



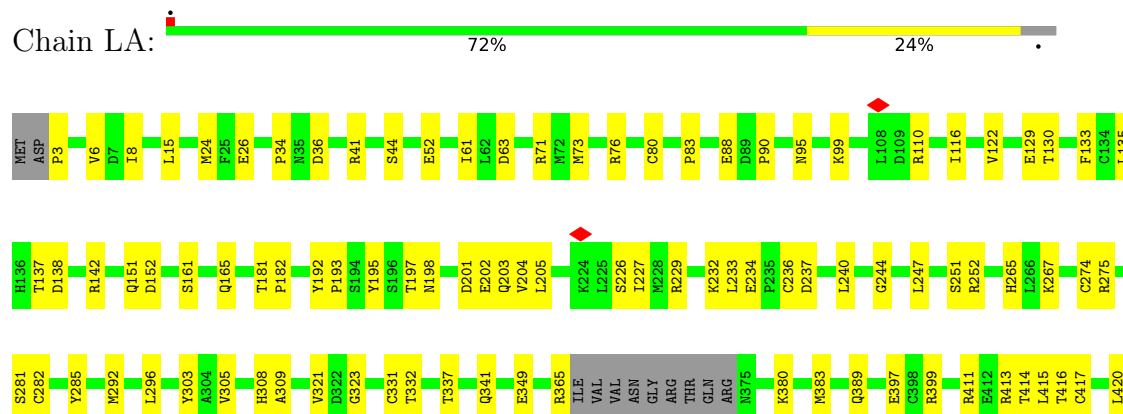
### • Molecule 1: Polyprotein P1234



• Molecule 1: Polyprotein P1234



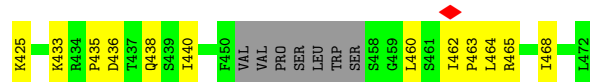
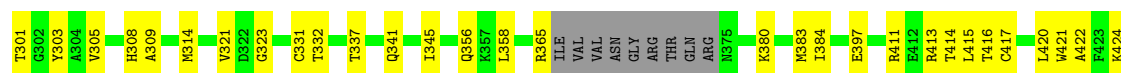
• Molecule 1: Polyprotein P1234





## • Molecule 1: Polyprotein P1234

Chain NA: 73% 23% .



## • Molecule 1: Polyprotein P1234

Chain PA: 76% 21% .



## • Molecule 1: Polyprotein P1234

Chain RA: 73% 23% .







## 4 Experimental information

| Property                             | Value                                                                                                                                                                                | Source    |
|--------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                                                                                                                                                      | Depositor |
| Imposed symmetry                     | POINT, D12                                                                                                                                                                           | Depositor |
| Number of particles used             | 47338                                                                                                                                                                                | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                                                                                                                                                    | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF was estimated from movie frames aligned without dose-weighting. Per particle CTF correction was also performed with polished particles. | Depositor |
| Microscope                           | FEI TITAN KRIOS                                                                                                                                                                      | Depositor |
| Voltage (kV)                         | 300                                                                                                                                                                                  | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 38.5                                                                                                                                                                                 | Depositor |
| Minimum defocus (nm)                 | 1000                                                                                                                                                                                 | Depositor |
| Maximum defocus (nm)                 | 2500                                                                                                                                                                                 | Depositor |
| Magnification                        | 165000                                                                                                                                                                               | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)                                                                                                                                                            | Depositor |
| Maximum map value                    | 0.091                                                                                                                                                                                | Depositor |
| Minimum map value                    | -0.069                                                                                                                                                                               | Depositor |
| Average map value                    | 0.001                                                                                                                                                                                | Depositor |
| Map value standard deviation         | 0.006                                                                                                                                                                                | Depositor |
| Recommended contour level            | 0.006                                                                                                                                                                                | Depositor |
| Map size ( $\text{\AA}$ )            | 248.1, 248.1, 248.1                                                                                                                                                                  | wwPDB     |
| Map dimensions                       | 300, 300, 300                                                                                                                                                                        | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                                                                                                                                                                     | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.827, 0.827, 0.827                                                                                                                                                                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | BA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | C     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | DA    | 0.29         | 0/3669  | 0.42        | 0/4975   |
| 1   | E     | 0.29         | 0/3669  | 0.42        | 0/4975   |
| 1   | FA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | G     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | HA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | I     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | JA    | 0.29         | 0/3669  | 0.42        | 0/4975   |
| 1   | K     | 0.29         | 0/3669  | 0.42        | 0/4975   |
| 1   | LA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | M     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | NA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | O     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | PA    | 0.29         | 0/3669  | 0.42        | 0/4975   |
| 1   | Q     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | RA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | S     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | TA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | V     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | VA    | 0.29         | 0/3669  | 0.43        | 0/4975   |
| 1   | X     | 0.29         | 0/3669  | 0.42        | 0/4975   |
| 1   | Z     | 0.29         | 0/3669  | 0.43        | 0/4975   |
| All | All   | 0.29         | 0/88056 | 0.43        | 0/119400 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3578  | 0        | 3536     | 90      | 0            |
| 1   | BA    | 3578  | 0        | 3536     | 86      | 0            |
| 1   | C     | 3578  | 0        | 3536     | 88      | 0            |
| 1   | DA    | 3578  | 0        | 3536     | 75      | 0            |
| 1   | E     | 3578  | 0        | 3536     | 75      | 0            |
| 1   | FA    | 3578  | 0        | 3536     | 91      | 0            |
| 1   | G     | 3578  | 0        | 3536     | 85      | 0            |
| 1   | HA    | 3578  | 0        | 3536     | 86      | 0            |
| 1   | I     | 3578  | 0        | 3536     | 87      | 0            |
| 1   | JA    | 3578  | 0        | 3536     | 78      | 0            |
| 1   | K     | 3578  | 0        | 3536     | 78      | 0            |
| 1   | LA    | 3578  | 0        | 3536     | 91      | 0            |
| 1   | M     | 3578  | 0        | 3536     | 92      | 0            |
| 1   | NA    | 3578  | 0        | 3536     | 87      | 0            |
| 1   | O     | 3578  | 0        | 3536     | 87      | 0            |
| 1   | PA    | 3578  | 0        | 3536     | 75      | 0            |
| 1   | Q     | 3578  | 0        | 3536     | 80      | 0            |
| 1   | RA    | 3578  | 0        | 3536     | 84      | 0            |
| 1   | S     | 3578  | 0        | 3536     | 92      | 0            |
| 1   | TA    | 3578  | 0        | 3536     | 89      | 0            |
| 1   | V     | 3578  | 0        | 3536     | 88      | 0            |
| 1   | VA    | 3578  | 0        | 3536     | 83      | 0            |
| 1   | X     | 3578  | 0        | 3536     | 75      | 0            |
| 1   | Z     | 3578  | 0        | 3536     | 89      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | BA    | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | DA    | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | FA    | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | HA    | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 1     | 0        | 0        | 0       | 0            |
| 2   | JA    | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | LA    | 1     | 0        | 0        | 0       | 0            |
| 2   | M     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | NA    | 1     | 0        | 0        | 0       | 0            |
| 2   | O     | 1     | 0        | 0        | 0       | 0            |
| 2   | PA    | 1     | 0        | 0        | 0       | 0            |
| 2   | Q     | 1     | 0        | 0        | 0       | 0            |
| 2   | RA    | 1     | 0        | 0        | 0       | 0            |
| 2   | S     | 1     | 0        | 0        | 0       | 0            |
| 2   | TA    | 1     | 0        | 0        | 0       | 0            |
| 2   | V     | 1     | 0        | 0        | 0       | 0            |
| 2   | VA    | 1     | 0        | 0        | 0       | 0            |
| 2   | X     | 1     | 0        | 0        | 0       | 0            |
| 2   | Z     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 59    | 0        | 0        | 4       | 0            |
| 3   | BA    | 58    | 0        | 0        | 3       | 0            |
| 3   | C     | 58    | 0        | 0        | 2       | 0            |
| 3   | DA    | 57    | 0        | 0        | 2       | 0            |
| 3   | E     | 57    | 0        | 0        | 2       | 0            |
| 3   | FA    | 59    | 0        | 0        | 4       | 0            |
| 3   | G     | 59    | 0        | 0        | 3       | 0            |
| 3   | HA    | 58    | 0        | 0        | 3       | 0            |
| 3   | I     | 58    | 0        | 0        | 3       | 0            |
| 3   | JA    | 57    | 0        | 0        | 2       | 0            |
| 3   | K     | 57    | 0        | 0        | 2       | 0            |
| 3   | LA    | 59    | 0        | 0        | 4       | 0            |
| 3   | M     | 59    | 0        | 0        | 4       | 0            |
| 3   | NA    | 58    | 0        | 0        | 3       | 0            |
| 3   | O     | 58    | 0        | 0        | 3       | 0            |
| 3   | PA    | 57    | 0        | 0        | 2       | 0            |
| 3   | Q     | 57    | 0        | 0        | 2       | 0            |
| 3   | RA    | 59    | 0        | 0        | 3       | 0            |
| 3   | S     | 58    | 0        | 0        | 4       | 0            |
| 3   | TA    | 58    | 0        | 0        | 3       | 0            |
| 3   | V     | 59    | 0        | 0        | 4       | 0            |
| 3   | VA    | 57    | 0        | 0        | 2       | 0            |
| 3   | X     | 57    | 0        | 0        | 2       | 0            |
| 3   | Z     | 59    | 0        | 0        | 4       | 0            |
| All | All   | 87288 | 0        | 84864    | 1761    | 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 10.

All (1761) 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:PA:52:GLU:O      | 1:PA:76:ARG:NH2  | 2.21                     | 0.74              |
| 1:E:52:GLU:O       | 1:E:76:ARG:NH2   | 2.21                     | 0.74              |
| 1:HA:232:LYS:HD3   | 1:HA:234:GLU:HG2 | 1.70                     | 0.73              |
| 1:V:232:LYS:HD3    | 1:V:234:GLU:HG2  | 1.70                     | 0.73              |
| 1:LA:52:GLU:O      | 1:LA:76:ARG:NH2  | 2.21                     | 0.73              |
| 1:A:52:GLU:O       | 1:A:76:ARG:NH2   | 2.21                     | 0.73              |
| 1:X:52:GLU:O       | 1:X:76:ARG:NH2   | 2.21                     | 0.73              |
| 1:RA:52:GLU:O      | 1:RA:76:ARG:NH2  | 2.21                     | 0.73              |
| 1:K:52:GLU:O       | 1:K:76:ARG:NH2   | 2.21                     | 0.73              |
| 1:M:52:GLU:O       | 1:M:76:ARG:NH2   | 2.21                     | 0.73              |
| 1:BA:232:LYS:HD3   | 1:BA:234:GLU:HG2 | 1.70                     | 0.73              |
| 1:G:52:GLU:O       | 1:G:76:ARG:NH2   | 2.21                     | 0.73              |
| 1:O:232:LYS:HD3    | 1:O:234:GLU:HG2  | 1.70                     | 0.73              |
| 1:Z:52:GLU:O       | 1:Z:76:ARG:NH2   | 2.21                     | 0.73              |
| 1:C:232:LYS:HD3    | 1:C:234:GLU:HG2  | 1.70                     | 0.73              |
| 1:NA:232:LYS:HD3   | 1:NA:234:GLU:HG2 | 1.70                     | 0.73              |
| 1:JA:52:GLU:O      | 1:JA:76:ARG:NH2  | 2.21                     | 0.72              |
| 1:Q:52:GLU:O       | 1:Q:76:ARG:NH2   | 2.21                     | 0.72              |
| 1:DA:52:GLU:O      | 1:DA:76:ARG:NH2  | 2.21                     | 0.72              |
| 1:G:232:LYS:HD3    | 1:G:234:GLU:HG2  | 1.70                     | 0.72              |
| 1:VA:52:GLU:O      | 1:VA:76:ARG:NH2  | 2.21                     | 0.72              |
| 1:A:232:LYS:HD3    | 1:A:234:GLU:HG2  | 1.71                     | 0.72              |
| 1:S:52:GLU:O       | 1:S:76:ARG:NH2   | 2.21                     | 0.72              |
| 1:LA:232:LYS:HD3   | 1:LA:234:GLU:HG2 | 1.70                     | 0.72              |
| 1:RA:232:LYS:HD3   | 1:RA:234:GLU:HG2 | 1.70                     | 0.72              |
| 1:FA:52:GLU:O      | 1:FA:76:ARG:NH2  | 2.21                     | 0.72              |
| 1:M:232:LYS:HD3    | 1:M:234:GLU:HG2  | 1.70                     | 0.72              |
| 1:TA:232:LYS:HD3   | 1:TA:234:GLU:HG2 | 1.70                     | 0.72              |
| 1:S:232:LYS:HD3    | 1:S:234:GLU:HG2  | 1.70                     | 0.72              |
| 1:I:232:LYS:HD3    | 1:I:234:GLU:HG2  | 1.70                     | 0.71              |
| 1:Z:232:LYS:HD3    | 1:Z:234:GLU:HG2  | 1.71                     | 0.71              |
| 1:I:52:GLU:O       | 1:I:76:ARG:NH2   | 2.23                     | 0.71              |
| 1:O:52:GLU:O       | 1:O:76:ARG:NH2   | 2.23                     | 0.71              |
| 1:BA:52:GLU:O      | 1:BA:76:ARG:NH2  | 2.23                     | 0.71              |
| 1:FA:232:LYS:HD3   | 1:FA:234:GLU:HG2 | 1.70                     | 0.71              |
| 1:HA:52:GLU:O      | 1:HA:76:ARG:NH2  | 2.23                     | 0.71              |
| 1:TA:52:GLU:O      | 1:TA:76:ARG:NH2  | 2.23                     | 0.71              |
| 1:V:52:GLU:O       | 1:V:76:ARG:NH2   | 2.23                     | 0.71              |
| 1:C:41[B]:ARG:NH2  | 3:C:1104:HOH:O   | 2.24                     | 0.71              |
| 1:Z:41[B]:ARG:NH2  | 3:Z:1104:HOH:O   | 2.24                     | 0.70              |
| 1:NA:41[B]:ARG:NH2 | 3:NA:1104:HOH:O  | 2.24                     | 0.70              |
| 1:M:41[B]:ARG:NH2  | 3:M:1104:HOH:O   | 2.24                     | 0.70              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:41[B]:ARG:NH2  | 3:A:1104:HOH:O    | 2.24                     | 0.70              |
| 1:C:52:GLU:O       | 1:C:76:ARG:NH2    | 2.23                     | 0.70              |
| 1:NA:52:GLU:O      | 1:NA:76:ARG:NH2   | 2.23                     | 0.70              |
| 1:LA:41[B]:ARG:NH2 | 3:LA:1104:HOH:O   | 2.24                     | 0.70              |
| 1:V:41[B]:ARG:NH2  | 3:V:1104:HOH:O    | 2.24                     | 0.70              |
| 1:HA:41[B]:ARG:NH2 | 3:HA:1104:HOH:O   | 2.24                     | 0.70              |
| 1:S:41[B]:ARG:NH2  | 3:S:1104:HOH:O    | 2.24                     | 0.70              |
| 1:X:41[B]:ARG:NH2  | 3:X:1104:HOH:O    | 2.25                     | 0.70              |
| 1:FA:41[B]:ARG:NH2 | 3:FA:1104:HOH:O   | 2.24                     | 0.70              |
| 1:JA:41[B]:ARG:NH2 | 3:JA:1104:HOH:O   | 2.25                     | 0.70              |
| 1:I:41[B]:ARG:NH2  | 3:I:1104:HOH:O    | 2.24                     | 0.69              |
| 1:K:41[B]:ARG:NH2  | 3:K:1104:HOH:O    | 2.25                     | 0.69              |
| 1:VA:41[B]:ARG:NH2 | 3:VA:1104:HOH:O   | 2.25                     | 0.69              |
| 1:TA:41[B]:ARG:NH2 | 3:TA:1104:HOH:O   | 2.24                     | 0.69              |
| 1:E:41[B]:ARG:NH2  | 3:E:1104:HOH:O    | 2.25                     | 0.69              |
| 1:PA:41[B]:ARG:NH2 | 3:PA:1104:HOH:O   | 2.25                     | 0.69              |
| 1:Q:203:GLN:NE2    | 1:Q:236:CYS:SG    | 2.66                     | 0.69              |
| 1:DA:41[B]:ARG:NH2 | 3:DA:1104:HOH:O   | 2.25                     | 0.69              |
| 1:DA:203:GLN:NE2   | 1:DA:236:CYS:SG   | 2.66                     | 0.69              |
| 1:Q:41[B]:ARG:NH2  | 3:Q:1104:HOH:O    | 2.25                     | 0.69              |
| 1:RA:41[B]:ARG:NH2 | 3:RA:1104:HOH:O   | 2.24                     | 0.68              |
| 1:G:41[B]:ARG:NH2  | 3:G:1104:HOH:O    | 2.24                     | 0.68              |
| 1:K:203:GLN:NE2    | 1:K:236:CYS:SG    | 2.66                     | 0.68              |
| 1:O:41[B]:ARG:NH2  | 3:O:1104:HOH:O    | 2.24                     | 0.68              |
| 1:VA:203:GLN:NE2   | 1:VA:236:CYS:SG   | 2.66                     | 0.68              |
| 1:BA:41[B]:ARG:NH2 | 3:BA:1104:HOH:O   | 2.24                     | 0.68              |
| 1:X:203:GLN:NE2    | 1:X:236:CYS:SG    | 2.66                     | 0.68              |
| 1:E:203:GLN:NE2    | 1:E:236:CYS:SG    | 2.66                     | 0.68              |
| 1:JA:203:GLN:NE2   | 1:JA:236:CYS:SG   | 2.66                     | 0.68              |
| 1:PA:203:GLN:NE2   | 1:PA:236:CYS:SG   | 2.66                     | 0.68              |
| 1:A:205:LEU:HD11   | 1:A:240:LEU:HD12  | 1.76                     | 0.68              |
| 1:G:205:LEU:HD11   | 1:G:240:LEU:HD12  | 1.76                     | 0.68              |
| 1:O:205:LEU:HD11   | 1:O:240:LEU:HD12  | 1.76                     | 0.68              |
| 1:BA:205:LEU:HD11  | 1:BA:240:LEU:HD12 | 1.76                     | 0.68              |
| 1:LA:205:LEU:HD11  | 1:LA:240:LEU:HD12 | 1.76                     | 0.68              |
| 1:RA:205:LEU:HD11  | 1:RA:240:LEU:HD12 | 1.76                     | 0.68              |
| 1:K:397:GLU:OE1    | 3:K:1101:HOH:O    | 2.12                     | 0.68              |
| 1:VA:397:GLU:OE1   | 3:VA:1101:HOH:O   | 2.12                     | 0.68              |
| 1:S:205:LEU:HD11   | 1:S:240:LEU:HD12  | 1.76                     | 0.67              |
| 1:HA:205:LEU:HD11  | 1:HA:240:LEU:HD12 | 1.76                     | 0.67              |
| 1:M:205:LEU:HD11   | 1:M:240:LEU:HD12  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:X:205:LEU:HD11  | 1:X:240:LEU:HD12  | 1.77                     | 0.67              |
| 1:Z:205:LEU:HD11  | 1:Z:240:LEU:HD12  | 1.76                     | 0.67              |
| 1:JA:205:LEU:HD11 | 1:JA:240:LEU:HD12 | 1.77                     | 0.67              |
| 1:V:205:LEU:HD11  | 1:V:240:LEU:HD12  | 1.77                     | 0.67              |
| 1:FA:205:LEU:HD11 | 1:FA:240:LEU:HD12 | 1.76                     | 0.67              |
| 1:Q:397:GLU:OE1   | 3:Q:1101:HOH:O    | 2.12                     | 0.67              |
| 1:DA:397:GLU:OE1  | 3:DA:1101:HOH:O   | 2.12                     | 0.67              |
| 1:I:205:LEU:HD11  | 1:I:240:LEU:HD12  | 1.76                     | 0.67              |
| 1:TA:205:LEU:HD11 | 1:TA:240:LEU:HD12 | 1.77                     | 0.67              |
| 1:O:397:GLU:OE1   | 3:O:1101:HOH:O    | 2.13                     | 0.66              |
| 1:BA:397:GLU:OE1  | 3:BA:1101:HOH:O   | 2.13                     | 0.66              |
| 1:PA:205:LEU:HD11 | 1:PA:240:LEU:HD12 | 1.77                     | 0.66              |
| 1:PA:397:GLU:OE1  | 3:PA:1101:HOH:O   | 2.12                     | 0.66              |
| 1:E:205:LEU:HD11  | 1:E:240:LEU:HD12  | 1.77                     | 0.66              |
| 1:E:397:GLU:OE1   | 3:E:1101:HOH:O    | 2.12                     | 0.66              |
| 1:C:205:LEU:HD11  | 1:C:240:LEU:HD12  | 1.76                     | 0.66              |
| 1:G:397:GLU:OE1   | 3:G:1101:HOH:O    | 2.13                     | 0.66              |
| 1:Q:205:LEU:HD11  | 1:Q:240:LEU:HD12  | 1.77                     | 0.66              |
| 1:DA:205:LEU:HD11 | 1:DA:240:LEU:HD12 | 1.77                     | 0.66              |
| 1:LA:397:GLU:OE1  | 3:LA:1101:HOH:O   | 2.13                     | 0.66              |
| 1:RA:397:GLU:OE1  | 3:RA:1101:HOH:O   | 2.13                     | 0.66              |
| 1:X:397:GLU:OE1   | 3:X:1101:HOH:O    | 2.12                     | 0.66              |
| 1:A:397:GLU:OE1   | 3:A:1101:HOH:O    | 2.13                     | 0.66              |
| 1:M:397:GLU:OE1   | 3:M:1101:HOH:O    | 2.13                     | 0.66              |
| 1:Z:397:GLU:OE1   | 3:Z:1101:HOH:O    | 2.13                     | 0.66              |
| 1:JA:397:GLU:OE1  | 3:JA:1101:HOH:O   | 2.12                     | 0.66              |
| 1:NA:205:LEU:HD11 | 1:NA:240:LEU:HD12 | 1.77                     | 0.66              |
| 1:E:232:LYS:HD3   | 1:E:234:GLU:HG2   | 1.78                     | 0.66              |
| 1:VA:205:LEU:HD11 | 1:VA:240:LEU:HD12 | 1.77                     | 0.66              |
| 1:K:232:LYS:HD3   | 1:K:234:GLU:HG2   | 1.78                     | 0.65              |
| 1:S:397:GLU:OE1   | 3:S:1101:HOH:O    | 2.13                     | 0.65              |
| 1:NA:397:GLU:OE1  | 3:NA:1101:HOH:O   | 2.13                     | 0.65              |
| 1:V:415:LEU:HG    | 1:V:417:CYS:H     | 1.61                     | 0.65              |
| 1:FA:397:GLU:OE1  | 3:FA:1101:HOH:O   | 2.13                     | 0.65              |
| 1:HA:415:LEU:HG   | 1:HA:417:CYS:H    | 1.61                     | 0.65              |
| 1:PA:232:LYS:HD3  | 1:PA:234:GLU:HG2  | 1.78                     | 0.65              |
| 1:VA:232:LYS:HD3  | 1:VA:234:GLU:HG2  | 1.78                     | 0.65              |
| 1:C:397:GLU:OE1   | 3:C:1101:HOH:O    | 2.13                     | 0.65              |
| 1:K:205:LEU:HD11  | 1:K:240:LEU:HD12  | 1.77                     | 0.65              |
| 1:V:397:GLU:OE1   | 3:V:1101:HOH:O    | 2.13                     | 0.65              |
| 1:X:415:LEU:HG    | 1:X:417:CYS:H     | 1.61                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:135:LEU:HD21 | 1:FA:460:LEU:HD13 | 1.78                     | 0.65              |
| 1:HA:397:GLU:OE1  | 3:HA:1101:HOH:O   | 2.13                     | 0.65              |
| 1:TA:397:GLU:OE1  | 3:TA:1101:HOH:O   | 2.13                     | 0.65              |
| 1:I:397:GLU:OE1   | 3:I:1101:HOH:O    | 2.13                     | 0.65              |
| 1:JA:415:LEU:HG   | 1:JA:417:CYS:H    | 1.62                     | 0.65              |
| 1:C:415:LEU:HG    | 1:C:417:CYS:H     | 1.61                     | 0.65              |
| 1:DA:415:LEU:HG   | 1:DA:417:CYS:H    | 1.61                     | 0.65              |
| 1:Z:135:LEU:HD21  | 1:Z:460:LEU:HD13  | 1.79                     | 0.64              |
| 1:M:135:LEU:HD21  | 1:M:460:LEU:HD13  | 1.79                     | 0.64              |
| 1:NA:415:LEU:HG   | 1:NA:417:CYS:H    | 1.61                     | 0.64              |
| 1:JA:232:LYS:HD3  | 1:JA:234:GLU:HG2  | 1.78                     | 0.64              |
| 1:O:415:LEU:HG    | 1:O:417:CYS:H     | 1.61                     | 0.64              |
| 1:X:232:LYS:HD3   | 1:X:234:GLU:HG2   | 1.78                     | 0.64              |
| 1:BA:415:LEU:HG   | 1:BA:417:CYS:H    | 1.61                     | 0.64              |
| 1:Q:232:LYS:HD3   | 1:Q:234:GLU:HG2   | 1.78                     | 0.64              |
| 1:S:135:LEU:HD21  | 1:S:460:LEU:HD13  | 1.79                     | 0.64              |
| 1:S:424:LYS:NZ    | 1:S:425:LYS:O     | 2.31                     | 0.64              |
| 1:G:135:LEU:HD21  | 1:G:460:LEU:HD13  | 1.78                     | 0.64              |
| 1:JA:414:THR:O    | 1:JA:422:ALA:N    | 2.31                     | 0.64              |
| 1:K:415:LEU:HG    | 1:K:417:CYS:H     | 1.61                     | 0.64              |
| 1:Q:415:LEU:HG    | 1:Q:417:CYS:H     | 1.62                     | 0.64              |
| 1:DA:232:LYS:HD3  | 1:DA:234:GLU:HG2  | 1.78                     | 0.64              |
| 1:X:414:THR:O     | 1:X:422:ALA:N     | 2.31                     | 0.64              |
| 1:RA:135:LEU:HD21 | 1:RA:460:LEU:HD13 | 1.79                     | 0.64              |
| 1:E:415:LEU:HG    | 1:E:417:CYS:H     | 1.62                     | 0.63              |
| 1:FA:193:PRO:O    | 1:FA:380:LYS:NZ   | 2.31                     | 0.63              |
| 1:TA:415:LEU:HG   | 1:TA:417:CYS:H    | 1.61                     | 0.63              |
| 1:VA:415:LEU:HG   | 1:VA:417:CYS:H    | 1.62                     | 0.63              |
| 1:I:415:LEU:HG    | 1:I:417:CYS:H     | 1.61                     | 0.63              |
| 1:PA:415:LEU:HG   | 1:PA:417:CYS:H    | 1.62                     | 0.63              |
| 1:S:193:PRO:O     | 1:S:380:LYS:NZ    | 2.31                     | 0.63              |
| 1:A:415:LEU:HG    | 1:A:417:CYS:H     | 1.63                     | 0.63              |
| 1:LA:193:PRO:O    | 1:LA:380:LYS:NZ   | 2.31                     | 0.63              |
| 1:LA:415:LEU:HG   | 1:LA:417:CYS:H    | 1.63                     | 0.63              |
| 1:A:193:PRO:O     | 1:A:380:LYS:NZ    | 2.31                     | 0.63              |
| 1:M:193:PRO:O     | 1:M:380:LYS:NZ    | 2.31                     | 0.63              |
| 1:S:90:PRO:HB3    | 1:S:464:LEU:HD11  | 1.81                     | 0.63              |
| 1:G:424:LYS:NZ    | 1:G:425:LYS:O     | 2.32                     | 0.62              |
| 1:Z:193:PRO:O     | 1:Z:380:LYS:NZ    | 2.31                     | 0.62              |
| 1:LA:135:LEU:HD21 | 1:LA:460:LEU:HD13 | 1.79                     | 0.62              |
| 1:RA:193:PRO:O    | 1:RA:380:LYS:NZ   | 2.31                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:135:LEU:HD21  | 1:A:460:LEU:HD13  | 1.79                     | 0.62              |
| 1:G:193:PRO:O     | 1:G:380:LYS:NZ    | 2.31                     | 0.62              |
| 1:M:424:LYS:NZ    | 1:M:425:LYS:O     | 2.32                     | 0.62              |
| 1:FA:415:LEU:HG   | 1:FA:417:CYS:H    | 1.63                     | 0.62              |
| 1:Z:424:LYS:NZ    | 1:Z:425:LYS:O     | 2.32                     | 0.62              |
| 1:LA:90:PRO:HB3   | 1:LA:464:LEU:HD11 | 1.81                     | 0.62              |
| 1:RA:424:LYS:NZ   | 1:RA:425:LYS:O    | 2.32                     | 0.62              |
| 1:TA:424:LYS:NZ   | 1:TA:425:LYS:O    | 2.33                     | 0.62              |
| 1:A:90:PRO:HB3    | 1:A:464:LEU:HD11  | 1.81                     | 0.62              |
| 1:I:424:LYS:NZ    | 1:I:425:LYS:O     | 2.33                     | 0.62              |
| 1:LA:424:LYS:NZ   | 1:LA:425:LYS:O    | 2.32                     | 0.62              |
| 1:A:424:LYS:NZ    | 1:A:425:LYS:O     | 2.32                     | 0.62              |
| 1:V:414:THR:O     | 1:V:422:ALA:N     | 2.33                     | 0.62              |
| 1:HA:414:THR:O    | 1:HA:422:ALA:N    | 2.33                     | 0.62              |
| 1:VA:460:LEU:HD21 | 1:VA:465:ARG:HB2  | 1.81                     | 0.62              |
| 1:K:460:LEU:HD21  | 1:K:465:ARG:HB2   | 1.81                     | 0.62              |
| 1:BA:203:GLN:NE2  | 1:BA:236:CYS:SG   | 2.72                     | 0.62              |
| 1:FA:90:PRO:HB3   | 1:FA:464:LEU:HD11 | 1.82                     | 0.62              |
| 1:FA:424:LYS:NZ   | 1:FA:425:LYS:O    | 2.32                     | 0.62              |
| 1:VA:414:THR:O    | 1:VA:422:ALA:N    | 2.31                     | 0.62              |
| 1:C:203:GLN:NE2   | 1:C:236:CYS:SG    | 2.73                     | 0.62              |
| 1:G:130:THR:OG1   | 1:G:133:PHE:O     | 2.18                     | 0.62              |
| 1:O:203:GLN:NE2   | 1:O:236:CYS:SG    | 2.73                     | 0.62              |
| 1:NA:203:GLN:NE2  | 1:NA:236:CYS:SG   | 2.72                     | 0.62              |
| 1:TA:203:GLN:NE2  | 1:TA:236:CYS:SG   | 2.73                     | 0.62              |
| 1:I:203:GLN:NE2   | 1:I:236:CYS:SG    | 2.73                     | 0.62              |
| 1:K:414:THR:O     | 1:K:422:ALA:N     | 2.31                     | 0.62              |
| 1:O:424:LYS:NZ    | 1:O:425:LYS:O     | 2.33                     | 0.62              |
| 1:V:424:LYS:NZ    | 1:V:425:LYS:O     | 2.33                     | 0.62              |
| 1:X:460:LEU:HD21  | 1:X:465:ARG:HB2   | 1.81                     | 0.62              |
| 1:BA:424:LYS:NZ   | 1:BA:425:LYS:O    | 2.33                     | 0.62              |
| 1:JA:90:PRO:HB3   | 1:JA:464:LEU:HD11 | 1.81                     | 0.62              |
| 1:A:203:GLN:NE2   | 1:A:236:CYS:SG    | 2.73                     | 0.62              |
| 1:C:414:THR:O     | 1:C:422:ALA:N     | 2.33                     | 0.62              |
| 1:E:414:THR:O     | 1:E:422:ALA:N     | 2.31                     | 0.62              |
| 1:E:460:LEU:HD21  | 1:E:465:ARG:HB2   | 1.81                     | 0.62              |
| 1:M:130:THR:OG1   | 1:M:133:PHE:O     | 2.18                     | 0.62              |
| 1:O:414:THR:O     | 1:O:422:ALA:N     | 2.33                     | 0.62              |
| 1:V:203:GLN:NE2   | 1:V:236:CYS:SG    | 2.73                     | 0.62              |
| 1:Z:130:THR:OG1   | 1:Z:133:PHE:O     | 2.18                     | 0.62              |
| 1:BA:414:THR:O    | 1:BA:422:ALA:N    | 2.33                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HA:203:GLN:NE2  | 1:HA:236:CYS:SG   | 2.73                     | 0.62              |
| 1:JA:460:LEU:HD21 | 1:JA:465:ARG:HB2  | 1.81                     | 0.62              |
| 1:LA:203:GLN:NE2  | 1:LA:236:CYS:SG   | 2.73                     | 0.62              |
| 1:RA:130:THR:OG1  | 1:RA:133:PHE:O    | 2.18                     | 0.62              |
| 1:S:415:LEU:HG    | 1:S:417:CYS:H     | 1.64                     | 0.61              |
| 1:HA:424:LYS:NZ   | 1:HA:425:LYS:O    | 2.33                     | 0.61              |
| 1:NA:414:THR:O    | 1:NA:422:ALA:N    | 2.33                     | 0.61              |
| 1:PA:460:LEU:HD21 | 1:PA:465:ARG:HB2  | 1.81                     | 0.61              |
| 1:S:203:GLN:NE2   | 1:S:236:CYS:SG    | 2.73                     | 0.61              |
| 1:DA:460:LEU:HD21 | 1:DA:465:ARG:HB2  | 1.81                     | 0.61              |
| 1:FA:203:GLN:NE2  | 1:FA:236:CYS:SG   | 2.73                     | 0.61              |
| 1:PA:414:THR:O    | 1:PA:422:ALA:N    | 2.31                     | 0.61              |
| 1:O:193:PRO:O     | 1:O:380:LYS:NZ    | 2.33                     | 0.61              |
| 1:Q:414:THR:O     | 1:Q:422:ALA:N     | 2.31                     | 0.61              |
| 1:Q:460:LEU:HD21  | 1:Q:465:ARG:HB2   | 1.81                     | 0.61              |
| 1:S:414:THR:O     | 1:S:422:ALA:N     | 2.34                     | 0.61              |
| 1:DA:414:THR:O    | 1:DA:422:ALA:N    | 2.31                     | 0.61              |
| 1:M:415:LEU:HG    | 1:M:417:CYS:H     | 1.63                     | 0.61              |
| 1:X:90:PRO:HB3    | 1:X:464:LEU:HD11  | 1.82                     | 0.61              |
| 1:BA:193:PRO:O    | 1:BA:380:LYS:NZ   | 2.33                     | 0.61              |
| 1:G:415:LEU:HG    | 1:G:417:CYS:H     | 1.63                     | 0.61              |
| 1:M:90:PRO:HB3    | 1:M:464:LEU:HD11  | 1.81                     | 0.61              |
| 1:Z:203:GLN:NE2   | 1:Z:236:CYS:SG    | 2.73                     | 0.61              |
| 1:DA:90:PRO:HB3   | 1:DA:464:LEU:HD11 | 1.82                     | 0.61              |
| 1:NA:424:LYS:NZ   | 1:NA:425:LYS:O    | 2.33                     | 0.61              |
| 1:RA:90:PRO:HB3   | 1:RA:464:LEU:HD11 | 1.81                     | 0.61              |
| 1:M:203:GLN:NE2   | 1:M:236:CYS:SG    | 2.73                     | 0.61              |
| 1:Z:90:PRO:HB3    | 1:Z:464:LEU:HD11  | 1.81                     | 0.61              |
| 1:Z:415:LEU:HG    | 1:Z:417:CYS:H     | 1.64                     | 0.61              |
| 1:FA:414:THR:O    | 1:FA:422:ALA:N    | 2.34                     | 0.61              |
| 1:A:265:HIS:ND1   | 1:A:446:GLU:OE1   | 2.30                     | 0.61              |
| 1:C:424:LYS:NZ    | 1:C:425:LYS:O     | 2.33                     | 0.61              |
| 1:G:203:GLN:NE2   | 1:G:236:CYS:SG    | 2.73                     | 0.61              |
| 1:A:130:THR:OG1   | 1:A:133:PHE:O     | 2.18                     | 0.61              |
| 1:A:414:THR:O     | 1:A:422:ALA:N     | 2.34                     | 0.61              |
| 1:Q:90:PRO:HB3    | 1:Q:464:LEU:HD11  | 1.82                     | 0.61              |
| 1:S:265:HIS:ND1   | 1:S:446:GLU:OE1   | 2.30                     | 0.61              |
| 1:LA:130:THR:OG1  | 1:LA:133:PHE:O    | 2.18                     | 0.61              |
| 1:VA:424:LYS:NZ   | 1:VA:425:LYS:O    | 2.34                     | 0.61              |
| 1:G:90:PRO:HB3    | 1:G:464:LEU:HD11  | 1.82                     | 0.60              |
| 1:K:424:LYS:NZ    | 1:K:425:LYS:O     | 2.34                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LA:414:THR:O    | 1:LA:422:ALA:N    | 2.34                     | 0.60              |
| 1:RA:203:GLN:NE2  | 1:RA:236:CYS:SG   | 2.73                     | 0.60              |
| 1:RA:415:LEU:HG   | 1:RA:417:CYS:H    | 1.64                     | 0.60              |
| 1:I:193:PRO:O     | 1:I:380:LYS:NZ    | 2.33                     | 0.60              |
| 1:O:416:THR:HG22  | 1:O:420:LEU:H     | 1.66                     | 0.60              |
| 1:Q:424:LYS:NZ    | 1:Q:425:LYS:O     | 2.34                     | 0.60              |
| 1:C:193:PRO:O     | 1:C:380:LYS:NZ    | 2.33                     | 0.60              |
| 1:I:416:THR:HG22  | 1:I:420:LEU:H     | 1.66                     | 0.60              |
| 1:K:90:PRO:HB3    | 1:K:464:LEU:HD11  | 1.82                     | 0.60              |
| 1:FA:265:HIS:ND1  | 1:FA:446:GLU:OE1  | 2.30                     | 0.60              |
| 1:LA:265:HIS:ND1  | 1:LA:446:GLU:OE1  | 2.30                     | 0.60              |
| 1:LA:337:THR:HG22 | 1:LA:341:GLN:HE21 | 1.66                     | 0.60              |
| 1:TA:193:PRO:O    | 1:TA:380:LYS:NZ   | 2.33                     | 0.60              |
| 1:TA:416:THR:HG22 | 1:TA:420:LEU:H    | 1.66                     | 0.60              |
| 1:A:337:THR:HG22  | 1:A:341:GLN:HE21  | 1.66                     | 0.60              |
| 1:C:416:THR:HG22  | 1:C:420:LEU:H     | 1.66                     | 0.60              |
| 1:S:130:THR:OG1   | 1:S:133:PHE:O     | 2.18                     | 0.60              |
| 1:V:193:PRO:O     | 1:V:380:LYS:NZ    | 2.33                     | 0.60              |
| 1:DA:424:LYS:NZ   | 1:DA:425:LYS:O    | 2.34                     | 0.60              |
| 1:JA:424:LYS:NZ   | 1:JA:425:LYS:O    | 2.34                     | 0.60              |
| 1:NA:193:PRO:O    | 1:NA:380:LYS:NZ   | 2.33                     | 0.60              |
| 1:E:424:LYS:NZ    | 1:E:425:LYS:O     | 2.34                     | 0.60              |
| 1:I:337:THR:HG22  | 1:I:341:GLN:HE21  | 1.67                     | 0.60              |
| 1:BA:416:THR:HG22 | 1:BA:420:LEU:H    | 1.66                     | 0.60              |
| 1:HA:193:PRO:O    | 1:HA:380:LYS:NZ   | 2.33                     | 0.60              |
| 1:NA:416:THR:HG22 | 1:NA:420:LEU:H    | 1.66                     | 0.60              |
| 1:X:337:THR:HG22  | 1:X:341:GLN:HE21  | 1.67                     | 0.60              |
| 1:X:424:LYS:NZ    | 1:X:425:LYS:O     | 2.34                     | 0.60              |
| 1:FA:130:THR:OG1  | 1:FA:133:PHE:O    | 2.18                     | 0.60              |
| 1:C:337:THR:HG22  | 1:C:341:GLN:HE21  | 1.67                     | 0.60              |
| 1:E:416:THR:HG22  | 1:E:420:LEU:H     | 1.66                     | 0.60              |
| 1:G:265:HIS:ND1   | 1:G:446:GLU:OE1   | 2.30                     | 0.60              |
| 1:K:416:THR:HG22  | 1:K:420:LEU:H     | 1.66                     | 0.60              |
| 1:BA:337:THR:HG22 | 1:BA:341:GLN:HE21 | 1.67                     | 0.60              |
| 1:JA:337:THR:HG22 | 1:JA:341:GLN:HE21 | 1.67                     | 0.60              |
| 1:PA:424:LYS:NZ   | 1:PA:425:LYS:O    | 2.34                     | 0.60              |
| 1:TA:337:THR:HG22 | 1:TA:341:GLN:HE21 | 1.67                     | 0.60              |
| 1:VA:342:MET:HE2  | 1:VA:345:ILE:HD13 | 1.82                     | 0.60              |
| 1:O:337:THR:HG22  | 1:O:341:GLN:HE21  | 1.67                     | 0.60              |
| 1:S:337:THR:HG22  | 1:S:341:GLN:HE21  | 1.66                     | 0.60              |
| 1:FA:337:THR:HG22 | 1:FA:341:GLN:HE21 | 1.66                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:NA:337:THR:HG22 | 1:NA:341:GLN:HE21 | 1.67                     | 0.60              |
| 1:PA:416:THR:HG22 | 1:PA:420:LEU:H    | 1.67                     | 0.60              |
| 1:RA:265:HIS:ND1  | 1:RA:446:GLU:OE1  | 2.30                     | 0.60              |
| 1:VA:90:PRO:HB3   | 1:VA:464:LEU:HD11 | 1.82                     | 0.60              |
| 1:E:90:PRO:HB3    | 1:E:464:LEU:HD11  | 1.82                     | 0.60              |
| 1:X:342:MET:HE2   | 1:X:345:ILE:HD13  | 1.82                     | 0.60              |
| 1:PA:90:PRO:HB3   | 1:PA:464:LEU:HD11 | 1.82                     | 0.60              |
| 1:I:130:THR:OG1   | 1:I:133:PHE:O     | 2.18                     | 0.60              |
| 1:I:414:THR:O     | 1:I:422:ALA:N     | 2.33                     | 0.60              |
| 1:JA:342:MET:HE2  | 1:JA:345:ILE:HD13 | 1.82                     | 0.60              |
| 1:TA:414:THR:O    | 1:TA:422:ALA:N    | 2.33                     | 0.60              |
| 1:VA:416:THR:HG22 | 1:VA:420:LEU:H    | 1.67                     | 0.60              |
| 1:G:337:THR:HG22  | 1:G:341:GLN:HE21  | 1.67                     | 0.59              |
| 1:K:342:MET:HE2   | 1:K:345:ILE:HD13  | 1.82                     | 0.59              |
| 1:RA:337:THR:HG22 | 1:RA:341:GLN:HE21 | 1.66                     | 0.59              |
| 1:E:337:THR:HG22  | 1:E:341:GLN:HE21  | 1.67                     | 0.59              |
| 1:E:342:MET:HE2   | 1:E:345:ILE:HD13  | 1.82                     | 0.59              |
| 1:Q:342:MET:HE2   | 1:Q:345:ILE:HD13  | 1.82                     | 0.59              |
| 1:PA:342:MET:HE2  | 1:PA:345:ILE:HD13 | 1.83                     | 0.59              |
| 1:TA:130:THR:OG1  | 1:TA:133:PHE:O    | 2.18                     | 0.59              |
| 1:K:337:THR:HG22  | 1:K:341:GLN:HE21  | 1.67                     | 0.59              |
| 1:X:416:THR:HG22  | 1:X:420:LEU:H     | 1.67                     | 0.59              |
| 1:JA:416:THR:HG22 | 1:JA:420:LEU:H    | 1.66                     | 0.59              |
| 1:PA:337:THR:HG22 | 1:PA:341:GLN:HE21 | 1.67                     | 0.59              |
| 1:VA:337:THR:HG22 | 1:VA:341:GLN:HE21 | 1.67                     | 0.59              |
| 1:Z:414:THR:O     | 1:Z:422:ALA:N     | 2.34                     | 0.59              |
| 1:I:438:GLN:NE2   | 1:K:244:GLY:O     | 2.35                     | 0.59              |
| 1:DA:342:MET:HE2  | 1:DA:345:ILE:HD13 | 1.82                     | 0.59              |
| 1:DA:130:THR:OG1  | 1:DA:133:PHE:O    | 2.17                     | 0.59              |
| 1:HA:416:THR:HG22 | 1:HA:420:LEU:H    | 1.66                     | 0.59              |
| 1:JA:193:PRO:O    | 1:JA:380:LYS:NZ   | 2.35                     | 0.59              |
| 1:TA:438:GLN:NE2  | 1:VA:244:GLY:O    | 2.35                     | 0.59              |
| 1:E:193:PRO:O     | 1:E:380:LYS:NZ    | 2.35                     | 0.59              |
| 1:M:414:THR:O     | 1:M:422:ALA:N     | 2.34                     | 0.59              |
| 1:Q:337:THR:HG22  | 1:Q:341:GLN:HE21  | 1.67                     | 0.59              |
| 1:V:416:THR:HG22  | 1:V:420:LEU:H     | 1.66                     | 0.59              |
| 1:Z:337:THR:HG22  | 1:Z:341:GLN:HE21  | 1.66                     | 0.59              |
| 1:RA:414:THR:O    | 1:RA:422:ALA:N    | 2.34                     | 0.59              |
| 1:DA:337:THR:HG22 | 1:DA:341:GLN:HE21 | 1.67                     | 0.59              |
| 1:G:44:SER:HB3    | 1:G:151:GLN:HE21  | 1.68                     | 0.59              |
| 1:M:337:THR:HG22  | 1:M:341:GLN:HE21  | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:X:193:PRO:O     | 1:X:380:LYS:NZ    | 2.35                     | 0.59              |
| 1:RA:44:SER:HB3   | 1:RA:151:GLN:HE21 | 1.68                     | 0.59              |
| 1:Q:130:THR:OG1   | 1:Q:133:PHE:O     | 2.18                     | 0.59              |
| 1:PA:193:PRO:O    | 1:PA:380:LYS:NZ   | 2.36                     | 0.59              |
| 1:S:416:THR:HG22  | 1:S:420:LEU:H     | 1.68                     | 0.58              |
| 1:V:337:THR:HG22  | 1:V:341:GLN:HE21  | 1.67                     | 0.58              |
| 1:RA:416:THR:HG22 | 1:RA:420:LEU:H    | 1.68                     | 0.58              |
| 1:Z:44:SER:HB3    | 1:Z:151:GLN:HE21  | 1.68                     | 0.58              |
| 1:HA:337:THR:HG22 | 1:HA:341:GLN:HE21 | 1.67                     | 0.58              |
| 1:G:414:THR:O     | 1:G:422:ALA:N     | 2.34                     | 0.58              |
| 1:M:44:SER:HB3    | 1:M:151:GLN:HE21  | 1.68                     | 0.58              |
| 1:Z:416:THR:HG22  | 1:Z:420:LEU:H     | 1.68                     | 0.58              |
| 1:S:44:SER:HB3    | 1:S:151:GLN:HE21  | 1.68                     | 0.58              |
| 1:DA:416:THR:HG22 | 1:DA:420:LEU:H    | 1.67                     | 0.58              |
| 1:FA:44:SER:HB3   | 1:FA:151:GLN:HE21 | 1.68                     | 0.58              |
| 1:K:130:THR:OG1   | 1:K:133:PHE:O     | 2.18                     | 0.58              |
| 1:Q:416:THR:HG22  | 1:Q:420:LEU:H     | 1.67                     | 0.58              |
| 1:FA:416:THR:HG22 | 1:FA:420:LEU:H    | 1.69                     | 0.58              |
| 1:A:44:SER:HB3    | 1:A:151:GLN:HE21  | 1.68                     | 0.58              |
| 1:HA:438:GLN:NE2  | 1:JA:244:GLY:O    | 2.35                     | 0.58              |
| 1:LA:416:THR:HG22 | 1:LA:420:LEU:H    | 1.69                     | 0.58              |
| 1:C:130:THR:OG1   | 1:C:133:PHE:O     | 2.18                     | 0.57              |
| 1:C:436:ASP:OD2   | 1:E:380:LYS:HE2   | 2.04                     | 0.57              |
| 1:LA:44:SER:HB3   | 1:LA:151:GLN:HE21 | 1.68                     | 0.57              |
| 1:G:416:THR:HG22  | 1:G:420:LEU:H     | 1.69                     | 0.57              |
| 1:I:436:ASP:OD2   | 1:K:380:LYS:HE2   | 2.04                     | 0.57              |
| 1:V:438:GLN:NE2   | 1:X:244:GLY:O     | 2.35                     | 0.57              |
| 1:Z:265:HIS:ND1   | 1:Z:446:GLU:OE1   | 2.30                     | 0.57              |
| 1:A:416:THR:HG22  | 1:A:420:LEU:H     | 1.69                     | 0.57              |
| 1:O:436:ASP:OD2   | 1:Q:380:LYS:HE2   | 2.05                     | 0.57              |
| 1:DA:193:PRO:O    | 1:DA:380:LYS:NZ   | 2.36                     | 0.57              |
| 1:NA:436:ASP:OD2  | 1:PA:380:LYS:HE2  | 2.05                     | 0.57              |
| 1:TA:436:ASP:OD2  | 1:VA:380:LYS:HE2  | 2.04                     | 0.57              |
| 1:M:416:THR:HG22  | 1:M:420:LEU:H     | 1.69                     | 0.57              |
| 1:V:436:ASP:OD2   | 1:X:380:LYS:HE2   | 2.05                     | 0.57              |
| 1:BA:436:ASP:OD2  | 1:DA:380:LYS:HE2  | 2.05                     | 0.57              |
| 1:K:193:PRO:O     | 1:K:380:LYS:NZ    | 2.36                     | 0.57              |
| 1:Q:193:PRO:O     | 1:Q:380:LYS:NZ    | 2.36                     | 0.57              |
| 1:HA:436:ASP:OD2  | 1:JA:380:LYS:HE2  | 2.05                     | 0.57              |
| 1:V:130:THR:OG1   | 1:V:133:PHE:O     | 2.18                     | 0.57              |
| 1:V:204:VAL:HG12  | 1:V:321:VAL:HG21  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:438:GLN:NE2   | 1:E:244:GLY:O     | 2.35                     | 0.57              |
| 1:RA:305:VAL:HG21 | 1:TA:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:VA:130:THR:OG1  | 1:VA:133:PHE:O    | 2.18                     | 0.57              |
| 1:G:305:VAL:HG21  | 1:I:247:LEU:HB2   | 1.87                     | 0.57              |
| 1:LA:305:VAL:HG21 | 1:NA:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:VA:193:PRO:O    | 1:VA:380:LYS:NZ   | 2.36                     | 0.57              |
| 1:M:265:HIS:ND1   | 1:M:446:GLU:OE1   | 2.30                     | 0.57              |
| 1:O:204:VAL:HG12  | 1:O:321:VAL:HG21  | 1.86                     | 0.57              |
| 1:Q:161:SER:O     | 1:Q:165:GLN:HG2   | 2.05                     | 0.57              |
| 1:BA:130:THR:OG1  | 1:BA:133:PHE:O    | 2.18                     | 0.57              |
| 1:HA:204:VAL:HG12 | 1:HA:321:VAL:HG21 | 1.87                     | 0.57              |
| 1:NA:438:GLN:NE2  | 1:PA:244:GLY:O    | 2.35                     | 0.57              |
| 1:O:438:GLN:NE2   | 1:Q:244:GLY:O     | 2.35                     | 0.56              |
| 1:DA:161:SER:O    | 1:DA:165:GLN:HG2  | 2.05                     | 0.56              |
| 1:NA:421:TRP:O    | 1:PA:226:SER:HB3  | 2.05                     | 0.56              |
| 1:K:161:SER:O     | 1:K:165:GLN:HG2   | 2.05                     | 0.56              |
| 1:O:130:THR:OG1   | 1:O:133:PHE:O     | 2.18                     | 0.56              |
| 1:BA:204:VAL:HG12 | 1:BA:321:VAL:HG21 | 1.86                     | 0.56              |
| 1:HA:130:THR:OG1  | 1:HA:133:PHE:O    | 2.18                     | 0.56              |
| 1:A:247:LEU:HB2   | 1:X:305:VAL:HG21  | 1.87                     | 0.56              |
| 1:A:305:VAL:HG21  | 1:C:247:LEU:HB2   | 1.88                     | 0.56              |
| 1:C:421:TRP:O     | 1:E:226:SER:HB3   | 2.05                     | 0.56              |
| 1:E:305:VAL:HG21  | 1:G:247:LEU:HB2   | 1.87                     | 0.56              |
| 1:I:204:VAL:HG12  | 1:I:321:VAL:HG21  | 1.86                     | 0.56              |
| 1:I:421:TRP:O     | 1:K:226:SER:HB3   | 2.05                     | 0.56              |
| 1:BA:152:ASP:OD1  | 1:BA:285:TYR:OH   | 2.24                     | 0.56              |
| 1:BA:438:GLN:NE2  | 1:DA:244:GLY:O    | 2.35                     | 0.56              |
| 1:JA:305:VAL:HG21 | 1:LA:247:LEU:HB2  | 1.87                     | 0.56              |
| 1:TA:204:VAL:HG12 | 1:TA:321:VAL:HG21 | 1.87                     | 0.56              |
| 1:VA:161:SER:O    | 1:VA:165:GLN:HG2  | 2.05                     | 0.56              |
| 1:O:152:ASP:OD1   | 1:O:285:TYR:OH    | 2.24                     | 0.56              |
| 1:V:161:SER:O     | 1:V:165:GLN:HG2   | 2.06                     | 0.56              |
| 1:HA:161:SER:O    | 1:HA:165:GLN:HG2  | 2.06                     | 0.56              |
| 1:JA:161:SER:O    | 1:JA:165:GLN:HG2  | 2.05                     | 0.56              |
| 1:PA:305:VAL:HG21 | 1:RA:247:LEU:HB2  | 1.87                     | 0.56              |
| 1:TA:421:TRP:O    | 1:VA:226:SER:HB3  | 2.05                     | 0.56              |
| 1:G:116:ILE:HG23  | 1:G:472:LEU:HD13  | 1.88                     | 0.56              |
| 1:X:161:SER:O     | 1:X:165:GLN:HG2   | 2.05                     | 0.56              |
| 1:BA:161:SER:O    | 1:BA:165:GLN:HG2  | 2.06                     | 0.56              |
| 1:O:161:SER:O     | 1:O:165:GLN:HG2   | 2.06                     | 0.56              |
| 1:FA:305:VAL:HG21 | 1:HA:247:LEU:HB2  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:NA:130:THR:OG1  | 1:NA:133:PHE:O    | 2.18                     | 0.56              |
| 1:S:305:VAL:HG21  | 1:V:247:LEU:HB2   | 1.87                     | 0.56              |
| 1:RA:116:ILE:HG23 | 1:RA:472:LEU:HD13 | 1.88                     | 0.56              |
| 1:C:204:VAL:HG12  | 1:C:321:VAL:HG21  | 1.86                     | 0.56              |
| 1:E:161:SER:O     | 1:E:165:GLN:HG2   | 2.05                     | 0.56              |
| 1:E:421:TRP:O     | 1:G:226:SER:HB3   | 2.06                     | 0.56              |
| 1:Z:305:VAL:HG21  | 1:BA:247:LEU:HB2  | 1.87                     | 0.56              |
| 1:FA:116:ILE:HG23 | 1:FA:472:LEU:HD13 | 1.88                     | 0.56              |
| 1:JA:130:THR:OG1  | 1:JA:133:PHE:O    | 2.18                     | 0.56              |
| 1:C:161:SER:O     | 1:C:165:GLN:HG2   | 2.06                     | 0.56              |
| 1:M:305:VAL:HG21  | 1:O:247:LEU:HB2   | 1.87                     | 0.56              |
| 1:NA:161:SER:O    | 1:NA:165:GLN:HG2  | 2.06                     | 0.56              |
| 1:NA:204:VAL:HG12 | 1:NA:321:VAL:HG21 | 1.87                     | 0.56              |
| 1:X:130:THR:OG1   | 1:X:133:PHE:O     | 2.18                     | 0.55              |
| 1:PA:161:SER:O    | 1:PA:165:GLN:HG2  | 2.06                     | 0.55              |
| 1:VA:44:SER:HB3   | 1:VA:151:GLN:HE21 | 1.71                     | 0.55              |
| 1:S:116:ILE:HG23  | 1:S:472:LEU:HD13  | 1.88                     | 0.55              |
| 1:PA:421:TRP:O    | 1:RA:226:SER:HB3  | 2.06                     | 0.55              |
| 1:X:44:SER:HB3    | 1:X:151:GLN:HE21  | 1.71                     | 0.55              |
| 1:TA:161:SER:O    | 1:TA:165:GLN:HG2  | 2.06                     | 0.55              |
| 1:I:161:SER:O     | 1:I:165:GLN:HG2   | 2.06                     | 0.55              |
| 1:Z:116:ILE:HG23  | 1:Z:472:LEU:HD13  | 1.88                     | 0.55              |
| 1:DA:421:TRP:O    | 1:FA:226:SER:HB3  | 2.06                     | 0.55              |
| 1:HA:421:TRP:O    | 1:JA:226:SER:HB3  | 2.05                     | 0.55              |
| 1:LA:129:GLU:HG3  | 1:LA:142:ARG:HB2  | 1.88                     | 0.55              |
| 1:A:129:GLU:HG3   | 1:A:142:ARG:HB2   | 1.88                     | 0.55              |
| 1:M:116:ILE:HG23  | 1:M:472:LEU:HD13  | 1.88                     | 0.55              |
| 1:V:421:TRP:O     | 1:X:226:SER:HB3   | 2.05                     | 0.55              |
| 1:DA:44:SER:HB3   | 1:DA:151:GLN:HE21 | 1.71                     | 0.55              |
| 1:K:44:SER:HB3    | 1:K:151:GLN:HE21  | 1.71                     | 0.55              |
| 1:S:129:GLU:HG3   | 1:S:142:ARG:HB2   | 1.88                     | 0.55              |
| 1:FA:129:GLU:HG3  | 1:FA:142:ARG:HB2  | 1.88                     | 0.55              |
| 1:K:305:VAL:HG21  | 1:M:247:LEU:HB2   | 1.87                     | 0.55              |
| 1:K:421:TRP:O     | 1:M:226:SER:HB3   | 2.06                     | 0.55              |
| 1:Q:44:SER:HB3    | 1:Q:151:GLN:HE21  | 1.71                     | 0.55              |
| 1:Q:421:TRP:O     | 1:S:226:SER:HB3   | 2.06                     | 0.55              |
| 1:Z:247:LEU:HB2   | 1:VA:305:VAL:HG21 | 1.87                     | 0.55              |
| 1:E:44:SER:HB3    | 1:E:151:GLN:HE21  | 1.71                     | 0.55              |
| 1:Z:129:GLU:HG3   | 1:Z:142:ARG:HB2   | 1.88                     | 0.55              |
| 1:BA:421:TRP:O    | 1:DA:226:SER:HB3  | 2.05                     | 0.55              |
| 1:FA:421:TRP:O    | 1:HA:226:SER:HB3  | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HA:413:ARG:HB3  | 1:HA:421:TRP:HB3  | 1.89                     | 0.55              |
| 1:JA:44:SER:HB3   | 1:JA:151:GLN:HE21 | 1.71                     | 0.55              |
| 1:A:226:SER:HB3   | 1:X:421:TRP:O     | 2.06                     | 0.55              |
| 1:G:421:TRP:O     | 1:I:226:SER:HB3   | 2.07                     | 0.55              |
| 1:M:129:GLU:HG3   | 1:M:142:ARG:HB2   | 1.88                     | 0.55              |
| 1:O:421:TRP:O     | 1:Q:226:SER:HB3   | 2.05                     | 0.55              |
| 1:Q:305:VAL:HG21  | 1:S:247:LEU:HB2   | 1.87                     | 0.55              |
| 1:S:421:TRP:O     | 1:V:226:SER:HB3   | 2.07                     | 0.55              |
| 1:V:413:ARG:HB3   | 1:V:421:TRP:HB3   | 1.89                     | 0.55              |
| 1:RA:421:TRP:O    | 1:TA:226:SER:HB3  | 2.07                     | 0.55              |
| 1:O:413:ARG:HB3   | 1:O:421:TRP:HB3   | 1.89                     | 0.55              |
| 1:DA:305:VAL:HG21 | 1:FA:247:LEU:HB2  | 1.87                     | 0.55              |
| 1:LA:116:ILE:HG23 | 1:LA:472:LEU:HD13 | 1.88                     | 0.55              |
| 1:PA:44:SER:HB3   | 1:PA:151:GLN:HE21 | 1.71                     | 0.55              |
| 1:A:116:ILE:HG23  | 1:A:472:LEU:HD13  | 1.88                     | 0.54              |
| 1:Q:152:ASP:OD1   | 1:Q:285:TYR:OH    | 2.24                     | 0.54              |
| 1:Z:226:SER:HB3   | 1:VA:421:TRP:O    | 2.06                     | 0.54              |
| 1:BA:413:ARG:HB3  | 1:BA:421:TRP:HB3  | 1.89                     | 0.54              |
| 1:JA:421:TRP:O    | 1:LA:226:SER:HB3  | 2.06                     | 0.54              |
| 1:G:129:GLU:HG3   | 1:G:142:ARG:HB2   | 1.89                     | 0.54              |
| 1:V:460:LEU:HD21  | 1:V:465:ARG:HB2   | 1.90                     | 0.54              |
| 1:DA:152:ASP:OD1  | 1:DA:285:TYR:OH   | 2.25                     | 0.54              |
| 1:C:460:LEU:HD21  | 1:C:465:ARG:HB2   | 1.90                     | 0.54              |
| 1:S:161:SER:O     | 1:S:165:GLN:HG2   | 2.08                     | 0.54              |
| 1:LA:152:ASP:OD1  | 1:LA:285:TYR:OH   | 2.25                     | 0.54              |
| 1:NA:460:LEU:HD21 | 1:NA:465:ARG:HB2  | 1.90                     | 0.54              |
| 1:A:152:ASP:OD1   | 1:A:285:TYR:OH    | 2.25                     | 0.54              |
| 1:FA:161:SER:O    | 1:FA:165:GLN:HG2  | 2.08                     | 0.54              |
| 1:A:421:TRP:O     | 1:C:226:SER:HB3   | 2.07                     | 0.54              |
| 1:M:152:ASP:OD1   | 1:M:285:TYR:OH    | 2.25                     | 0.54              |
| 1:X:116:ILE:HG23  | 1:X:472:LEU:HD13  | 1.89                     | 0.54              |
| 1:Z:421:TRP:O     | 1:BA:226:SER:HB3  | 2.07                     | 0.54              |
| 1:FA:152:ASP:OD1  | 1:FA:285:TYR:OH   | 2.25                     | 0.54              |
| 1:HA:460:LEU:HD21 | 1:HA:465:ARG:HB2  | 1.90                     | 0.54              |
| 1:LA:421:TRP:O    | 1:NA:226:SER:HB3  | 2.07                     | 0.54              |
| 1:RA:129:GLU:HG3  | 1:RA:142:ARG:HB2  | 1.89                     | 0.54              |
| 1:M:421:TRP:O     | 1:O:226:SER:HB3   | 2.07                     | 0.54              |
| 1:HA:152:ASP:OD1  | 1:HA:285:TYR:OH   | 2.24                     | 0.54              |
| 1:TA:460:LEU:HD21 | 1:TA:465:ARG:HB2  | 1.89                     | 0.54              |
| 1:A:161:SER:O     | 1:A:165:GLN:HG2   | 2.08                     | 0.54              |
| 1:C:413:ARG:HB3   | 1:C:421:TRP:HB3   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:V:152:ASP:OD1   | 1:V:285:TYR:OH    | 2.24                     | 0.54              |
| 1:LA:161:SER:O    | 1:LA:165:GLN:HG2  | 2.08                     | 0.54              |
| 1:NA:413:ARG:HB3  | 1:NA:421:TRP:HB3  | 1.89                     | 0.54              |
| 1:A:83:PRO:HB3    | 1:A:137:THR:HG22  | 1.90                     | 0.54              |
| 1:E:116:ILE:HG23  | 1:E:472:LEU:HD13  | 1.89                     | 0.54              |
| 1:O:460:LEU:HD21  | 1:O:465:ARG:HB2   | 1.90                     | 0.54              |
| 1:PA:116:ILE:HG23 | 1:PA:472:LEU:HD13 | 1.89                     | 0.54              |
| 1:I:152:ASP:OD1   | 1:I:285:TYR:OH    | 2.24                     | 0.54              |
| 1:K:116:ILE:HG23  | 1:K:472:LEU:HD13  | 1.89                     | 0.54              |
| 1:LA:83:PRO:HB3   | 1:LA:137:THR:HG22 | 1.90                     | 0.54              |
| 1:NA:305:VAL:HG21 | 1:PA:247:LEU:HB2  | 1.90                     | 0.54              |
| 1:C:305:VAL:HG21  | 1:E:247:LEU:HB2   | 1.90                     | 0.53              |
| 1:I:460:LEU:HD21  | 1:I:465:ARG:HB2   | 1.90                     | 0.53              |
| 1:S:204:VAL:HG12  | 1:S:321:VAL:HG21  | 1.90                     | 0.53              |
| 1:TA:152:ASP:OD1  | 1:TA:285:TYR:OH   | 2.24                     | 0.53              |
| 1:K:303:TYR:HB3   | 1:K:440:ILE:HD11  | 1.90                     | 0.53              |
| 1:BA:460:LEU:HD21 | 1:BA:465:ARG:HB2  | 1.90                     | 0.53              |
| 1:DA:204:VAL:HG12 | 1:DA:321:VAL:HG21 | 1.90                     | 0.53              |
| 1:JA:303:TYR:HB3  | 1:JA:440:ILE:HD11 | 1.91                     | 0.53              |
| 1:VA:303:TYR:HB3  | 1:VA:440:ILE:HD11 | 1.91                     | 0.53              |
| 1:E:303:TYR:HB3   | 1:E:440:ILE:HD11  | 1.91                     | 0.53              |
| 1:G:83:PRO:HB3    | 1:G:137:THR:HG22  | 1.90                     | 0.53              |
| 1:Q:303:TYR:HB3   | 1:Q:440:ILE:HD11  | 1.91                     | 0.53              |
| 1:X:303:TYR:HB3   | 1:X:440:ILE:HD11  | 1.91                     | 0.53              |
| 1:DA:303:TYR:HB3  | 1:DA:440:ILE:HD11 | 1.91                     | 0.53              |
| 1:FA:204:VAL:HG12 | 1:FA:321:VAL:HG21 | 1.90                     | 0.53              |
| 1:PA:303:TYR:HB3  | 1:PA:440:ILE:HD11 | 1.91                     | 0.53              |
| 1:RA:83:PRO:HB3   | 1:RA:137:THR:HG22 | 1.90                     | 0.53              |
| 1:M:161:SER:O     | 1:M:165:GLN:HG2   | 2.08                     | 0.53              |
| 1:Z:161:SER:O     | 1:Z:165:GLN:HG2   | 2.07                     | 0.53              |
| 1:I:275:ARG:NH2   | 1:K:88:GLU:OE2    | 2.42                     | 0.53              |
| 1:VA:204:VAL:HG12 | 1:VA:321:VAL:HG21 | 1.90                     | 0.53              |
| 1:E:152:ASP:OD1   | 1:E:285:TYR:OH    | 2.24                     | 0.53              |
| 1:I:413:ARG:HB3   | 1:I:421:TRP:HB3   | 1.89                     | 0.53              |
| 1:TA:275:ARG:NH2  | 1:VA:88:GLU:OE2   | 2.42                     | 0.53              |
| 1:TA:413:ARG:HB3  | 1:TA:421:TRP:HB3  | 1.89                     | 0.53              |
| 1:VA:152:ASP:OD1  | 1:VA:285:TYR:OH   | 2.25                     | 0.53              |
| 1:G:420:LEU:HD22  | 1:I:227:ILE:HA    | 1.91                     | 0.53              |
| 1:I:305:VAL:HG21  | 1:K:247:LEU:HB2   | 1.90                     | 0.53              |
| 1:Q:204:VAL:HG12  | 1:Q:321:VAL:HG21  | 1.90                     | 0.53              |
| 1:G:152:ASP:OD1   | 1:G:285:TYR:OH    | 2.25                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:152:ASP:OD1   | 1:K:285:TYR:OH    | 2.25                     | 0.53              |
| 1:M:83:PRO:HB3    | 1:M:137:THR:HG22  | 1.90                     | 0.53              |
| 1:X:204:VAL:HG12  | 1:X:321:VAL:HG21  | 1.90                     | 0.53              |
| 1:RA:152:ASP:OD1  | 1:RA:285:TYR:OH   | 2.25                     | 0.53              |
| 1:G:161:SER:O     | 1:G:165:GLN:HG2   | 2.08                     | 0.53              |
| 1:K:204:VAL:HG12  | 1:K:321:VAL:HG21  | 1.90                     | 0.53              |
| 1:Z:83:PRO:HB3    | 1:Z:137:THR:HG22  | 1.90                     | 0.53              |
| 1:PA:152:ASP:OD1  | 1:PA:285:TYR:OH   | 2.25                     | 0.53              |
| 1:A:204:VAL:HG12  | 1:A:321:VAL:HG21  | 1.90                     | 0.53              |
| 1:O:275:ARG:NH2   | 1:Q:88:GLU:OE2    | 2.42                     | 0.53              |
| 1:V:305:VAL:HG21  | 1:X:247:LEU:HB2   | 1.90                     | 0.53              |
| 1:BA:464:LEU:O    | 1:BA:468:ILE:HG12 | 2.09                     | 0.53              |
| 1:HA:305:VAL:HG21 | 1:JA:247:LEU:HB2  | 1.90                     | 0.53              |
| 1:O:464:LEU:O     | 1:O:468:ILE:HG12  | 2.09                     | 0.52              |
| 1:LA:204:VAL:HG12 | 1:LA:321:VAL:HG21 | 1.90                     | 0.52              |
| 1:RA:161:SER:O    | 1:RA:165:GLN:HG2  | 2.08                     | 0.52              |
| 1:RA:420:LEU:HD22 | 1:TA:227:ILE:HA   | 1.91                     | 0.52              |
| 1:TA:305:VAL:HG21 | 1:VA:247:LEU:HB2  | 1.91                     | 0.52              |
| 1:DA:116:ILE:HG23 | 1:DA:472:LEU:HD13 | 1.89                     | 0.52              |
| 1:JA:204:VAL:HG12 | 1:JA:321:VAL:HG21 | 1.90                     | 0.52              |
| 1:TA:464:LEU:O    | 1:TA:468:ILE:HG12 | 2.09                     | 0.52              |
| 1:I:464:LEU:O     | 1:I:468:ILE:HG12  | 2.09                     | 0.52              |
| 1:BA:275:ARG:NH2  | 1:DA:88:GLU:OE2   | 2.42                     | 0.52              |
| 1:E:204:VAL:HG12  | 1:E:321:VAL:HG21  | 1.90                     | 0.52              |
| 1:G:204:VAL:HG12  | 1:G:321:VAL:HG21  | 1.90                     | 0.52              |
| 1:V:129:GLU:HG3   | 1:V:142:ARG:HB2   | 1.92                     | 0.52              |
| 1:BA:305:VAL:HG21 | 1:DA:247:LEU:HB2  | 1.90                     | 0.52              |
| 1:HA:341:GLN:HE22 | 1:HA:365:ARG:HH22 | 1.58                     | 0.52              |
| 1:NA:152:ASP:OD1  | 1:NA:285:TYR:OH   | 2.24                     | 0.52              |
| 1:C:152:ASP:OD1   | 1:C:285:TYR:OH    | 2.24                     | 0.52              |
| 1:M:204:VAL:HG12  | 1:M:321:VAL:HG21  | 1.90                     | 0.52              |
| 1:M:420:LEU:HD22  | 1:O:227:ILE:HA    | 1.91                     | 0.52              |
| 1:O:305:VAL:HG21  | 1:Q:247:LEU:HB2   | 1.90                     | 0.52              |
| 1:O:341:GLN:HE22  | 1:O:365:ARG:HH22  | 1.58                     | 0.52              |
| 1:BA:341:GLN:HE22 | 1:BA:365:ARG:HH22 | 1.58                     | 0.52              |
| 1:HA:129:GLU:HG3  | 1:HA:142:ARG:HB2  | 1.92                     | 0.52              |
| 1:HA:275:ARG:NH2  | 1:JA:88:GLU:OE2   | 2.42                     | 0.52              |
| 1:JA:185:TYR:HB3  | 1:JA:314:MET:SD   | 2.50                     | 0.52              |
| 1:RA:204:VAL:HG12 | 1:RA:321:VAL:HG21 | 1.90                     | 0.52              |
| 1:X:185:TYR:HB3   | 1:X:314:MET:SD    | 2.50                     | 0.52              |
| 1:Z:204:VAL:HG12  | 1:Z:321:VAL:HG21  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Z:420:LEU:HD22  | 1:BA:227:ILE:HA   | 1.91                     | 0.52              |
| 1:DA:185:TYR:HB3  | 1:DA:314:MET:SD   | 2.50                     | 0.52              |
| 1:FA:83:PRO:HB3   | 1:FA:137:THR:HG22 | 1.90                     | 0.52              |
| 1:NA:129:GLU:HG3  | 1:NA:142:ARG:HB2  | 1.92                     | 0.52              |
| 1:Q:185:TYR:HB3   | 1:Q:314:MET:SD    | 2.50                     | 0.52              |
| 1:V:275:ARG:NH2   | 1:X:88:GLU:OE2    | 2.42                     | 0.52              |
| 1:V:341:GLN:HE22  | 1:V:365:ARG:HH22  | 1.58                     | 0.52              |
| 1:V:464:LEU:O     | 1:V:468:ILE:HG12  | 2.09                     | 0.52              |
| 1:HA:464:LEU:O    | 1:HA:468:ILE:HG12 | 2.09                     | 0.52              |
| 1:A:138:ASP:OD2   | 1:A:161:SER:OG    | 2.26                     | 0.52              |
| 1:S:83:PRO:HB3    | 1:S:137:THR:HG22  | 1.90                     | 0.52              |
| 1:X:413:ARG:HB3   | 1:X:421:TRP:HB3   | 1.92                     | 0.52              |
| 1:PA:204:VAL:HG12 | 1:PA:321:VAL:HG21 | 1.90                     | 0.52              |
| 1:C:129:GLU:HG3   | 1:C:142:ARG:HB2   | 1.92                     | 0.52              |
| 1:M:341:GLN:HE22  | 1:M:365:ARG:HH22  | 1.59                     | 0.52              |
| 1:DA:413:ARG:HB3  | 1:DA:421:TRP:HB3  | 1.92                     | 0.52              |
| 1:FA:138:ASP:OD2  | 1:FA:161:SER:OG   | 2.26                     | 0.52              |
| 1:NA:275:ARG:NH2  | 1:PA:88:GLU:OE2   | 2.42                     | 0.52              |
| 1:A:281:SER:OG    | 3:A:1102:HOH:O    | 2.19                     | 0.51              |
| 1:I:129:GLU:HG3   | 1:I:142:ARG:HB2   | 1.92                     | 0.51              |
| 1:K:413:ARG:HB3   | 1:K:421:TRP:HB3   | 1.92                     | 0.51              |
| 1:S:138:ASP:OD2   | 1:S:161:SER:OG    | 2.26                     | 0.51              |
| 1:S:152:ASP:OD1   | 1:S:285:TYR:OH    | 2.25                     | 0.51              |
| 1:Z:227:ILE:HA    | 1:VA:420:LEU:HD22 | 1.92                     | 0.51              |
| 1:Z:341:GLN:HE22  | 1:Z:365:ARG:HH22  | 1.59                     | 0.51              |
| 1:LA:138:ASP:OD2  | 1:LA:161:SER:OG   | 2.26                     | 0.51              |
| 1:C:195:TYR:OH    | 1:C:282:CYS:O     | 2.28                     | 0.51              |
| 1:X:341:GLN:OE1   | 1:X:365:ARG:NH2   | 2.44                     | 0.51              |
| 1:PA:185:TYR:HB3  | 1:PA:314:MET:SD   | 2.50                     | 0.51              |
| 1:C:275:ARG:NH2   | 1:E:88:GLU:OE2    | 2.42                     | 0.51              |
| 1:Q:413:ARG:HB3   | 1:Q:421:TRP:HB3   | 1.93                     | 0.51              |
| 1:JA:341:GLN:OE1  | 1:JA:365:ARG:NH2  | 2.44                     | 0.51              |
| 1:TA:129:GLU:HG3  | 1:TA:142:ARG:HB2  | 1.92                     | 0.51              |
| 1:A:413:ARG:HB3   | 1:A:421:TRP:HB3   | 1.93                     | 0.51              |
| 1:M:138:ASP:OD2   | 1:M:161:SER:OG    | 2.26                     | 0.51              |
| 1:V:135:LEU:HD21  | 1:V:460:LEU:HD13  | 1.93                     | 0.51              |
| 1:FA:341:GLN:HE22 | 1:FA:365:ARG:HH22 | 1.59                     | 0.51              |
| 1:FA:413:ARG:HB3  | 1:FA:421:TRP:HB3  | 1.93                     | 0.51              |
| 1:LA:281:SER:OG   | 3:LA:1102:HOH:O   | 2.19                     | 0.51              |
| 1:NA:195:TYR:OH   | 1:NA:282:CYS:O    | 2.28                     | 0.51              |
| 1:BA:135:LEU:HD21 | 1:BA:460:LEU:HD13 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HA:135:LEU:HD21 | 1:HA:460:LEU:HD13 | 1.93                     | 0.51              |
| 1:LA:413:ARG:HB3  | 1:LA:421:TRP:HB3  | 1.93                     | 0.51              |
| 1:LA:420:LEU:HD22 | 1:NA:227:ILE:HA   | 1.91                     | 0.51              |
| 1:TA:135:LEU:HD21 | 1:TA:460:LEU:HD13 | 1.93                     | 0.51              |
| 1:A:420:LEU:HD22  | 1:C:227:ILE:HA    | 1.91                     | 0.51              |
| 1:E:185:TYR:HB3   | 1:E:314:MET:SD    | 2.50                     | 0.51              |
| 1:M:413:ARG:HB3   | 1:M:421:TRP:HB3   | 1.93                     | 0.51              |
| 1:S:341:GLN:HE22  | 1:S:365:ARG:HH22  | 1.59                     | 0.51              |
| 1:S:413:ARG:HB3   | 1:S:421:TRP:HB3   | 1.93                     | 0.51              |
| 1:S:420:LEU:HD22  | 1:V:227:ILE:HA    | 1.91                     | 0.51              |
| 1:Z:138:ASP:OD2   | 1:Z:161:SER:OG    | 2.26                     | 0.51              |
| 1:JA:413:ARG:HB3  | 1:JA:421:TRP:HB3  | 1.93                     | 0.51              |
| 1:LA:341:GLN:HE22 | 1:LA:365:ARG:HH22 | 1.59                     | 0.51              |
| 1:VA:413:ARG:HB3  | 1:VA:421:TRP:HB3  | 1.93                     | 0.51              |
| 1:A:341:GLN:HE22  | 1:A:365:ARG:HH22  | 1.59                     | 0.51              |
| 1:C:135:LEU:HD21  | 1:C:460:LEU:HD13  | 1.93                     | 0.51              |
| 1:I:341:GLN:HE22  | 1:I:365:ARG:HH22  | 1.58                     | 0.51              |
| 1:O:135:LEU:HD21  | 1:O:460:LEU:HD13  | 1.93                     | 0.51              |
| 1:NA:425:LYS:HB3  | 1:PA:220:GLY:HA2  | 1.92                     | 0.51              |
| 1:NA:464:LEU:O    | 1:NA:468:ILE:HG12 | 2.09                     | 0.51              |
| 1:TA:341:GLN:HE22 | 1:TA:365:ARG:HH22 | 1.58                     | 0.51              |
| 1:VA:185:TYR:HB3  | 1:VA:314:MET:SD   | 2.50                     | 0.51              |
| 1:G:413:ARG:HB3   | 1:G:421:TRP:HB3   | 1.93                     | 0.51              |
| 1:M:281:SER:OG    | 3:M:1102:HOH:O    | 2.19                     | 0.51              |
| 1:BA:129:GLU:HG3  | 1:BA:142:ARG:HB2  | 1.92                     | 0.51              |
| 1:FA:420:LEU:HD22 | 1:HA:227:ILE:HA   | 1.91                     | 0.51              |
| 1:NA:135:LEU:HD21 | 1:NA:460:LEU:HD13 | 1.93                     | 0.51              |
| 1:PA:413:ARG:HB3  | 1:PA:421:TRP:HB3  | 1.93                     | 0.51              |
| 1:RA:341:GLN:HE22 | 1:RA:365:ARG:HH22 | 1.58                     | 0.51              |
| 1:E:341:GLN:OE1   | 1:E:365:ARG:NH2   | 2.44                     | 0.51              |
| 1:E:413:ARG:HB3   | 1:E:421:TRP:HB3   | 1.93                     | 0.51              |
| 1:G:438:GLN:NE2   | 1:I:244:GLY:O     | 2.44                     | 0.51              |
| 1:I:135:LEU:HD21  | 1:I:460:LEU:HD13  | 1.93                     | 0.51              |
| 1:O:425:LYS:HB3   | 1:Q:220:GLY:HA2   | 1.93                     | 0.51              |
| 1:S:95:ASN:O      | 1:S:99:LYS:HG2    | 2.11                     | 0.51              |
| 1:Z:152:ASP:OD1   | 1:Z:285:TYR:OH    | 2.25                     | 0.51              |
| 1:Z:438:GLN:OE1   | 1:BA:198:ASN:ND2  | 2.37                     | 0.51              |
| 1:FA:95:ASN:O     | 1:FA:99:LYS:HG2   | 2.11                     | 0.51              |
| 1:PA:341:GLN:OE1  | 1:PA:365:ARG:NH2  | 2.44                     | 0.51              |
| 1:RA:413:ARG:HB3  | 1:RA:421:TRP:HB3  | 1.93                     | 0.51              |
| 1:C:341:GLN:HE22  | 1:C:365:ARG:HH22  | 1.58                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:464:LEU:O     | 1:C:468:ILE:HG12  | 2.09                     | 0.51              |
| 1:K:420:LEU:HD22  | 1:M:227:ILE:HA    | 1.93                     | 0.51              |
| 1:M:438:GLN:OE1   | 1:O:198:ASN:ND2   | 2.37                     | 0.51              |
| 1:O:129:GLU:HG3   | 1:O:142:ARG:HB2   | 1.92                     | 0.51              |
| 1:X:152:ASP:OD1   | 1:X:285:TYR:OH    | 2.25                     | 0.51              |
| 1:Z:413:ARG:HB3   | 1:Z:421:TRP:HB3   | 1.93                     | 0.51              |
| 1:LA:438:GLN:OE1  | 1:NA:198:ASN:ND2  | 2.37                     | 0.51              |
| 1:RA:438:GLN:NE2  | 1:TA:244:GLY:O    | 2.44                     | 0.51              |
| 1:G:341:GLN:HE22  | 1:G:365:ARG:HH22  | 1.59                     | 0.50              |
| 1:BA:425:LYS:HB3  | 1:DA:220:GLY:HA2  | 1.93                     | 0.50              |
| 1:JA:152:ASP:OD1  | 1:JA:285:TYR:OH   | 2.25                     | 0.50              |
| 1:NA:341:GLN:HE22 | 1:NA:365:ARG:HH22 | 1.58                     | 0.50              |
| 1:C:425:LYS:HB3   | 1:E:220:GLY:HA2   | 1.93                     | 0.50              |
| 1:K:185:TYR:HB3   | 1:K:314:MET:SD    | 2.50                     | 0.50              |
| 1:A:95:ASN:O      | 1:A:99:LYS:HG2    | 2.11                     | 0.50              |
| 1:Q:341:GLN:OE1   | 1:Q:365:ARG:NH2   | 2.44                     | 0.50              |
| 1:DA:341:GLN:OE1  | 1:DA:365:ARG:NH2  | 2.44                     | 0.50              |
| 1:A:438:GLN:OE1   | 1:C:198:ASN:ND2   | 2.37                     | 0.50              |
| 1:C:117:GLY:HA2   | 1:C:120:GLN:HG2   | 1.94                     | 0.50              |
| 1:K:341:GLN:OE1   | 1:K:365:ARG:NH2   | 2.44                     | 0.50              |
| 1:Z:281:SER:OG    | 3:Z:1102:HOH:O    | 2.19                     | 0.50              |
| 1:HA:117:GLY:HA2  | 1:HA:120:GLN:HG2  | 1.94                     | 0.50              |
| 1:LA:95:ASN:O     | 1:LA:99:LYS:HG2   | 2.11                     | 0.50              |
| 1:V:117:GLY:HA2   | 1:V:120:GLN:HG2   | 1.94                     | 0.50              |
| 1:DA:420:LEU:HD22 | 1:FA:227:ILE:HA   | 1.92                     | 0.50              |
| 1:NA:117:GLY:HA2  | 1:NA:120:GLN:HG2  | 1.94                     | 0.50              |
| 1:I:425:LYS:HB3   | 1:K:220:GLY:HA2   | 1.92                     | 0.50              |
| 1:S:281:SER:OG    | 3:S:1102:HOH:O    | 2.19                     | 0.50              |
| 1:JA:116:ILE:HG23 | 1:JA:472:LEU:HD13 | 1.93                     | 0.50              |
| 1:Q:420:LEU:HD22  | 1:S:227:ILE:HA    | 1.92                     | 0.50              |
| 1:V:425:LYS:HB3   | 1:X:220:GLY:HA2   | 1.93                     | 0.50              |
| 1:TA:182:PRO:HB3  | 1:TA:331:CYS:SG   | 2.52                     | 0.50              |
| 1:VA:341:GLN:OE1  | 1:VA:365:ARG:NH2  | 2.44                     | 0.50              |
| 1:I:182:PRO:HB3   | 1:I:331:CYS:SG    | 2.52                     | 0.50              |
| 1:Z:95:ASN:O      | 1:Z:99:LYS:HG2    | 2.11                     | 0.50              |
| 1:PA:420:LEU:HD22 | 1:RA:227:ILE:HA   | 1.92                     | 0.50              |
| 1:A:460:LEU:HD21  | 1:A:465:ARG:HB2   | 1.94                     | 0.49              |
| 1:M:95:ASN:O      | 1:M:99:LYS:HG2    | 2.11                     | 0.49              |
| 1:O:182:PRO:HB3   | 1:O:331:CYS:SG    | 2.52                     | 0.49              |
| 1:S:438:GLN:NE2   | 1:V:244:GLY:O     | 2.44                     | 0.49              |
| 1:BA:182:PRO:HB3  | 1:BA:331:CYS:SG   | 2.52                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:438:GLN:NE2  | 1:HA:244:GLY:O    | 2.44                     | 0.49              |
| 1:NA:182:PRO:HB3  | 1:NA:331:CYS:SG   | 2.52                     | 0.49              |
| 1:O:341:GLN:NE2   | 1:O:365:ARG:HH22  | 2.10                     | 0.49              |
| 1:LA:460:LEU:HD21 | 1:LA:465:ARG:HB2  | 1.94                     | 0.49              |
| 1:RA:460:LEU:HD21 | 1:RA:465:ARG:HB2  | 1.94                     | 0.49              |
| 1:A:227:ILE:HA    | 1:X:420:LEU:HD22  | 1.93                     | 0.49              |
| 1:S:460:LEU:HD21  | 1:S:465:ARG:HB2   | 1.94                     | 0.49              |
| 1:BA:341:GLN:NE2  | 1:BA:365:ARG:HH22 | 2.10                     | 0.49              |
| 1:HA:425:LYS:HB3  | 1:JA:220:GLY:HA2  | 1.93                     | 0.49              |
| 1:TA:425:LYS:HB3  | 1:VA:220:GLY:HA2  | 1.93                     | 0.49              |
| 1:C:182:PRO:HB3   | 1:C:331:CYS:SG    | 2.52                     | 0.49              |
| 1:RA:332:THR:HB   | 1:RA:383:MET:HE2  | 1.95                     | 0.49              |
| 1:C:301:THR:HG22  | 1:C:303:TYR:HD2   | 1.78                     | 0.49              |
| 1:G:332:THR:HB    | 1:G:383:MET:HE2   | 1.95                     | 0.49              |
| 1:M:460:LEU:HD21  | 1:M:465:ARG:HB2   | 1.94                     | 0.49              |
| 1:Z:460:LEU:HD21  | 1:Z:465:ARG:HB2   | 1.94                     | 0.49              |
| 1:HA:182:PRO:HB3  | 1:HA:331:CYS:SG   | 2.52                     | 0.49              |
| 1:JA:420:LEU:HD22 | 1:LA:227:ILE:HA   | 1.93                     | 0.49              |
| 1:LA:332:THR:HB   | 1:LA:383:MET:HE2  | 1.95                     | 0.49              |
| 1:NA:192:TYR:HB2  | 1:NA:197:THR:HB   | 1.95                     | 0.49              |
| 1:NA:301:THR:HG22 | 1:NA:303:TYR:HD2  | 1.78                     | 0.49              |
| 1:RA:438:GLN:OE1  | 1:TA:198:ASN:ND2  | 2.37                     | 0.49              |
| 1:A:332:THR:HB    | 1:A:383:MET:HE2   | 1.95                     | 0.49              |
| 1:G:438:GLN:OE1   | 1:I:198:ASN:ND2   | 2.37                     | 0.49              |
| 1:I:341:GLN:NE2   | 1:I:365:ARG:HH22  | 2.10                     | 0.49              |
| 1:V:341:GLN:NE2   | 1:V:365:ARG:HH22  | 2.10                     | 0.49              |
| 1:PA:130:THR:OG1  | 1:PA:133:PHE:O    | 2.18                     | 0.49              |
| 1:RA:95:ASN:O     | 1:RA:99:LYS:HG2   | 2.11                     | 0.49              |
| 1:G:95:ASN:O      | 1:G:99:LYS:HG2    | 2.11                     | 0.49              |
| 1:K:421:TRP:CD1   | 1:M:229:ARG:HB3   | 2.48                     | 0.49              |
| 1:HA:341:GLN:NE2  | 1:HA:365:ARG:HH22 | 2.10                     | 0.49              |
| 1:TA:341:GLN:NE2  | 1:TA:365:ARG:HH22 | 2.10                     | 0.49              |
| 1:VA:182:PRO:HB3  | 1:VA:331:CYS:SG   | 2.53                     | 0.49              |
| 1:A:229:ARG:HB3   | 1:X:421:TRP:CD1   | 2.48                     | 0.49              |
| 1:C:192:TYR:HB2   | 1:C:197:THR:HB    | 1.95                     | 0.49              |
| 1:O:195:TYR:OH    | 1:O:282:CYS:O     | 2.29                     | 0.49              |
| 1:V:182:PRO:HB3   | 1:V:331:CYS:SG    | 2.52                     | 0.49              |
| 1:DA:182:PRO:HB3  | 1:DA:331:CYS:SG   | 2.53                     | 0.49              |
| 1:DA:421:TRP:CD1  | 1:FA:229:ARG:HB3  | 2.48                     | 0.49              |
| 1:FA:281:SER:OG   | 3:FA:1102:HOH:O   | 2.19                     | 0.49              |
| 1:G:460:LEU:HD21  | 1:G:465:ARG:HB2   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:K:182:PRO:HB3   | 1:K:331:CYS:SG     | 2.53                     | 0.49              |
| 1:Q:421:TRP:CD1   | 1:S:229:ARG:HB3    | 2.48                     | 0.49              |
| 1:Z:229:ARG:HB3   | 1:VA:421:TRP:CD1   | 2.48                     | 0.49              |
| 1:BA:195:TYR:OH   | 1:BA:282:CYS:O     | 2.28                     | 0.49              |
| 1:FA:332:THR:HB   | 1:FA:383:MET:HE2   | 1.95                     | 0.49              |
| 1:FA:460:LEU:HD21 | 1:FA:465:ARG:HB2   | 1.95                     | 0.49              |
| 1:JA:421:TRP:CD1  | 1:LA:229:ARG:HB3   | 2.48                     | 0.49              |
| 1:RA:63:ASP:HB2   | 1:RA:80:CYS:HA     | 1.95                     | 0.49              |
| 1:RA:341:GLN:NE2  | 1:RA:365:ARG:HH22  | 2.10                     | 0.49              |
| 1:A:192:TYR:HB2   | 1:A:197:THR:HB     | 1.95                     | 0.49              |
| 1:E:130:THR:OG1   | 1:E:133:PHE:O      | 2.18                     | 0.49              |
| 1:E:420:LEU:HD22  | 1:G:227:ILE:HA     | 1.93                     | 0.49              |
| 1:E:421:TRP:CD1   | 1:G:229:ARG:HB3    | 2.48                     | 0.49              |
| 1:Q:182:PRO:HB3   | 1:Q:331:CYS:SG     | 2.53                     | 0.49              |
| 1:S:332:THR:HB    | 1:S:383:MET:HE2    | 1.95                     | 0.49              |
| 1:Z:341:GLN:NE2   | 1:Z:365:ARG:HH22   | 2.11                     | 0.49              |
| 1:LA:192:TYR:HB2  | 1:LA:197:THR:HB    | 1.95                     | 0.49              |
| 1:G:63:ASP:HB2    | 1:G:80:CYS:HA      | 1.95                     | 0.48              |
| 1:G:341:GLN:NE2   | 1:G:365:ARG:HH22   | 2.11                     | 0.48              |
| 1:K:438:GLN:NE2   | 1:M:244:GLY:O      | 2.46                     | 0.48              |
| 1:M:341:GLN:NE2   | 1:M:365:ARG:HH22   | 2.11                     | 0.48              |
| 1:O:117:GLY:HA2   | 1:O:120:GLN:HG2    | 1.93                     | 0.48              |
| 1:Z:244:GLY:O     | 1:VA:438:GLN:NE2   | 2.46                     | 0.48              |
| 1:FA:341:GLN:NE2  | 1:FA:365:ARG:HH22  | 2.11                     | 0.48              |
| 1:LA:438:GLN:NE2  | 1:NA:244:GLY:O     | 2.44                     | 0.48              |
| 1:TA:117:GLY:HA2  | 1:TA:120:GLN:HG2   | 1.94                     | 0.48              |
| 1:C:44:SER:HB3    | 1:C:151:GLN:HE21   | 1.79                     | 0.48              |
| 1:I:117:GLY:HA2   | 1:I:120:GLN:HG2    | 1.94                     | 0.48              |
| 1:S:192:TYR:HB2   | 1:S:197:THR:HB     | 1.95                     | 0.48              |
| 1:S:341:GLN:NE2   | 1:S:365:ARG:HH22   | 2.11                     | 0.48              |
| 1:V:192:TYR:HB2   | 1:V:197:THR:HB     | 1.95                     | 0.48              |
| 1:V:301:THR:HG22  | 1:V:303:TYR:HD2    | 1.78                     | 0.48              |
| 1:FA:41[B]:ARG:HA | 1:FA:41[B]:ARG:HD2 | 1.71                     | 0.48              |
| 1:HA:192:TYR:HB2  | 1:HA:197:THR:HB    | 1.95                     | 0.48              |
| 1:HA:301:THR:HG22 | 1:HA:303:TYR:HD2   | 1.78                     | 0.48              |
| 1:NA:44:SER:HB3   | 1:NA:151:GLN:HE21  | 1.79                     | 0.48              |
| 1:NA:341:GLN:NE2  | 1:NA:365:ARG:HH22  | 2.10                     | 0.48              |
| 1:PA:421:TRP:CD1  | 1:RA:229:ARG:HB3   | 2.48                     | 0.48              |
| 1:A:438:GLN:NE2   | 1:C:244:GLY:O      | 2.44                     | 0.48              |
| 1:C:341:GLN:NE2   | 1:C:365:ARG:HH22   | 2.10                     | 0.48              |
| 1:M:449:SER:O     | 1:M:449:SER:OG     | 2.32                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:O:192:TYR:HB2   | 1:O:197:THR:HB     | 1.95                     | 0.48              |
| 1:X:182:PRO:HB3   | 1:X:331:CYS:SG     | 2.53                     | 0.48              |
| 1:PA:41[B]:ARG:HA | 1:PA:41[B]:ARG:HD2 | 1.68                     | 0.48              |
| 1:E:182:PRO:HB3   | 1:E:331:CYS:SG     | 2.53                     | 0.48              |
| 1:I:185:TYR:HB3   | 1:I:314:MET:SD     | 2.53                     | 0.48              |
| 1:I:301:THR:HG22  | 1:I:303:TYR:HD2    | 1.78                     | 0.48              |
| 1:M:438:GLN:NE2   | 1:O:244:GLY:O      | 2.44                     | 0.48              |
| 1:Q:345:ILE:HG21  | 1:Q:358:LEU:HD13   | 1.96                     | 0.48              |
| 1:S:63:ASP:HB2    | 1:S:80:CYS:HA      | 1.95                     | 0.48              |
| 1:Z:438:GLN:NE2   | 1:BA:244:GLY:O     | 2.44                     | 0.48              |
| 1:Z:449:SER:O     | 1:Z:449:SER:OG     | 2.32                     | 0.48              |
| 1:BA:192:TYR:HB2  | 1:BA:197:THR:HB    | 1.95                     | 0.48              |
| 1:FA:192:TYR:HB2  | 1:FA:197:THR:HB    | 1.96                     | 0.48              |
| 1:HA:44:SER:HB3   | 1:HA:151:GLN:HE21  | 1.79                     | 0.48              |
| 1:JA:182:PRO:HB3  | 1:JA:331:CYS:SG    | 2.53                     | 0.48              |
| 1:A:303:TYR:HB3   | 1:A:440:ILE:HD11   | 1.96                     | 0.48              |
| 1:V:3:PRO:HA      | 1:V:26:GLU:HB2     | 1.96                     | 0.48              |
| 1:V:44:SER:HB3    | 1:V:151:GLN:HE21   | 1.79                     | 0.48              |
| 1:BA:44:SER:HB3   | 1:BA:151:GLN:HE21  | 1.79                     | 0.48              |
| 1:BA:117:GLY:HA2  | 1:BA:120:GLN:HG2   | 1.94                     | 0.48              |
| 1:DA:345:ILE:HG21 | 1:DA:358:LEU:HD13  | 1.96                     | 0.48              |
| 1:FA:63:ASP:HB2   | 1:FA:80:CYS:HA     | 1.95                     | 0.48              |
| 1:HA:3:PRO:HA     | 1:HA:26:GLU:HB2    | 1.96                     | 0.48              |
| 1:PA:182:PRO:HB3  | 1:PA:331:CYS:SG    | 2.53                     | 0.48              |
| 1:TA:301:THR:HG22 | 1:TA:303:TYR:HD2   | 1.78                     | 0.48              |
| 1:VA:345:ILE:HG21 | 1:VA:358:LEU:HD13  | 1.95                     | 0.48              |
| 1:I:44:SER:HB3    | 1:I:151:GLN:HE21   | 1.79                     | 0.48              |
| 1:K:345:ILE:HG21  | 1:K:358:LEU:HD13   | 1.96                     | 0.48              |
| 1:O:3:PRO:HA      | 1:O:26:GLU:HB2     | 1.96                     | 0.48              |
| 1:O:44:SER:HB3    | 1:O:151:GLN:HE21   | 1.79                     | 0.48              |
| 1:O:301:THR:HG22  | 1:O:303:TYR:HD2    | 1.78                     | 0.48              |
| 1:S:41[B]:ARG:HA  | 1:S:41[B]:ARG:HD2  | 1.71                     | 0.48              |
| 1:Z:332:THR:HB    | 1:Z:383:MET:HE2    | 1.95                     | 0.48              |
| 1:BA:185:TYR:HB3  | 1:BA:314:MET:SD    | 2.53                     | 0.48              |
| 1:HA:185:TYR:HB3  | 1:HA:314:MET:SD    | 2.53                     | 0.48              |
| 1:LA:341:GLN:NE2  | 1:LA:365:ARG:HH22  | 2.11                     | 0.48              |
| 1:PA:345:ILE:HG21 | 1:PA:358:LEU:HD13  | 1.96                     | 0.48              |
| 1:E:345:ILE:HG21  | 1:E:358:LEU:HD13   | 1.96                     | 0.48              |
| 1:O:185:TYR:HB3   | 1:O:314:MET:SD     | 2.53                     | 0.48              |
| 1:V:185:TYR:HB3   | 1:V:314:MET:SD     | 2.53                     | 0.48              |
| 1:X:345:ILE:HG21  | 1:X:358:LEU:HD13   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BA:301:THR:HG22 | 1:BA:303:TYR:HD2  | 1.78                     | 0.48              |
| 1:PA:438:GLN:OE1  | 1:RA:198:ASN:ND2  | 2.37                     | 0.48              |
| 1:TA:44:SER:HB3   | 1:TA:151:GLN:HE21 | 1.79                     | 0.48              |
| 1:E:41[B]:ARG:HA  | 1:E:41[B]:ARG:HD2 | 1.68                     | 0.48              |
| 1:JA:345:ILE:HG21 | 1:JA:358:LEU:HD13 | 1.96                     | 0.48              |
| 1:RA:192:TYR:HB2  | 1:RA:197:THR:HB   | 1.95                     | 0.48              |
| 1:TA:185:TYR:HB3  | 1:TA:314:MET:SD   | 2.54                     | 0.48              |
| 1:A:63:ASP:HB2    | 1:A:80:CYS:HA     | 1.95                     | 0.48              |
| 1:A:341:GLN:NE2   | 1:A:365:ARG:HH22  | 2.11                     | 0.48              |
| 1:C:185:TYR:HB3   | 1:C:314:MET:SD    | 2.53                     | 0.48              |
| 1:C:275:ARG:HD2   | 1:E:88:GLU:HG3    | 1.96                     | 0.48              |
| 1:M:332:THR:HB    | 1:M:383:MET:HE2   | 1.95                     | 0.48              |
| 1:LA:63:ASP:HB2   | 1:LA:80:CYS:HA    | 1.95                     | 0.48              |
| 1:TA:192:TYR:HB2  | 1:TA:197:THR:HB   | 1.95                     | 0.48              |
| 1:TA:438:GLN:OE1  | 1:VA:198:ASN:ND2  | 2.39                     | 0.48              |
| 1:C:3:PRO:HA      | 1:C:26:GLU:HB2    | 1.96                     | 0.48              |
| 1:E:438:GLN:OE1   | 1:G:198:ASN:ND2   | 2.37                     | 0.48              |
| 1:G:192:TYR:HB2   | 1:G:197:THR:HB    | 1.95                     | 0.48              |
| 1:M:192:TYR:HB2   | 1:M:197:THR:HB    | 1.95                     | 0.48              |
| 1:BA:3:PRO:HA     | 1:BA:26:GLU:HB2   | 1.96                     | 0.48              |
| 1:HA:275:ARG:HD2  | 1:JA:88:GLU:HG3   | 1.96                     | 0.48              |
| 1:NA:185:TYR:HB3  | 1:NA:314:MET:SD   | 2.53                     | 0.48              |
| 1:NA:275:ARG:HD2  | 1:PA:88:GLU:HG3   | 1.96                     | 0.48              |
| 1:RA:464:LEU:O    | 1:RA:468:ILE:HG12 | 2.14                     | 0.48              |
| 1:A:244:GLY:O     | 1:X:438:GLN:NE2   | 2.46                     | 0.47              |
| 1:I:192:TYR:HB2   | 1:I:197:THR:HB    | 1.95                     | 0.47              |
| 1:V:275:ARG:HD2   | 1:X:88:GLU:HG3    | 1.96                     | 0.47              |
| 1:Z:63:ASP:HB2    | 1:Z:80:CYS:HA     | 1.95                     | 0.47              |
| 1:NA:3:PRO:HA     | 1:NA:26:GLU:HB2   | 1.95                     | 0.47              |
| 1:Q:438:GLN:NE2   | 1:S:244:GLY:O     | 2.46                     | 0.47              |
| 1:Z:192:TYR:HB2   | 1:Z:197:THR:HB    | 1.96                     | 0.47              |
| 1:VA:116:ILE:HG23 | 1:VA:472:LEU:HD13 | 1.96                     | 0.47              |
| 1:M:63:ASP:HB2    | 1:M:80:CYS:HA     | 1.95                     | 0.47              |
| 1:FA:265:HIS:CD2  | 1:FA:296:LEU:HD22 | 2.49                     | 0.47              |
| 1:FA:434:ARG:O    | 1:FA:437:THR:OG1  | 2.32                     | 0.47              |
| 1:A:265:HIS:CD2   | 1:A:296:LEU:HD22  | 2.49                     | 0.47              |
| 1:S:265:HIS:CD2   | 1:S:296:LEU:HD22  | 2.49                     | 0.47              |
| 1:RA:265:HIS:CD2  | 1:RA:296:LEU:HD22 | 2.49                     | 0.47              |
| 1:E:237:ASP:OD2   | 1:E:251:SER:HB2   | 2.15                     | 0.47              |
| 1:G:265:HIS:CD2   | 1:G:296:LEU:HD22  | 2.49                     | 0.47              |
| 1:K:237:ASP:OD2   | 1:K:251:SER:HB2   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:O:438:GLN:OE1  | 1:Q:198:ASN:ND2   | 2.38                     | 0.47              |
| 1:S:303:TYR:HB3  | 1:S:440:ILE:HD11  | 1.97                     | 0.47              |
| 1:HA:337:THR:O   | 1:HA:341:GLN:HG3  | 2.15                     | 0.47              |
| 1:JA:438:GLN:NE2 | 1:LA:244:GLY:O    | 2.46                     | 0.47              |
| 1:LA:265:HIS:CD2 | 1:LA:296:LEU:HD22 | 2.49                     | 0.47              |
| 1:VA:237:ASP:OD2 | 1:VA:251:SER:HB2  | 2.15                     | 0.47              |
| 1:M:267:LYS:HZ1  | 1:M:446:GLU:HB3   | 1.79                     | 0.47              |
| 1:Q:337:THR:O    | 1:Q:341:GLN:HG3   | 2.15                     | 0.47              |
| 1:V:337:THR:O    | 1:V:341:GLN:HG3   | 2.15                     | 0.47              |
| 1:BA:337:THR:O   | 1:BA:341:GLN:HG3  | 2.15                     | 0.47              |
| 1:DA:8:ILE:HD11  | 1:DA:15:LEU:HD13  | 1.97                     | 0.47              |
| 1:DA:337:THR:O   | 1:DA:341:GLN:HG3  | 2.15                     | 0.47              |
| 1:DA:438:GLN:NE2 | 1:FA:244:GLY:O    | 2.46                     | 0.47              |
| 1:FA:303:TYR:HB3 | 1:FA:440:ILE:HD11 | 1.97                     | 0.47              |
| 1:PA:237:ASP:OD2 | 1:PA:251:SER:HB2  | 2.15                     | 0.47              |
| 1:I:3:PRO:HA     | 1:I:26:GLU:HB2    | 1.95                     | 0.47              |
| 1:I:195:TYR:OH   | 1:I:282:CYS:O     | 2.28                     | 0.47              |
| 1:M:195:TYR:OH   | 1:M:282:CYS:O     | 2.31                     | 0.47              |
| 1:O:275:ARG:HD2  | 1:Q:88:GLU:HG3    | 1.96                     | 0.47              |
| 1:S:341:GLN:OE1  | 1:S:365:ARG:NH2   | 2.48                     | 0.47              |
| 1:X:8:ILE:HD11   | 1:X:15:LEU:HD13   | 1.97                     | 0.47              |
| 1:Z:88:GLU:OE2   | 1:VA:275:ARG:NH2  | 2.48                     | 0.47              |
| 1:BA:275:ARG:HD2 | 1:DA:88:GLU:HG3   | 1.96                     | 0.47              |
| 1:DA:275:ARG:NH2 | 1:FA:88:GLU:OE2   | 2.48                     | 0.47              |
| 1:FA:341:GLN:OE1 | 1:FA:365:ARG:NH2  | 2.48                     | 0.47              |
| 1:JA:8:ILE:HD11  | 1:JA:15:LEU:HD13  | 1.97                     | 0.47              |
| 1:JA:129:GLU:HG3 | 1:JA:142:ARG:HB2  | 1.97                     | 0.47              |
| 1:TA:195:TYR:OH  | 1:TA:282:CYS:O    | 2.28                     | 0.47              |
| 1:K:275:ARG:NH2  | 1:M:88:GLU:OE2    | 2.48                     | 0.47              |
| 1:O:337:THR:O    | 1:O:341:GLN:HG3   | 2.15                     | 0.47              |
| 1:X:129:GLU:HG3  | 1:X:142:ARG:HB2   | 1.97                     | 0.47              |
| 1:TA:3:PRO:HA    | 1:TA:26:GLU:HB2   | 1.95                     | 0.47              |
| 1:A:341:GLN:OE1  | 1:A:365:ARG:NH2   | 2.48                     | 0.47              |
| 1:Q:8:ILE:HD11   | 1:Q:15:LEU:HD13   | 1.97                     | 0.47              |
| 1:LA:341:GLN:OE1 | 1:LA:365:ARG:NH2  | 2.48                     | 0.47              |
| 1:PA:8:ILE:HD11  | 1:PA:15:LEU:HD13  | 1.97                     | 0.47              |
| 1:E:8:ILE:HD11   | 1:E:15:LEU:HD13   | 1.97                     | 0.47              |
| 1:K:337:THR:O    | 1:K:341:GLN:HG3   | 2.15                     | 0.47              |
| 1:M:341:GLN:OE1  | 1:M:365:ARG:NH2   | 2.48                     | 0.47              |
| 1:Q:275:ARG:NH2  | 1:S:88:GLU:OE2    | 2.48                     | 0.47              |
| 1:Z:195:TYR:OH   | 1:Z:282:CYS:O     | 2.31                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:Z:341:GLN:OE1    | 1:Z:365:ARG:NH2   | 2.48                     | 0.47              |
| 1:VA:337:THR:O     | 1:VA:341:GLN:HG3  | 2.15                     | 0.47              |
| 1:I:61:ILE:HD13    | 1:I:76:ARG:HB3    | 1.98                     | 0.46              |
| 1:O:117:GLY:HA2    | 1:O:120:GLN:HE21  | 1.80                     | 0.46              |
| 1:S:44:SER:HB3     | 1:S:151:GLN:NE2   | 2.30                     | 0.46              |
| 1:Z:265:HIS:CD2    | 1:Z:296:LEU:HD22  | 2.49                     | 0.46              |
| 1:Z:303:TYR:HB3    | 1:Z:440:ILE:HD11  | 1.97                     | 0.46              |
| 1:BA:117:GLY:HA2   | 1:BA:120:GLN:HE21 | 1.80                     | 0.46              |
| 1:FA:44:SER:HB3    | 1:FA:151:GLN:NE2  | 2.30                     | 0.46              |
| 1:PA:337:THR:O     | 1:PA:341:GLN:HG3  | 2.15                     | 0.46              |
| 1:C:61:ILE:HD13    | 1:C:76:ARG:HB3    | 1.98                     | 0.46              |
| 1:E:337:THR:O      | 1:E:341:GLN:HG3   | 2.15                     | 0.46              |
| 1:I:146:ASP:HA     | 1:I:170:VAL:HA    | 1.98                     | 0.46              |
| 1:K:129:GLU:HG3    | 1:K:142:ARG:HB2   | 1.97                     | 0.46              |
| 1:Q:116:ILE:HG23   | 1:Q:472:LEU:HD13  | 1.96                     | 0.46              |
| 1:BA:118:ASP:OD1   | 1:BA:130:THR:OG1  | 2.33                     | 0.46              |
| 1:LA:303:TYR:HB3   | 1:LA:440:ILE:HD11 | 1.97                     | 0.46              |
| 1:NA:61:ILE:HD13   | 1:NA:76:ARG:HB3   | 1.98                     | 0.46              |
| 1:TA:61:ILE:HD13   | 1:TA:76:ARG:HB3   | 1.98                     | 0.46              |
| 1:TA:117:GLY:HA2   | 1:TA:120:GLN:HE21 | 1.80                     | 0.46              |
| 1:I:117:GLY:HA2    | 1:I:120:GLN:HE21  | 1.80                     | 0.46              |
| 1:O:118:ASP:OD1    | 1:O:130:THR:OG1   | 2.33                     | 0.46              |
| 1:V:118:ASP:OD1    | 1:V:130:THR:OG1   | 2.33                     | 0.46              |
| 1:V:341:GLN:OE1    | 1:V:365:ARG:NH2   | 2.49                     | 0.46              |
| 1:X:337:THR:O      | 1:X:341:GLN:HG3   | 2.15                     | 0.46              |
| 1:HA:118:ASP:OD1   | 1:HA:130:THR:OG1  | 2.33                     | 0.46              |
| 1:JA:337:THR:O     | 1:JA:341:GLN:HG3  | 2.15                     | 0.46              |
| 1:RA:341:GLN:OE1   | 1:RA:365:ARG:NH2  | 2.48                     | 0.46              |
| 1:TA:146:ASP:HA    | 1:TA:170:VAL:HA   | 1.98                     | 0.46              |
| 1:A:88:GLU:OE2     | 1:X:275:ARG:NH2   | 2.48                     | 0.46              |
| 1:C:138:ASP:OD2    | 1:C:161:SER:OG    | 2.29                     | 0.46              |
| 1:G:281:SER:OG     | 3:G:1102:HOH:O    | 2.19                     | 0.46              |
| 1:G:341:GLN:OE1    | 1:G:365:ARG:NH2   | 2.48                     | 0.46              |
| 1:I:337:THR:O      | 1:I:341:GLN:HG3   | 2.15                     | 0.46              |
| 1:M:232:LYS:CD     | 1:M:234:GLU:HG2   | 2.43                     | 0.46              |
| 1:V:117:GLY:HA2    | 1:V:120:GLN:HE21  | 1.80                     | 0.46              |
| 1:BA:41[B]:ARG:HD2 | 1:BA:41[B]:ARG:HA | 1.71                     | 0.46              |
| 1:BA:332:THR:HB    | 1:BA:383:MET:HE2  | 1.98                     | 0.46              |
| 1:FA:337:THR:O     | 1:FA:341:GLN:HG3  | 2.16                     | 0.46              |
| 1:NA:341:GLN:OE1   | 1:NA:365:ARG:NH2  | 2.49                     | 0.46              |
| 1:PA:438:GLN:NE2   | 1:RA:244:GLY:O    | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:TA:118:ASP:OD1  | 1:TA:130:THR:OG1  | 2.33                     | 0.46              |
| 1:VA:129:GLU:HG3  | 1:VA:142:ARG:HB2  | 1.97                     | 0.46              |
| 1:C:341:GLN:OE1   | 1:C:365:ARG:NH2   | 2.49                     | 0.46              |
| 1:G:41[B]:ARG:HD2 | 1:G:41[B]:ARG:HA  | 1.71                     | 0.46              |
| 1:I:275:ARG:HD2   | 1:K:88:GLU:HG3    | 1.96                     | 0.46              |
| 1:M:303:TYR:HB3   | 1:M:440:ILE:HD11  | 1.97                     | 0.46              |
| 1:S:337:THR:O     | 1:S:341:GLN:HG3   | 2.16                     | 0.46              |
| 1:HA:117:GLY:HA2  | 1:HA:120:GLN:HE21 | 1.80                     | 0.46              |
| 1:HA:146:ASP:HA   | 1:HA:170:VAL:HA   | 1.97                     | 0.46              |
| 1:HA:341:GLN:OE1  | 1:HA:365:ARG:NH2  | 2.49                     | 0.46              |
| 1:JA:275:ARG:NH2  | 1:LA:88:GLU:OE2   | 2.48                     | 0.46              |
| 1:RA:281:SER:OG   | 3:RA:1102:HOH:O   | 2.19                     | 0.46              |
| 1:TA:275:ARG:HD2  | 1:VA:88:GLU:HG3   | 1.96                     | 0.46              |
| 1:C:411:ARG:NH2   | 1:E:233:LEU:HD13  | 2.31                     | 0.46              |
| 1:E:129:GLU:HG3   | 1:E:142:ARG:HB2   | 1.97                     | 0.46              |
| 1:I:118:ASP:OD1   | 1:I:130:THR:OG1   | 2.34                     | 0.46              |
| 1:K:8:ILE:HD11    | 1:K:15:LEU:HD13   | 1.97                     | 0.46              |
| 1:V:146:ASP:HA    | 1:V:170:VAL:HA    | 1.98                     | 0.46              |
| 1:V:411:ARG:NH2   | 1:X:233:LEU:HD13  | 2.31                     | 0.46              |
| 1:DA:192:TYR:HB2  | 1:DA:197:THR:HB   | 1.98                     | 0.46              |
| 1:DA:438:GLN:OE1  | 1:FA:198:ASN:ND2  | 2.37                     | 0.46              |
| 1:HA:411:ARG:NH2  | 1:JA:233:LEU:HD13 | 2.31                     | 0.46              |
| 1:LA:337:THR:O    | 1:LA:341:GLN:HG3  | 2.16                     | 0.46              |
| 1:NA:411:ARG:NH2  | 1:PA:233:LEU:HD13 | 2.31                     | 0.46              |
| 1:PA:129:GLU:HG3  | 1:PA:142:ARG:HB2  | 1.97                     | 0.46              |
| 1:TA:337:THR:O    | 1:TA:341:GLN:HG3  | 2.15                     | 0.46              |
| 1:A:337:THR:O     | 1:A:341:GLN:HG3   | 2.16                     | 0.46              |
| 1:E:438:GLN:NE2   | 1:G:244:GLY:O     | 2.46                     | 0.46              |
| 1:O:332:THR:HB    | 1:O:383:MET:HE2   | 1.98                     | 0.46              |
| 1:Q:232:LYS:CD    | 1:Q:234:GLU:HG2   | 2.46                     | 0.46              |
| 1:S:8:ILE:HD11    | 1:S:15:LEU:HD13   | 1.98                     | 0.46              |
| 1:FA:8:ILE:HD11   | 1:FA:15:LEU:HD13  | 1.98                     | 0.46              |
| 1:LA:8:ILE:HD11   | 1:LA:15:LEU:HD13  | 1.98                     | 0.46              |
| 1:PA:192:TYR:HB2  | 1:PA:197:THR:HB   | 1.98                     | 0.46              |
| 1:RA:8:ILE:HD11   | 1:RA:15:LEU:HD13  | 1.98                     | 0.46              |
| 1:VA:8:ILE:HD11   | 1:VA:15:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:8:ILE:HD11    | 1:A:15:LEU:HD13   | 1.98                     | 0.46              |
| 1:C:337:THR:O     | 1:C:341:GLN:HG3   | 2.15                     | 0.46              |
| 1:O:411:ARG:NH2   | 1:Q:233:LEU:HD13  | 2.31                     | 0.46              |
| 1:X:192:TYR:HB2   | 1:X:197:THR:HB    | 1.98                     | 0.46              |
| 1:Z:232:LYS:CD    | 1:Z:234:GLU:HG2   | 2.43                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:BA:411:ARG:NH2   | 1:DA:233:LEU:HD13 | 2.31                     | 0.46              |
| 1:JA:192:TYR:HB2   | 1:JA:197:THR:HB   | 1.98                     | 0.46              |
| 1:NA:138:ASP:OD2   | 1:NA:161:SER:OG   | 2.29                     | 0.46              |
| 1:TA:332:THR:HB    | 1:TA:383:MET:HE2  | 1.98                     | 0.46              |
| 1:C:146:ASP:HA     | 1:C:170:VAL:HA    | 1.98                     | 0.46              |
| 1:E:192:TYR:HB2    | 1:E:197:THR:HB    | 1.98                     | 0.46              |
| 1:G:8:ILE:HD11     | 1:G:15:LEU:HD13   | 1.98                     | 0.46              |
| 1:G:303:TYR:HB3    | 1:G:440:ILE:HD11  | 1.97                     | 0.46              |
| 1:I:232:LYS:CD     | 1:I:234:GLU:HG2   | 2.43                     | 0.46              |
| 1:I:332:THR:HB     | 1:I:383:MET:HE2   | 1.98                     | 0.46              |
| 1:O:341:GLN:OE1    | 1:O:365:ARG:NH2   | 2.49                     | 0.46              |
| 1:O:421:TRP:CD1    | 1:Q:229:ARG:HB3   | 2.51                     | 0.46              |
| 1:Q:438:GLN:OE1    | 1:S:198:ASN:ND2   | 2.37                     | 0.46              |
| 1:Z:8:ILE:HD11     | 1:Z:15:LEU:HD13   | 1.98                     | 0.46              |
| 1:DA:118:ASP:OD1   | 1:DA:130:THR:OG1  | 2.34                     | 0.46              |
| 1:DA:232:LYS:CD    | 1:DA:234:GLU:HG2  | 2.46                     | 0.46              |
| 1:JA:237:ASP:OD2   | 1:JA:251:SER:HB2  | 2.15                     | 0.46              |
| 1:NA:117:GLY:HA2   | 1:NA:120:GLN:HE21 | 1.80                     | 0.46              |
| 1:RA:303:TYR:HB3   | 1:RA:440:ILE:HD11 | 1.96                     | 0.46              |
| 1:A:182:PRO:HB3    | 1:A:331:CYS:SG    | 2.56                     | 0.46              |
| 1:G:138:ASP:OD2    | 1:G:161:SER:OG    | 2.26                     | 0.46              |
| 1:K:118:ASP:OD1    | 1:K:130:THR:OG1   | 2.34                     | 0.46              |
| 1:O:184:MET:HG3    | 1:O:259:HIS:ND1   | 2.31                     | 0.46              |
| 1:Q:118:ASP:OD1    | 1:Q:130:THR:OG1   | 2.35                     | 0.46              |
| 1:BA:341:GLN:OE1   | 1:BA:365:ARG:NH2  | 2.49                     | 0.46              |
| 1:BA:421:TRP:CD1   | 1:DA:229:ARG:HB3  | 2.51                     | 0.46              |
| 1:NA:146:ASP:HA    | 1:NA:170:VAL:HA   | 1.97                     | 0.46              |
| 1:RA:41[B]:ARG:HD2 | 1:RA:41[B]:ARG:HA | 1.71                     | 0.46              |
| 1:C:301:THR:HG22   | 1:C:303:TYR:CD2   | 2.51                     | 0.45              |
| 1:I:301:THR:HG22   | 1:I:303:TYR:CD2   | 2.51                     | 0.45              |
| 1:M:8:ILE:HD11     | 1:M:15:LEU:HD13   | 1.98                     | 0.45              |
| 1:O:232:LYS:CD     | 1:O:234:GLU:HG2   | 2.43                     | 0.45              |
| 1:Q:192:TYR:HB2    | 1:Q:197:THR:HB    | 1.98                     | 0.45              |
| 1:Q:237:ASP:OD2    | 1:Q:251:SER:HB2   | 2.15                     | 0.45              |
| 1:V:332:THR:HB     | 1:V:383:MET:HE2   | 1.98                     | 0.45              |
| 1:X:237:ASP:OD2    | 1:X:251:SER:HB2   | 2.15                     | 0.45              |
| 1:BA:146:ASP:HA    | 1:BA:170:VAL:HA   | 1.97                     | 0.45              |
| 1:BA:184:MET:HG3   | 1:BA:259:HIS:ND1  | 2.31                     | 0.45              |
| 1:BA:232:LYS:CD    | 1:BA:234:GLU:HG2  | 2.43                     | 0.45              |
| 1:HA:332:THR:HB    | 1:HA:383:MET:HE2  | 1.98                     | 0.45              |
| 1:LA:182:PRO:HB3   | 1:LA:331:CYS:SG   | 2.56                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:NA:337:THR:O    | 1:NA:341:GLN:HG3   | 2.15                     | 0.45              |
| 1:TA:232:LYS:CD   | 1:TA:234:GLU:HG2   | 2.43                     | 0.45              |
| 1:TA:301:THR:HG22 | 1:TA:303:TYR:CD2   | 2.51                     | 0.45              |
| 1:TA:341:GLN:OE1  | 1:TA:365:ARG:NH2   | 2.49                     | 0.45              |
| 1:VA:41[B]:ARG:HA | 1:VA:41[B]:ARG:HD2 | 1.68                     | 0.45              |
| 1:VA:195:TYR:OH   | 1:VA:282:CYS:O     | 2.33                     | 0.45              |
| 1:C:117:GLY:HA2   | 1:C:120:GLN:HE21   | 1.80                     | 0.45              |
| 1:I:421:TRP:CD1   | 1:K:229:ARG:HB3    | 2.51                     | 0.45              |
| 1:M:275:ARG:NH2   | 1:O:88:GLU:OE2     | 2.49                     | 0.45              |
| 1:V:61:ILE:HD13   | 1:V:76:ARG:HB3     | 1.97                     | 0.45              |
| 1:VA:118:ASP:OD1  | 1:VA:130:THR:OG1   | 2.35                     | 0.45              |
| 1:VA:192:TYR:HB2  | 1:VA:197:THR:HB    | 1.98                     | 0.45              |
| 1:E:275:ARG:NH2   | 1:G:88:GLU:OE2     | 2.48                     | 0.45              |
| 1:I:341:GLN:OE1   | 1:I:365:ARG:NH2    | 2.49                     | 0.45              |
| 1:O:146:ASP:HA    | 1:O:170:VAL:HA     | 1.98                     | 0.45              |
| 1:DA:237:ASP:OD2  | 1:DA:251:SER:HB2   | 2.15                     | 0.45              |
| 1:HA:61:ILE:HD13  | 1:HA:76:ARG:HB3    | 1.98                     | 0.45              |
| 1:HA:301:THR:HG22 | 1:HA:303:TYR:CD2   | 2.51                     | 0.45              |
| 1:NA:301:THR:HG22 | 1:NA:303:TYR:CD2   | 2.51                     | 0.45              |
| 1:NA:421:TRP:CD1  | 1:PA:229:ARG:HB3   | 2.51                     | 0.45              |
| 1:RA:337:THR:O    | 1:RA:341:GLN:HG3   | 2.16                     | 0.45              |
| 1:TA:6:VAL:HG23   | 1:TA:8:ILE:HG12    | 1.99                     | 0.45              |
| 1:A:44:SER:HB3    | 1:A:151:GLN:NE2    | 2.30                     | 0.45              |
| 1:C:6:VAL:HG23    | 1:C:8:ILE:HG12     | 1.99                     | 0.45              |
| 1:C:421:TRP:CD1   | 1:E:229:ARG:HB3    | 2.51                     | 0.45              |
| 1:E:232:LYS:CD    | 1:E:234:GLU:HG2    | 2.46                     | 0.45              |
| 1:G:337:THR:O     | 1:G:341:GLN:HG3    | 2.16                     | 0.45              |
| 1:G:411:ARG:NH2   | 1:I:233:LEU:HD13   | 2.32                     | 0.45              |
| 1:I:6:VAL:HG23    | 1:I:8:ILE:HG12     | 1.99                     | 0.45              |
| 1:K:192:TYR:HB2   | 1:K:197:THR:HB     | 1.98                     | 0.45              |
| 1:M:265:HIS:CD2   | 1:M:296:LEU:HD22   | 2.51                     | 0.45              |
| 1:M:337:THR:O     | 1:M:341:GLN:HG3    | 2.16                     | 0.45              |
| 1:V:301:THR:HG22  | 1:V:303:TYR:CD2    | 2.51                     | 0.45              |
| 1:Z:275:ARG:NH2   | 1:BA:88:GLU:OE2    | 2.50                     | 0.45              |
| 1:Z:337:THR:O     | 1:Z:341:GLN:HG3    | 2.16                     | 0.45              |
| 1:BA:61:ILE:HD13  | 1:BA:76:ARG:HB3    | 1.98                     | 0.45              |
| 1:BA:138:ASP:OD2  | 1:BA:161:SER:OG    | 2.29                     | 0.45              |
| 1:HA:6:VAL:HG23   | 1:HA:8:ILE:HG12    | 1.99                     | 0.45              |
| 1:TA:421:TRP:CD1  | 1:VA:229:ARG:HB3   | 2.52                     | 0.45              |
| 1:C:118:ASP:OD1   | 1:C:130:THR:OG1    | 2.33                     | 0.45              |
| 1:G:182:PRO:HB3   | 1:G:331:CYS:SG     | 2.56                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:M:182:PRO:HB3   | 1:M:331:CYS:SG     | 2.56                     | 0.45              |
| 1:O:301:THR:HG22  | 1:O:303:TYR:CD2    | 2.51                     | 0.45              |
| 1:Q:341:GLN:NE2   | 1:Q:365:ARG:HH22   | 2.15                     | 0.45              |
| 1:V:6:VAL:HG23    | 1:V:8:ILE:HG12     | 1.99                     | 0.45              |
| 1:Z:44:SER:HB3    | 1:Z:151:GLN:NE2    | 2.30                     | 0.45              |
| 1:BA:301:THR:HG22 | 1:BA:303:TYR:CD2   | 2.51                     | 0.45              |
| 1:DA:129:GLU:HG3  | 1:DA:142:ARG:HB2   | 1.97                     | 0.45              |
| 1:DA:341:GLN:NE2  | 1:DA:365:ARG:HH22  | 2.15                     | 0.45              |
| 1:FA:182:PRO:HB3  | 1:FA:331:CYS:SG    | 2.56                     | 0.45              |
| 1:FA:275:ARG:NH2  | 1:HA:88:GLU:OE2    | 2.50                     | 0.45              |
| 1:LA:44:SER:HB3   | 1:LA:151:GLN:NE2   | 2.30                     | 0.45              |
| 1:RA:411:ARG:NH2  | 1:TA:233:LEU:HD13  | 2.32                     | 0.45              |
| 1:TA:411:ARG:NH2  | 1:VA:233:LEU:HD13  | 2.31                     | 0.45              |
| 1:I:184:MET:HG3   | 1:I:259:HIS:ND1    | 2.31                     | 0.45              |
| 1:O:61:ILE:HD13   | 1:O:76:ARG:HB3     | 1.98                     | 0.45              |
| 1:S:182:PRO:HB3   | 1:S:331:CYS:SG     | 2.56                     | 0.45              |
| 1:V:421:TRP:CD1   | 1:X:229:ARG:HB3    | 2.51                     | 0.45              |
| 1:Z:182:PRO:HB3   | 1:Z:331:CYS:SG     | 2.57                     | 0.45              |
| 1:Z:198:ASN:ND2   | 1:VA:438:GLN:OE1   | 2.37                     | 0.45              |
| 1:JA:118:ASP:OD1  | 1:JA:130:THR:OG1   | 2.34                     | 0.45              |
| 1:JA:232:LYS:CD   | 1:JA:234:GLU:HG2   | 2.46                     | 0.45              |
| 1:NA:6:VAL:HG23   | 1:NA:8:ILE:HG12    | 1.99                     | 0.45              |
| 1:PA:232:LYS:CD   | 1:PA:234:GLU:HG2   | 2.46                     | 0.45              |
| 1:PA:275:ARG:NH2  | 1:RA:88:GLU:OE2    | 2.48                     | 0.45              |
| 1:RA:138:ASP:OD2  | 1:RA:161:SER:OG    | 2.26                     | 0.45              |
| 1:VA:341:GLN:NE2  | 1:VA:365:ARG:HH22  | 2.15                     | 0.45              |
| 1:C:184:MET:HG3   | 1:C:259:HIS:ND1    | 2.31                     | 0.45              |
| 1:I:411:ARG:NH2   | 1:K:233:LEU:HD13   | 2.31                     | 0.45              |
| 1:K:41[B]:ARG:HA  | 1:K:41[B]:ARG:HD2  | 1.68                     | 0.45              |
| 1:K:195:TYR:OH    | 1:K:282:CYS:O      | 2.33                     | 0.45              |
| 1:M:44:SER:HB3    | 1:M:151:GLN:NE2    | 2.30                     | 0.45              |
| 1:Q:138:ASP:OD1   | 1:Q:138:ASP:N      | 2.49                     | 0.45              |
| 1:S:275:ARG:NH2   | 1:V:88:GLU:OE2     | 2.50                     | 0.45              |
| 1:X:232:LYS:CD    | 1:X:234:GLU:HG2    | 2.46                     | 0.45              |
| 1:DA:138:ASP:OD1  | 1:DA:138:ASP:N     | 2.49                     | 0.45              |
| 1:HA:421:TRP:CD1  | 1:JA:229:ARG:HB3   | 2.51                     | 0.45              |
| 1:JA:41[B]:ARG:HA | 1:JA:41[B]:ARG:HD2 | 1.68                     | 0.45              |
| 1:NA:118:ASP:OD1  | 1:NA:130:THR:OG1   | 2.34                     | 0.45              |
| 1:RA:182:PRO:HB3  | 1:RA:331:CYS:SG    | 2.56                     | 0.45              |
| 1:K:341:GLN:NE2   | 1:K:365:ARG:HH22   | 2.15                     | 0.45              |
| 1:K:438:GLN:OE1   | 1:M:198:ASN:ND2    | 2.37                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:6:VAL:HG23    | 1:O:8:ILE:HG12    | 1.99                     | 0.45              |
| 1:V:281:SER:OG    | 3:V:1102:HOH:O    | 2.15                     | 0.45              |
| 1:DA:341:GLN:HE22 | 1:DA:365:ARG:HH22 | 1.65                     | 0.45              |
| 1:NA:184:MET:HG3  | 1:NA:259:HIS:ND1  | 2.31                     | 0.45              |
| 1:RA:462:ILE:N    | 1:RA:463:PRO:HD2  | 2.32                     | 0.45              |
| 1:TA:184:MET:HG3  | 1:TA:259:HIS:ND1  | 2.31                     | 0.45              |
| 1:C:332:THR:HB    | 1:C:383:MET:HE2   | 1.98                     | 0.45              |
| 1:G:275:ARG:NH2   | 1:I:88:GLU:OE2    | 2.50                     | 0.45              |
| 1:Q:341:GLN:HE22  | 1:Q:365:ARG:HH22  | 1.65                     | 0.45              |
| 1:X:118:ASP:OD1   | 1:X:130:THR:OG1   | 2.34                     | 0.45              |
| 1:BA:6:VAL:HG23   | 1:BA:8:ILE:HG12   | 1.99                     | 0.45              |
| 1:G:195:TYR:OH    | 1:G:282:CYS:O     | 2.31                     | 0.45              |
| 1:G:462:ILE:N     | 1:G:463:PRO:HD2   | 2.33                     | 0.45              |
| 1:Q:129:GLU:HG3   | 1:Q:142:ARG:HB2   | 1.97                     | 0.45              |
| 1:NA:332:THR:HB   | 1:NA:383:MET:HE2  | 1.98                     | 0.45              |
| 1:PA:411:ARG:NH2  | 1:RA:233:LEU:HD13 | 2.32                     | 0.45              |
| 1:RA:275:ARG:NH2  | 1:TA:88:GLU:OE2   | 2.50                     | 0.45              |
| 1:E:118:ASP:OD1   | 1:E:130:THR:OG1   | 2.34                     | 0.44              |
| 1:E:411:ARG:NH2   | 1:G:233:LEU:HD13  | 2.32                     | 0.44              |
| 1:K:411:ARG:NH2   | 1:M:233:LEU:HD13  | 2.32                     | 0.44              |
| 1:M:411:ARG:NH2   | 1:O:233:LEU:HD13  | 2.32                     | 0.44              |
| 1:Z:233:LEU:HD13  | 1:VA:411:ARG:NH2  | 2.32                     | 0.44              |
| 1:BA:8:ILE:HD11   | 1:BA:15:LEU:HD13  | 1.99                     | 0.44              |
| 1:PA:118:ASP:OD1  | 1:PA:130:THR:OG1  | 2.34                     | 0.44              |
| 1:O:8:ILE:HD11    | 1:O:15:LEU:HD13   | 2.00                     | 0.44              |
| 1:S:434:ARG:O     | 1:S:437:THR:OG1   | 2.32                     | 0.44              |
| 1:S:462:ILE:N     | 1:S:463:PRO:HD2   | 2.32                     | 0.44              |
| 1:X:41[B]:ARG:HA  | 1:X:41[B]:ARG:HD2 | 1.68                     | 0.44              |
| 1:X:341:GLN:NE2   | 1:X:365:ARG:HH22  | 2.15                     | 0.44              |
| 1:Z:411:ARG:NH2   | 1:BA:233:LEU:HD13 | 2.32                     | 0.44              |
| 1:Z:462:ILE:N     | 1:Z:463:PRO:HD2   | 2.32                     | 0.44              |
| 1:JA:341:GLN:NE2  | 1:JA:365:ARG:HH22 | 2.15                     | 0.44              |
| 1:JA:438:GLN:OE1  | 1:LA:198:ASN:ND2  | 2.37                     | 0.44              |
| 1:LA:411:ARG:NH2  | 1:NA:233:LEU:HD13 | 2.32                     | 0.44              |
| 1:A:411:ARG:NH2   | 1:C:233:LEU:HD13  | 2.32                     | 0.44              |
| 1:C:8:ILE:HD11    | 1:C:15:LEU:HD13   | 1.99                     | 0.44              |
| 1:G:71:ARG:NH1    | 1:G:151:GLN:OE1   | 2.41                     | 0.44              |
| 1:I:8:ILE:HD11    | 1:I:15:LEU:HD13   | 2.00                     | 0.44              |
| 1:M:462:ILE:N     | 1:M:463:PRO:HD2   | 2.32                     | 0.44              |
| 1:S:411:ARG:NH2   | 1:V:233:LEU:HD13  | 2.32                     | 0.44              |
| 1:V:41[B]:ARG:HA  | 1:V:41[B]:ARG:HD2 | 1.71                     | 0.44              |

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| Atom-1            | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 1:V:184:MET:HG3   | 1:V:259:HIS:ND1      | 2.31                     | 0.44              |
| 1:Z:434:ARG:O     | 1:Z:437:THR:OG1      | 2.32                     | 0.44              |
| 1:DA:201:ASP:HB2  | 1:DA:252:ARG:HH11    | 1.82                     | 0.44              |
| 1:FA:411:ARG:NH2  | 1:HA:233:LEU:HD13    | 2.32                     | 0.44              |
| 1:JA:341:GLN:HE22 | 1:JA:365:ARG:HH22    | 1.65                     | 0.44              |
| 1:RA:195:TYR:OH   | 1:RA:282:CYS:O       | 2.31                     | 0.44              |
| 1:M:201:ASP:HB2   | 1:M:252:ARG:HH11     | 1.83                     | 0.44              |
| 1:S:201:ASP:HB2   | 1:S:252:ARG:HH11     | 1.83                     | 0.44              |
| 1:V:8:ILE:HD11    | 1:V:15:LEU:HD13      | 1.99                     | 0.44              |
| 1:Z:201:ASP:HB2   | 1:Z:252:ARG:HH11     | 1.83                     | 0.44              |
| 1:JA:138:ASP:OD1  | 1:JA:138:ASP:N       | 2.49                     | 0.44              |
| 1:LA:462:ILE:N    | 1:LA:463:PRO:HD2     | 2.32                     | 0.44              |
| 1:NA:8:ILE:HD11   | 1:NA:15:LEU:HD13     | 1.99                     | 0.44              |
| 1:A:462:ILE:N     | 1:A:463:PRO:HD2      | 2.32                     | 0.44              |
| 1:E:402:MET:HE2   | 1:G:389[A]:GLN:HE21  | 1.83                     | 0.44              |
| 1:G:464:LEU:O     | 1:G:468:ILE:HG12     | 2.18                     | 0.44              |
| 1:M:434:ARG:O     | 1:M:437:THR:OG1      | 2.32                     | 0.44              |
| 1:V:43:PHE:CE2    | 1:V:282:CYS:HB3      | 2.53                     | 0.44              |
| 1:X:341:GLN:HE22  | 1:X:365:ARG:HH22     | 1.65                     | 0.44              |
| 1:HA:184:MET:HG3  | 1:HA:259:HIS:ND1     | 2.31                     | 0.44              |
| 1:HA:345:ILE:HG21 | 1:HA:358:LEU:HD13    | 2.00                     | 0.44              |
| 1:NA:345:ILE:HG21 | 1:NA:358:LEU:HD13    | 2.00                     | 0.44              |
| 1:TA:8:ILE:HD11   | 1:TA:15:LEU:HD13     | 2.00                     | 0.44              |
| 1:VA:341:GLN:HE22 | 1:VA:365:ARG:HH22    | 1.65                     | 0.44              |
| 1:C:345:ILE:HG21  | 1:C:358:LEU:HD13     | 2.00                     | 0.44              |
| 1:X:201:ASP:HB2   | 1:X:252:ARG:HH11     | 1.82                     | 0.44              |
| 1:FA:201:ASP:HB2  | 1:FA:252:ARG:HH11    | 1.83                     | 0.44              |
| 1:HA:8:ILE:HD11   | 1:HA:15:LEU:HD13     | 1.99                     | 0.44              |
| 1:HA:281:SER:OG   | 3:HA:1102:HOH:O      | 2.15                     | 0.44              |
| 1:JA:201:ASP:HB2  | 1:JA:252:ARG:HH11    | 1.82                     | 0.44              |
| 1:RA:71:ARG:NH1   | 1:RA:151:GLN:OE1     | 2.41                     | 0.44              |
| 1:A:275:ARG:NH2   | 1:C:88:GLU:OE2       | 2.50                     | 0.44              |
| 1:E:9:ASP:OD1     | 1:E:12:SER:HB2       | 2.18                     | 0.44              |
| 1:Q:201:ASP:HB2   | 1:Q:252:ARG:HH11     | 1.83                     | 0.44              |
| 1:Q:449:SER:O     | 1:Q:449:SER:OG       | 2.30                     | 0.44              |
| 1:V:345:ILE:HG21  | 1:V:358:LEU:HD13     | 2.00                     | 0.44              |
| 1:X:138:ASP:OD1   | 1:X:138:ASP:N        | 2.49                     | 0.44              |
| 1:FA:462:ILE:N    | 1:FA:463:PRO:HD2     | 2.33                     | 0.44              |
| 1:HA:43:PHE:CE2   | 1:HA:282:CYS:HB3     | 2.53                     | 0.44              |
| 1:PA:9:ASP:OD1    | 1:PA:12:SER:HB2      | 2.18                     | 0.44              |
| 1:PA:402:MET:HE2  | 1:RA:389[A]:GLN:HE21 | 1.83                     | 0.44              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:A:198:ASN:ND2     | 1:X:438:GLN:OE1      | 2.37                     | 0.44              |
| 1:K:332:THR:HB      | 1:K:383:MET:HE2      | 2.00                     | 0.44              |
| 1:K:341:GLN:HE22    | 1:K:365:ARG:HH22     | 1.65                     | 0.44              |
| 1:O:138:ASP:OD2     | 1:O:161:SER:OG       | 2.28                     | 0.44              |
| 1:V:117:GLY:HA2     | 1:V:120:GLN:NE2      | 2.33                     | 0.44              |
| 1:JA:402:MET:HE2    | 1:LA:389[A]:GLN:HE21 | 1.83                     | 0.44              |
| 1:JA:411:ARG:NH2    | 1:LA:233:LEU:HD13    | 2.32                     | 0.44              |
| 1:LA:275:ARG:NH2    | 1:NA:88:GLU:OE2      | 2.50                     | 0.44              |
| 1:A:389[A]:GLN:HE21 | 1:X:402:MET:HE2      | 1.83                     | 0.44              |
| 1:G:202:GLU:HA      | 1:G:205:LEU:HG       | 2.00                     | 0.44              |
| 1:I:345:ILE:HG21    | 1:I:358:LEU:HD13     | 2.00                     | 0.44              |
| 1:I:438:GLN:OE1     | 1:K:198:ASN:ND2      | 2.42                     | 0.44              |
| 1:K:402:MET:HE2     | 1:M:389[A]:GLN:HE21  | 1.83                     | 0.44              |
| 1:DA:449:SER:O      | 1:DA:449:SER:OG      | 2.30                     | 0.44              |
| 1:A:233:LEU:HD13    | 1:X:411:ARG:NH2      | 2.32                     | 0.43              |
| 1:E:195:TYR:OH      | 1:E:282:CYS:O        | 2.32                     | 0.43              |
| 1:G:232:LYS:CD      | 1:G:234:GLU:HG2      | 2.43                     | 0.43              |
| 1:M:464:LEU:O       | 1:M:468:ILE:HG12     | 2.18                     | 0.43              |
| 1:O:117:GLY:HA2     | 1:O:120:GLN:NE2      | 2.33                     | 0.43              |
| 1:Z:389[A]:GLN:HE21 | 1:VA:402:MET:HE2     | 1.83                     | 0.43              |
| 1:BA:43:PHE:CE2     | 1:BA:282:CYS:HB3     | 2.53                     | 0.43              |
| 1:BA:117:GLY:HA2    | 1:BA:120:GLN:NE2     | 2.33                     | 0.43              |
| 1:HA:117:GLY:HA2    | 1:HA:120:GLN:NE2     | 2.33                     | 0.43              |
| 1:JA:425:LYS:HG3    | 1:LA:323:GLY:HA3     | 2.00                     | 0.43              |
| 1:RA:202:GLU:HA     | 1:RA:205:LEU:HG      | 2.00                     | 0.43              |
| 1:TA:267:LYS:HE3    | 1:TA:267:LYS:HB2     | 1.76                     | 0.43              |
| 1:TA:345:ILE:HG21   | 1:TA:358:LEU:HD13    | 2.00                     | 0.43              |
| 1:VA:332:THR:HB     | 1:VA:383:MET:HE2     | 2.00                     | 0.43              |
| 1:A:195:TYR:OH      | 1:A:282:CYS:O        | 2.31                     | 0.43              |
| 1:A:323:GLY:HA3     | 1:X:425:LYS:HG3      | 2.00                     | 0.43              |
| 1:E:341:GLN:NE2     | 1:E:365:ARG:HH22     | 2.15                     | 0.43              |
| 1:I:281:SER:OG      | 3:I:1102:HOH:O       | 2.15                     | 0.43              |
| 1:Q:402:MET:HE2     | 1:S:389[A]:GLN:HE21  | 1.83                     | 0.43              |
| 1:S:232:LYS:CD      | 1:S:234:GLU:HG2      | 2.43                     | 0.43              |
| 1:X:9:ASP:OD1       | 1:X:12:SER:HB2       | 2.18                     | 0.43              |
| 1:Z:464:LEU:O       | 1:Z:468:ILE:HG12     | 2.18                     | 0.43              |
| 1:FA:3:PRO:HA       | 1:FA:26:GLU:HB2      | 2.01                     | 0.43              |
| 1:JA:9:ASP:OD1      | 1:JA:12:SER:HB2      | 2.18                     | 0.43              |
| 1:LA:202:GLU:HA     | 1:LA:205:LEU:HG      | 2.00                     | 0.43              |
| 1:PA:341:GLN:NE2    | 1:PA:365:ARG:HH22    | 2.15                     | 0.43              |
| 1:A:3:PRO:HA        | 1:A:26:GLU:HB2       | 2.00                     | 0.43              |

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| Atom-1            | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 1:A:202:GLU:HA    | 1:A:205:LEU:HG       | 2.00                     | 0.43              |
| 1:G:434:ARG:O     | 1:G:437:THR:OG1      | 2.32                     | 0.43              |
| 1:Q:425:LYS:HG3   | 1:S:323:GLY:HA3      | 2.00                     | 0.43              |
| 1:S:3:PRO:HA      | 1:S:26:GLU:HB2       | 2.01                     | 0.43              |
| 1:DA:332:THR:HB   | 1:DA:383:MET:HE2     | 2.00                     | 0.43              |
| 1:DA:402:MET:HE2  | 1:FA:389[A]:GLN:HE21 | 1.83                     | 0.43              |
| 1:RA:232:LYS:CD   | 1:RA:234:GLU:HG2     | 2.43                     | 0.43              |
| 1:I:267:LYS:HE3   | 1:I:267:LYS:HB2      | 1.76                     | 0.43              |
| 1:M:24:MET:SD     | 1:M:24:MET:N         | 2.90                     | 0.43              |
| 1:X:332:THR:HB    | 1:X:383:MET:HE2      | 2.00                     | 0.43              |
| 1:BA:345:ILE:HG21 | 1:BA:358:LEU:HD13    | 2.00                     | 0.43              |
| 1:DA:411:ARG:NH2  | 1:FA:233:LEU:HD13    | 2.32                     | 0.43              |
| 1:DA:425:LYS:HG3  | 1:FA:323:GLY:HA3     | 2.00                     | 0.43              |
| 1:FA:232:LYS:CD   | 1:FA:234:GLU:HG2     | 2.43                     | 0.43              |
| 1:PA:201:ASP:HB2  | 1:PA:252:ARG:HH11    | 1.82                     | 0.43              |
| 1:PA:341:GLN:HE22 | 1:PA:365:ARG:HH22    | 1.65                     | 0.43              |
| 1:VA:184:MET:HG3  | 1:VA:259:HIS:ND1     | 2.34                     | 0.43              |
| 1:E:341:GLN:HE22  | 1:E:365:ARG:HH22     | 1.65                     | 0.43              |
| 1:E:462:ILE:N     | 1:E:463:PRO:HD2      | 2.34                     | 0.43              |
| 1:G:44:SER:HB3    | 1:G:151:GLN:NE2      | 2.30                     | 0.43              |
| 1:I:117:GLY:HA2   | 1:I:120:GLN:NE2      | 2.33                     | 0.43              |
| 1:K:462:ILE:N     | 1:K:463:PRO:HD2      | 2.34                     | 0.43              |
| 1:O:345:ILE:HG21  | 1:O:358:LEU:HD13     | 2.00                     | 0.43              |
| 1:Q:411:ARG:NH2   | 1:S:233:LEU:HD13     | 2.32                     | 0.43              |
| 1:V:146:ASP:OD1   | 1:V:146:ASP:N        | 2.51                     | 0.43              |
| 1:V:303:TYR:HB3   | 1:V:440:ILE:HD11     | 2.01                     | 0.43              |
| 1:X:181:THR:N     | 1:X:182:PRO:HD2      | 2.34                     | 0.43              |
| 1:JA:181:THR:N    | 1:JA:182:PRO:HD2     | 2.34                     | 0.43              |
| 1:LA:3:PRO:HA     | 1:LA:26:GLU:HB2      | 2.01                     | 0.43              |
| 1:LA:195:TYR:OH   | 1:LA:282:CYS:O       | 2.31                     | 0.43              |
| 1:PA:332:THR:HB   | 1:PA:383:MET:HE2     | 2.00                     | 0.43              |
| 1:PA:462:ILE:N    | 1:PA:463:PRO:HD2     | 2.34                     | 0.43              |
| 1:TA:30:ARG:O     | 1:TA:32:VAL:HG13     | 2.19                     | 0.43              |
| 1:TA:117:GLY:HA2  | 1:TA:120:GLN:NE2     | 2.33                     | 0.43              |
| 1:TA:281:SER:OG   | 3:TA:1102:HOH:O      | 2.15                     | 0.43              |
| 1:VA:9:ASP:OD1    | 1:VA:12:SER:HB2      | 2.18                     | 0.43              |
| 1:VA:462:ILE:N    | 1:VA:463:PRO:HD2     | 2.34                     | 0.43              |
| 1:A:201:ASP:HB2   | 1:A:252:ARG:HH11     | 1.83                     | 0.43              |
| 1:A:464:LEU:O     | 1:A:468:ILE:HG12     | 2.18                     | 0.43              |
| 1:E:332:THR:HB    | 1:E:383:MET:HE2      | 2.00                     | 0.43              |
| 1:G:349:GLU:HG3   | 1:G:399[A]:ARG:HG3   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:K:9:ASP:OD1    | 1:K:12:SER:HB2      | 2.18                     | 0.43              |
| 1:K:184:MET:HG3  | 1:K:259:HIS:ND1     | 2.34                     | 0.43              |
| 1:O:30:ARG:O     | 1:O:32:VAL:HG13     | 2.19                     | 0.43              |
| 1:BA:303:TYR:HB3 | 1:BA:440:ILE:HD11   | 2.01                     | 0.43              |
| 1:FA:349:GLU:HG3 | 1:FA:399[A]:ARG:HG3 | 2.01                     | 0.43              |
| 1:HA:146:ASP:OD1 | 1:HA:146:ASP:N      | 2.51                     | 0.43              |
| 1:HA:303:TYR:HB3 | 1:HA:440:ILE:HD11   | 2.01                     | 0.43              |
| 1:JA:332:THR:HB  | 1:JA:383:MET:HE2    | 2.01                     | 0.43              |
| 1:LA:464:LEU:O   | 1:LA:468:ILE:HG12   | 2.18                     | 0.43              |
| 1:RA:44:SER:HB3  | 1:RA:151:GLN:NE2    | 2.30                     | 0.43              |
| 1:RA:349:GLU:HG3 | 1:RA:399[A]:ARG:HG3 | 2.01                     | 0.43              |
| 1:E:181:THR:N    | 1:E:182:PRO:HD2     | 2.34                     | 0.43              |
| 1:E:201:ASP:HB2  | 1:E:252:ARG:HH11    | 1.83                     | 0.43              |
| 1:G:201:ASP:HB2  | 1:G:252:ARG:HH11    | 1.83                     | 0.43              |
| 1:I:30:ARG:O     | 1:I:32:VAL:HG13     | 2.19                     | 0.43              |
| 1:K:232:LYS:CD   | 1:K:234:GLU:HG2     | 2.46                     | 0.43              |
| 1:Q:332:THR:HB   | 1:Q:383:MET:HE2     | 2.01                     | 0.43              |
| 1:S:349:GLU:HG3  | 1:S:399[A]:ARG:HG3  | 2.01                     | 0.43              |
| 1:BA:30:ARG:O    | 1:BA:32:VAL:HG13    | 2.19                     | 0.43              |
| 1:HA:195:TYR:OH  | 1:HA:282:CYS:O      | 2.28                     | 0.43              |
| 1:RA:201:ASP:HB2 | 1:RA:252:ARG:HH11   | 1.83                     | 0.43              |
| 1:RA:434:ARG:O   | 1:RA:437:THR:OG1    | 2.32                     | 0.43              |
| 1:VA:449:SER:O   | 1:VA:449:SER:OG     | 2.30                     | 0.43              |
| 1:E:425:LYS:HG3  | 1:G:323:GLY:HA3     | 2.00                     | 0.43              |
| 1:O:303:TYR:HB3  | 1:O:440:ILE:HD11    | 2.01                     | 0.43              |
| 1:X:462:ILE:N    | 1:X:463:PRO:HD2     | 2.34                     | 0.43              |
| 1:Z:349:GLU:HG3  | 1:Z:399[A]:ARG:HG3  | 2.01                     | 0.43              |
| 1:DA:44:SER:HB3  | 1:DA:151:GLN:NE2    | 2.34                     | 0.43              |
| 1:JA:462:ILE:N   | 1:JA:463:PRO:HD2    | 2.34                     | 0.43              |
| 1:LA:129:GLU:N   | 3:LA:1109:HOH:O     | 2.51                     | 0.43              |
| 1:LA:201:ASP:HB2 | 1:LA:252:ARG:HH11   | 1.83                     | 0.43              |
| 1:LA:349:GLU:HG3 | 1:LA:399[A]:ARG:HG3 | 2.01                     | 0.43              |
| 1:PA:181:THR:N   | 1:PA:182:PRO:HD2    | 2.34                     | 0.43              |
| 1:PA:425:LYS:HG3 | 1:RA:323:GLY:HA3    | 2.00                     | 0.43              |
| 1:A:349:GLU:HG3  | 1:A:399[A]:ARG:HG3  | 2.01                     | 0.43              |
| 1:K:201:ASP:HB2  | 1:K:252:ARG:HH11    | 1.82                     | 0.43              |
| 1:M:129:GLU:N    | 3:M:1108:HOH:O      | 2.51                     | 0.43              |
| 1:X:44:SER:HB3   | 1:X:151:GLN:NE2     | 2.34                     | 0.43              |
| 1:NA:117:GLY:HA2 | 1:NA:120:GLN:NE2    | 2.33                     | 0.43              |
| 1:VA:232:LYS:CD  | 1:VA:234:GLU:HG2    | 2.46                     | 0.43              |
| 1:A:129:GLU:N    | 3:A:1109:HOH:O      | 2.51                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:138:ASP:OD1   | 1:A:138:ASP:N      | 2.52                     | 0.43              |
| 1:I:146:ASP:OD1   | 1:I:146:ASP:N      | 2.51                     | 0.43              |
| 1:M:349:GLU:HG3   | 1:M:399[A]:ARG:HG3 | 2.01                     | 0.43              |
| 1:O:265:HIS:CD2   | 1:O:296:LEU:HD22   | 2.54                     | 0.43              |
| 1:Q:63:ASP:HB2    | 1:Q:80:CYS:HA      | 2.00                     | 0.43              |
| 1:Z:129:GLU:N     | 3:Z:1109:HOH:O     | 2.51                     | 0.43              |
| 1:Z:202:GLU:HA    | 1:Z:205:LEU:HG     | 2.00                     | 0.43              |
| 1:DA:181:THR:N    | 1:DA:182:PRO:HD2   | 2.34                     | 0.43              |
| 1:FA:438:GLN:OE1  | 1:HA:198:ASN:ND2   | 2.37                     | 0.43              |
| 1:FA:464:LEU:O    | 1:FA:468:ILE:HG12  | 2.18                     | 0.43              |
| 1:TA:146:ASP:OD1  | 1:TA:146:ASP:N     | 2.52                     | 0.43              |
| 1:VA:201:ASP:HB2  | 1:VA:252:ARG:HH11  | 1.83                     | 0.43              |
| 1:C:202:GLU:HA    | 1:C:205:LEU:HG     | 2.01                     | 0.42              |
| 1:Q:44:SER:HB3    | 1:Q:151:GLN:NE2    | 2.34                     | 0.42              |
| 1:Q:181:THR:N     | 1:Q:182:PRO:HD2    | 2.34                     | 0.42              |
| 1:Q:184:MET:HG3   | 1:Q:259:HIS:ND1    | 2.34                     | 0.42              |
| 1:Q:462:ILE:N     | 1:Q:463:PRO:HD2    | 2.34                     | 0.42              |
| 1:BA:265:HIS:CD2  | 1:BA:296:LEU:HD22  | 2.54                     | 0.42              |
| 1:BA:267:LYS:HB2  | 1:BA:267:LYS:HE3   | 1.76                     | 0.42              |
| 1:JA:63:ASP:HB2   | 1:JA:80:CYS:HA     | 2.01                     | 0.42              |
| 1:LA:138:ASP:OD1  | 1:LA:138:ASP:N     | 2.52                     | 0.42              |
| 1:NA:41[B]:ARG:HA | 1:NA:41[B]:ARG:HD2 | 1.71                     | 0.42              |
| 1:TA:415:LEU:HD12 | 1:TA:420:LEU:O     | 2.19                     | 0.42              |
| 1:C:117:GLY:HA2   | 1:C:120:GLN:NE2    | 2.33                     | 0.42              |
| 1:C:303:TYR:HB3   | 1:C:440:ILE:HD11   | 2.01                     | 0.42              |
| 1:I:415:LEU:HD12  | 1:I:420:LEU:O      | 2.20                     | 0.42              |
| 1:M:3:PRO:HA      | 1:M:26:GLU:HB2     | 2.01                     | 0.42              |
| 1:Q:9:ASP:OD1     | 1:Q:12:SER:HB2     | 2.18                     | 0.42              |
| 1:Q:263:VAL:HG12  | 1:Q:300:THR:HG22   | 2.02                     | 0.42              |
| 1:S:202:GLU:HA    | 1:S:205:LEU:HG     | 2.01                     | 0.42              |
| 1:Z:3:PRO:HA      | 1:Z:26:GLU:HB2     | 2.01                     | 0.42              |
| 1:BA:146:ASP:N    | 1:BA:146:ASP:OD1   | 2.51                     | 0.42              |
| 1:DA:9:ASP:OD1    | 1:DA:12:SER:HB2    | 2.18                     | 0.42              |
| 1:FA:202:GLU:HA   | 1:FA:205:LEU:HG    | 2.00                     | 0.42              |
| 1:JA:44:SER:HB3   | 1:JA:151:GLN:NE2   | 2.34                     | 0.42              |
| 1:NA:202:GLU:HA   | 1:NA:205:LEU:HG    | 2.01                     | 0.42              |
| 1:NA:415:LEU:HD12 | 1:NA:420:LEU:O     | 2.19                     | 0.42              |
| 1:PA:195:TYR:OH   | 1:PA:282:CYS:O     | 2.33                     | 0.42              |
| 1:RA:305:VAL:HA   | 1:RA:439:SER:O     | 2.19                     | 0.42              |
| 1:A:434:ARG:O     | 1:A:437:THR:OG1    | 2.32                     | 0.42              |
| 1:C:43:PHE:CE2    | 1:C:282:CYS:HB3    | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:415:LEU:HD12  | 1:C:420:LEU:O     | 2.20                     | 0.42              |
| 1:C:438:GLN:OE1   | 1:E:198:ASN:ND2   | 2.38                     | 0.42              |
| 1:C:462:ILE:N     | 1:C:463:PRO:HD2   | 2.35                     | 0.42              |
| 1:I:41[B]:ARG:HD2 | 1:I:41[B]:ARG:HA  | 1.71                     | 0.42              |
| 1:I:202:GLU:HA    | 1:I:205:LEU:HG    | 2.01                     | 0.42              |
| 1:I:462:ILE:N     | 1:I:463:PRO:HD2   | 2.35                     | 0.42              |
| 1:M:202:GLU:HA    | 1:M:205:LEU:HG    | 2.00                     | 0.42              |
| 1:O:146:ASP:N     | 1:O:146:ASP:OD1   | 2.51                     | 0.42              |
| 1:O:267:LYS:HB2   | 1:O:267:LYS:HE3   | 1.76                     | 0.42              |
| 1:S:414:THR:N     | 1:S:422:ALA:O     | 2.43                     | 0.42              |
| 1:S:464:LEU:O     | 1:S:468:ILE:HG12  | 2.18                     | 0.42              |
| 1:V:232:LYS:CD    | 1:V:234:GLU:HG2   | 2.43                     | 0.42              |
| 1:X:63:ASP:HB2    | 1:X:80:CYS:HA     | 2.01                     | 0.42              |
| 1:BA:421:TRP:CE2  | 1:DA:229:ARG:HD2  | 2.55                     | 0.42              |
| 1:DA:184:MET:HG3  | 1:DA:259:HIS:ND1  | 2.34                     | 0.42              |
| 1:DA:263:VAL:HG12 | 1:DA:300:THR:HG22 | 2.02                     | 0.42              |
| 1:NA:462:ILE:N    | 1:NA:463:PRO:HD2  | 2.35                     | 0.42              |
| 1:TA:202:GLU:HA   | 1:TA:205:LEU:HG   | 2.01                     | 0.42              |
| 1:C:41[B]:ARG:HA  | 1:C:41[B]:ARG:HD2 | 1.71                     | 0.42              |
| 1:C:421:TRP:CE2   | 1:E:229:ARG:HD2   | 2.55                     | 0.42              |
| 1:G:3:PRO:HA      | 1:G:26:GLU:HB2    | 2.00                     | 0.42              |
| 1:G:305:VAL:HA    | 1:G:439:SER:O     | 2.19                     | 0.42              |
| 1:O:138:ASP:OD1   | 1:O:138:ASP:N     | 2.53                     | 0.42              |
| 1:O:421:TRP:CE2   | 1:Q:229:ARG:HD2   | 2.55                     | 0.42              |
| 1:S:267:LYS:HZ1   | 1:S:446:GLU:HB3   | 1.84                     | 0.42              |
| 1:V:415:LEU:HD12  | 1:V:420:LEU:O     | 2.19                     | 0.42              |
| 1:Z:138:ASP:OD1   | 1:Z:138:ASP:N     | 2.52                     | 0.42              |
| 1:DA:63:ASP:HB2   | 1:DA:80:CYS:HA    | 2.01                     | 0.42              |
| 1:FA:267:LYS:HZ1  | 1:FA:446:GLU:HB3  | 1.84                     | 0.42              |
| 1:NA:421:TRP:CE2  | 1:PA:229:ARG:HD2  | 2.55                     | 0.42              |
| 1:PA:184:MET:HG3  | 1:PA:259:HIS:ND1  | 2.33                     | 0.42              |
| 1:RA:308:HIS:CD2  | 1:RA:433:LYS:HB3  | 2.55                     | 0.42              |
| 1:TA:462:ILE:N    | 1:TA:463:PRO:HD2  | 2.35                     | 0.42              |
| 1:A:181:THR:N     | 1:A:182:PRO:HD2   | 2.35                     | 0.42              |
| 1:A:232:LYS:CD    | 1:A:234:GLU:HG2   | 2.43                     | 0.42              |
| 1:G:110:ARG:O     | 1:G:115:LYS:NZ    | 2.53                     | 0.42              |
| 1:G:181:THR:N     | 1:G:182:PRO:HD2   | 2.35                     | 0.42              |
| 1:S:71:ARG:NH1    | 1:S:151:GLN:OE1   | 2.41                     | 0.42              |
| 1:S:90:PRO:HB3    | 1:S:464:LEU:CD1   | 2.49                     | 0.42              |
| 1:S:181:THR:N     | 1:S:182:PRO:HD2   | 2.35                     | 0.42              |
| 1:S:195:TYR:OH    | 1:S:282:CYS:O     | 2.31                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:S:305:VAL:HA    | 1:S:439:SER:O      | 2.19                     | 0.42              |
| 1:X:195:TYR:OH    | 1:X:282:CYS:O      | 2.33                     | 0.42              |
| 1:Z:36:ASP:N      | 1:Z:36:ASP:OD1     | 2.53                     | 0.42              |
| 1:FA:181:THR:N    | 1:FA:182:PRO:HD2   | 2.35                     | 0.42              |
| 1:JA:184:MET:HG3  | 1:JA:259:HIS:ND1   | 2.34                     | 0.42              |
| 1:LA:181:THR:N    | 1:LA:182:PRO:HD2   | 2.35                     | 0.42              |
| 1:NA:303:TYR:HB3  | 1:NA:440:ILE:HD11  | 2.01                     | 0.42              |
| 1:RA:181:THR:N    | 1:RA:182:PRO:HD2   | 2.35                     | 0.42              |
| 1:TA:43:PHE:CE2   | 1:TA:282:CYS:HB3   | 2.53                     | 0.42              |
| 1:C:265:HIS:CD2   | 1:C:296:LEU:HD22   | 2.54                     | 0.42              |
| 1:E:63:ASP:HB2    | 1:E:80:CYS:HA      | 2.00                     | 0.42              |
| 1:E:184:MET:HG3   | 1:E:259:HIS:ND1    | 2.33                     | 0.42              |
| 1:E:202:GLU:HA    | 1:E:205:LEU:HG     | 2.02                     | 0.42              |
| 1:G:308:HIS:CD2   | 1:G:433:LYS:HB3    | 2.55                     | 0.42              |
| 1:M:36:ASP:OD1    | 1:M:36:ASP:N       | 2.53                     | 0.42              |
| 1:M:138:ASP:OD1   | 1:M:138:ASP:N      | 2.52                     | 0.42              |
| 1:M:421:TRP:CE2   | 1:O:229:ARG:HD2    | 2.55                     | 0.42              |
| 1:Q:90:PRO:HB3    | 1:Q:464:LEU:CD1    | 2.49                     | 0.42              |
| 1:Q:111:ASN:HB3   | 1:Q:115:LYS:HZ2    | 1.84                     | 0.42              |
| 1:S:438:GLN:OE1   | 1:V:198:ASN:ND2    | 2.37                     | 0.42              |
| 1:V:462:ILE:N     | 1:V:463:PRO:HD2    | 2.35                     | 0.42              |
| 1:X:61:ILE:HD13   | 1:X:76:ARG:HB3     | 2.02                     | 0.42              |
| 1:X:184:MET:HG3   | 1:X:259:HIS:ND1    | 2.34                     | 0.42              |
| 1:DA:462:ILE:N    | 1:DA:463:PRO:HD2   | 2.34                     | 0.42              |
| 1:FA:71:ARG:NH1   | 1:FA:151:GLN:OE1   | 2.41                     | 0.42              |
| 1:FA:305:VAL:HA   | 1:FA:439:SER:O     | 2.19                     | 0.42              |
| 1:HA:202:GLU:HA   | 1:HA:205:LEU:HG    | 2.01                     | 0.42              |
| 1:HA:232:LYS:CD   | 1:HA:234:GLU:HG2   | 2.43                     | 0.42              |
| 1:HA:415:LEU:HD12 | 1:HA:420:LEU:O     | 2.20                     | 0.42              |
| 1:HA:462:ILE:N    | 1:HA:463:PRO:HD2   | 2.35                     | 0.42              |
| 1:NA:30:ARG:O     | 1:NA:32:VAL:HG13   | 2.19                     | 0.42              |
| 1:NA:265:HIS:CD2  | 1:NA:296:LEU:HD22  | 2.54                     | 0.42              |
| 1:A:308:HIS:CD2   | 1:A:433:LYS:HB3    | 2.55                     | 0.42              |
| 1:K:61:ILE:HD13   | 1:K:76:ARG:HB3     | 2.02                     | 0.42              |
| 1:V:195:TYR:OH    | 1:V:282:CYS:O      | 2.28                     | 0.42              |
| 1:V:421:TRP:CE2   | 1:X:229:ARG:HD2    | 2.55                     | 0.42              |
| 1:X:263:VAL:HG12  | 1:X:300:THR:HG22   | 2.02                     | 0.42              |
| 1:Z:181:THR:N     | 1:Z:182:PRO:HD2    | 2.35                     | 0.42              |
| 1:BA:138:ASP:OD1  | 1:BA:138:ASP:N     | 2.53                     | 0.42              |
| 1:DA:41[B]:ARG:HA | 1:DA:41[B]:ARG:HD2 | 1.68                     | 0.42              |
| 1:JA:263:VAL:HG12 | 1:JA:300:THR:HG22  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LA:308:HIS:CD2  | 1:LA:433:LYS:HB3  | 2.55                     | 0.42              |
| 1:LA:415:LEU:HD12 | 1:LA:420:LEU:O    | 2.20                     | 0.42              |
| 1:RA:3:PRO:HA     | 1:RA:26:GLU:HB2   | 2.01                     | 0.42              |
| 1:VA:61:ILE:HD13  | 1:VA:76:ARG:HB3   | 2.02                     | 0.42              |
| 1:A:36:ASP:OD1    | 1:A:36:ASP:N      | 2.53                     | 0.42              |
| 1:A:415:LEU:HD12  | 1:A:420:LEU:O     | 2.20                     | 0.42              |
| 1:C:146:ASP:OD1   | 1:C:146:ASP:N     | 2.51                     | 0.42              |
| 1:I:308:HIS:CD2   | 1:I:433:LYS:HB3   | 2.55                     | 0.42              |
| 1:I:421:TRP:CE2   | 1:K:229:ARG:HD2   | 2.55                     | 0.42              |
| 1:M:181:THR:N     | 1:M:182:PRO:HD2   | 2.35                     | 0.42              |
| 1:M:308:HIS:CD2   | 1:M:433:LYS:HB3   | 2.55                     | 0.42              |
| 1:Q:61:ILE:HD13   | 1:Q:76:ARG:HB3    | 2.02                     | 0.42              |
| 1:S:425:LYS:HG3   | 1:V:323:GLY:HA3   | 2.01                     | 0.42              |
| 1:V:202:GLU:HA    | 1:V:205:LEU:HG    | 2.01                     | 0.42              |
| 1:V:265:HIS:CD2   | 1:V:296:LEU:HD22  | 2.54                     | 0.42              |
| 1:DA:90:PRO:HB3   | 1:DA:464:LEU:CD1  | 2.50                     | 0.42              |
| 1:HA:421:TRP:CE2  | 1:JA:229:ARG:HD2  | 2.55                     | 0.42              |
| 1:LA:305:VAL:HA   | 1:LA:439:SER:O    | 2.19                     | 0.42              |
| 1:LA:434:ARG:O    | 1:LA:437:THR:OG1  | 2.32                     | 0.42              |
| 1:PA:63:ASP:HB2   | 1:PA:80:CYS:HA    | 2.00                     | 0.42              |
| 1:PA:202:GLU:HA   | 1:PA:205:LEU:HG   | 2.02                     | 0.42              |
| 1:TA:263:VAL:HG12 | 1:TA:300:THR:HG22 | 2.02                     | 0.42              |
| 1:TA:308:HIS:CD2  | 1:TA:433:LYS:HB3  | 2.55                     | 0.42              |
| 1:VA:181:THR:N    | 1:VA:182:PRO:HD2  | 2.34                     | 0.42              |
| 1:E:61:ILE:HD13   | 1:E:76:ARG:HB3    | 2.02                     | 0.42              |
| 1:G:421:TRP:CE2   | 1:I:229:ARG:HD2   | 2.55                     | 0.42              |
| 1:I:265:HIS:CD2   | 1:I:296:LEU:HD22  | 2.54                     | 0.42              |
| 1:I:303:TYR:HB3   | 1:I:440:ILE:HD11  | 2.01                     | 0.42              |
| 1:I:356:GLN:HG3   | 1:I:384:ILE:HG22  | 2.02                     | 0.42              |
| 1:M:41[B]:ARG:HA  | 1:M:41[B]:ARG:HD2 | 1.71                     | 0.42              |
| 1:O:308:HIS:CD2   | 1:O:433:LYS:HB3   | 2.55                     | 0.42              |
| 1:S:421:TRP:CZ2   | 1:V:229:ARG:HD2   | 2.55                     | 0.42              |
| 1:Z:308:HIS:CD2   | 1:Z:433:LYS:HB3   | 2.55                     | 0.42              |
| 1:Z:323:GLY:HA3   | 1:VA:425:LYS:HG3  | 2.00                     | 0.42              |
| 1:FA:90:PRO:HB3   | 1:FA:464:LEU:CD1  | 2.50                     | 0.42              |
| 1:FA:195:TYR:OH   | 1:FA:282:CYS:O    | 2.31                     | 0.42              |
| 1:JA:195:TYR:OH   | 1:JA:282:CYS:O    | 2.33                     | 0.42              |
| 1:JA:434:ARG:O    | 1:JA:437:THR:OG1  | 2.37                     | 0.42              |
| 1:LA:24:MET:SD    | 1:LA:24:MET:N     | 2.90                     | 0.42              |
| 1:LA:36:ASP:OD1   | 1:LA:36:ASP:N     | 2.53                     | 0.42              |
| 1:LA:232:LYS:CD   | 1:LA:234:GLU:HG2  | 2.43                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:NA:308:HIS:CD2 | 1:NA:433:LYS:HB3  | 2.55                     | 0.42              |
| 1:PA:61:ILE:HD13 | 1:PA:76:ARG:HB3   | 2.02                     | 0.42              |
| 1:TA:421:TRP:CE2 | 1:VA:229:ARG:HD2  | 2.55                     | 0.42              |
| 1:VA:63:ASP:HB2  | 1:VA:80:CYS:HA    | 2.00                     | 0.42              |
| 1:A:421:TRP:CZ2  | 1:C:229:ARG:HD2   | 2.55                     | 0.42              |
| 1:C:30:ARG:O     | 1:C:32:VAL:HG13   | 2.19                     | 0.42              |
| 1:C:308:HIS:CD2  | 1:C:433:LYS:HB3   | 2.55                     | 0.42              |
| 1:G:421:TRP:CZ2  | 1:I:229:ARG:HD2   | 2.55                     | 0.42              |
| 1:K:181:THR:N    | 1:K:182:PRO:HD2   | 2.34                     | 0.42              |
| 1:K:425:LYS:HG3  | 1:M:323:GLY:HA3   | 2.00                     | 0.42              |
| 1:M:415:LEU:HD12 | 1:M:420:LEU:O     | 2.20                     | 0.42              |
| 1:S:129:GLU:N    | 3:S:1109:HOH:O    | 2.51                     | 0.42              |
| 1:Z:41[B]:ARG:HA | 1:Z:41[B]:ARG:HD2 | 1.71                     | 0.42              |
| 1:BA:308:HIS:CD2 | 1:BA:433:LYS:HB3  | 2.55                     | 0.42              |
| 1:HA:265:HIS:CD2 | 1:HA:296:LEU:HD22 | 2.54                     | 0.42              |
| 1:JA:61:ILE:HD13 | 1:JA:76:ARG:HB3   | 2.02                     | 0.42              |
| 1:LA:414:THR:N   | 1:LA:422:ALA:O    | 2.43                     | 0.42              |
| 1:NA:146:ASP:OD1 | 1:NA:146:ASP:N    | 2.52                     | 0.42              |
| 1:NA:356:GLN:HG3 | 1:NA:384:ILE:HG22 | 2.02                     | 0.42              |
| 1:RA:309:ALA:O   | 1:RA:435:PRO:HB3  | 2.20                     | 0.42              |
| 1:RA:421:TRP:CZ2 | 1:TA:229:ARG:HD2  | 2.55                     | 0.42              |
| 1:G:309:ALA:O    | 1:G:435:PRO:HB3   | 2.20                     | 0.41              |
| 1:I:263:VAL:HG12 | 1:I:300:THR:HG22  | 2.02                     | 0.41              |
| 1:O:43:PHE:CE2   | 1:O:282:CYS:HB3   | 2.55                     | 0.41              |
| 1:V:138:ASP:OD1  | 1:V:138:ASP:N     | 2.53                     | 0.41              |
| 1:Z:421:TRP:CE2  | 1:BA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:FA:421:TRP:CZ2 | 1:HA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:FA:421:TRP:CE2 | 1:HA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:HA:138:ASP:OD1 | 1:HA:138:ASP:N    | 2.53                     | 0.41              |
| 1:LA:421:TRP:CZ2 | 1:NA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:PA:6:VAL:HG23  | 1:PA:8:ILE:HG12   | 2.02                     | 0.41              |
| 1:RA:421:TRP:CE2 | 1:TA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:TA:265:HIS:CD2 | 1:TA:296:LEU:HD22 | 2.54                     | 0.41              |
| 1:TA:356:GLN:HG3 | 1:TA:384:ILE:HG22 | 2.02                     | 0.41              |
| 1:C:356:GLN:HG3  | 1:C:384:ILE:HG22  | 2.02                     | 0.41              |
| 1:M:421:TRP:CD1  | 1:O:229:ARG:HB3   | 2.56                     | 0.41              |
| 1:O:421:TRP:CZ2  | 1:Q:229:ARG:HD2   | 2.55                     | 0.41              |
| 1:S:73:MET:HA    | 1:S:110:ARG:HG3   | 2.02                     | 0.41              |
| 1:V:30:ARG:O     | 1:V:32:VAL:HG13   | 2.19                     | 0.41              |
| 1:Z:309:ALA:O    | 1:Z:435:PRO:HB3   | 2.20                     | 0.41              |
| 1:Z:415:LEU:HD12 | 1:Z:420:LEU:O     | 2.20                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:BA:201:ASP:HB2   | 1:BA:252:ARG:HH11 | 1.86                     | 0.41              |
| 1:BA:421:TRP:CZ2   | 1:DA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:BA:462:ILE:N     | 1:BA:463:PRO:HD2  | 2.35                     | 0.41              |
| 1:DA:61:ILE:HD13   | 1:DA:76:ARG:HB3   | 2.02                     | 0.41              |
| 1:FA:129:GLU:N     | 3:FA:1109:HOH:O   | 2.51                     | 0.41              |
| 1:FA:415:LEU:HD12  | 1:FA:420:LEU:O    | 2.20                     | 0.41              |
| 1:TA:303:TYR:HB3   | 1:TA:440:ILE:HD11 | 2.01                     | 0.41              |
| 1:TA:309:ALA:O     | 1:TA:435:PRO:HB3  | 2.21                     | 0.41              |
| 1:TA:421:TRP:CZ2   | 1:VA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:A:24:MET:SD      | 1:A:24:MET:N      | 2.90                     | 0.41              |
| 1:A:421:TRP:CE2    | 1:C:229:ARG:HD2   | 2.55                     | 0.41              |
| 1:E:6:VAL:HG23     | 1:E:8:ILE:HG12    | 2.02                     | 0.41              |
| 1:G:73:MET:HA      | 1:G:110:ARG:HG3   | 2.02                     | 0.41              |
| 1:G:421:TRP:CD1    | 1:I:229:ARG:HB3   | 2.56                     | 0.41              |
| 1:I:421:TRP:CZ2    | 1:K:229:ARG:HD2   | 2.55                     | 0.41              |
| 1:K:263:VAL:HG12   | 1:K:300:THR:HG22  | 2.02                     | 0.41              |
| 1:M:110:ARG:O      | 1:M:115:LYS:NZ    | 2.53                     | 0.41              |
| 1:O:41[B]:ARG:HA   | 1:O:41[B]:ARG:HD2 | 1.71                     | 0.41              |
| 1:O:201:ASP:HB2    | 1:O:252:ARG:HH11  | 1.86                     | 0.41              |
| 1:O:462:ILE:N      | 1:O:463:PRO:HD2   | 2.34                     | 0.41              |
| 1:Q:41[B]:ARG:HA   | 1:Q:41[B]:ARG:HD2 | 1.68                     | 0.41              |
| 1:X:267:LYS:NZ     | 1:X:446:GLU:HB3   | 2.35                     | 0.41              |
| 1:Z:110:ARG:O      | 1:Z:115:LYS:NZ    | 2.53                     | 0.41              |
| 1:Z:305:VAL:HA     | 1:Z:439:SER:O     | 2.19                     | 0.41              |
| 1:Z:421:TRP:CZ2    | 1:BA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:DA:267:LYS:NZ    | 1:DA:446:GLU:HB3  | 2.35                     | 0.41              |
| 1:FA:73:MET:HA     | 1:FA:110:ARG:HG3  | 2.02                     | 0.41              |
| 1:HA:30:ARG:O      | 1:HA:32:VAL:HG13  | 2.19                     | 0.41              |
| 1:TA:41[B]:ARG:HD2 | 1:TA:41[B]:ARG:HA | 1.71                     | 0.41              |
| 1:A:6:VAL:HG23     | 1:A:8:ILE:HG12    | 2.03                     | 0.41              |
| 1:M:305:VAL:HA     | 1:M:439:SER:O     | 2.19                     | 0.41              |
| 1:M:309:ALA:O      | 1:M:435:PRO:HB3   | 2.20                     | 0.41              |
| 1:O:202:GLU:HA     | 1:O:205:LEU:HG    | 2.01                     | 0.41              |
| 1:O:263:VAL:HG12   | 1:O:300:THR:HG22  | 2.02                     | 0.41              |
| 1:Q:267:LYS:NZ     | 1:Q:446:GLU:HB3   | 2.35                     | 0.41              |
| 1:S:415:LEU:HD12   | 1:S:420:LEU:O     | 2.20                     | 0.41              |
| 1:V:308:HIS:CD2    | 1:V:433:LYS:HB3   | 2.55                     | 0.41              |
| 1:X:202:GLU:HA     | 1:X:205:LEU:HG    | 2.02                     | 0.41              |
| 1:BA:415:LEU:HD12  | 1:BA:420:LEU:O    | 2.19                     | 0.41              |
| 1:HA:308:HIS:CD2   | 1:HA:433:LYS:HB3  | 2.55                     | 0.41              |
| 1:JA:267:LYS:NZ    | 1:JA:446:GLU:HB3  | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LA:73:MET:HA    | 1:LA:110:ARG:HG3  | 2.02                     | 0.41              |
| 1:LA:421:TRP:CE2  | 1:NA:229:ARG:HD2  | 2.55                     | 0.41              |
| 1:RA:73:MET:HA    | 1:RA:110:ARG:HG3  | 2.02                     | 0.41              |
| 1:A:71:ARG:NH1    | 1:A:151:GLN:OE1   | 2.41                     | 0.41              |
| 1:A:73:MET:HA     | 1:A:110:ARG:HG3   | 2.02                     | 0.41              |
| 1:C:232:LYS:CD    | 1:C:234:GLU:HG2   | 2.43                     | 0.41              |
| 1:K:63:ASP:HB2    | 1:K:80:CYS:HA     | 2.01                     | 0.41              |
| 1:M:421:TRP:CZ2   | 1:O:229:ARG:HD2   | 2.55                     | 0.41              |
| 1:O:415:LEU:HD12  | 1:O:420:LEU:O     | 2.19                     | 0.41              |
| 1:S:421:TRP:CE2   | 1:V:229:ARG:HD2   | 2.55                     | 0.41              |
| 1:JA:202:GLU:HA   | 1:JA:205:LEU:HG   | 2.02                     | 0.41              |
| 1:LA:6:VAL:HG23   | 1:LA:8:ILE:HG12   | 2.03                     | 0.41              |
| 1:VA:263:VAL:HG12 | 1:VA:300:THR:HG22 | 2.02                     | 0.41              |
| 1:A:305:VAL:HA    | 1:A:439:SER:O     | 2.20                     | 0.41              |
| 1:G:274:CYS:SG    | 1:G:292:MET:HG2   | 2.61                     | 0.41              |
| 1:I:273:THR:HG21  | 1:I:297:TYR:HB2   | 2.03                     | 0.41              |
| 1:K:202:GLU:HA    | 1:K:205:LEU:HG    | 2.02                     | 0.41              |
| 1:M:267:LYS:NZ    | 1:M:446:GLU:HB3   | 2.36                     | 0.41              |
| 1:X:36:ASP:OD1    | 1:X:36:ASP:N      | 2.54                     | 0.41              |
| 1:Z:421:TRP:CD1   | 1:BA:229:ARG:HB3  | 2.56                     | 0.41              |
| 1:BA:263:VAL:HG12 | 1:BA:300:THR:HG22 | 2.02                     | 0.41              |
| 1:FA:24:MET:SD    | 1:FA:24:MET:N     | 2.90                     | 0.41              |
| 1:FA:274:CYS:SG   | 1:FA:292:MET:HG2  | 2.61                     | 0.41              |
| 1:JA:36:ASP:OD1   | 1:JA:36:ASP:N     | 2.54                     | 0.41              |
| 1:RA:6:VAL:HG23   | 1:RA:8:ILE:HG12   | 2.03                     | 0.41              |
| 1:RA:274:CYS:SG   | 1:RA:292:MET:HG2  | 2.61                     | 0.41              |
| 1:RA:421:TRP:CD1  | 1:TA:229:ARG:HB3  | 2.56                     | 0.41              |
| 1:VA:44:SER:HB3   | 1:VA:151:GLN:NE2  | 2.34                     | 0.41              |
| 1:C:309:ALA:O     | 1:C:435:PRO:HB3   | 2.21                     | 0.41              |
| 1:I:309:ALA:O     | 1:I:435:PRO:HB3   | 2.21                     | 0.41              |
| 1:O:356:GLN:HG3   | 1:O:384:ILE:HG22  | 2.02                     | 0.41              |
| 1:S:138:ASP:OD1   | 1:S:138:ASP:N     | 2.52                     | 0.41              |
| 1:S:309:ALA:O     | 1:S:435:PRO:HB3   | 2.20                     | 0.41              |
| 1:V:201:ASP:HB2   | 1:V:252:ARG:HH11  | 1.86                     | 0.41              |
| 1:X:6:VAL:HG23    | 1:X:8:ILE:HG12    | 2.02                     | 0.41              |
| 1:Z:273:THR:HG21  | 1:Z:297:TYR:HB2   | 2.03                     | 0.41              |
| 1:BA:273:THR:HG21 | 1:BA:297:TYR:HB2  | 2.03                     | 0.41              |
| 1:FA:309:ALA:O    | 1:FA:435:PRO:HB3  | 2.20                     | 0.41              |
| 1:HA:201:ASP:HB2  | 1:HA:252:ARG:HH11 | 1.86                     | 0.41              |
| 1:NA:281:SER:OG   | 3:NA:1102:HOH:O   | 2.15                     | 0.41              |
| 1:TA:414:THR:N    | 1:TA:422:ALA:O    | 2.43                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:VA:6:VAL:HG23   | 1:VA:8:ILE:HG12     | 2.02                     | 0.41              |
| 1:VA:202:GLU:HA   | 1:VA:205:LEU:HG     | 2.02                     | 0.41              |
| 1:VA:464:LEU:O    | 1:VA:468:ILE:HG12   | 2.21                     | 0.41              |
| 1:C:263:VAL:HG12  | 1:C:300:THR:HG22    | 2.02                     | 0.41              |
| 1:E:263:VAL:HG12  | 1:E:300:THR:HG22    | 2.01                     | 0.41              |
| 1:M:273:THR:HG21  | 1:M:297:TYR:HB2     | 2.03                     | 0.41              |
| 1:S:274:CYS:SG    | 1:S:292:MET:HG2     | 2.61                     | 0.41              |
| 1:S:436:ASP:OD1   | 1:V:196:SER:OG      | 2.33                     | 0.41              |
| 1:V:36:ASP:OD1    | 1:V:36:ASP:N        | 2.54                     | 0.41              |
| 1:Z:6:VAL:HG23    | 1:Z:8:ILE:HG12      | 2.03                     | 0.41              |
| 1:Z:73:MET:HA     | 1:Z:110:ARG:HG3     | 2.02                     | 0.41              |
| 1:BA:202:GLU:HA   | 1:BA:205:LEU:HG     | 2.01                     | 0.41              |
| 1:FA:6:VAL:HG23   | 1:FA:8:ILE:HG12     | 2.03                     | 0.41              |
| 1:FA:138:ASP:OD1  | 1:FA:138:ASP:N      | 2.52                     | 0.41              |
| 1:FA:436:ASP:OD1  | 1:HA:196:SER:OG     | 2.33                     | 0.41              |
| 1:NA:263:VAL:HG12 | 1:NA:300:THR:HG22   | 2.02                     | 0.41              |
| 1:PA:263:VAL:HG12 | 1:PA:300:THR:HG22   | 2.01                     | 0.41              |
| 1:RA:122:VAL:HG11 | 1:RA:133:PHE:CD2    | 2.56                     | 0.41              |
| 1:A:90:PRO:HB3    | 1:A:464:LEU:CD1     | 2.49                     | 0.41              |
| 1:C:273:THR:HG21  | 1:C:297:TYR:HB2     | 2.03                     | 0.41              |
| 1:C:421:TRP:CZ2   | 1:E:229:ARG:HD2     | 2.55                     | 0.41              |
| 1:E:267:LYS:NZ    | 1:E:446:GLU:HB3     | 2.36                     | 0.41              |
| 1:G:6:VAL:HG23    | 1:G:8:ILE:HG12      | 2.03                     | 0.41              |
| 1:G:61:ILE:HD13   | 1:G:76:ARG:HB3      | 2.03                     | 0.41              |
| 1:I:349:GLU:HG3   | 1:I:399[A]:ARG:HG3  | 2.03                     | 0.41              |
| 1:K:6:VAL:HG23    | 1:K:8:ILE:HG12      | 2.02                     | 0.41              |
| 1:K:44:SER:HB3    | 1:K:151:GLN:NE2     | 2.34                     | 0.41              |
| 1:M:61:ILE:HD13   | 1:M:76:ARG:HB3      | 2.03                     | 0.41              |
| 1:O:273:THR:HG21  | 1:O:297:TYR:HB2     | 2.03                     | 0.41              |
| 1:S:24:MET:SD     | 1:S:24:MET:N        | 2.90                     | 0.41              |
| 1:V:273:THR:HG21  | 1:V:297:TYR:HB2     | 2.03                     | 0.41              |
| 1:V:356:GLN:HG3   | 1:V:384:ILE:HG22    | 2.02                     | 0.41              |
| 1:Z:61:ILE:HD13   | 1:Z:76:ARG:HB3      | 2.03                     | 0.41              |
| 1:Z:122:VAL:HG11  | 1:Z:133:PHE:CD2     | 2.56                     | 0.41              |
| 1:Z:267:LYS:NZ    | 1:Z:446:GLU:HB3     | 2.36                     | 0.41              |
| 1:BA:356:GLN:HG3  | 1:BA:384:ILE:HG22   | 2.03                     | 0.41              |
| 1:HA:36:ASP:OD1   | 1:HA:36:ASP:N       | 2.54                     | 0.41              |
| 1:HA:273:THR:HG21 | 1:HA:297:TYR:HB2    | 2.03                     | 0.41              |
| 1:HA:349:GLU:HG3  | 1:HA:399[A]:ARG:HG3 | 2.03                     | 0.41              |
| 1:HA:356:GLN:HG3  | 1:HA:384:ILE:HG22   | 2.02                     | 0.41              |
| 1:JA:6:VAL:HG23   | 1:JA:8:ILE:HG12     | 2.02                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:LA:71:ARG:NH1   | 1:LA:151:GLN:OE1    | 2.41                     | 0.41              |
| 1:LA:267:LYS:NZ   | 1:LA:446:GLU:HB3    | 2.36                     | 0.41              |
| 1:NA:232:LYS:CD   | 1:NA:234:GLU:HG2    | 2.43                     | 0.41              |
| 1:NA:267:LYS:HE3  | 1:NA:267:LYS:HB2    | 1.76                     | 0.41              |
| 1:NA:273:THR:HG21 | 1:NA:297:TYR:HB2    | 2.03                     | 0.41              |
| 1:NA:421:TRP:CZ2  | 1:PA:229:ARG:HD2    | 2.55                     | 0.41              |
| 1:PA:267:LYS:NZ   | 1:PA:446:GLU:HB3    | 2.35                     | 0.41              |
| 1:RA:61:ILE:HD13  | 1:RA:76:ARG:HB3     | 2.03                     | 0.41              |
| 1:TA:273:THR:HG21 | 1:TA:297:TYR:HB2    | 2.03                     | 0.41              |
| 1:TA:349:GLU:HG3  | 1:TA:399[A]:ARG:HG3 | 2.03                     | 0.41              |
| 1:VA:267:LYS:NZ   | 1:VA:446:GLU:HB3    | 2.35                     | 0.41              |
| 1:A:61:ILE:HD13   | 1:A:76:ARG:HB3      | 2.03                     | 0.41              |
| 1:A:267:LYS:NZ    | 1:A:446:GLU:HB3     | 2.36                     | 0.41              |
| 1:C:267:LYS:HE3   | 1:C:267:LYS:HB2     | 1.76                     | 0.41              |
| 1:E:44:SER:HB3    | 1:E:151:GLN:NE2     | 2.34                     | 0.41              |
| 1:G:415:LEU:HD12  | 1:G:420:LEU:O       | 2.20                     | 0.41              |
| 1:I:414:THR:N     | 1:I:422:ALA:O       | 2.43                     | 0.41              |
| 1:K:308:HIS:CD2   | 1:K:433:LYS:HB3     | 2.56                     | 0.41              |
| 1:M:73:MET:HA     | 1:M:110:ARG:HG3     | 2.02                     | 0.41              |
| 1:M:122:VAL:HG11  | 1:M:133:PHE:CD2     | 2.56                     | 0.41              |
| 1:M:406:LYS:HA    | 1:M:406:LYS:HD3     | 1.86                     | 0.41              |
| 1:O:349:GLU:HG3   | 1:O:399[A]:ARG:HG3  | 2.03                     | 0.41              |
| 1:Q:195:TYR:OH    | 1:Q:282:CYS:O       | 2.33                     | 0.41              |
| 1:Q:202:GLU:HA    | 1:Q:205:LEU:HG      | 2.02                     | 0.41              |
| 1:V:349:GLU:HG3   | 1:V:399[A]:ARG:HG3  | 2.03                     | 0.41              |
| 1:FA:425:LYS:HG3  | 1:HA:323:GLY:HA3    | 2.03                     | 0.41              |
| 1:HA:263:VAL:HG12 | 1:HA:300:THR:HG22   | 2.02                     | 0.41              |
| 1:LA:61:ILE:HD13  | 1:LA:76:ARG:HB3     | 2.03                     | 0.41              |
| 1:NA:43:PHE:CE2   | 1:NA:282:CYS:HB3    | 2.55                     | 0.41              |
| 1:NA:309:ALA:O    | 1:NA:435:PRO:HB3    | 2.21                     | 0.41              |
| 1:TA:181:THR:N    | 1:TA:182:PRO:HD2    | 2.36                     | 0.41              |
| 1:TA:201:ASP:HB2  | 1:TA:252:ARG:HH11   | 1.86                     | 0.41              |
| 1:A:122:VAL:HG11  | 1:A:133:PHE:CD2     | 2.56                     | 0.40              |
| 1:A:309:ALA:O     | 1:A:435:PRO:HB3     | 2.20                     | 0.40              |
| 1:A:425:LYS:HG3   | 1:C:323:GLY:HA3     | 2.03                     | 0.40              |
| 1:C:36:ASP:OD1    | 1:C:36:ASP:N        | 2.54                     | 0.40              |
| 1:M:349:GLU:HG3   | 1:M:399[B]:ARG:HG3  | 2.04                     | 0.40              |
| 1:V:421:TRP:CZ2   | 1:X:229:ARG:HD2     | 2.55                     | 0.40              |
| 1:Z:349:GLU:HG3   | 1:Z:399[B]:ARG:HG3  | 2.04                     | 0.40              |
| 1:BA:129:GLU:N    | 3:BA:1109:HOH:O     | 2.53                     | 0.40              |
| 1:LA:90:PRO:HB3   | 1:LA:464:LEU:CD1    | 2.49                     | 0.40              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:LA:122:VAL:HG11 | 1:LA:133:PHE:CD2    | 2.56                     | 0.40              |
| 1:LA:421:TRP:CD1  | 1:NA:229:ARG:HB3    | 2.56                     | 0.40              |
| 1:LA:425:LYS:HG3  | 1:NA:323:GLY:HA3    | 2.03                     | 0.40              |
| 1:A:421:TRP:CD1   | 1:C:229:ARG:HB3     | 2.56                     | 0.40              |
| 1:C:181:THR:N     | 1:C:182:PRO:HD2     | 2.37                     | 0.40              |
| 1:E:21:ALA:O      | 1:G:34:PRO:HG3      | 2.22                     | 0.40              |
| 1:I:181:THR:N     | 1:I:182:PRO:HD2     | 2.37                     | 0.40              |
| 1:I:201:ASP:HB2   | 1:I:252:ARG:HH11    | 1.86                     | 0.40              |
| 1:K:267:LYS:NZ    | 1:K:446:GLU:HB3     | 2.36                     | 0.40              |
| 1:K:273:THR:HG21  | 1:K:297:TYR:HB2     | 2.04                     | 0.40              |
| 1:O:129:GLU:N     | 3:O:1109:HOH:O      | 2.54                     | 0.40              |
| 1:Q:83:PRO:HB3    | 1:Q:137:THR:HA      | 2.03                     | 0.40              |
| 1:BA:349:GLU:HG3  | 1:BA:399[A]:ARG:HG3 | 2.03                     | 0.40              |
| 1:FA:110:ARG:O    | 1:FA:115:LYS:NZ     | 2.53                     | 0.40              |
| 1:FA:308:HIS:CD2  | 1:FA:433:LYS:HB3    | 2.55                     | 0.40              |
| 1:LA:309:ALA:O    | 1:LA:435:PRO:HB3    | 2.20                     | 0.40              |
| 1:NA:181:THR:N    | 1:NA:182:PRO:HD2    | 2.37                     | 0.40              |
| 1:PA:21:ALA:O     | 1:RA:34:PRO:HG3     | 2.22                     | 0.40              |
| 1:PA:44:SER:HB3   | 1:PA:151:GLN:NE2    | 2.34                     | 0.40              |
| 1:PA:308:HIS:CD2  | 1:PA:433:LYS:HB3    | 2.56                     | 0.40              |
| 1:VA:138:ASP:OD1  | 1:VA:138:ASP:N      | 2.49                     | 0.40              |
| 1:VA:273:THR:HG21 | 1:VA:297:TYR:HB2    | 2.04                     | 0.40              |
| 1:VA:308:HIS:CD2  | 1:VA:433:LYS:HB3    | 2.56                     | 0.40              |
| 1:A:34:PRO:HG3    | 1:X:21:ALA:O        | 2.22                     | 0.40              |
| 1:K:21:ALA:O      | 1:M:34:PRO:HG3      | 2.22                     | 0.40              |
| 1:M:6:VAL:HG23    | 1:M:8:ILE:HG12      | 2.03                     | 0.40              |
| 1:S:6:VAL:HG23    | 1:S:8:ILE:HG12      | 2.03                     | 0.40              |
| 1:S:308:HIS:CD2   | 1:S:433:LYS:HB3     | 2.55                     | 0.40              |
| 1:V:263:VAL:HG12  | 1:V:300:THR:HG22    | 2.02                     | 0.40              |
| 1:DA:202:GLU:HA   | 1:DA:205:LEU:HG     | 2.02                     | 0.40              |
| 1:HA:309:ALA:O    | 1:HA:435:PRO:HB3    | 2.21                     | 0.40              |
| 1:HA:421:TRP:CZ2  | 1:JA:229:ARG:HD2    | 2.55                     | 0.40              |
| 1:LA:274:CYS:SG   | 1:LA:292:MET:HG2    | 2.61                     | 0.40              |
| 1:NA:201:ASP:HB2  | 1:NA:252:ARG:HH11   | 1.86                     | 0.40              |
| 1:RA:273:THR:HG21 | 1:RA:297:TYR:HB2    | 2.03                     | 0.40              |
| 1:RA:415:LEU:HD12 | 1:RA:420:LEU:O      | 2.20                     | 0.40              |
| 1:VA:83:PRO:HB3   | 1:VA:137:THR:HA     | 2.03                     | 0.40              |
| 1:A:274:CYS:SG    | 1:A:292:MET:HG2     | 2.61                     | 0.40              |
| 1:G:122:VAL:HG11  | 1:G:133:PHE:CD2     | 2.56                     | 0.40              |
| 1:G:273:THR:HG21  | 1:G:297:TYR:HB2     | 2.03                     | 0.40              |
| 1:I:43:PHE:CE2    | 1:I:282:CYS:HB3     | 2.55                     | 0.40              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:K:138:ASP:OD1   | 1:K:138:ASP:N       | 2.49                     | 0.40              |
| 1:M:274:CYS:SG    | 1:M:292:MET:HG2     | 2.61                     | 0.40              |
| 1:O:181:THR:N     | 1:O:182:PRO:HD2     | 2.36                     | 0.40              |
| 1:Q:9:ASP:HB3     | 1:Q:31:GLN:OE1      | 2.22                     | 0.40              |
| 1:Q:273:THR:HG21  | 1:Q:297:TYR:HB2     | 2.04                     | 0.40              |
| 1:S:61:ILE:HD13   | 1:S:76:ARG:HB3      | 2.03                     | 0.40              |
| 1:S:110:ARG:O     | 1:S:115:LYS:NZ      | 2.53                     | 0.40              |
| 1:V:309:ALA:O     | 1:V:435:PRO:HB3     | 2.21                     | 0.40              |
| 1:Z:34:PRO:HG3    | 1:VA:21:ALA:O       | 2.22                     | 0.40              |
| 1:Z:274:CYS:SG    | 1:Z:292:MET:HG2     | 2.61                     | 0.40              |
| 1:BA:414:THR:N    | 1:BA:422:ALA:O      | 2.43                     | 0.40              |
| 1:FA:61:ILE:HD13  | 1:FA:76:ARG:HB3     | 2.03                     | 0.40              |
| 1:FA:237:ASP:OD2  | 1:FA:251:SER:HB2    | 2.21                     | 0.40              |
| 1:JA:21:ALA:O     | 1:LA:34:PRO:HG3     | 2.22                     | 0.40              |
| 1:A:237:ASP:OD2   | 1:A:251:SER:HB2     | 2.21                     | 0.40              |
| 1:A:275:ARG:HD2   | 1:C:88:GLU:HG3      | 2.04                     | 0.40              |
| 1:C:201:ASP:HB2   | 1:C:252:ARG:HH11    | 1.86                     | 0.40              |
| 1:E:9:ASP:HB3     | 1:E:31:GLN:OE1      | 2.22                     | 0.40              |
| 1:G:449:SER:O     | 1:G:449:SER:OG      | 2.32                     | 0.40              |
| 1:K:349:GLU:HG3   | 1:K:399[B]:ARG:HG3  | 2.04                     | 0.40              |
| 1:Q:21:ALA:O      | 1:S:34:PRO:HG3      | 2.22                     | 0.40              |
| 1:S:237:ASP:OD2   | 1:S:251:SER:HB2     | 2.21                     | 0.40              |
| 1:S:267:LYS:NZ    | 1:S:446:GLU:HB3     | 2.36                     | 0.40              |
| 1:S:421:TRP:CD1   | 1:V:229:ARG:HB3     | 2.56                     | 0.40              |
| 1:V:129:GLU:N     | 3:V:1109:HOH:O      | 2.54                     | 0.40              |
| 1:DA:9:ASP:HB3    | 1:DA:31:GLN:OE1     | 2.22                     | 0.40              |
| 1:DA:21:ALA:O     | 1:FA:34:PRO:HG3     | 2.22                     | 0.40              |
| 1:FA:273:THR:HG21 | 1:FA:297:TYR:HB2    | 2.03                     | 0.40              |
| 1:FA:421:TRP:CD1  | 1:HA:229:ARG:HB3    | 2.56                     | 0.40              |
| 1:JA:9:ASP:HB3    | 1:JA:31:GLN:OE1     | 2.22                     | 0.40              |
| 1:JA:90:PRO:HB3   | 1:JA:464:LEU:CD1    | 2.49                     | 0.40              |
| 1:LA:237:ASP:OD2  | 1:LA:251:SER:HB2    | 2.21                     | 0.40              |
| 1:LA:275:ARG:HD2  | 1:NA:88:GLU:HG3     | 2.04                     | 0.40              |
| 1:PA:9:ASP:HB3    | 1:PA:31:GLN:OE1     | 2.22                     | 0.40              |
| 1:RA:421:TRP:CG   | 1:TA:229:ARG:HB3    | 2.57                     | 0.40              |
| 1:TA:421:TRP:CG   | 1:VA:229:ARG:HB3    | 2.57                     | 0.40              |
| 1:VA:349:GLU:HG3  | 1:VA:399[B]:ARG:HG3 | 2.04                     | 0.40              |
| 1:VA:415:LEU:HD12 | 1:VA:420:LEU:O      | 2.22                     | 0.40              |

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

### 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     | 259/409 (63%) | 259 (100%) | 0        | 100         | 100 |
| 1   | BA    | 184/409 (45%) | 184 (100%) | 0        | 100         | 100 |
| 1   | C     | 302/409 (74%) | 302 (100%) | 0        | 100         | 100 |
| 1   | E     | 56/409 (14%)  | 56 (100%)  | 0        | 100         | 100 |
| 1   | FA    | 141/409 (34%) | 141 (100%) | 0        | 100         | 100 |
| 1   | G     | 344/409 (84%) | 344 (100%) | 0        | 100         | 100 |
| 1   | HA    | 5/409 (1%)    | 5 (100%)   | 0        | 100         | 100 |
| 1   | I     | 346/409 (85%) | 346 (100%) | 0        | 100         | 100 |
| 1   | JA    | 274/409 (67%) | 274 (100%) | 0        | 100         | 100 |
| 1   | K     | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | LA    | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | M     | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | NA    | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | O     | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | PA    | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | Q     | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | RA    | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | S     | 337/409 (82%) | 337 (100%) | 0        | 100         | 100 |
| 1   | TA    | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |
| 1   | V     | 5/409 (1%)    | 5 (100%)   | 0        | 100         | 100 |
| 1   | VA    | 386/409 (94%) | 386 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | Z     | 228/409 (56%)   | 228 (100%)  | 0        | 100         | 100 |
| All | All   | 6341/8998 (70%) | 6341 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 39  | ASN  |
| 1   | A     | 53  | GLN  |
| 1   | A     | 95  | ASN  |
| 1   | A     | 136 | HIS  |
| 1   | A     | 157 | HIS  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 203 | GLN  |
| 1   | A     | 259 | HIS  |
| 1   | A     | 441 | GLN  |
| 1   | C     | 39  | ASN  |
| 1   | C     | 120 | GLN  |
| 1   | C     | 136 | HIS  |
| 1   | C     | 165 | GLN  |
| 1   | C     | 203 | GLN  |
| 1   | C     | 259 | HIS  |
| 1   | C     | 341 | GLN  |
| 1   | E     | 426 | GLN  |
| 1   | G     | 39  | ASN  |
| 1   | G     | 53  | GLN  |
| 1   | G     | 95  | ASN  |
| 1   | G     | 136 | HIS  |
| 1   | G     | 157 | HIS  |
| 1   | G     | 165 | GLN  |
| 1   | G     | 203 | GLN  |
| 1   | G     | 259 | HIS  |
| 1   | G     | 341 | GLN  |
| 1   | I     | 39  | ASN  |
| 1   | I     | 120 | GLN  |
| 1   | I     | 136 | HIS  |
| 1   | I     | 203 | GLN  |
| 1   | I     | 259 | HIS  |
| 1   | I     | 341 | GLN  |
| 1   | I     | 441 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 39  | ASN  |
| 1   | K     | 95  | ASN  |
| 1   | K     | 120 | GLN  |
| 1   | K     | 157 | HIS  |
| 1   | K     | 165 | GLN  |
| 1   | K     | 203 | GLN  |
| 1   | K     | 259 | HIS  |
| 1   | K     | 426 | GLN  |
| 1   | M     | 39  | ASN  |
| 1   | M     | 53  | GLN  |
| 1   | M     | 95  | ASN  |
| 1   | M     | 136 | HIS  |
| 1   | M     | 157 | HIS  |
| 1   | M     | 165 | GLN  |
| 1   | M     | 203 | GLN  |
| 1   | M     | 259 | HIS  |
| 1   | M     | 341 | GLN  |
| 1   | M     | 441 | GLN  |
| 1   | O     | 39  | ASN  |
| 1   | O     | 120 | GLN  |
| 1   | O     | 136 | HIS  |
| 1   | O     | 157 | HIS  |
| 1   | O     | 165 | GLN  |
| 1   | O     | 203 | GLN  |
| 1   | O     | 259 | HIS  |
| 1   | O     | 341 | GLN  |
| 1   | O     | 441 | GLN  |
| 1   | Q     | 39  | ASN  |
| 1   | Q     | 95  | ASN  |
| 1   | Q     | 157 | HIS  |
| 1   | Q     | 165 | GLN  |
| 1   | Q     | 203 | GLN  |
| 1   | Q     | 259 | HIS  |
| 1   | Q     | 426 | GLN  |
| 1   | S     | 39  | ASN  |
| 1   | S     | 95  | ASN  |
| 1   | S     | 136 | HIS  |
| 1   | S     | 157 | HIS  |
| 1   | S     | 165 | GLN  |
| 1   | S     | 203 | GLN  |
| 1   | S     | 259 | HIS  |
| 1   | S     | 341 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z     | 203 | GLN  |
| 1   | Z     | 259 | HIS  |
| 1   | Z     | 341 | GLN  |
| 1   | Z     | 441 | GLN  |
| 1   | BA    | 120 | GLN  |
| 1   | BA    | 136 | HIS  |
| 1   | BA    | 157 | HIS  |
| 1   | BA    | 165 | GLN  |
| 1   | BA    | 341 | GLN  |
| 1   | FA    | 341 | GLN  |
| 1   | FA    | 441 | GLN  |
| 1   | JA    | 157 | HIS  |
| 1   | JA    | 165 | GLN  |
| 1   | JA    | 203 | GLN  |
| 1   | JA    | 259 | HIS  |
| 1   | JA    | 426 | GLN  |
| 1   | LA    | 39  | ASN  |
| 1   | LA    | 53  | GLN  |
| 1   | LA    | 95  | ASN  |
| 1   | LA    | 136 | HIS  |
| 1   | LA    | 157 | HIS  |
| 1   | LA    | 165 | GLN  |
| 1   | LA    | 203 | GLN  |
| 1   | LA    | 259 | HIS  |
| 1   | LA    | 341 | GLN  |
| 1   | LA    | 441 | GLN  |
| 1   | NA    | 39  | ASN  |
| 1   | NA    | 120 | GLN  |
| 1   | NA    | 136 | HIS  |
| 1   | NA    | 165 | GLN  |
| 1   | NA    | 203 | GLN  |
| 1   | NA    | 341 | GLN  |
| 1   | NA    | 441 | GLN  |
| 1   | PA    | 39  | ASN  |
| 1   | PA    | 95  | ASN  |
| 1   | PA    | 120 | GLN  |
| 1   | PA    | 165 | GLN  |
| 1   | PA    | 203 | GLN  |
| 1   | PA    | 259 | HIS  |
| 1   | PA    | 426 | GLN  |
| 1   | RA    | 39  | ASN  |
| 1   | RA    | 53  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | RA    | 95  | ASN  |
| 1   | RA    | 136 | HIS  |
| 1   | RA    | 157 | HIS  |
| 1   | RA    | 165 | GLN  |
| 1   | RA    | 203 | GLN  |
| 1   | RA    | 259 | HIS  |
| 1   | RA    | 341 | GLN  |
| 1   | RA    | 441 | GLN  |
| 1   | TA    | 39  | ASN  |
| 1   | TA    | 120 | GLN  |
| 1   | TA    | 136 | HIS  |
| 1   | TA    | 157 | HIS  |
| 1   | TA    | 165 | GLN  |
| 1   | TA    | 203 | GLN  |
| 1   | TA    | 259 | HIS  |
| 1   | TA    | 341 | GLN  |
| 1   | TA    | 441 | GLN  |
| 1   | VA    | 39  | ASN  |
| 1   | VA    | 95  | ASN  |
| 1   | VA    | 157 | HIS  |
| 1   | VA    | 165 | GLN  |
| 1   | VA    | 203 | GLN  |
| 1   | VA    | 259 | HIS  |
| 1   | VA    | 426 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

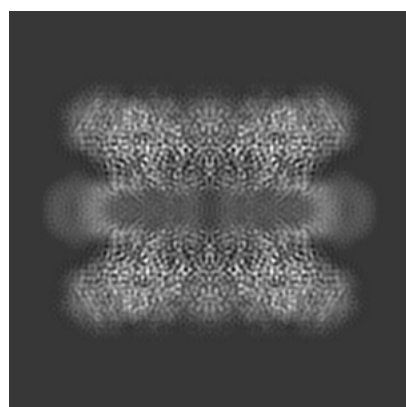
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11023. These allow visual inspection of the internal detail of the map and identification of artifacts.

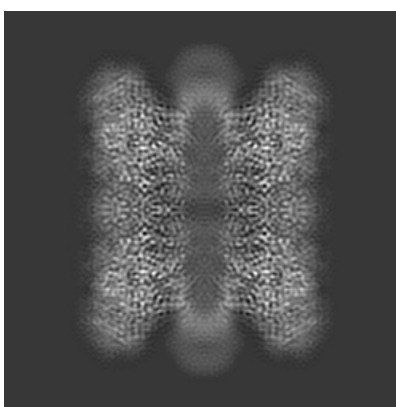
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

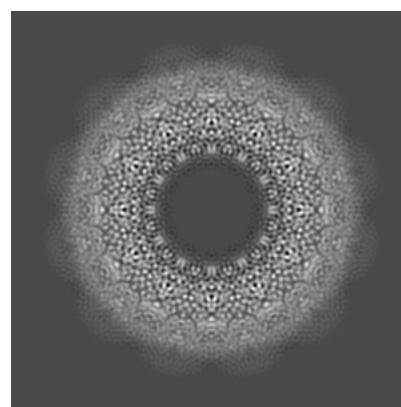
#### 6.1.1 Primary map



X



Y

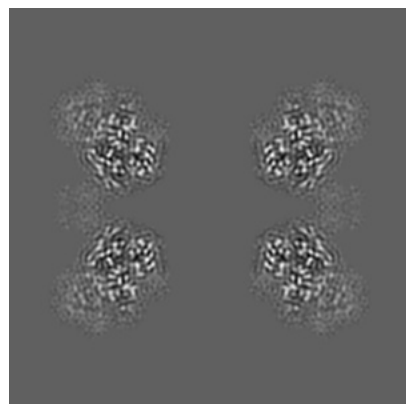


Z

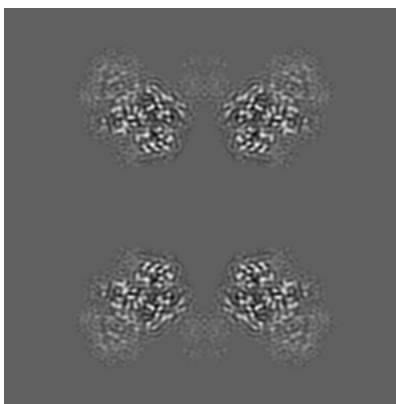
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

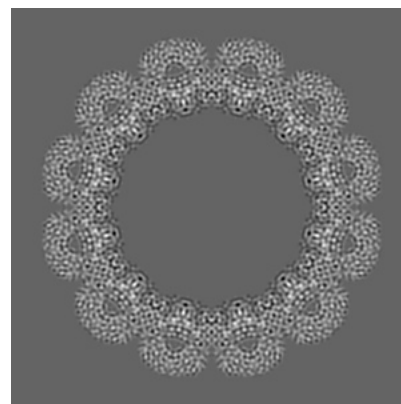
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

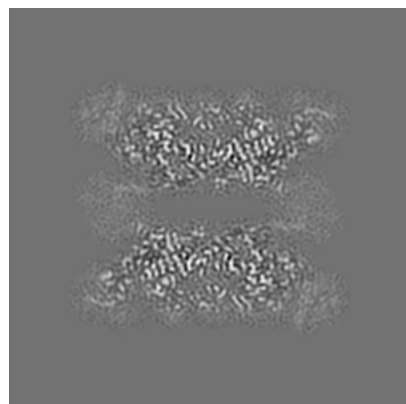


Z Index: 150

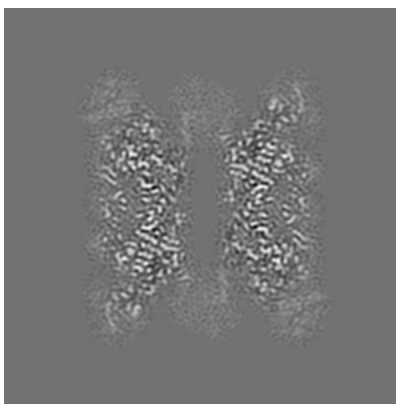
The images above show central slices of the map in three orthogonal directions.

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

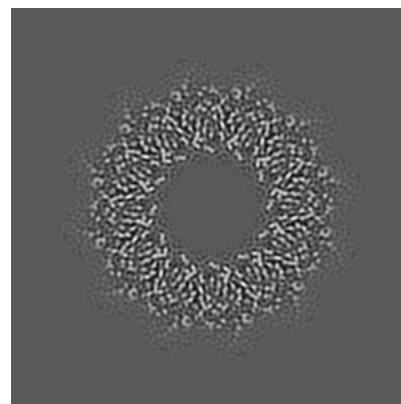
### 6.3.1 Primary map



X Index: 209



Y Index: 91

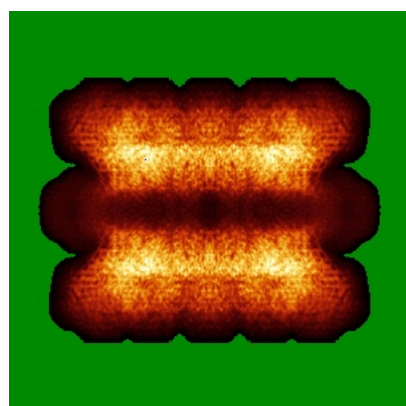


Z Index: 107

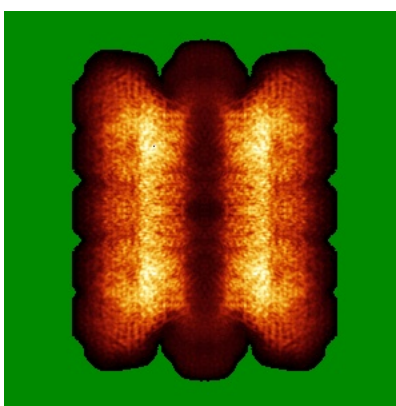
The images above show the largest variance slices of the map in three orthogonal directions.

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

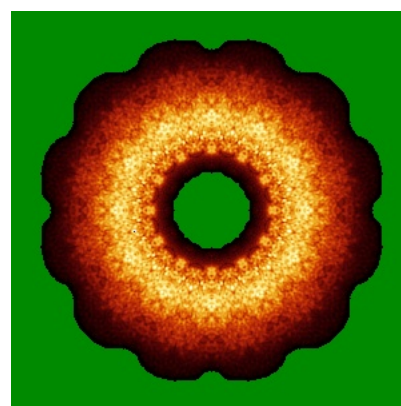
### 6.4.1 Primary map



X



Y



Z

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

This section was not generated.

## 6.6 Mask visualisation

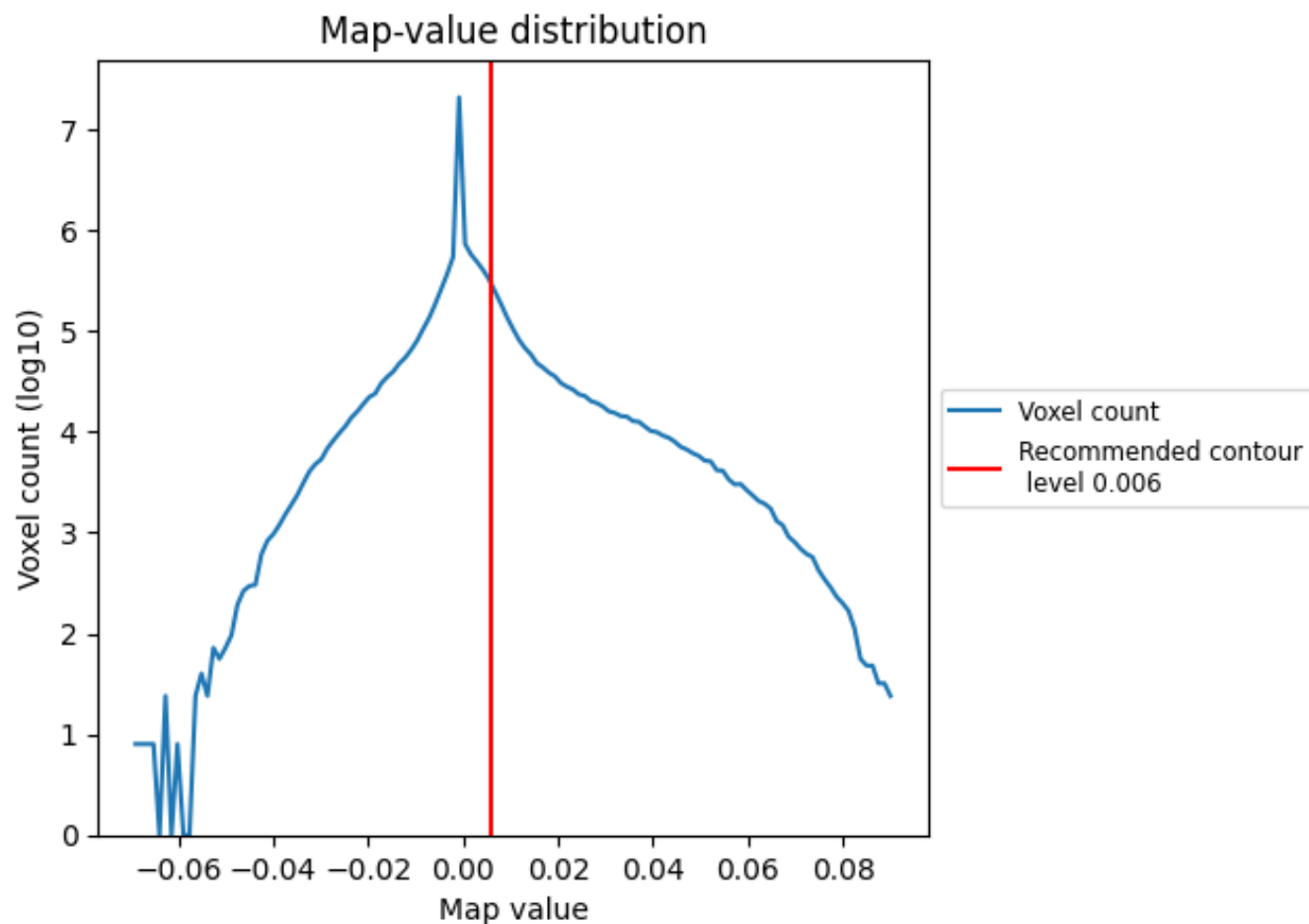
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

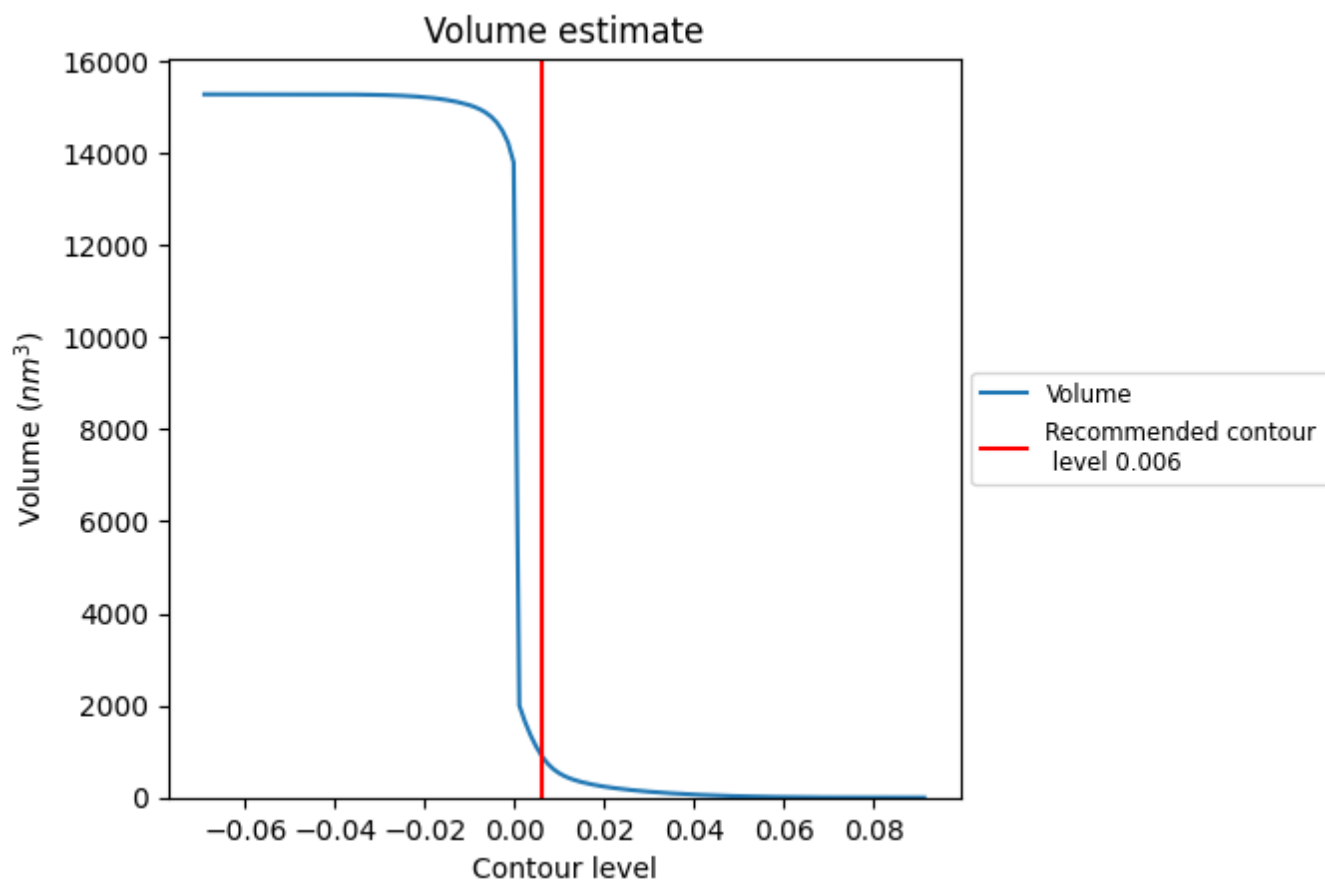
This section contains the results of statistical analysis of the map.

### 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.

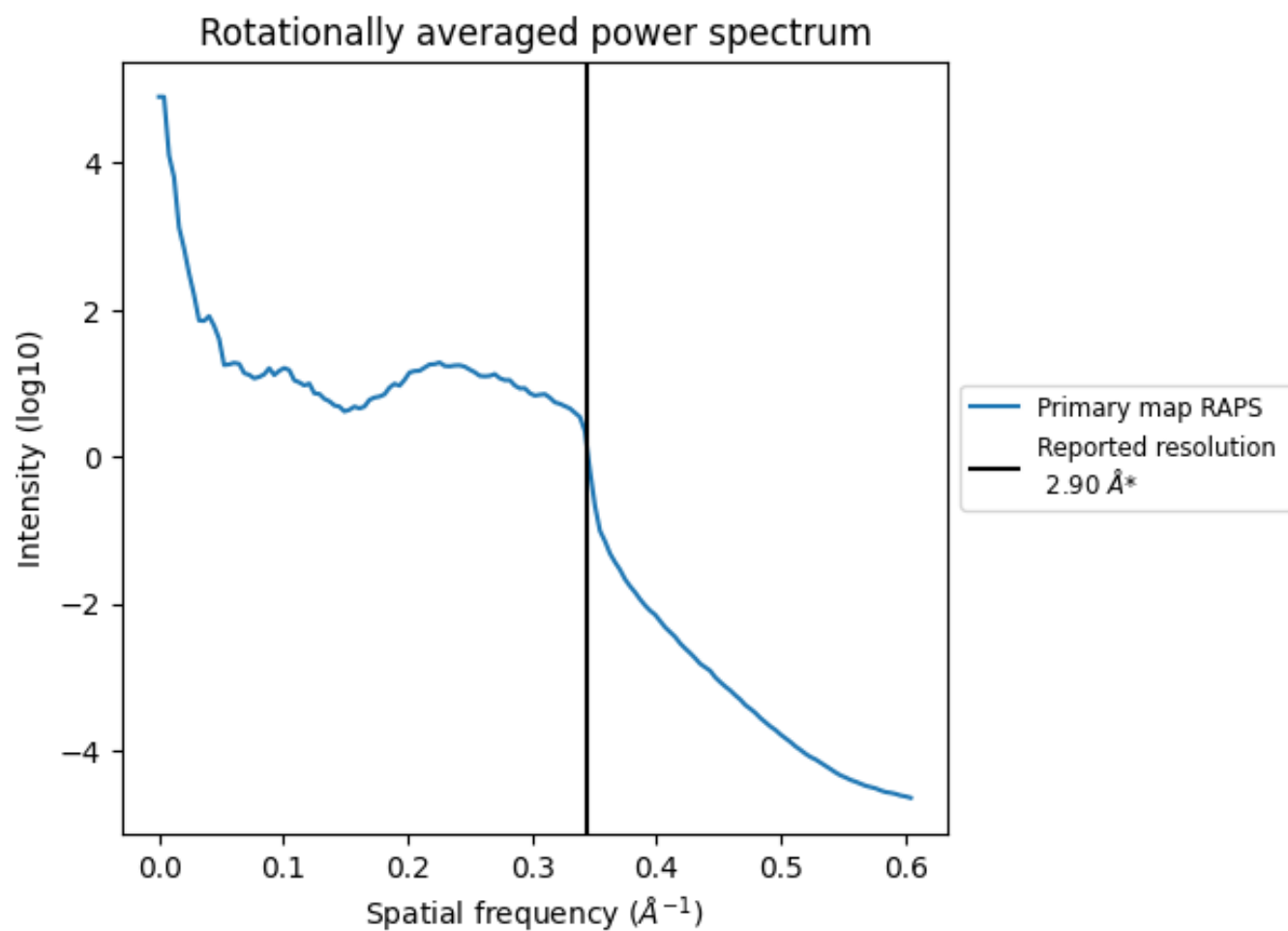
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 921 nm<sup>3</sup>; this corresponds to an approximate mass of 832 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 ⓘ

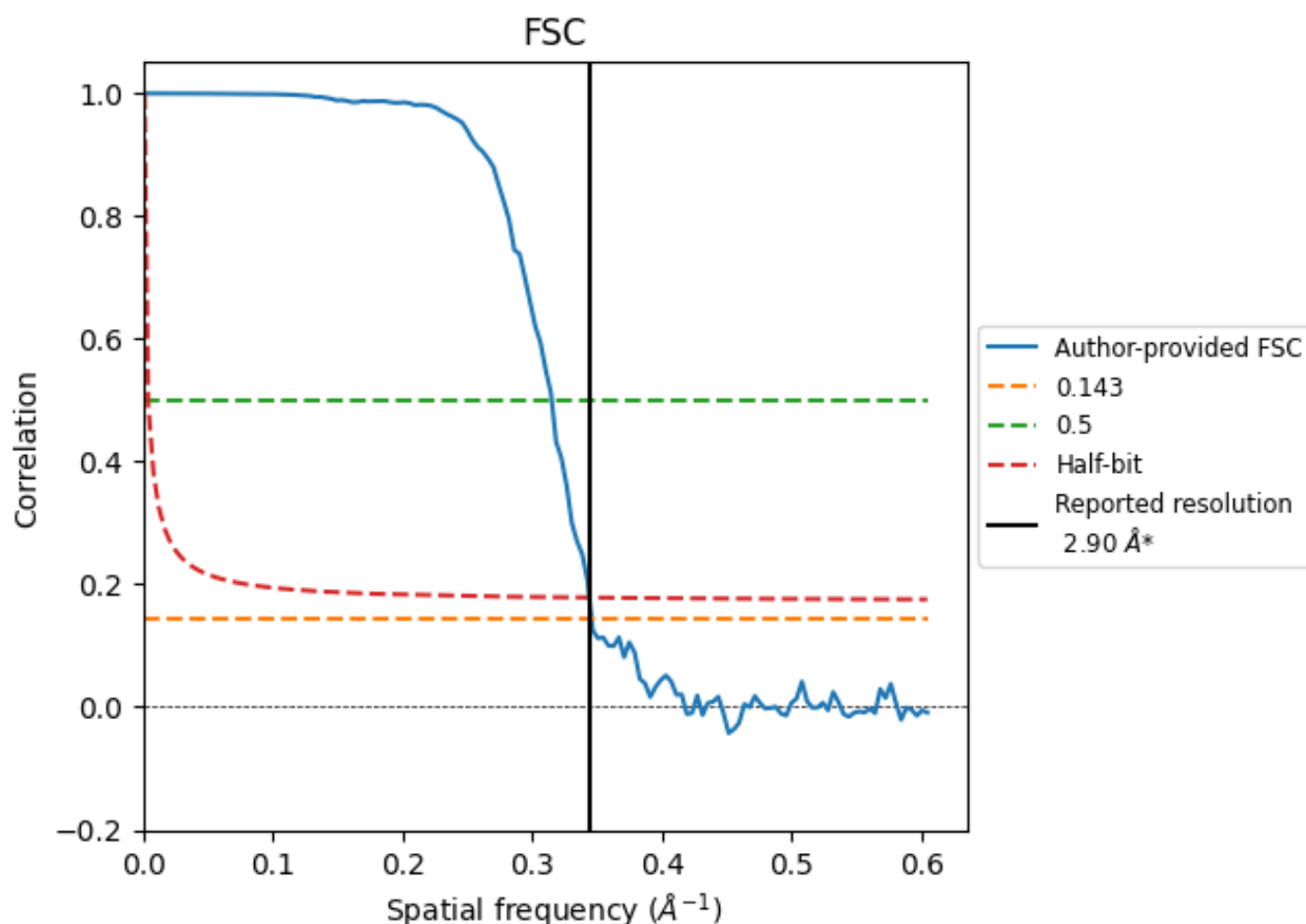


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | 2.89                               | 3.17 | 2.91     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

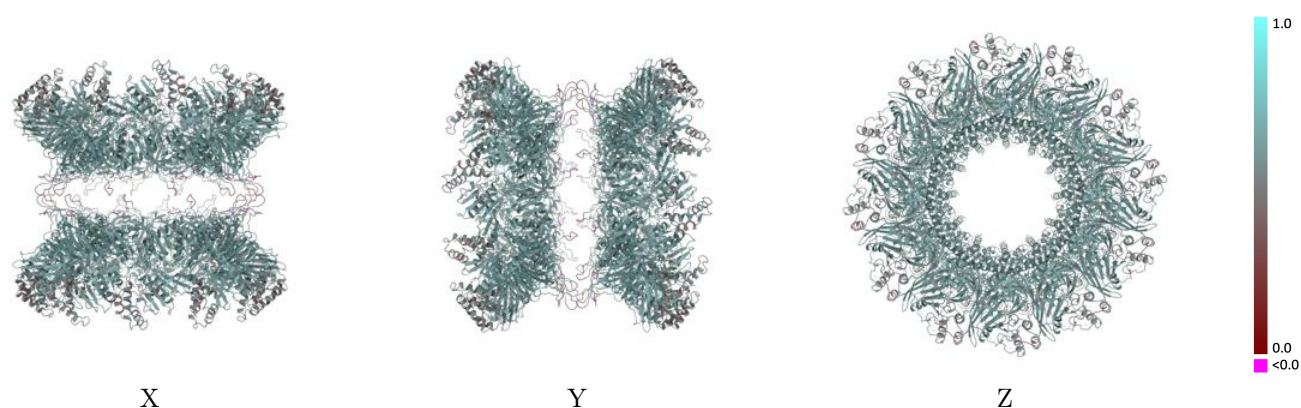
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-11023 and PDB model 6Z0U. Per-residue inclusion information can be found in section 3 on page 8.

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

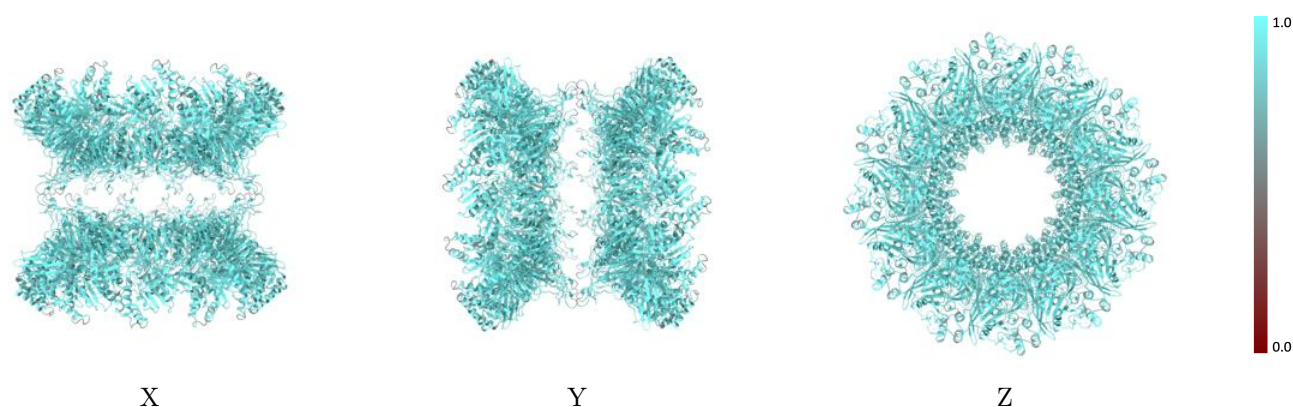
This section was not generated.

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



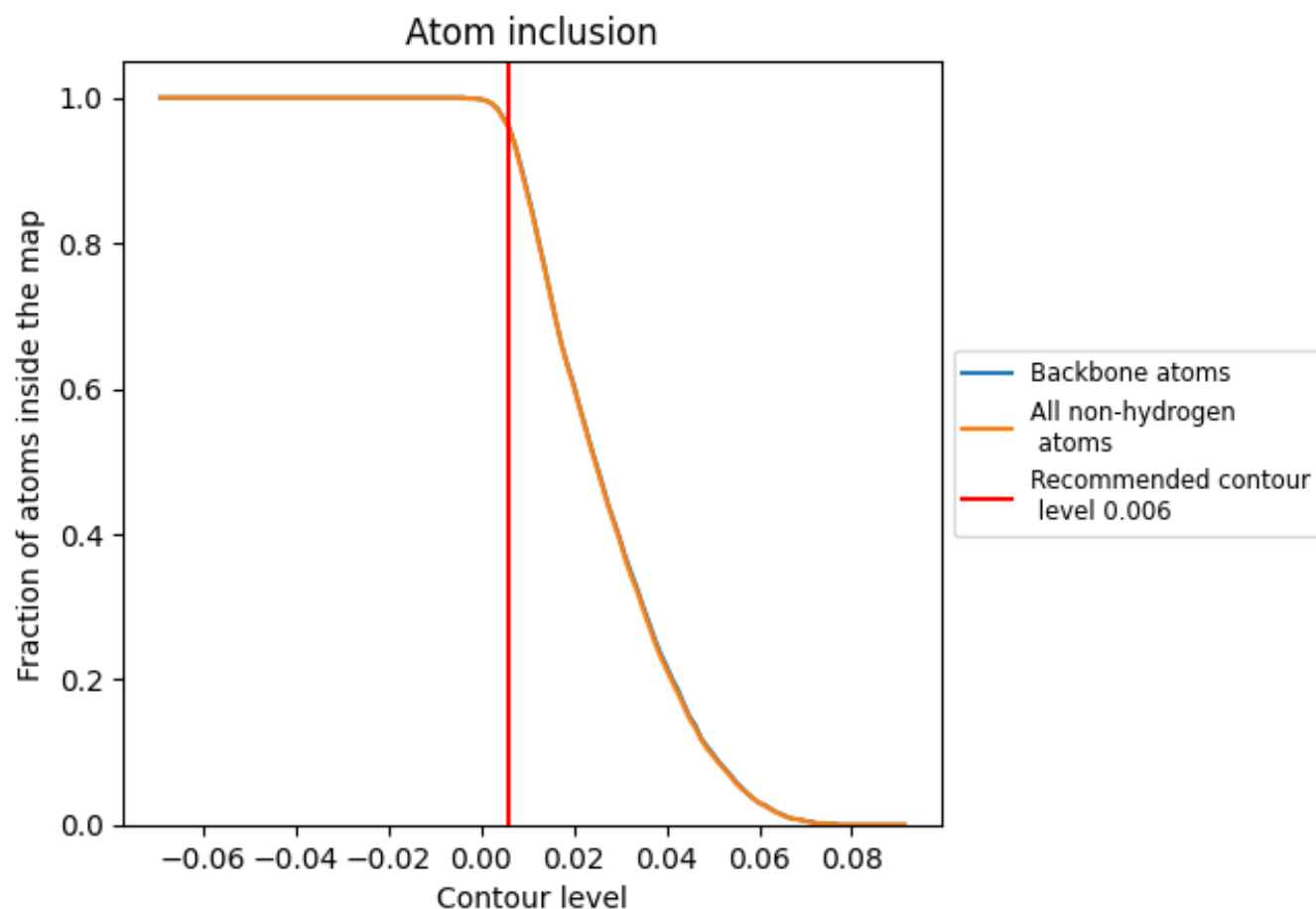
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9580   |  0.5950   |
| A     |  0.9590   |  0.5960   |
| BA    |  0.9600   |  0.5950   |
| C     |  0.9600   |  0.5960   |
| DA    |  0.9590   |  0.5940   |
| E     |  0.9580   |  0.5950   |
| FA    |  0.9590   |  0.5950   |
| G     |  0.9590   |  0.5960   |
| HA    |  0.9600   |  0.5950   |
| I     |  0.9600   |  0.5950   |
| JA    |  0.9580   |  0.5940   |
| K     |  0.9580   |  0.5950   |
| LA    |  0.9590   |  0.5960   |
| M     |  0.9590   |  0.5960   |
| NA    |  0.9600  |  0.5950  |
| O     |  0.9600 |  0.5950 |
| PA    |  0.9580 |  0.5950 |
| Q     |  0.9590 |  0.5930 |
| RA    |  0.9590 |  0.5950 |
| S     |  0.9590 |  0.5960 |
| TA    |  0.9600 |  0.5960 |
| V     |  0.9600 |  0.5940 |
| VA    |  0.9590 |  0.5950 |
| X     |  0.9590 |  0.5950 |
| Z     |  0.9590 |  0.5960 |

