



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:29 PM UTC

PDB ID : 7QG0 / pdb\_00007qg0  
EMDB ID : EMD-13951  
Title : Inhibitor-induced hSARM1 duplex  
Authors : Zalk, R.; Kahzma, T.; Guez-Haddad, J.  
Deposited on : 2021-12-07  
Resolution : 4.02 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:

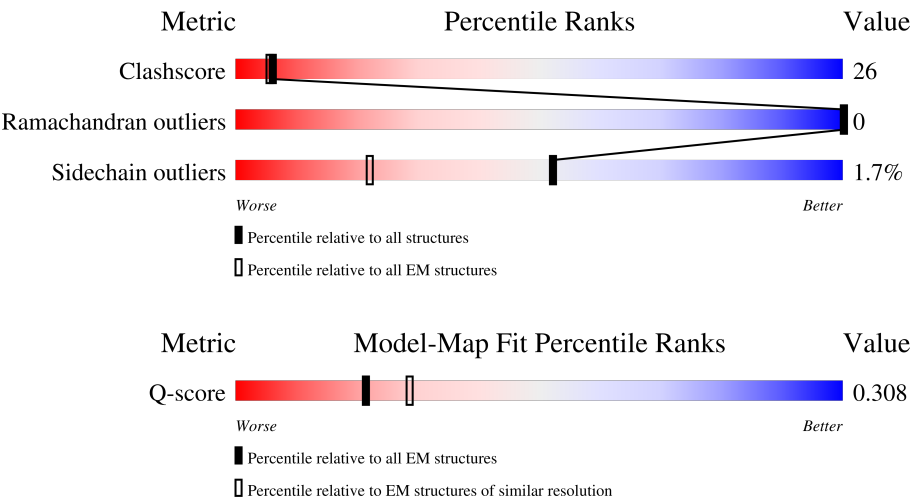
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.02 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 6727 ( 3.52 - 4.52 )                                     |

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     | 726    |                  |
| 1   | B     | 726    |                  |
| 1   | C     | 726    |                  |
| 1   | D     | 726    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 726    |                  |
| 1   | F     | 726    |                  |
| 1   | G     | 726    |                  |
| 1   | H     | 726    |                  |
| 1   | I     | 726    |                  |
| 1   | J     | 726    |                  |
| 1   | K     | 726    |                  |
| 1   | L     | 726    |                  |
| 1   | M     | 726    |                  |
| 1   | N     | 726    |                  |
| 1   | O     | 726    |                  |
| 1   | P     | 726    |                  |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 78880 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 NAD(+) hydrolase SARM1.

| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1   | A     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | B     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | C     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | D     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | E     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | F     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | G     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | H     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | I     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | J     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | K     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | L     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | M     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | N     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | O     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |
| 1   | P     | 631      | Total<br>4930 | C<br>3116 | N<br>885 | O<br>905 | S<br>24 | 0       | 0     |

There are 448 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| A     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| A     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| A     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| A     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| A     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| A     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| A     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| A     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| A     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| A     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| A     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| A     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| A     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| A     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| A     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| A     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| A     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| A     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| A     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| A     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| A     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| A     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| A     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| A     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| A     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| A     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| A     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| B     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| B     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| B     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| B     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| B     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| B     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| B     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| B     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| B     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| B     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| B     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| B     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| B     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| B     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| B     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| B     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| B     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| B     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| B     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| B     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| B     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| B     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| B     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| B     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| B     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| B     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| B     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| C     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| C     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| C     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| C     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| C     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| C     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| C     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| C     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| C     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| C     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| C     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| C     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| C     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| C     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| C     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| C     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| C     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| C     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| C     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| C     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| C     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| C     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| C     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| C     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| C     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| C     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| C     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| C     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| D     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| D     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| D     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| D     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| D     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| D     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| D     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| D     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| D     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| D     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| D     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| D     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| D     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| D     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| D     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| D     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| D     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| D     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| D     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| D     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| D     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| D     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| D     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| D     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| D     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| D     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| D     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| D     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| E     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| E     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| E     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| E     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| E     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| E     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| E     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| E     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| E     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| E     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| E     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| E     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| E     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| E     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| E     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| E     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| E     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| E     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| E     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| E     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| E     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| E     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| E     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| E     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| E     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| E     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| E     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| E     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| F     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| F     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| F     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| F     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| F     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| F     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| F     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| F     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| F     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| F     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| F     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| F     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| F     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| F     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| F     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| F     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| F     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| F     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| F     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| F     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| F     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| F     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| F     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| F     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| F     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| F     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| F     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| F     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| G     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| G     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| G     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| G     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| G     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| G     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| G     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| G     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| G     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| G     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| G     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| G     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| G     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| G     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| G     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| G     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| G     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| G     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| G     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| G     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| G     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| G     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| G     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| G     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| G     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| G     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| G     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| G     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| H     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| H     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| H     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| H     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| H     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| H     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| H     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| H     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| H     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| H     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| H     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| H     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| H     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| H     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| H     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| H     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| H     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| H     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| H     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| H     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| H     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| H     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| H     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| H     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| H     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| H     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| H     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
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| I     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| I     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| I     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| I     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| I     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| I     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| I     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| I     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| I     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| I     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| I     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| I     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| I     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| I     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| I     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| I     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| I     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| I     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
| I     | 20      | GLN      | -      | expression tag        | UNP Q6SZW1 |
| I     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| I     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| I     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| I     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| I     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| I     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| J     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| J     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| J     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
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| J     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| J     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
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| J     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| J     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| J     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
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| J     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| J     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| J     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| J     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
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| J     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
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| K     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
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| K     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| K     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| K     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| K     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| K     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| K     | 10      | ASP      | -      | expression tag        | UNP Q6SZW1 |
| K     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| K     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| K     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| K     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
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| K     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| K     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
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| K     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
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| K     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| K     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| K     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| K     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| K     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| L     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| L     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| L     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| L     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| L     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| L     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| L     | 5       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| L     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| L     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| L     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
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| L     | 11      | ILE      | -      | expression tag        | UNP Q6SZW1 |
| L     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
| L     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| L     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| L     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| L     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
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| L     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| L     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| L     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| L     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| M     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| M     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| M     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
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| M     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| M     | 4       | HIS      | -      | expression tag        | UNP Q6SZW1 |
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| M     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| M     | 8       | ASP      | -      | expression tag        | UNP Q6SZW1 |
| M     | 9       | TYR      | -      | expression tag        | UNP Q6SZW1 |
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| M     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| M     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
| M     | 16      | ASN      | -      | expression tag        | UNP Q6SZW1 |
| M     | 17      | LEU      | -      | expression tag        | UNP Q6SZW1 |
| M     | 18      | TYR      | -      | expression tag        | UNP Q6SZW1 |
| M     | 19      | PHE      | -      | expression tag        | UNP Q6SZW1 |
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| M     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| N     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |
| N     | 0       | SER      | -      | expression tag        | UNP Q6SZW1 |
| N     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| N     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
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| N     | 12      | PRO      | -      | expression tag        | UNP Q6SZW1 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| N     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
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| N     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| N     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
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| N     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| N     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| N     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
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| O     | 1       | TYR      | -      | expression tag        | UNP Q6SZW1 |
| O     | 2       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| O     | 3       | HIS      | -      | expression tag        | UNP Q6SZW1 |
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| O     | 6       | HIS      | -      | expression tag        | UNP Q6SZW1 |
| O     | 7       | HIS      | -      | expression tag        | UNP Q6SZW1 |
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| O     | 13      | THR      | -      | expression tag        | UNP Q6SZW1 |
| O     | 14      | THR      | -      | expression tag        | UNP Q6SZW1 |
| O     | 15      | GLU      | -      | expression tag        | UNP Q6SZW1 |
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| O     | 21      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| O     | 22      | ALA      | -      | expression tag        | UNP Q6SZW1 |
| O     | 23      | MET      | -      | expression tag        | UNP Q6SZW1 |
| O     | 24      | GLY      | -      | expression tag        | UNP Q6SZW1 |
| O     | 25      | SER      | -      | expression tag        | UNP Q6SZW1 |
| O     | 642     | GLN      | GLU    | conflict              | UNP Q6SZW1 |
| P     | -1      | MET      | -      | initiating methionine | UNP Q6SZW1 |

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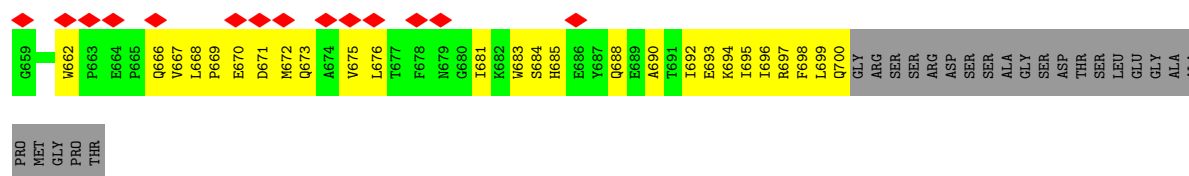


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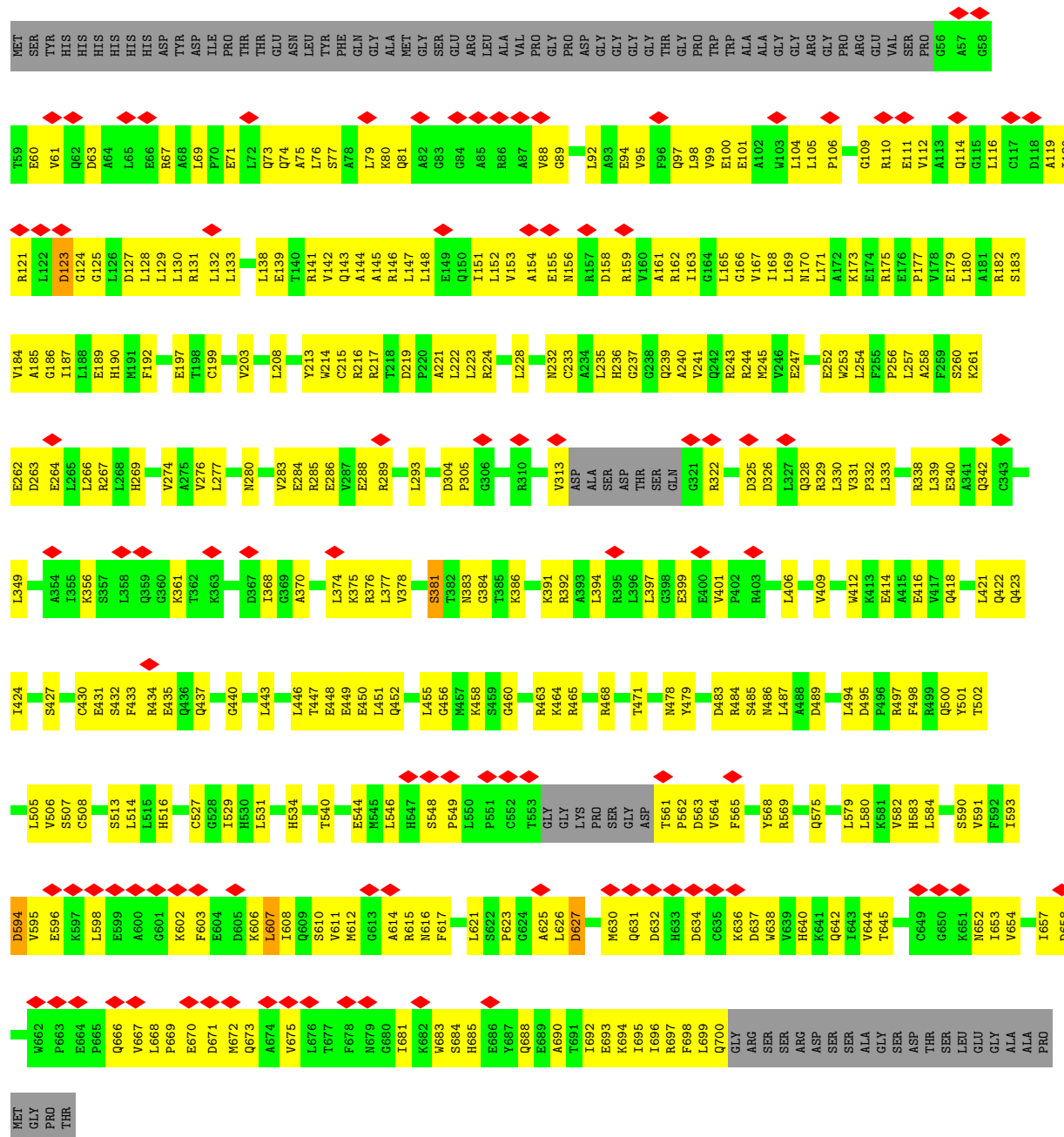
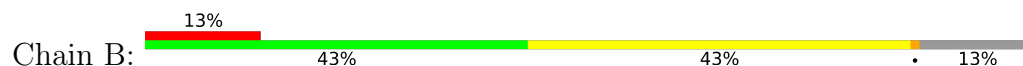
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
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| P     | 1       | TYR      | -      | expression tag | UNP Q6SZW1 |
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| P     | 11      | ILE      | -      | expression tag | UNP Q6SZW1 |
| P     | 12      | PRO      | -      | expression tag | UNP Q6SZW1 |
| P     | 13      | THR      | -      | expression tag | UNP Q6SZW1 |
| P     | 14      | THR      | -      | expression tag | UNP Q6SZW1 |
| P     | 15      | GLU      | -      | expression tag | UNP Q6SZW1 |
| P     | 16      | ASN      | -      | expression tag | UNP Q6SZW1 |
| P     | 17      | LEU      | -      | expression tag | UNP Q6SZW1 |
| P     | 18      | TYR      | -      | expression tag | UNP Q6SZW1 |
| P     | 19      | PHE      | -      | expression tag | UNP Q6SZW1 |
| P     | 20      | GLN      | -      | expression tag | UNP Q6SZW1 |
| P     | 21      | GLY      | -      | expression tag | UNP Q6SZW1 |
| P     | 22      | ALA      | -      | expression tag | UNP Q6SZW1 |
| P     | 23      | MET      | -      | expression tag | UNP Q6SZW1 |
| P     | 24      | GLY      | -      | expression tag | UNP Q6SZW1 |
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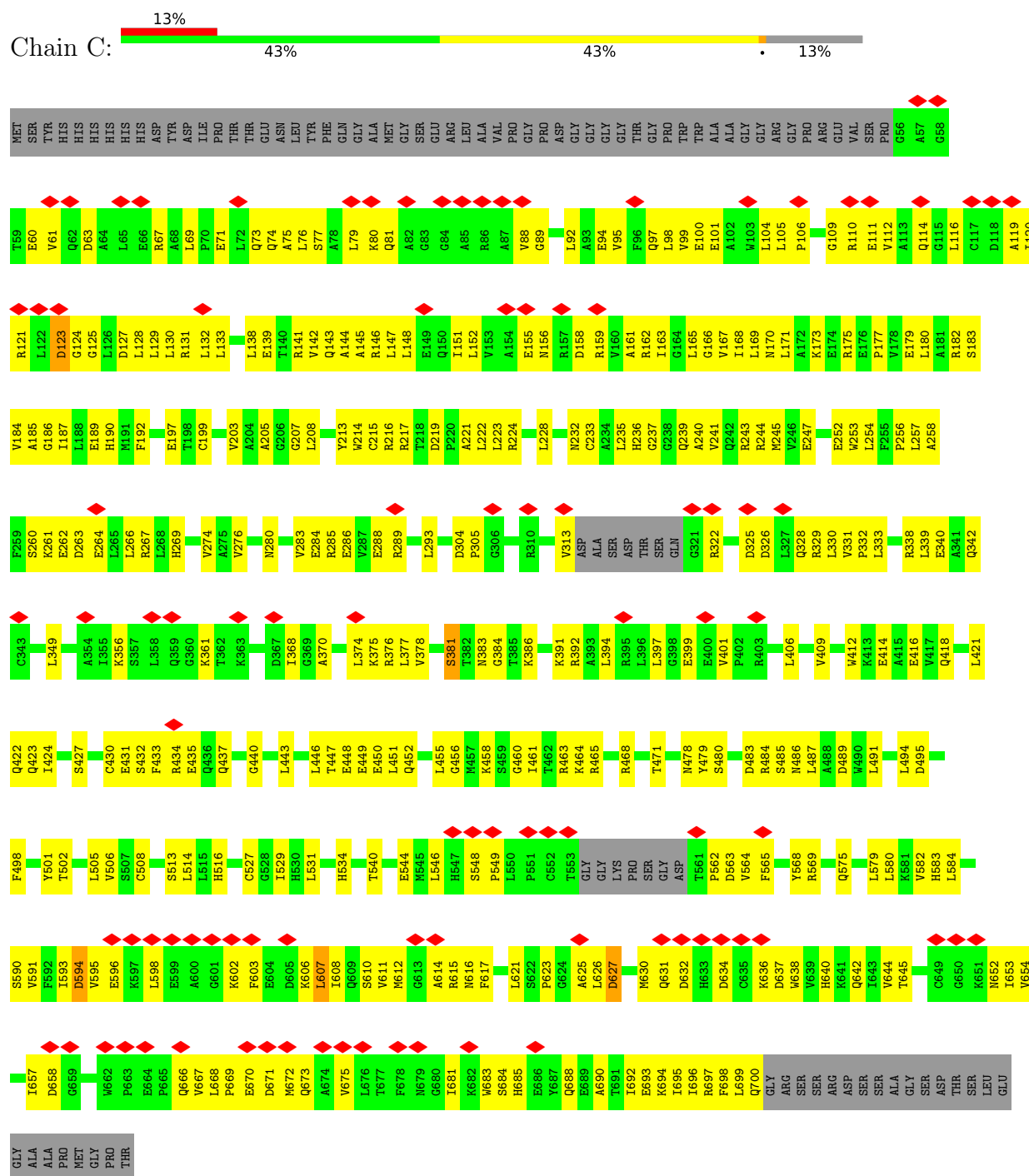




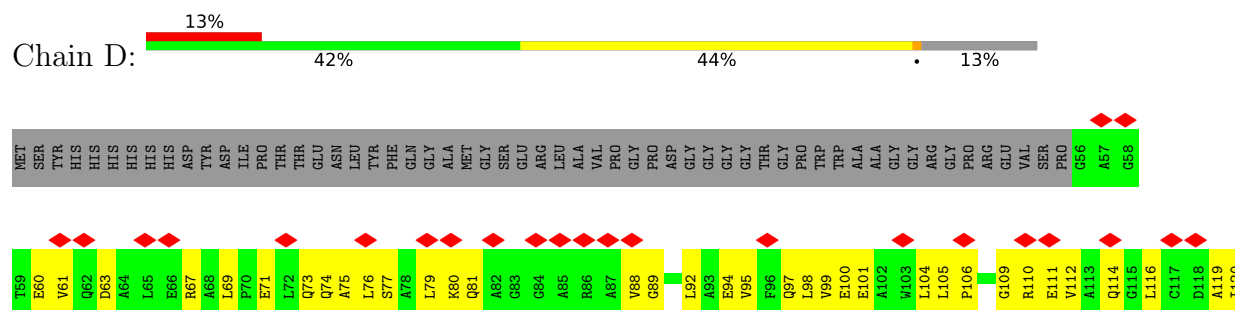
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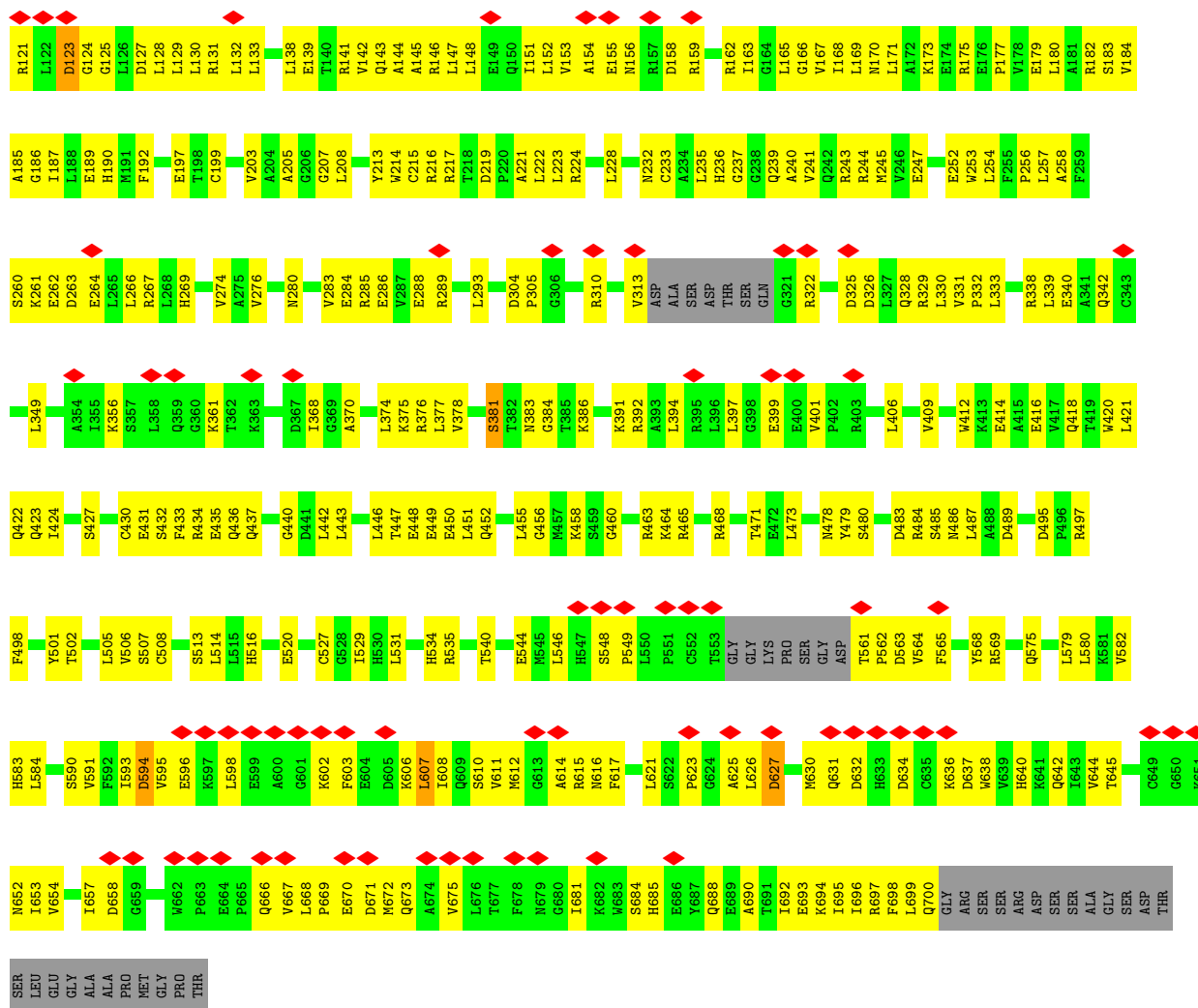


• Molecule 1: NAD(+) hydrolase SARM1

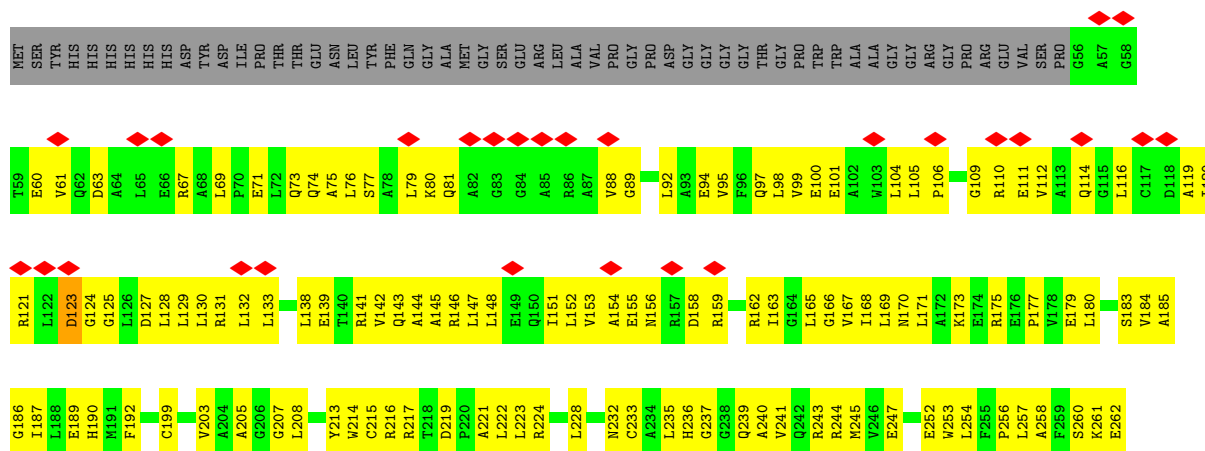
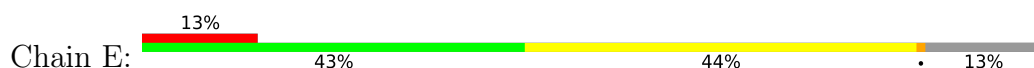


• Molecule 1: NAD(+) hydrolase SARM1

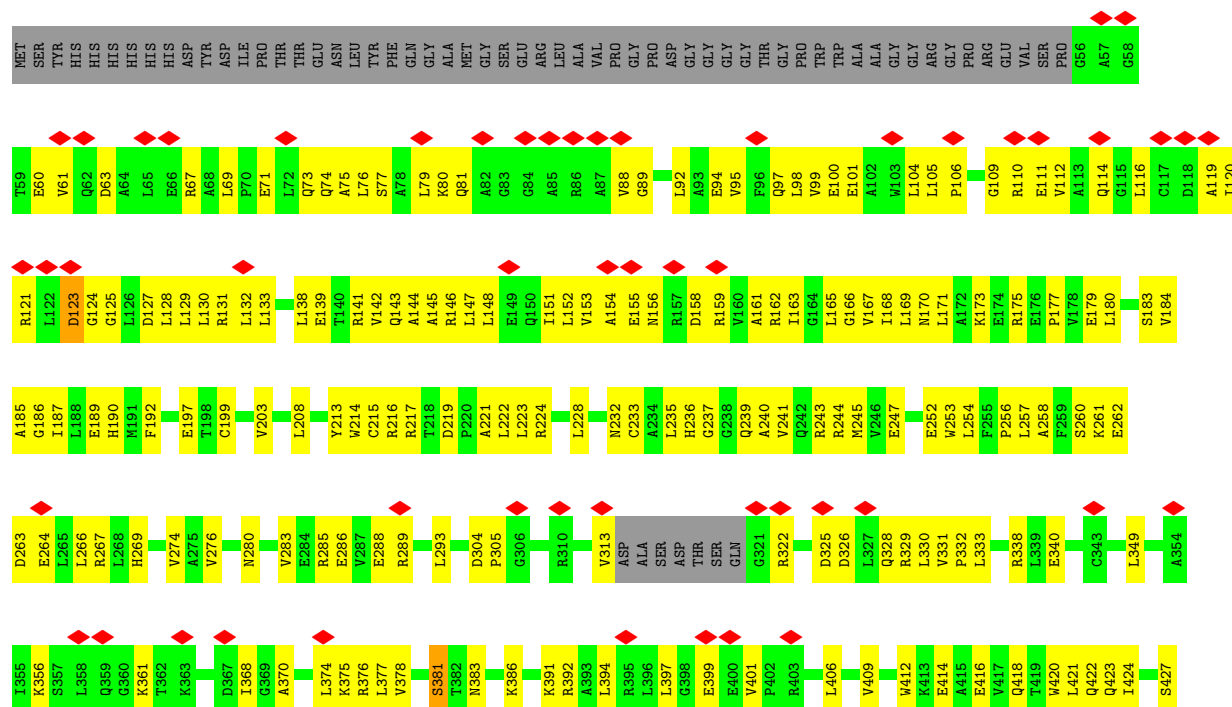
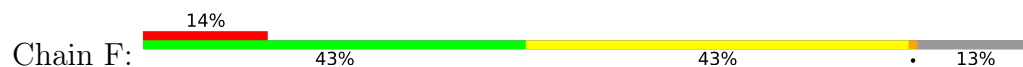


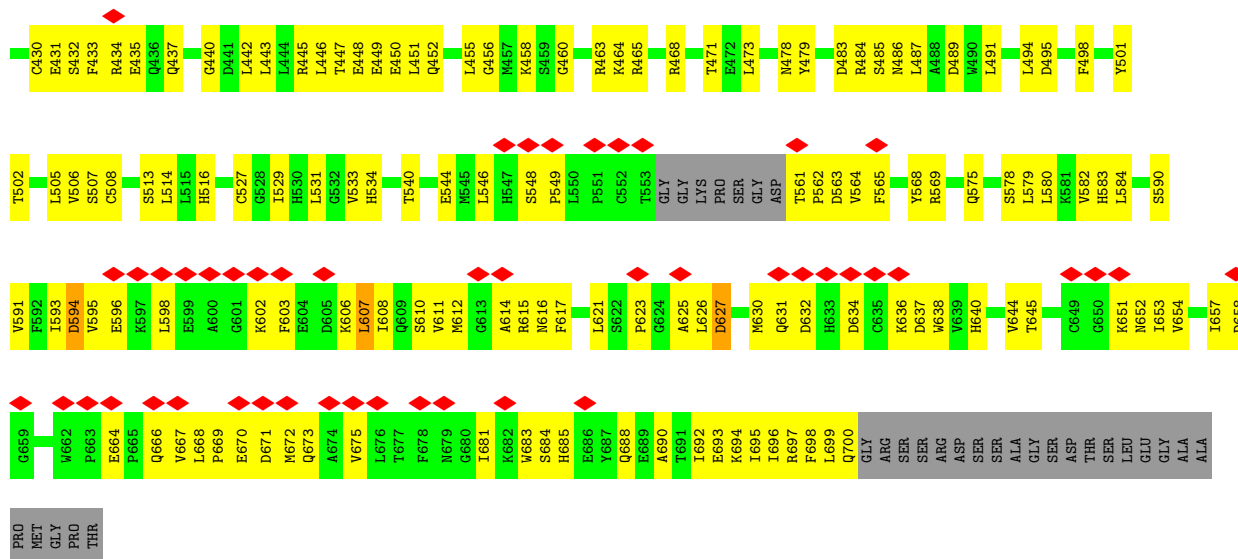


• Molecule 1: NAD(+) hydrolase SARM1

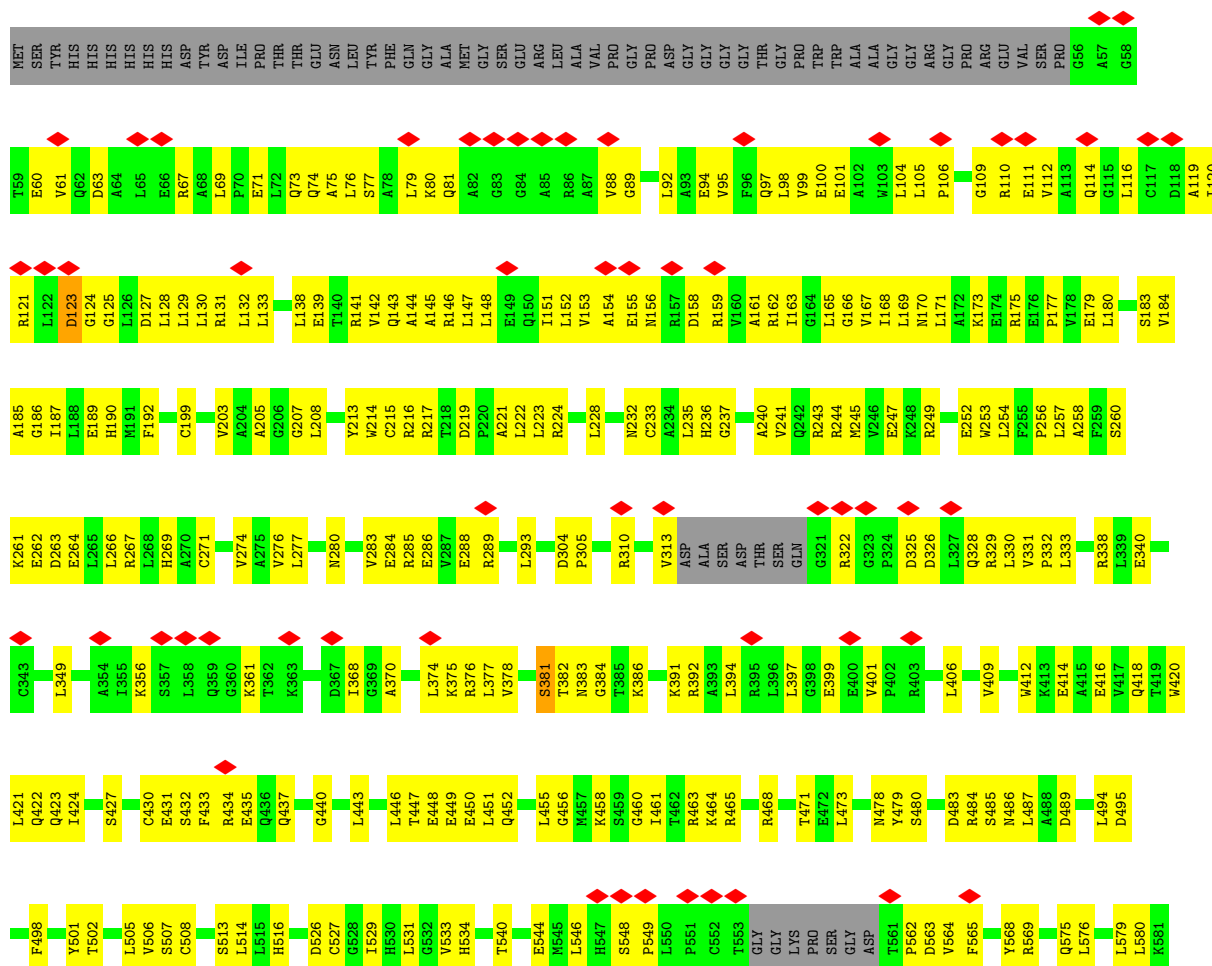
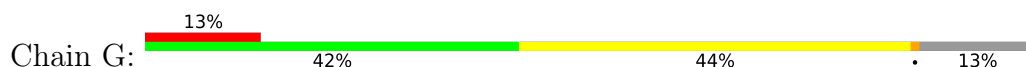


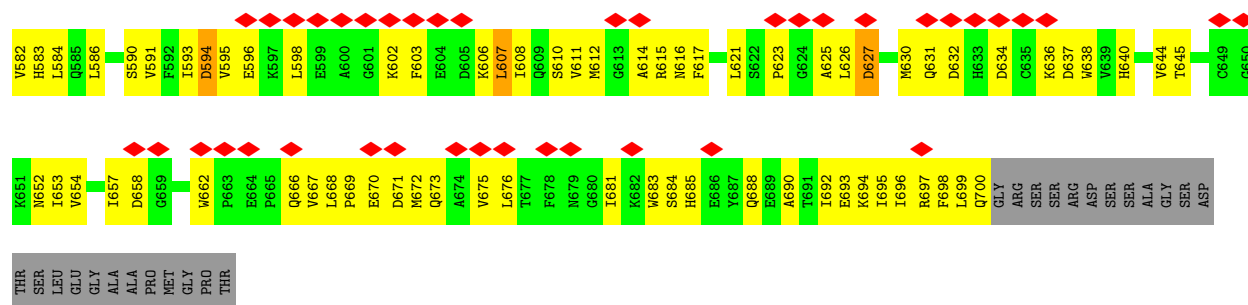
- Molecule 1: NAD(+) hydrolase SARM1



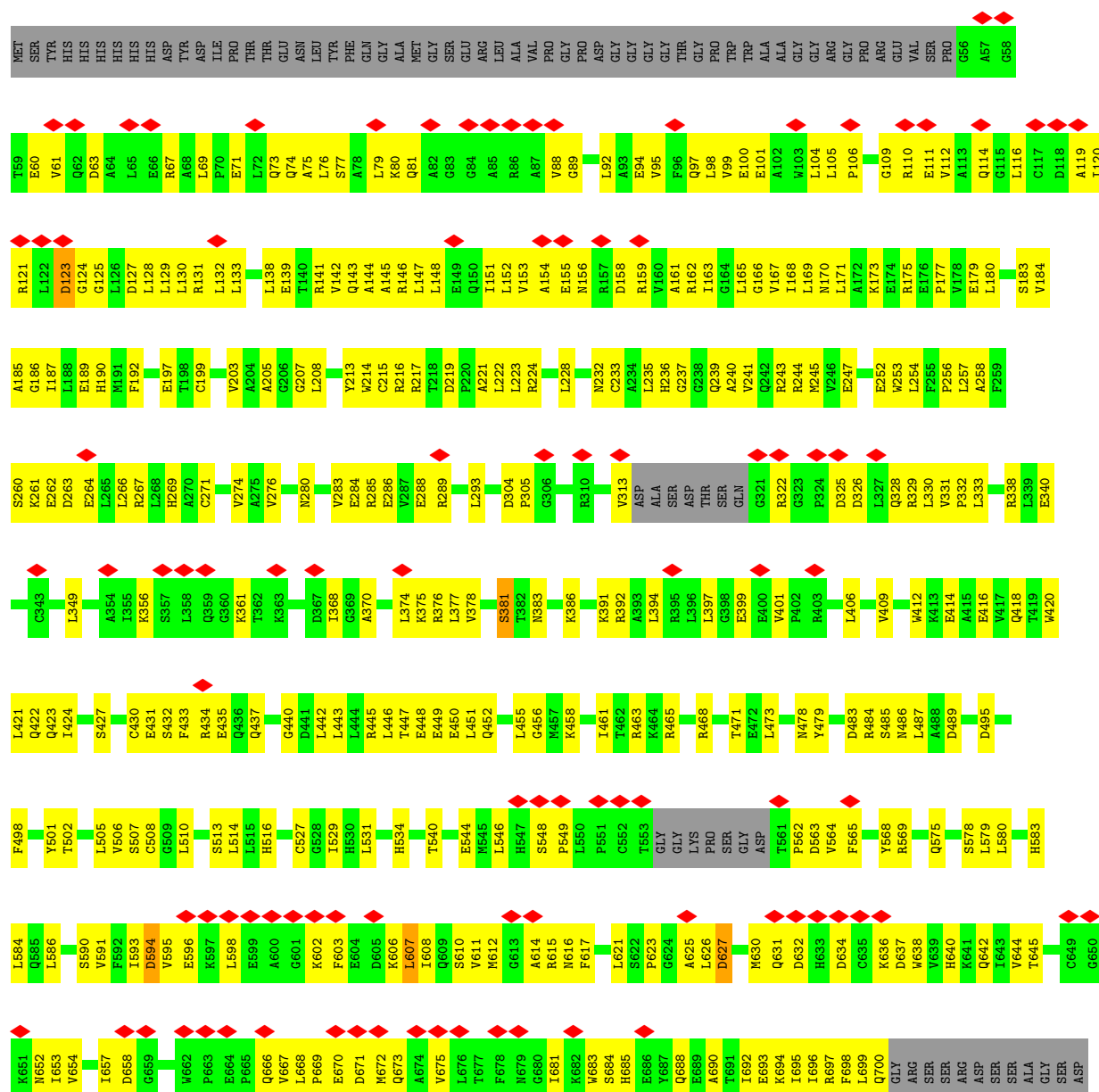
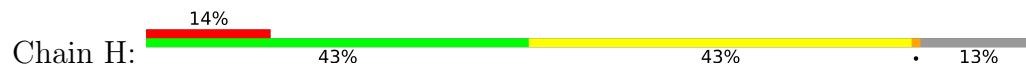


• Molecule 1: NAD(+) hydrolase SARM1





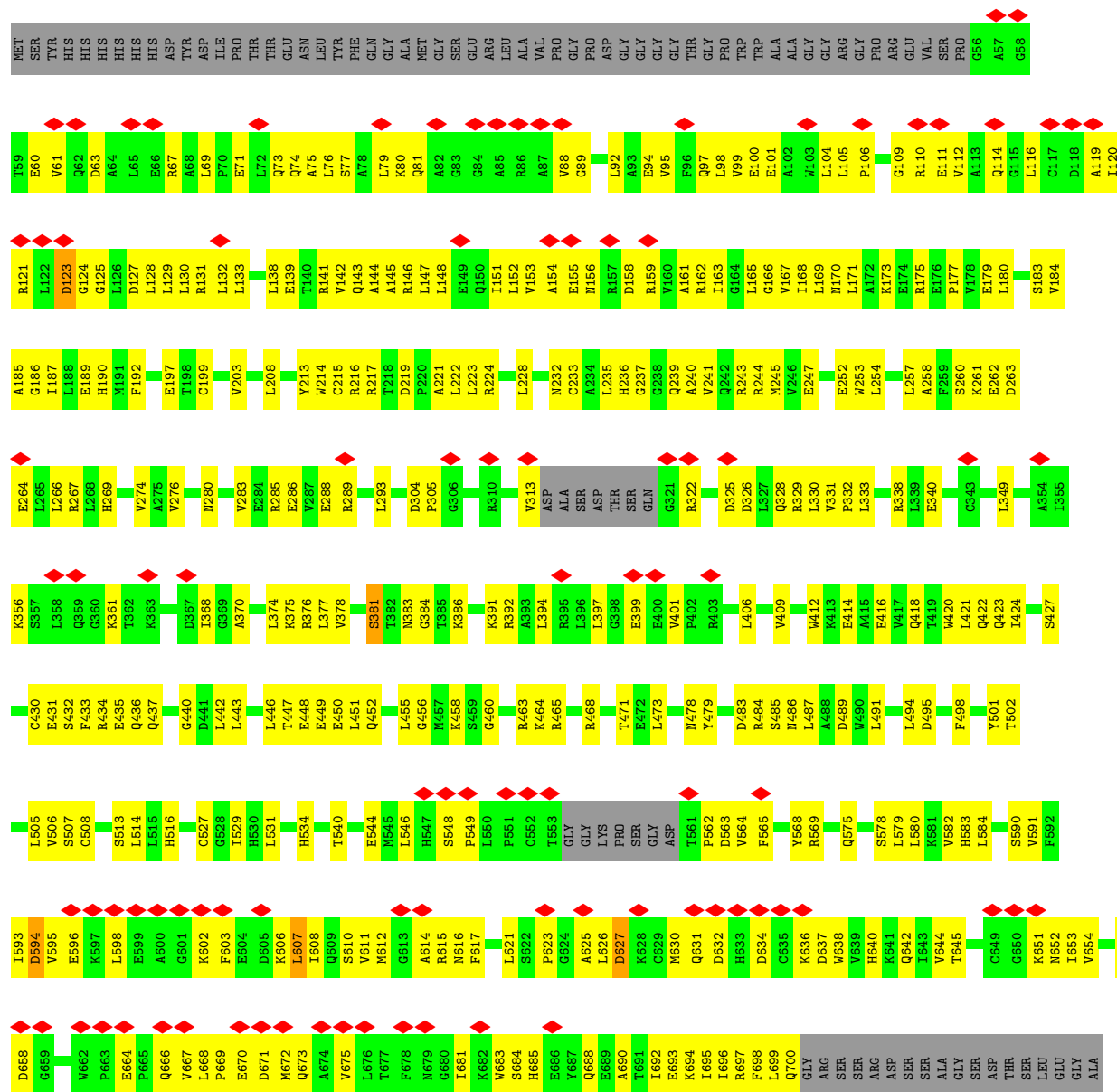
● Molecule 1: NAD(+) hydrolase SARM1



THR  
SER  
LEU  
GLY  
GLY  
ALA  
ALA  
PRO  
MET  
GLY  
PRO  
THR

• Molecule 1: NAD(+) hydrolase SARM1

Chain I: 13% 43% 43% 13%



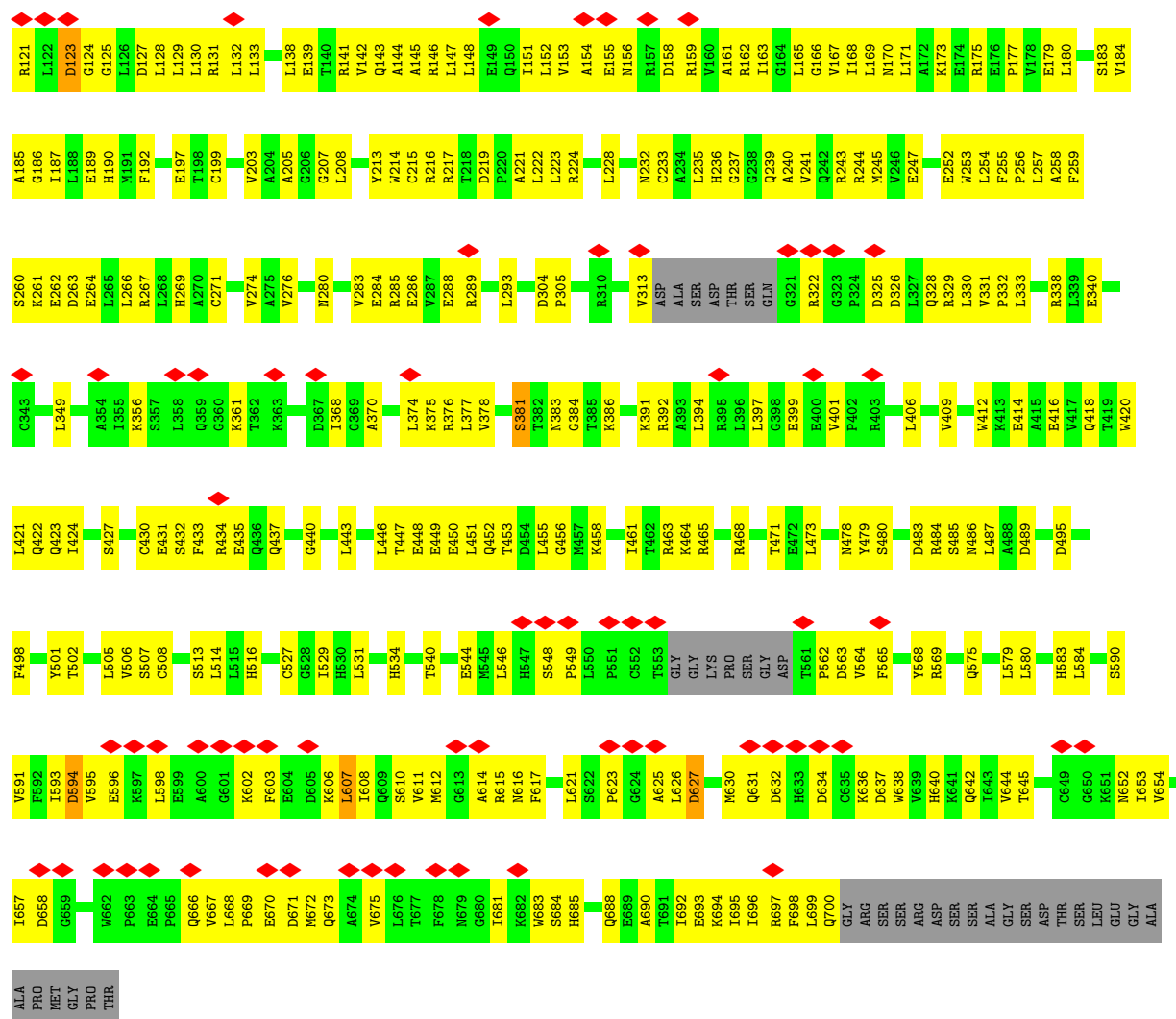
ALA  
PRO  
MET  
GLY  
PRO  
THR

• Molecule 1: NAD(+) hydrolase SARM1

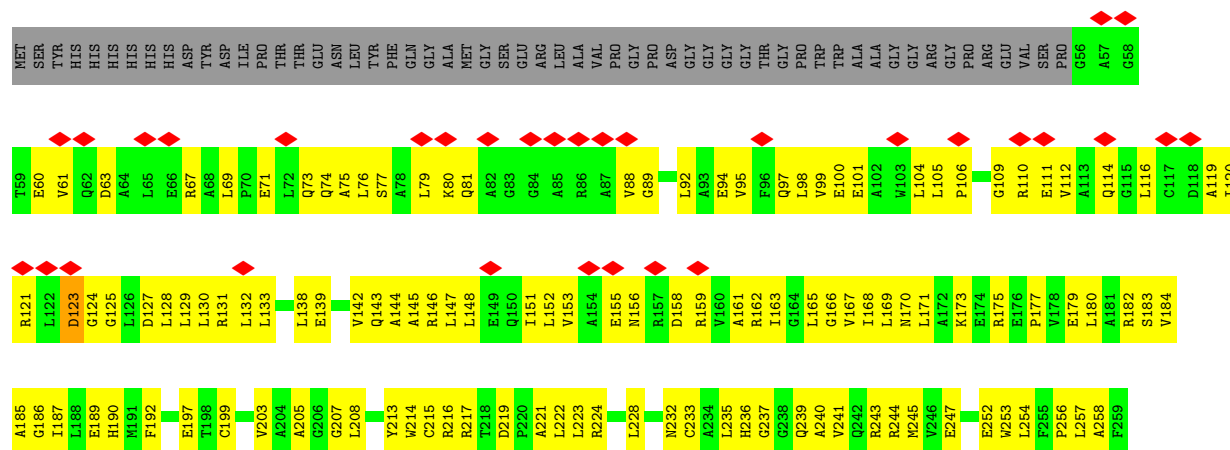
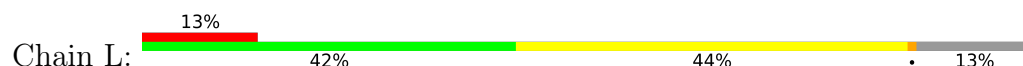
Chain J: 13% 42% 44% 13%

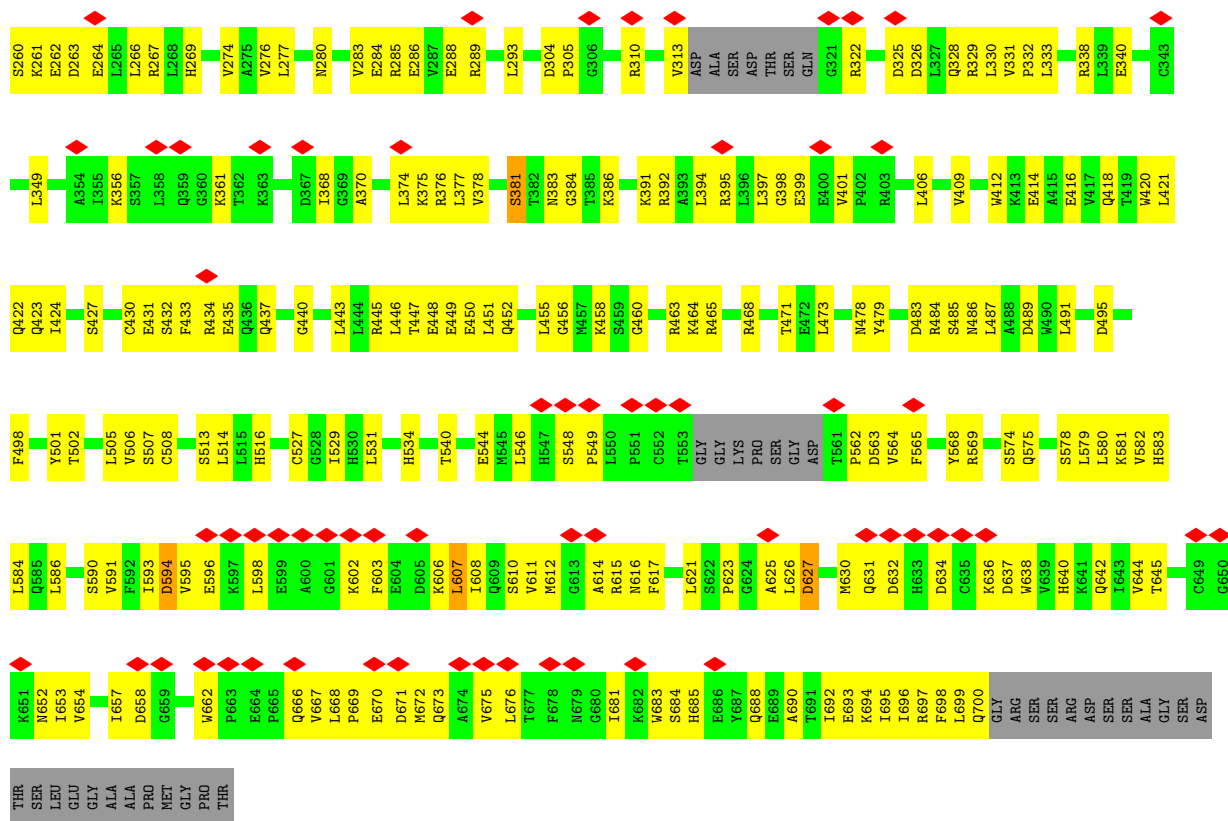




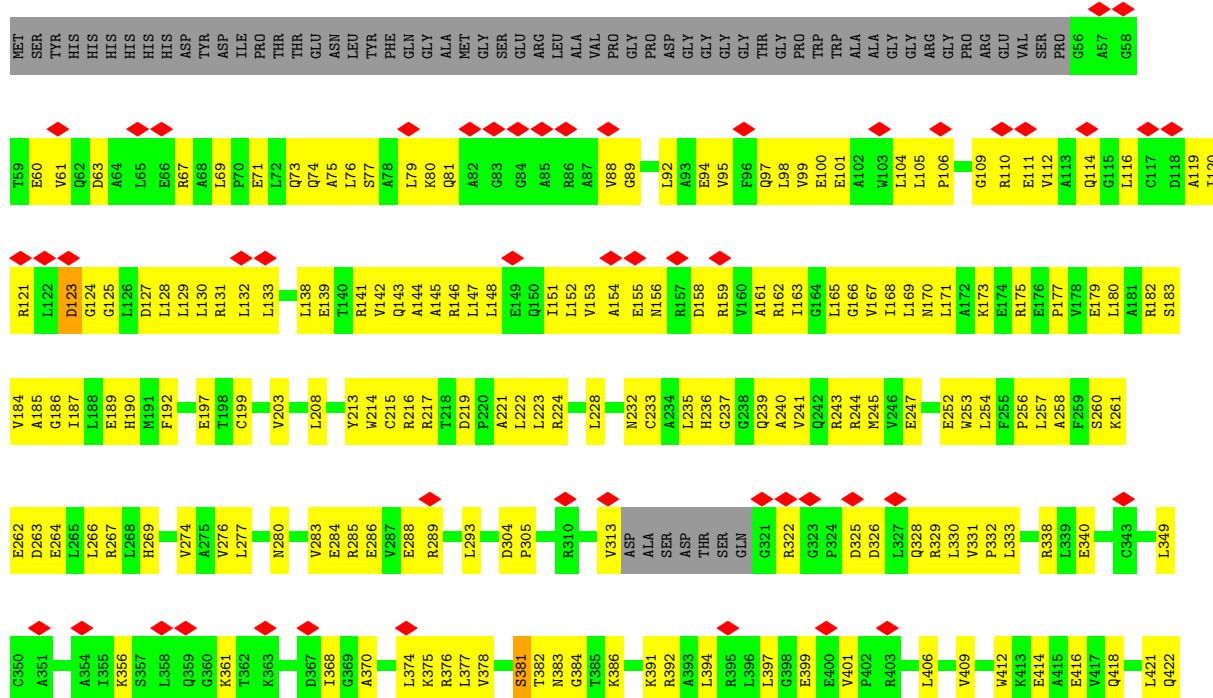


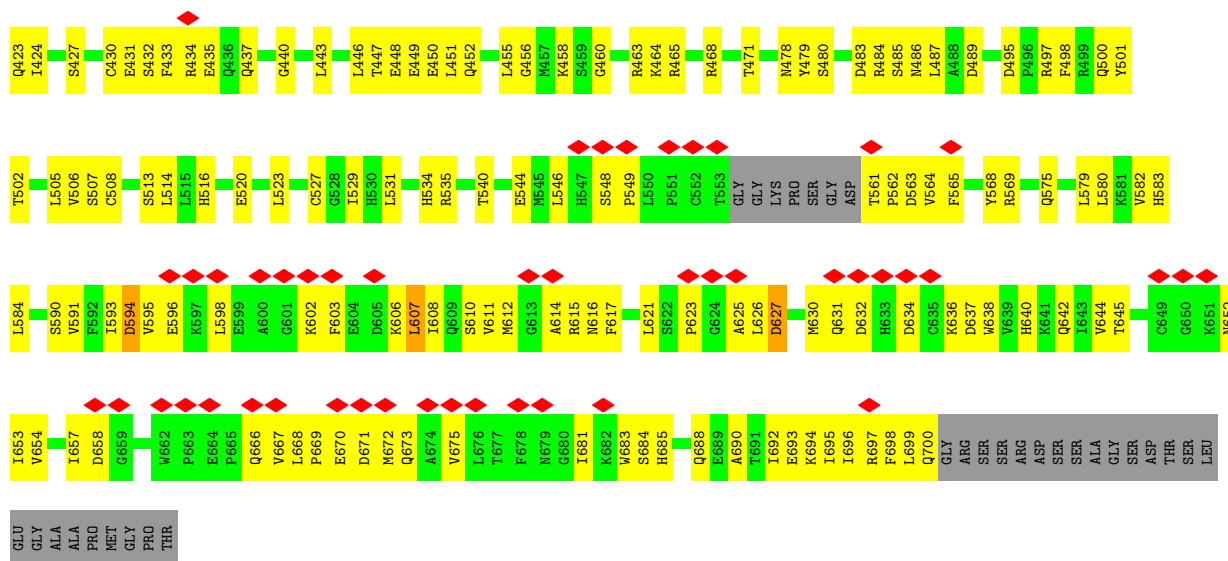
• Molecule 1: NAD(+) hydrolase SARM1



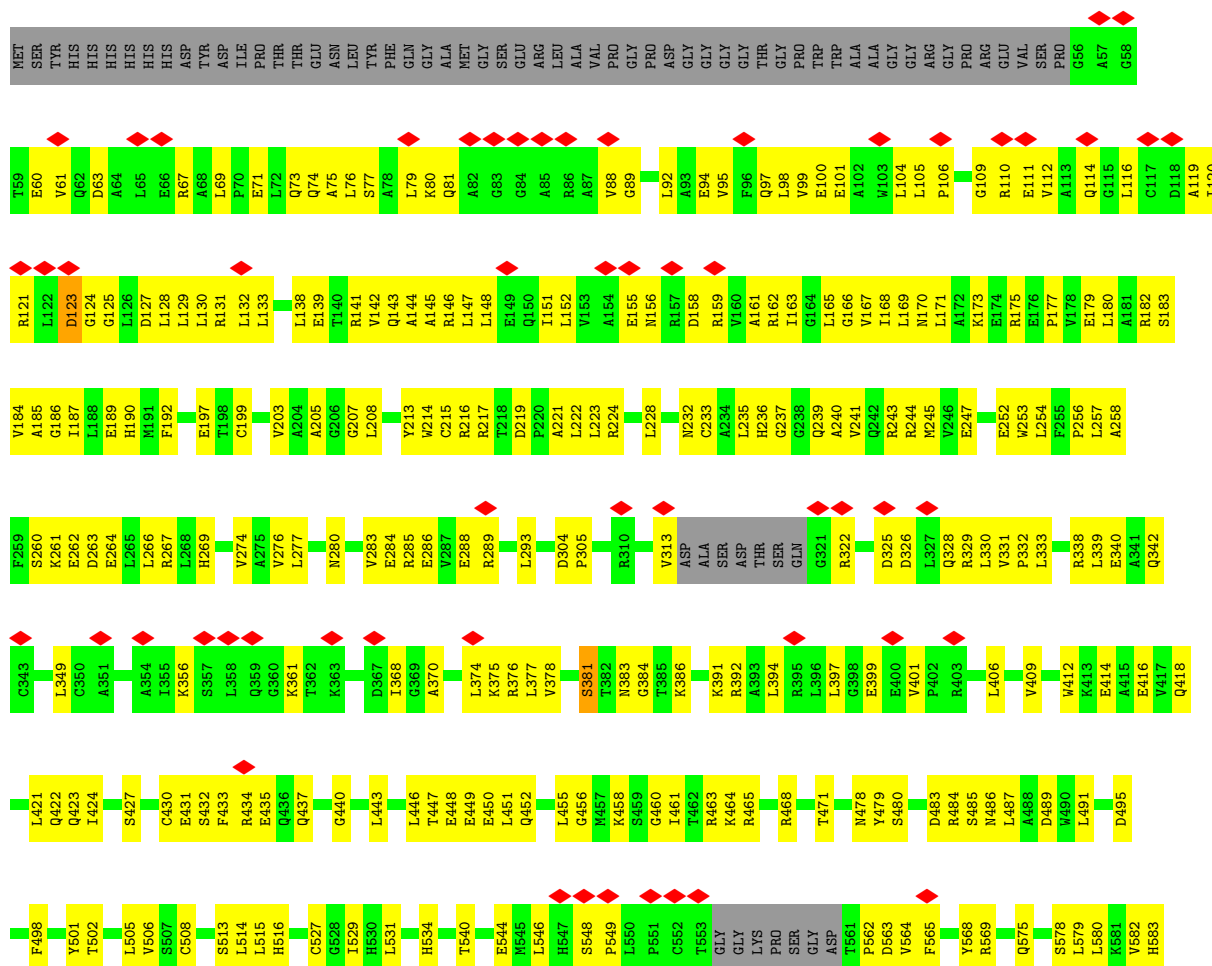
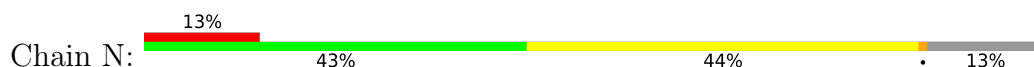


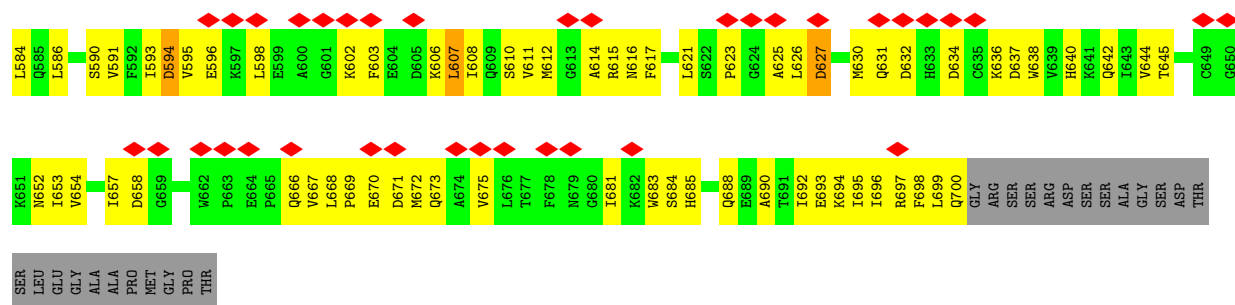
• Molecule 1: NAD(+) hydrolase SARM1



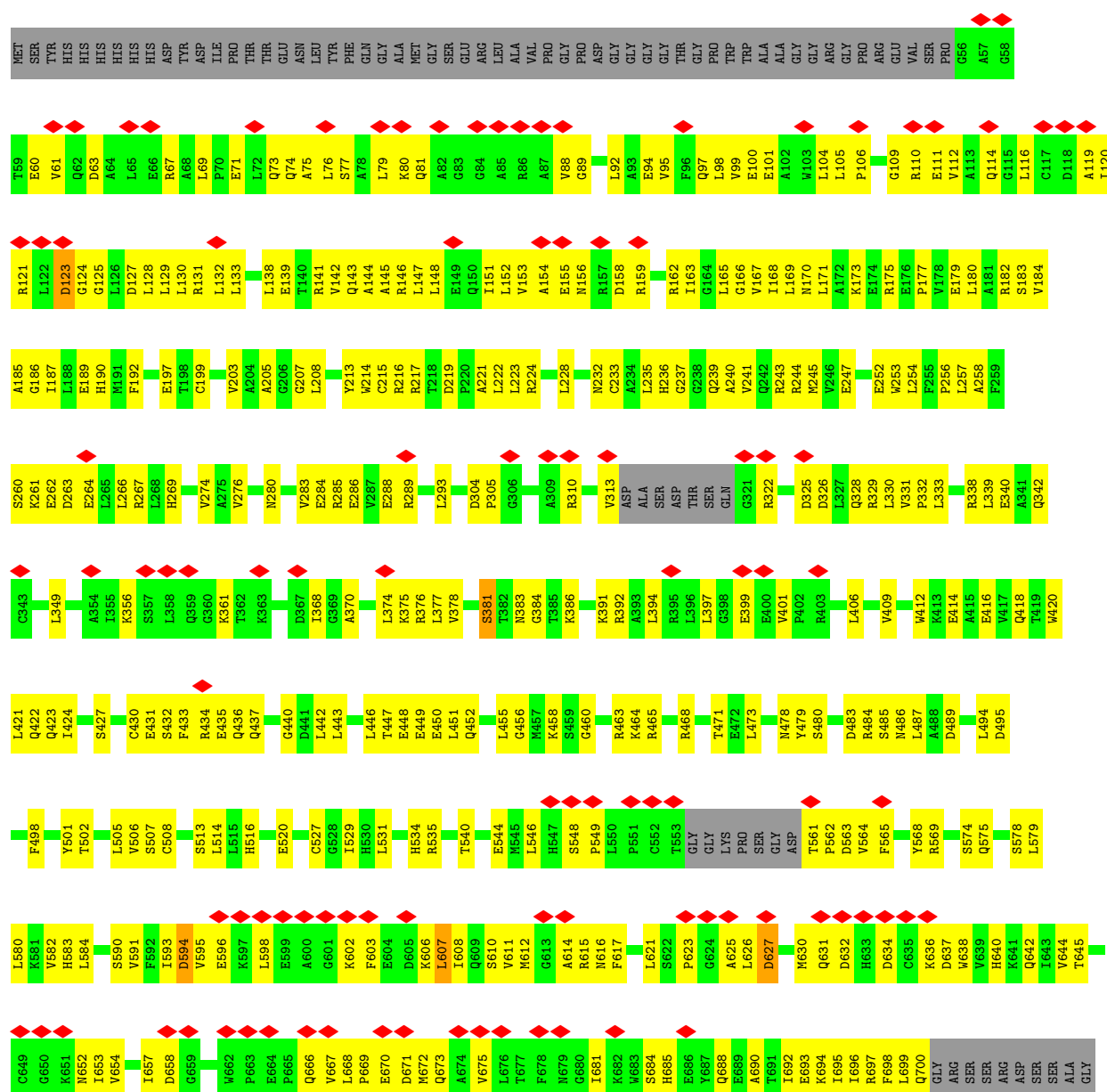


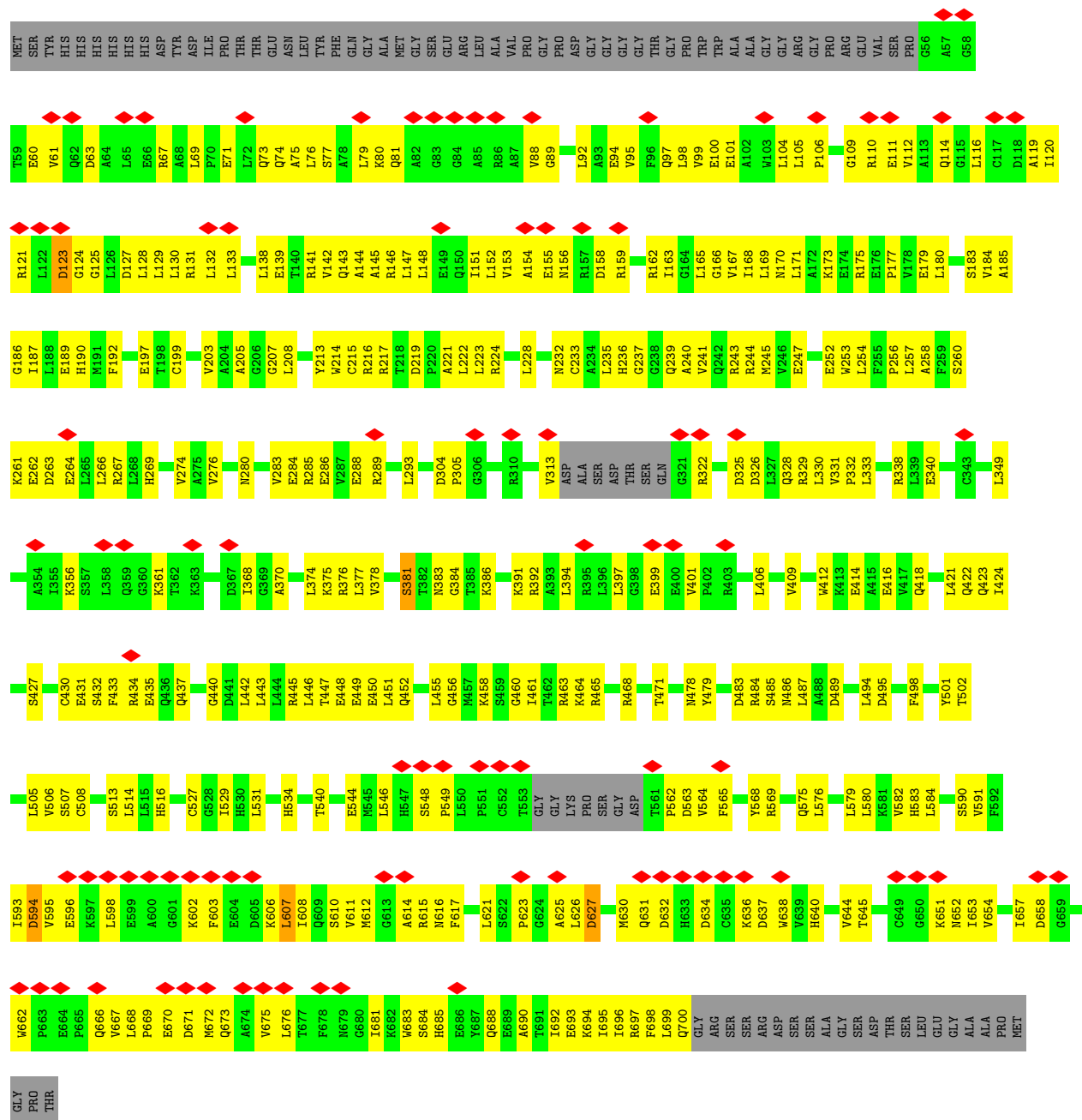
• Molecule 1: NAD(+) hydrolase SARM1





● Molecule 1: NAD(+) hydrolase SARM1





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 28303                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.749                                   | Depositor |
| Minimum map value                    | -0.361                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.035                                   | Depositor |
| Recommended contour level            | 0.13                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 335.6, 335.6, 335.6                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.839, 0.839, 0.839                     | Depositor |

## 5 Model quality [i](#)

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

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     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | B     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | C     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | D     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | E     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | F     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | G     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | H     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | I     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | J     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | K     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | L     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | M     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | N     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | O     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| 1   | P     | 0.30         | 0/5012      | 0.52        | 0/6776      |
| All | All   | 0.30         | 0/80192     | 0.52        | 0/108416    |

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 [i](#)

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



| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4930  | 0        | 5018     | 262     | 0            |
| 1   | B     | 4930  | 0        | 5018     | 260     | 0            |
| 1   | C     | 4930  | 0        | 5018     | 266     | 0            |
| 1   | D     | 4930  | 0        | 5018     | 271     | 0            |
| 1   | E     | 4930  | 0        | 5018     | 272     | 0            |
| 1   | F     | 4930  | 0        | 5018     | 275     | 0            |
| 1   | G     | 4930  | 0        | 5018     | 279     | 0            |
| 1   | H     | 4930  | 0        | 5018     | 268     | 0            |
| 1   | I     | 4930  | 0        | 5018     | 267     | 0            |
| 1   | J     | 4930  | 0        | 5018     | 268     | 0            |
| 1   | K     | 4930  | 0        | 5018     | 276     | 0            |
| 1   | L     | 4930  | 0        | 5018     | 280     | 0            |
| 1   | M     | 4930  | 0        | 5018     | 272     | 0            |
| 1   | N     | 4930  | 0        | 5018     | 278     | 0            |
| 1   | O     | 4930  | 0        | 5018     | 274     | 0            |
| 1   | P     | 4930  | 0        | 5018     | 269     | 0            |
| All | All   | 78880 | 0        | 80288    | 4157    | 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 26.

All (4157) 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:D:430:CYS:HB3 | 1:D:434:ARG:HH21 | 1.27                     | 0.99              |
| 1:E:430:CYS:HB3 | 1:E:434:ARG:HH21 | 1.27                     | 0.99              |
| 1:O:430:CYS:HB3 | 1:O:434:ARG:HH21 | 1.27                     | 0.99              |
| 1:P:430:CYS:HB3 | 1:P:434:ARG:HH21 | 1.27                     | 0.99              |
| 1:C:430:CYS:HB3 | 1:C:434:ARG:HH21 | 1.27                     | 0.99              |
| 1:M:430:CYS:HB3 | 1:M:434:ARG:HH21 | 1.27                     | 0.99              |
| 1:N:430:CYS:HB3 | 1:N:434:ARG:HH21 | 1.27                     | 0.99              |
| 1:B:430:CYS:HB3 | 1:B:434:ARG:HH21 | 1.27                     | 0.98              |
| 1:L:430:CYS:HB3 | 1:L:434:ARG:HH21 | 1.27                     | 0.98              |
| 1:F:430:CYS:HB3 | 1:F:434:ARG:HH21 | 1.27                     | 0.98              |
| 1:I:430:CYS:HB3 | 1:I:434:ARG:HH21 | 1.27                     | 0.98              |
| 1:K:430:CYS:HB3 | 1:K:434:ARG:HH21 | 1.27                     | 0.98              |
| 1:A:430:CYS:HB3 | 1:A:434:ARG:HH21 | 1.27                     | 0.98              |
| 1:G:430:CYS:HB3 | 1:G:434:ARG:HH21 | 1.27                     | 0.97              |
| 1:H:430:CYS:HB3 | 1:H:434:ARG:HH21 | 1.27                     | 0.97              |
| 1:J:430:CYS:HB3 | 1:J:434:ARG:HH21 | 1.27                     | 0.97              |
| 1:C:465:ARG:NH2 | 1:D:437:GLN:OE1  | 2.06                     | 0.87              |
| 1:I:437:GLN:OE1 | 1:P:465:ARG:NH2  | 2.07                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:239:GLN:HB2  | 1:K:478:ASN:HD21 | 1.41                     | 0.84              |
| 1:N:465:ARG:NH2  | 1:O:437:GLN:OE1  | 2.11                     | 0.83              |
| 1:B:276:VAL:HA   | 1:B:333:LEU:HD21 | 1.62                     | 0.81              |
| 1:M:276:VAL:HA   | 1:M:333:LEU:HD21 | 1.62                     | 0.81              |
| 1:N:276:VAL:HA   | 1:N:333:LEU:HD21 | 1.62                     | 0.81              |
| 1:C:276:VAL:HA   | 1:C:333:LEU:HD21 | 1.62                     | 0.81              |
| 1:E:276:VAL:HA   | 1:E:333:LEU:HD21 | 1.62                     | 0.81              |
| 1:P:276:VAL:HA   | 1:P:333:LEU:HD21 | 1.62                     | 0.80              |
| 1:D:276:VAL:HA   | 1:D:333:LEU:HD21 | 1.62                     | 0.80              |
| 1:O:276:VAL:HA   | 1:O:333:LEU:HD21 | 1.62                     | 0.80              |
| 1:G:276:VAL:HA   | 1:G:333:LEU:HD21 | 1.62                     | 0.80              |
| 1:J:276:VAL:HA   | 1:J:333:LEU:HD21 | 1.62                     | 0.80              |
| 1:J:465:ARG:NH2  | 1:K:437:GLN:OE1  | 2.14                     | 0.80              |
| 1:A:276:VAL:HA   | 1:A:333:LEU:HD21 | 1.62                     | 0.79              |
| 1:F:276:VAL:HA   | 1:F:333:LEU:HD21 | 1.62                     | 0.79              |
| 1:L:276:VAL:HA   | 1:L:333:LEU:HD21 | 1.62                     | 0.79              |
| 1:I:276:VAL:HA   | 1:I:333:LEU:HD21 | 1.62                     | 0.79              |
| 1:H:276:VAL:HA   | 1:H:333:LEU:HD21 | 1.62                     | 0.79              |
| 1:K:276:VAL:HA   | 1:K:333:LEU:HD21 | 1.62                     | 0.79              |
| 1:J:197:GLU:OE1  | 1:K:384:GLY:N    | 2.15                     | 0.78              |
| 1:D:328:GLN:NE2  | 1:E:416:GLU:OE2  | 2.16                     | 0.77              |
| 1:L:197:GLU:OE1  | 1:M:384:GLY:N    | 2.16                     | 0.77              |
| 1:K:235:LEU:O    | 1:K:329:ARG:NH1  | 2.18                     | 0.77              |
| 1:H:235:LEU:O    | 1:H:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:L:235:LEU:O    | 1:L:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:B:235:LEU:O    | 1:B:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:E:217:ARG:HH12 | 1:F:685:HIS:HB3  | 1.51                     | 0.76              |
| 1:J:235:LEU:O    | 1:J:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:M:235:LEU:O    | 1:M:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:N:235:LEU:O    | 1:N:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:A:235:LEU:O    | 1:A:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:C:235:LEU:O    | 1:C:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:G:235:LEU:O    | 1:G:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:F:235:LEU:O    | 1:F:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:I:235:LEU:O    | 1:I:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:E:235:LEU:O    | 1:E:329:ARG:NH1  | 2.18                     | 0.76              |
| 1:F:239:GLN:HB2  | 1:G:478:ASN:HD21 | 1.50                     | 0.75              |
| 1:O:235:LEU:O    | 1:O:329:ARG:NH1  | 2.18                     | 0.75              |
| 1:P:235:LEU:O    | 1:P:329:ARG:NH1  | 2.18                     | 0.75              |
| 1:A:437:GLN:OE1  | 1:H:465:ARG:NH2  | 2.19                     | 0.75              |
| 1:D:235:LEU:O    | 1:D:329:ARG:NH1  | 2.18                     | 0.75              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:127:ASP:HB2 | 1:O:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:C:127:ASP:HB2 | 1:C:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:D:127:ASP:HB2 | 1:D:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:P:127:ASP:HB2 | 1:P:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:B:127:ASP:HB2 | 1:B:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:E:127:ASP:HB2 | 1:E:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:N:127:ASP:HB2 | 1:N:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:M:127:ASP:HB2 | 1:M:131:ARG:HH12 | 1.52                     | 0.75              |
| 1:A:127:ASP:HB2 | 1:A:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:A:384:GLY:N   | 1:H:197:GLU:OE1  | 2.19                     | 0.74              |
| 1:I:127:ASP:HB2 | 1:I:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:L:127:ASP:HB2 | 1:L:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:F:127:ASP:HB2 | 1:F:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:H:127:ASP:HB2 | 1:H:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:J:127:ASP:HB2 | 1:J:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:K:127:ASP:HB2 | 1:K:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:A:465:ARG:NH2 | 1:B:437:GLN:OE1  | 2.21                     | 0.74              |
| 1:G:127:ASP:HB2 | 1:G:131:ARG:HH12 | 1.52                     | 0.74              |
| 1:L:239:GLN:HB2 | 1:M:478:ASN:HD21 | 1.51                     | 0.74              |
| 1:I:328:GLN:NE2 | 1:J:416:GLU:OE2  | 2.20                     | 0.72              |
| 1:A:583:HIS:CG  | 1:A:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:F:583:HIS:CG  | 1:F:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:K:583:HIS:CG  | 1:K:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:L:583:HIS:CG  | 1:L:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:I:583:HIS:CG  | 1:I:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:A:328:GLN:NE2 | 1:B:416:GLU:OE2  | 2.23                     | 0.71              |
| 1:D:583:HIS:CG  | 1:D:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:H:583:HIS:CG  | 1:H:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:E:583:HIS:CG  | 1:E:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:J:583:HIS:CG  | 1:J:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:P:583:HIS:CG  | 1:P:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:G:583:HIS:CG  | 1:G:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:O:583:HIS:CG  | 1:O:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:F:465:ARG:NH2 | 1:G:437:GLN:OE1  | 2.23                     | 0.71              |
| 1:B:583:HIS:CG  | 1:B:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:M:583:HIS:CG  | 1:M:692:ILE:HG13 | 2.25                     | 0.71              |
| 1:P:483:ASP:OD1 | 1:P:486:ASN:N    | 2.24                     | 0.71              |
| 1:D:197:GLU:OE1 | 1:E:384:GLY:N    | 2.24                     | 0.70              |
| 1:E:483:ASP:OD1 | 1:E:486:ASN:N    | 2.24                     | 0.70              |
| 1:I:416:GLU:OE2 | 1:P:328:GLN:NE2  | 2.23                     | 0.70              |
| 1:N:583:HIS:CG  | 1:N:692:ILE:HG13 | 2.25                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:583:HIS:CG   | 1:C:692:ILE:HG13 | 2.25                     | 0.70              |
| 1:E:615:ARG:NH2  | 1:E:700:GLN:O    | 2.24                     | 0.70              |
| 1:P:615:ARG:NH2  | 1:P:700:GLN:O    | 2.24                     | 0.70              |
| 1:J:159:ARG:HH21 | 1:J:163:ILE:HG21 | 1.57                     | 0.70              |
| 1:O:166:GLY:HA2  | 1:O:169:LEU:HD12 | 1.74                     | 0.70              |
| 1:A:159:ARG:HH21 | 1:A:163:ILE:HG21 | 1.57                     | 0.70              |
| 1:G:159:ARG:HH21 | 1:G:163:ILE:HG21 | 1.57                     | 0.70              |
| 1:I:483:ASP:OD1  | 1:I:486:ASN:N    | 2.24                     | 0.70              |
| 1:I:615:ARG:NH2  | 1:I:700:GLN:O    | 2.24                     | 0.70              |
| 1:D:166:GLY:HA2  | 1:D:169:LEU:HD12 | 1.74                     | 0.70              |
| 1:F:483:ASP:OD1  | 1:F:486:ASN:N    | 2.24                     | 0.70              |
| 1:F:615:ARG:NH2  | 1:F:700:GLN:O    | 2.24                     | 0.70              |
| 1:L:159:ARG:HH21 | 1:L:163:ILE:HG21 | 1.57                     | 0.70              |
| 1:M:159:ARG:HH21 | 1:M:163:ILE:HG21 | 1.57                     | 0.70              |
| 1:B:159:ARG:HH21 | 1:B:163:ILE:HG21 | 1.57                     | 0.70              |
| 1:L:483:ASP:OD1  | 1:L:486:ASN:N    | 2.24                     | 0.69              |
| 1:N:166:GLY:HA2  | 1:N:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:B:166:GLY:HA2  | 1:B:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:F:239:GLN:HG3  | 1:G:480:SER:HB2  | 1.74                     | 0.69              |
| 1:M:483:ASP:OD1  | 1:M:486:ASN:N    | 2.24                     | 0.69              |
| 1:A:145:ALA:HA   | 1:A:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:A:483:ASP:OD1  | 1:A:486:ASN:N    | 2.24                     | 0.69              |
| 1:C:166:GLY:HA2  | 1:C:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:K:145:ALA:HA   | 1:K:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:L:145:ALA:HA   | 1:L:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:N:217:ARG:HH12 | 1:O:685:HIS:HB3  | 1.57                     | 0.69              |
| 1:E:166:GLY:HA2  | 1:E:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:F:159:ARG:HH21 | 1:F:163:ILE:HG21 | 1.57                     | 0.69              |
| 1:H:145:ALA:HA   | 1:H:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:I:159:ARG:HH21 | 1:I:163:ILE:HG21 | 1.57                     | 0.69              |
| 1:J:483:ASP:OD1  | 1:J:486:ASN:N    | 2.24                     | 0.69              |
| 1:K:483:ASP:OD1  | 1:K:486:ASN:N    | 2.24                     | 0.69              |
| 1:M:166:GLY:HA2  | 1:M:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:P:166:GLY:HA2  | 1:P:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:A:617:PHE:O    | 1:A:654:VAL:N    | 2.26                     | 0.69              |
| 1:B:328:GLN:NE2  | 1:C:416:GLU:OE2  | 2.25                     | 0.69              |
| 1:H:483:ASP:OD1  | 1:H:486:ASN:N    | 2.24                     | 0.69              |
| 1:N:145:ALA:HA   | 1:N:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:B:483:ASP:OD1  | 1:B:486:ASN:N    | 2.24                     | 0.69              |
| 1:K:256:PRO:HG3  | 1:L:582:VAL:HG21 | 1.72                     | 0.69              |
| 1:M:145:ALA:HA   | 1:M:148:LEU:HD12 | 1.75                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:145:ALA:HA   | 1:B:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:C:145:ALA:HA   | 1:C:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:O:615:ARG:NH2  | 1:O:700:GLN:O    | 2.24                     | 0.69              |
| 1:A:166:GLY:HA2  | 1:A:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:A:478:ASN:HD21 | 1:H:239:GLN:HB2  | 1.58                     | 0.69              |
| 1:C:617:PHE:O    | 1:C:654:VAL:N    | 2.26                     | 0.69              |
| 1:E:465:ARG:NH2  | 1:F:437:GLN:OE1  | 2.25                     | 0.69              |
| 1:G:483:ASP:OD1  | 1:G:486:ASN:N    | 2.24                     | 0.69              |
| 1:H:617:PHE:O    | 1:H:654:VAL:N    | 2.26                     | 0.69              |
| 1:J:145:ALA:HA   | 1:J:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:K:617:PHE:O    | 1:K:654:VAL:N    | 2.26                     | 0.69              |
| 1:L:617:PHE:O    | 1:L:654:VAL:N    | 2.26                     | 0.69              |
| 1:M:617:PHE:O    | 1:M:654:VAL:N    | 2.26                     | 0.69              |
| 1:N:617:PHE:O    | 1:N:654:VAL:N    | 2.26                     | 0.69              |
| 1:B:197:GLU:OE1  | 1:C:384:GLY:N    | 2.26                     | 0.69              |
| 1:D:615:ARG:NH2  | 1:D:700:GLN:O    | 2.24                     | 0.69              |
| 1:G:145:ALA:HA   | 1:G:148:LEU:HD12 | 1.75                     | 0.69              |
| 1:J:286:GLU:HG3  | 1:J:289:ARG:HH12 | 1.58                     | 0.69              |
| 1:L:166:GLY:HA2  | 1:L:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:B:617:PHE:O    | 1:B:654:VAL:N    | 2.26                     | 0.69              |
| 1:G:286:GLU:HG3  | 1:G:289:ARG:HH12 | 1.58                     | 0.69              |
| 1:I:166:GLY:HA2  | 1:I:169:LEU:HD12 | 1.74                     | 0.69              |
| 1:A:615:ARG:NH2  | 1:A:700:GLN:O    | 2.24                     | 0.68              |
| 1:K:286:GLU:HG3  | 1:K:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:L:286:GLU:HG3  | 1:L:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:H:286:GLU:HG3  | 1:H:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:M:615:ARG:NH2  | 1:M:700:GLN:O    | 2.24                     | 0.68              |
| 1:P:286:GLU:HG3  | 1:P:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:A:286:GLU:HG3  | 1:A:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:B:615:ARG:NH2  | 1:B:700:GLN:O    | 2.24                     | 0.68              |
| 1:E:286:GLU:HG3  | 1:E:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:F:166:GLY:HA2  | 1:F:169:LEU:HD12 | 1.74                     | 0.68              |
| 1:L:615:ARG:NH2  | 1:L:700:GLN:O    | 2.24                     | 0.68              |
| 1:O:145:ALA:HA   | 1:O:148:LEU:HD12 | 1.75                     | 0.68              |
| 1:C:159:ARG:HH21 | 1:C:163:ILE:HG21 | 1.57                     | 0.68              |
| 1:D:145:ALA:HA   | 1:D:148:LEU:HD12 | 1.75                     | 0.68              |
| 1:N:159:ARG:HH21 | 1:N:163:ILE:HG21 | 1.57                     | 0.68              |
| 1:H:166:GLY:HA2  | 1:H:169:LEU:HD12 | 1.74                     | 0.68              |
| 1:K:166:GLY:HA2  | 1:K:169:LEU:HD12 | 1.74                     | 0.68              |
| 1:D:286:GLU:HG3  | 1:D:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:E:145:ALA:HA   | 1:E:148:LEU:HD12 | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:159:ARG:HH21 | 1:E:163:ILE:HG21 | 1.57                     | 0.68              |
| 1:F:617:PHE:O    | 1:F:654:VAL:N    | 2.26                     | 0.68              |
| 1:G:617:PHE:O    | 1:G:654:VAL:N    | 2.26                     | 0.68              |
| 1:H:159:ARG:HH21 | 1:H:163:ILE:HG21 | 1.57                     | 0.68              |
| 1:J:166:GLY:HA2  | 1:J:169:LEU:HD12 | 1.74                     | 0.68              |
| 1:J:617:PHE:O    | 1:J:654:VAL:N    | 2.26                     | 0.68              |
| 1:N:483:ASP:OD1  | 1:N:486:ASN:N    | 2.24                     | 0.68              |
| 1:F:286:GLU:HG3  | 1:F:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:H:615:ARG:NH2  | 1:H:700:GLN:O    | 2.24                     | 0.68              |
| 1:I:617:PHE:O    | 1:I:654:VAL:N    | 2.26                     | 0.68              |
| 1:P:159:ARG:HH21 | 1:P:163:ILE:HG21 | 1.57                     | 0.68              |
| 1:G:166:GLY:HA2  | 1:G:169:LEU:HD12 | 1.74                     | 0.68              |
| 1:G:328:GLN:HG3  | 1:G:368:ILE:HG23 | 1.76                     | 0.68              |
| 1:J:239:GLN:HB2  | 1:K:478:ASN:ND2  | 2.09                     | 0.68              |
| 1:J:328:GLN:HG3  | 1:J:368:ILE:HG23 | 1.76                     | 0.68              |
| 1:K:159:ARG:HH21 | 1:K:163:ILE:HG21 | 1.57                     | 0.68              |
| 1:P:145:ALA:HA   | 1:P:148:LEU:HD12 | 1.75                     | 0.68              |
| 1:B:328:GLN:HG3  | 1:B:368:ILE:HG23 | 1.76                     | 0.68              |
| 1:I:286:GLU:HG3  | 1:I:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:I:328:GLN:HG3  | 1:I:368:ILE:HG23 | 1.76                     | 0.68              |
| 1:K:615:ARG:NH2  | 1:K:700:GLN:O    | 2.24                     | 0.68              |
| 1:O:159:ARG:HH21 | 1:O:163:ILE:HG21 | 1.57                     | 0.68              |
| 1:O:286:GLU:HG3  | 1:O:289:ARG:HH12 | 1.58                     | 0.68              |
| 1:C:197:GLU:OE1  | 1:D:384:GLY:N    | 2.27                     | 0.67              |
| 1:C:483:ASP:OD1  | 1:C:486:ASN:N    | 2.24                     | 0.67              |
| 1:F:328:GLN:HG3  | 1:F:368:ILE:HG23 | 1.76                     | 0.67              |
| 1:M:286:GLU:HG3  | 1:M:289:ARG:HH12 | 1.58                     | 0.67              |
| 1:M:328:GLN:HG3  | 1:M:368:ILE:HG23 | 1.76                     | 0.67              |
| 1:B:286:GLU:HG3  | 1:B:289:ARG:HH12 | 1.58                     | 0.67              |
| 1:D:159:ARG:HH21 | 1:D:163:ILE:HG21 | 1.57                     | 0.67              |
| 1:E:617:PHE:O    | 1:E:654:VAL:N    | 2.26                     | 0.67              |
| 1:F:145:ALA:HA   | 1:F:148:LEU:HD12 | 1.75                     | 0.67              |
| 1:I:145:ALA:HA   | 1:I:148:LEU:HD12 | 1.75                     | 0.67              |
| 1:P:617:PHE:O    | 1:P:654:VAL:N    | 2.26                     | 0.67              |
| 1:B:465:ARG:NH2  | 1:C:437:GLN:OE1  | 2.27                     | 0.67              |
| 1:N:615:ARG:NH2  | 1:N:700:GLN:O    | 2.24                     | 0.67              |
| 1:C:615:ARG:NH2  | 1:C:700:GLN:O    | 2.24                     | 0.67              |
| 1:D:617:PHE:O    | 1:D:654:VAL:N    | 2.26                     | 0.67              |
| 1:E:186:GLY:O    | 1:E:190:HIS:ND1  | 2.28                     | 0.67              |
| 1:O:328:GLN:HG3  | 1:O:368:ILE:HG23 | 1.76                     | 0.67              |
| 1:E:328:GLN:HG3  | 1:E:368:ILE:HG23 | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:186:GLY:O    | 1:P:190:HIS:ND1  | 2.28                     | 0.67              |
| 1:P:328:GLN:HG3  | 1:P:368:ILE:HG23 | 1.76                     | 0.67              |
| 1:D:328:GLN:HG3  | 1:D:368:ILE:HG23 | 1.76                     | 0.67              |
| 1:H:186:GLY:O    | 1:H:190:HIS:ND1  | 2.28                     | 0.67              |
| 1:J:615:ARG:NH2  | 1:J:700:GLN:O    | 2.24                     | 0.67              |
| 1:K:186:GLY:O    | 1:K:190:HIS:ND1  | 2.28                     | 0.67              |
| 1:G:186:GLY:O    | 1:G:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:K:328:GLN:HG3  | 1:K:368:ILE:HG23 | 1.76                     | 0.66              |
| 1:N:286:GLU:HG3  | 1:N:289:ARG:HH12 | 1.58                     | 0.66              |
| 1:O:617:PHE:O    | 1:O:654:VAL:N    | 2.26                     | 0.66              |
| 1:H:328:GLN:HG3  | 1:H:368:ILE:HG23 | 1.76                     | 0.66              |
| 1:J:186:GLY:O    | 1:J:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:C:286:GLU:HG3  | 1:C:289:ARG:HH12 | 1.58                     | 0.66              |
| 1:C:328:GLN:HG3  | 1:C:368:ILE:HG23 | 1.76                     | 0.66              |
| 1:J:328:GLN:NE2  | 1:K:416:GLU:OE2  | 2.28                     | 0.66              |
| 1:G:615:ARG:NH2  | 1:G:700:GLN:O    | 2.24                     | 0.66              |
| 1:N:328:GLN:HG3  | 1:N:368:ILE:HG23 | 1.76                     | 0.66              |
| 1:L:233:CYS:O    | 1:L:237:GLY:N    | 2.29                     | 0.66              |
| 1:A:233:CYS:O    | 1:A:237:GLY:N    | 2.29                     | 0.66              |
| 1:C:256:PRO:HG3  | 1:D:582:VAL:HG21 | 1.76                     | 0.66              |
| 1:D:186:GLY:O    | 1:D:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:I:186:GLY:O    | 1:I:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:L:186:GLY:O    | 1:L:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:N:569:ARG:NH2  | 1:N:625:ALA:O    | 2.29                     | 0.66              |
| 1:C:611:VAL:HG11 | 1:C:645:THR:HG23 | 1.78                     | 0.66              |
| 1:H:569:ARG:NH2  | 1:H:625:ALA:O    | 2.29                     | 0.66              |
| 1:K:468:ARG:O    | 1:K:471:THR:OG1  | 2.14                     | 0.66              |
| 1:N:611:VAL:HG11 | 1:N:645:THR:HG23 | 1.78                     | 0.66              |
| 1:A:186:GLY:O    | 1:A:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:A:569:ARG:NH2  | 1:A:625:ALA:O    | 2.29                     | 0.66              |
| 1:B:569:ARG:NH2  | 1:B:625:ALA:O    | 2.29                     | 0.66              |
| 1:C:186:GLY:O    | 1:C:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:D:233:CYS:O    | 1:D:237:GLY:N    | 2.29                     | 0.66              |
| 1:D:611:VAL:HG11 | 1:D:645:THR:HG23 | 1.78                     | 0.66              |
| 1:F:197:GLU:OE1  | 1:G:384:GLY:N    | 2.29                     | 0.66              |
| 1:H:233:CYS:O    | 1:H:237:GLY:N    | 2.29                     | 0.66              |
| 1:H:468:ARG:O    | 1:H:471:THR:OG1  | 2.14                     | 0.66              |
| 1:M:569:ARG:NH2  | 1:M:625:ALA:O    | 2.29                     | 0.66              |
| 1:N:186:GLY:O    | 1:N:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:N:233:CYS:O    | 1:N:237:GLY:N    | 2.29                     | 0.66              |
| 1:O:186:GLY:O    | 1:O:190:HIS:ND1  | 2.28                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:186:GLY:O    | 1:B:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:B:233:CYS:O    | 1:B:237:GLY:N    | 2.29                     | 0.66              |
| 1:B:611:VAL:HG11 | 1:B:645:THR:HG23 | 1.78                     | 0.66              |
| 1:F:186:GLY:O    | 1:F:190:HIS:ND1  | 2.28                     | 0.66              |
| 1:K:233:CYS:O    | 1:K:237:GLY:N    | 2.29                     | 0.66              |
| 1:K:449:GLU:OE1  | 1:K:449:GLU:N    | 2.29                     | 0.66              |
| 1:K:569:ARG:NH2  | 1:K:625:ALA:O    | 2.29                     | 0.66              |
| 1:L:569:ARG:NH2  | 1:L:625:ALA:O    | 2.29                     | 0.66              |
| 1:M:233:CYS:O    | 1:M:237:GLY:N    | 2.29                     | 0.66              |
| 1:M:611:VAL:HG11 | 1:M:645:THR:HG23 | 1.78                     | 0.66              |
| 1:O:233:CYS:O    | 1:O:237:GLY:N    | 2.29                     | 0.66              |
| 1:O:611:VAL:HG11 | 1:O:645:THR:HG23 | 1.78                     | 0.66              |
| 1:A:328:GLN:HG3  | 1:A:368:ILE:HG23 | 1.76                     | 0.65              |
| 1:A:468:ARG:O    | 1:A:471:THR:OG1  | 2.14                     | 0.65              |
| 1:C:328:GLN:NE2  | 1:D:416:GLU:OE2  | 2.29                     | 0.65              |
| 1:F:233:CYS:O    | 1:F:237:GLY:N    | 2.29                     | 0.65              |
| 1:I:233:CYS:O    | 1:I:237:GLY:N    | 2.29                     | 0.65              |
| 1:L:328:GLN:HG3  | 1:L:368:ILE:HG23 | 1.76                     | 0.65              |
| 1:L:468:ARG:O    | 1:L:471:THR:OG1  | 2.14                     | 0.65              |
| 1:C:233:CYS:O    | 1:C:237:GLY:N    | 2.29                     | 0.65              |
| 1:C:569:ARG:NH2  | 1:C:625:ALA:O    | 2.29                     | 0.65              |
| 1:E:233:CYS:O    | 1:E:237:GLY:N    | 2.29                     | 0.65              |
| 1:M:186:GLY:O    | 1:M:190:HIS:ND1  | 2.28                     | 0.65              |
| 1:P:233:CYS:O    | 1:P:237:GLY:N    | 2.29                     | 0.65              |
| 1:B:449:GLU:OE1  | 1:B:449:GLU:N    | 2.29                     | 0.65              |
| 1:G:468:ARG:O    | 1:G:471:THR:OG1  | 2.14                     | 0.65              |
| 1:J:468:ARG:O    | 1:J:471:THR:OG1  | 2.14                     | 0.65              |
| 1:A:611:VAL:HG11 | 1:A:645:THR:HG23 | 1.78                     | 0.65              |
| 1:C:468:ARG:O    | 1:C:471:THR:OG1  | 2.14                     | 0.65              |
| 1:G:233:CYS:O    | 1:G:237:GLY:N    | 2.29                     | 0.65              |
| 1:M:449:GLU:OE1  | 1:M:449:GLU:N    | 2.29                     | 0.65              |
| 1:C:239:GLN:HB2  | 1:D:478:ASN:HD21 | 1.62                     | 0.65              |
| 1:N:468:ARG:O    | 1:N:471:THR:OG1  | 2.14                     | 0.65              |
| 1:O:449:GLU:OE1  | 1:O:449:GLU:N    | 2.29                     | 0.65              |
| 1:E:468:ARG:O    | 1:E:471:THR:OG1  | 2.14                     | 0.65              |
| 1:E:611:VAL:HG11 | 1:E:645:THR:HG23 | 1.78                     | 0.65              |
| 1:J:233:CYS:O    | 1:J:237:GLY:N    | 2.29                     | 0.65              |
| 1:L:611:VAL:HG11 | 1:L:645:THR:HG23 | 1.78                     | 0.65              |
| 1:M:468:ARG:O    | 1:M:471:THR:OG1  | 2.14                     | 0.65              |
| 1:O:637:ASP:HB3  | 1:O:640:HIS:HB3  | 1.79                     | 0.65              |
| 1:A:197:GLU:OE1  | 1:B:384:GLY:N    | 2.30                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:449:GLU:OE1  | 1:C:449:GLU:N    | 2.29                     | 0.65              |
| 1:D:449:GLU:OE1  | 1:D:449:GLU:N    | 2.29                     | 0.65              |
| 1:D:637:ASP:HB3  | 1:D:640:HIS:HB3  | 1.79                     | 0.65              |
| 1:N:449:GLU:N    | 1:N:449:GLU:OE1  | 2.29                     | 0.65              |
| 1:O:468:ARG:O    | 1:O:471:THR:OG1  | 2.14                     | 0.65              |
| 1:O:483:ASP:OD1  | 1:O:486:ASN:N    | 2.24                     | 0.65              |
| 1:C:637:ASP:HB3  | 1:C:640:HIS:HB3  | 1.79                     | 0.65              |
| 1:N:637:ASP:HB3  | 1:N:640:HIS:HB3  | 1.79                     | 0.65              |
| 1:B:468:ARG:O    | 1:B:471:THR:OG1  | 2.14                     | 0.65              |
| 1:C:621:LEU:HD12 | 1:C:657:ILE:HD13 | 1.79                     | 0.65              |
| 1:D:468:ARG:O    | 1:D:471:THR:OG1  | 2.14                     | 0.65              |
| 1:G:449:GLU:OE1  | 1:G:449:GLU:N    | 2.29                     | 0.65              |
| 1:H:611:VAL:HG11 | 1:H:645:THR:HG23 | 1.78                     | 0.65              |
| 1:I:468:ARG:O    | 1:I:471:THR:OG1  | 2.14                     | 0.65              |
| 1:O:569:ARG:NH2  | 1:O:625:ALA:O    | 2.29                     | 0.65              |
| 1:P:468:ARG:O    | 1:P:471:THR:OG1  | 2.14                     | 0.65              |
| 1:P:611:VAL:HG11 | 1:P:645:THR:HG23 | 1.78                     | 0.65              |
| 1:A:177:PRO:HB2  | 1:A:180:LEU:HB3  | 1.79                     | 0.64              |
| 1:D:569:ARG:NH2  | 1:D:625:ALA:O    | 2.29                     | 0.64              |
| 1:E:569:ARG:NH2  | 1:E:625:ALA:O    | 2.29                     | 0.64              |
| 1:L:177:PRO:HB2  | 1:L:180:LEU:HB3  | 1.79                     | 0.64              |
| 1:L:328:GLN:NE2  | 1:M:416:GLU:OE2  | 2.29                     | 0.64              |
| 1:N:621:LEU:HD12 | 1:N:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:O:197:GLU:OE1  | 1:P:384:GLY:N    | 2.29                     | 0.64              |
| 1:P:569:ARG:NH2  | 1:P:625:ALA:O    | 2.29                     | 0.64              |
| 1:D:621:LEU:HD12 | 1:D:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:F:468:ARG:O    | 1:F:471:THR:OG1  | 2.14                     | 0.64              |
| 1:G:569:ARG:NH2  | 1:G:625:ALA:O    | 2.29                     | 0.64              |
| 1:J:449:GLU:OE1  | 1:J:449:GLU:N    | 2.29                     | 0.64              |
| 1:P:637:ASP:HB3  | 1:P:640:HIS:HB3  | 1.79                     | 0.64              |
| 1:D:483:ASP:OD1  | 1:D:486:ASN:N    | 2.24                     | 0.64              |
| 1:E:637:ASP:HB3  | 1:E:640:HIS:HB3  | 1.79                     | 0.64              |
| 1:K:217:ARG:HH12 | 1:L:685:HIS:HB3  | 1.62                     | 0.64              |
| 1:K:611:VAL:HG11 | 1:K:645:THR:HG23 | 1.78                     | 0.64              |
| 1:O:621:LEU:HD12 | 1:O:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:E:449:GLU:OE1  | 1:E:449:GLU:N    | 2.29                     | 0.64              |
| 1:E:621:LEU:HD12 | 1:E:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:F:304:ASP:OD1  | 1:F:392:ARG:NH1  | 2.29                     | 0.64              |
| 1:J:569:ARG:NH2  | 1:J:625:ALA:O    | 2.29                     | 0.64              |
| 1:P:621:LEU:HD12 | 1:P:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:A:77:SER:HA    | 1:A:80:LYS:HD2   | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:77:SER:HA    | 1:B:80:LYS:HD2   | 1.79                     | 0.64              |
| 1:B:177:PRO:HB2  | 1:B:180:LEU:HB3  | 1.79                     | 0.64              |
| 1:K:177:PRO:HB2  | 1:K:180:LEU:HB3  | 1.79                     | 0.64              |
| 1:B:621:LEU:HD12 | 1:B:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:F:569:ARG:NH2  | 1:F:625:ALA:O    | 2.29                     | 0.64              |
| 1:H:177:PRO:HB2  | 1:H:180:LEU:HB3  | 1.79                     | 0.64              |
| 1:J:611:VAL:HG11 | 1:J:645:THR:HG23 | 1.78                     | 0.64              |
| 1:L:77:SER:HA    | 1:L:80:LYS:HD2   | 1.80                     | 0.64              |
| 1:M:177:PRO:HB2  | 1:M:180:LEU:HB3  | 1.79                     | 0.64              |
| 1:P:449:GLU:OE1  | 1:P:449:GLU:N    | 2.29                     | 0.64              |
| 1:D:105:LEU:HB3  | 1:D:109:GLY:HA3  | 1.80                     | 0.64              |
| 1:E:105:LEU:HB3  | 1:E:109:GLY:HA3  | 1.80                     | 0.64              |
| 1:F:611:VAL:HG11 | 1:F:645:THR:HG23 | 1.78                     | 0.64              |
| 1:I:304:ASP:OD1  | 1:I:392:ARG:NH1  | 2.29                     | 0.64              |
| 1:I:569:ARG:NH2  | 1:I:625:ALA:O    | 2.29                     | 0.64              |
| 1:I:611:VAL:HG11 | 1:I:645:THR:HG23 | 1.78                     | 0.64              |
| 1:M:77:SER:HA    | 1:M:80:LYS:HD2   | 1.80                     | 0.64              |
| 1:M:621:LEU:HD12 | 1:M:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:B:240:ALA:HA   | 1:B:243:ARG:HE   | 1.63                     | 0.64              |
| 1:G:611:VAL:HG11 | 1:G:645:THR:HG23 | 1.78                     | 0.64              |
| 1:H:77:SER:HA    | 1:H:80:LYS:HD2   | 1.80                     | 0.64              |
| 1:M:240:ALA:HA   | 1:M:243:ARG:HE   | 1.63                     | 0.64              |
| 1:O:105:LEU:HB3  | 1:O:109:GLY:HA3  | 1.80                     | 0.64              |
| 1:P:105:LEU:HB3  | 1:P:109:GLY:HA3  | 1.80                     | 0.64              |
| 1:C:240:ALA:HA   | 1:C:243:ARG:HE   | 1.63                     | 0.64              |
| 1:F:105:LEU:HB3  | 1:F:109:GLY:HA3  | 1.80                     | 0.64              |
| 1:G:217:ARG:HH12 | 1:H:685:HIS:HB3  | 1.63                     | 0.64              |
| 1:H:637:ASP:HB3  | 1:H:640:HIS:HB3  | 1.79                     | 0.64              |
| 1:I:240:ALA:HA   | 1:I:243:ARG:HE   | 1.63                     | 0.64              |
| 1:I:621:LEU:HD12 | 1:I:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:K:621:LEU:HD12 | 1:K:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:L:240:ALA:HA   | 1:L:243:ARG:HE   | 1.63                     | 0.64              |
| 1:N:77:SER:HA    | 1:N:80:LYS:HD2   | 1.80                     | 0.64              |
| 1:A:240:ALA:HA   | 1:A:243:ARG:HE   | 1.63                     | 0.64              |
| 1:F:621:LEU:HD12 | 1:F:657:ILE:HD13 | 1.79                     | 0.64              |
| 1:G:240:ALA:HA   | 1:G:243:ARG:HE   | 1.63                     | 0.64              |
| 1:G:464:LYS:HE2  | 1:H:445:ARG:NH2  | 2.12                     | 0.64              |
| 1:J:240:ALA:HA   | 1:J:243:ARG:HE   | 1.63                     | 0.64              |
| 1:K:77:SER:HA    | 1:K:80:LYS:HD2   | 1.80                     | 0.64              |
| 1:K:637:ASP:HB3  | 1:K:640:HIS:HB3  | 1.79                     | 0.64              |
| 1:L:449:GLU:OE1  | 1:L:449:GLU:N    | 2.29                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:240:ALA:HA   | 1:N:243:ARG:HE   | 1.63                     | 0.64              |
| 1:N:256:PRO:HG3  | 1:O:582:VAL:HG21 | 1.80                     | 0.64              |
| 1:C:105:LEU:HB3  | 1:C:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:F:240:ALA:HA   | 1:F:243:ARG:HE   | 1.63                     | 0.63              |
| 1:G:105:LEU:HB3  | 1:G:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:G:177:PRO:HB2  | 1:G:180:LEU:HB3  | 1.79                     | 0.63              |
| 1:G:637:ASP:HB3  | 1:G:640:HIS:HB3  | 1.79                     | 0.63              |
| 1:H:240:ALA:HA   | 1:H:243:ARG:HE   | 1.63                     | 0.63              |
| 1:I:105:LEU:HB3  | 1:I:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:J:105:LEU:HB3  | 1:J:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:J:177:PRO:HB2  | 1:J:180:LEU:HB3  | 1.79                     | 0.63              |
| 1:N:105:LEU:HB3  | 1:N:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:A:449:GLU:N    | 1:A:449:GLU:OE1  | 2.29                     | 0.63              |
| 1:C:77:SER:HA    | 1:C:80:LYS:HD2   | 1.80                     | 0.63              |
| 1:H:105:LEU:HB3  | 1:H:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:H:621:LEU:HD12 | 1:H:657:ILE:HD13 | 1.79                     | 0.63              |
| 1:J:637:ASP:HB3  | 1:J:640:HIS:HB3  | 1.79                     | 0.63              |
| 1:K:240:ALA:HA   | 1:K:243:ARG:HE   | 1.63                     | 0.63              |
| 1:N:177:PRO:HB2  | 1:N:180:LEU:HB3  | 1.79                     | 0.63              |
| 1:E:304:ASP:OD1  | 1:E:392:ARG:NH1  | 2.29                     | 0.63              |
| 1:I:637:ASP:HB3  | 1:I:640:HIS:HB3  | 1.79                     | 0.63              |
| 1:K:105:LEU:HB3  | 1:K:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:A:105:LEU:HB3  | 1:A:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:B:105:LEU:HB3  | 1:B:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:B:637:ASP:HB3  | 1:B:640:HIS:HB3  | 1.79                     | 0.63              |
| 1:C:177:PRO:HB2  | 1:C:180:LEU:HB3  | 1.79                     | 0.63              |
| 1:P:177:PRO:HB2  | 1:P:180:LEU:HB3  | 1.79                     | 0.63              |
| 1:D:240:ALA:HA   | 1:D:243:ARG:HE   | 1.63                     | 0.63              |
| 1:E:177:PRO:HB2  | 1:E:180:LEU:HB3  | 1.79                     | 0.63              |
| 1:F:637:ASP:HB3  | 1:F:640:HIS:HB3  | 1.79                     | 0.63              |
| 1:J:77:SER:HA    | 1:J:80:LYS:HD2   | 1.80                     | 0.63              |
| 1:L:105:LEU:HB3  | 1:L:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:L:621:LEU:HD12 | 1:L:657:ILE:HD13 | 1.79                     | 0.63              |
| 1:P:304:ASP:OD1  | 1:P:392:ARG:NH1  | 2.29                     | 0.63              |
| 1:A:621:LEU:HD12 | 1:A:657:ILE:HD13 | 1.79                     | 0.63              |
| 1:E:77:SER:HA    | 1:E:80:LYS:HD2   | 1.80                     | 0.63              |
| 1:I:77:SER:HA    | 1:I:80:LYS:HD2   | 1.80                     | 0.63              |
| 1:O:240:ALA:HA   | 1:O:243:ARG:HE   | 1.63                     | 0.63              |
| 1:P:77:SER:HA    | 1:P:80:LYS:HD2   | 1.80                     | 0.63              |
| 1:F:77:SER:HA    | 1:F:80:LYS:HD2   | 1.80                     | 0.63              |
| 1:G:77:SER:HA    | 1:G:80:LYS:HD2   | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:105:LEU:HB3  | 1:M:109:GLY:HA3  | 1.80                     | 0.63              |
| 1:O:77:SER:HA    | 1:O:80:LYS:HD2   | 1.80                     | 0.63              |
| 1:O:465:ARG:NH2  | 1:P:437:GLN:OE1  | 2.32                     | 0.63              |
| 1:G:77:SER:O     | 1:G:81:GLN:NE2   | 2.32                     | 0.63              |
| 1:J:77:SER:O     | 1:J:81:GLN:NE2   | 2.32                     | 0.63              |
| 1:P:240:ALA:HA   | 1:P:243:ARG:HE   | 1.63                     | 0.63              |
| 1:E:240:ALA:HA   | 1:E:243:ARG:HE   | 1.63                     | 0.62              |
| 1:F:177:PRO:HB2  | 1:F:180:LEU:HB3  | 1.79                     | 0.62              |
| 1:F:449:GLU:N    | 1:F:449:GLU:OE1  | 2.29                     | 0.62              |
| 1:I:449:GLU:N    | 1:I:449:GLU:OE1  | 2.29                     | 0.62              |
| 1:M:637:ASP:HB3  | 1:M:640:HIS:HB3  | 1.79                     | 0.62              |
| 1:D:77:SER:HA    | 1:D:80:LYS:HD2   | 1.80                     | 0.62              |
| 1:I:177:PRO:HB2  | 1:I:180:LEU:HB3  | 1.79                     | 0.62              |
| 1:M:465:ARG:NH2  | 1:N:437:GLN:OE1  | 2.33                     | 0.62              |
| 1:G:621:LEU:HD12 | 1:G:657:ILE:HD13 | 1.79                     | 0.62              |
| 1:H:77:SER:O     | 1:H:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:A:77:SER:O     | 1:A:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:A:637:ASP:HB3  | 1:A:640:HIS:HB3  | 1.79                     | 0.62              |
| 1:D:177:PRO:HB2  | 1:D:180:LEU:HB3  | 1.79                     | 0.62              |
| 1:J:239:GLN:HG3  | 1:K:480:SER:HB2  | 1.80                     | 0.62              |
| 1:J:621:LEU:HD12 | 1:J:657:ILE:HD13 | 1.79                     | 0.62              |
| 1:M:77:SER:O     | 1:M:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:K:77:SER:O     | 1:K:81:GLN:NE2   | 2.33                     | 0.62              |
| 1:L:637:ASP:HB3  | 1:L:640:HIS:HB3  | 1.79                     | 0.62              |
| 1:B:77:SER:O     | 1:B:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:L:77:SER:O     | 1:L:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:M:657:ILE:N    | 1:M:681:ILE:O    | 2.33                     | 0.62              |
| 1:O:328:GLN:NE2  | 1:P:416:GLU:OE2  | 2.33                     | 0.62              |
| 1:A:657:ILE:N    | 1:A:681:ILE:O    | 2.33                     | 0.62              |
| 1:I:77:SER:O     | 1:I:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:O:177:PRO:HB2  | 1:O:180:LEU:HB3  | 1.79                     | 0.62              |
| 1:A:105:LEU:HD12 | 1:A:106:PRO:HD2  | 1.81                     | 0.62              |
| 1:B:657:ILE:N    | 1:B:681:ILE:O    | 2.33                     | 0.62              |
| 1:F:77:SER:O     | 1:F:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:L:657:ILE:N    | 1:L:681:ILE:O    | 2.33                     | 0.62              |
| 1:C:105:LEU:HD12 | 1:C:106:PRO:HD2  | 1.82                     | 0.62              |
| 1:D:239:GLN:HB2  | 1:E:478:ASN:HD21 | 1.64                     | 0.62              |
| 1:G:505:LEU:HD23 | 1:G:527:CYS:SG   | 2.40                     | 0.62              |
| 1:H:505:LEU:HD23 | 1:H:527:CYS:SG   | 2.40                     | 0.62              |
| 1:K:505:LEU:HD23 | 1:K:527:CYS:SG   | 2.40                     | 0.62              |
| 1:N:105:LEU:HD12 | 1:N:106:PRO:HD2  | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:416:GLU:OE2  | 1:H:328:GLN:NE2  | 2.32                     | 0.62              |
| 1:G:257:LEU:HD12 | 1:G:266:LEU:HD21 | 1.82                     | 0.62              |
| 1:J:505:LEU:HD23 | 1:J:527:CYS:SG   | 2.40                     | 0.62              |
| 1:K:465:ARG:NH2  | 1:L:437:GLN:OE1  | 2.33                     | 0.62              |
| 1:M:256:PRO:HG3  | 1:N:582:VAL:HG21 | 1.82                     | 0.62              |
| 1:N:77:SER:O     | 1:N:81:GLN:NE2   | 2.32                     | 0.62              |
| 1:P:657:ILE:N    | 1:P:681:ILE:O    | 2.33                     | 0.62              |
| 1:B:505:LEU:HD23 | 1:B:527:CYS:SG   | 2.40                     | 0.61              |
| 1:C:77:SER:O     | 1:C:81:GLN:NE2   | 2.32                     | 0.61              |
| 1:E:657:ILE:N    | 1:E:681:ILE:O    | 2.33                     | 0.61              |
| 1:G:465:ARG:NH2  | 1:H:437:GLN:HB2  | 2.15                     | 0.61              |
| 1:J:257:LEU:HD12 | 1:J:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:K:257:LEU:HD12 | 1:K:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:L:105:LEU:HD12 | 1:L:106:PRO:HD2  | 1.82                     | 0.61              |
| 1:L:505:LEU:HD23 | 1:L:527:CYS:SG   | 2.40                     | 0.61              |
| 1:A:257:LEU:HD12 | 1:A:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:505:LEU:HD23 | 1:A:527:CYS:SG   | 2.40                     | 0.61              |
| 1:D:657:ILE:N    | 1:D:681:ILE:O    | 2.33                     | 0.61              |
| 1:E:340:GLU:OE1  | 1:E:340:GLU:N    | 2.30                     | 0.61              |
| 1:F:657:ILE:N    | 1:F:681:ILE:O    | 2.33                     | 0.61              |
| 1:H:257:LEU:HD12 | 1:H:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:H:657:ILE:N    | 1:H:681:ILE:O    | 2.33                     | 0.61              |
| 1:I:105:LEU:HD12 | 1:I:106:PRO:HD2  | 1.82                     | 0.61              |
| 1:I:257:LEU:HD12 | 1:I:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:I:657:ILE:N    | 1:I:681:ILE:O    | 2.33                     | 0.61              |
| 1:K:657:ILE:N    | 1:K:681:ILE:O    | 2.33                     | 0.61              |
| 1:L:257:LEU:HD12 | 1:L:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:N:657:ILE:N    | 1:N:681:ILE:O    | 2.33                     | 0.61              |
| 1:O:657:ILE:N    | 1:O:681:ILE:O    | 2.33                     | 0.61              |
| 1:C:657:ILE:N    | 1:C:681:ILE:O    | 2.33                     | 0.61              |
| 1:F:105:LEU:HD12 | 1:F:106:PRO:HD2  | 1.82                     | 0.61              |
| 1:F:257:LEU:HD12 | 1:F:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:F:340:GLU:OE1  | 1:F:340:GLU:N    | 2.30                     | 0.61              |
| 1:H:449:GLU:OE1  | 1:H:449:GLU:N    | 2.29                     | 0.61              |
| 1:I:340:GLU:OE1  | 1:I:340:GLU:N    | 2.30                     | 0.61              |
| 1:M:505:LEU:HD23 | 1:M:527:CYS:SG   | 2.40                     | 0.61              |
| 1:P:340:GLU:OE1  | 1:P:340:GLU:N    | 2.30                     | 0.61              |
| 1:D:77:SER:O     | 1:D:81:GLN:NE2   | 2.32                     | 0.61              |
| 1:D:505:LEU:HD23 | 1:D:527:CYS:SG   | 2.40                     | 0.61              |
| 1:F:607:LEU:HD23 | 1:F:607:LEU:H    | 1.66                     | 0.61              |
| 1:H:596:GLU:HG2  | 1:H:598:LEU:H    | 1.66                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:465:ARG:NH2  | 1:J:437:GLN:OE1  | 2.34                     | 0.61              |
| 1:I:607:LEU:HD23 | 1:I:607:LEU:H    | 1.66                     | 0.61              |
| 1:J:105:LEU:HD12 | 1:J:106:PRO:HD2  | 1.81                     | 0.61              |
| 1:O:505:LEU:HD23 | 1:O:527:CYS:SG   | 2.40                     | 0.61              |
| 1:C:505:LEU:HD23 | 1:C:527:CYS:SG   | 2.40                     | 0.61              |
| 1:G:105:LEU:HD12 | 1:G:106:PRO:HD2  | 1.82                     | 0.61              |
| 1:G:657:ILE:N    | 1:G:681:ILE:O    | 2.33                     | 0.61              |
| 1:I:197:GLU:OE1  | 1:J:384:GLY:N    | 2.31                     | 0.61              |
| 1:J:657:ILE:N    | 1:J:681:ILE:O    | 2.33                     | 0.61              |
| 1:K:596:GLU:HG2  | 1:K:598:LEU:H    | 1.66                     | 0.61              |
| 1:M:105:LEU:HD12 | 1:M:106:PRO:HD2  | 1.82                     | 0.61              |
| 1:M:607:LEU:HD23 | 1:M:607:LEU:H    | 1.66                     | 0.61              |
| 1:O:77:SER:O     | 1:O:81:GLN:NE2   | 2.32                     | 0.61              |
| 1:B:105:LEU:HD12 | 1:B:106:PRO:HD2  | 1.82                     | 0.61              |
| 1:B:239:GLN:HB2  | 1:C:478:ASN:HD21 | 1.65                     | 0.61              |
| 1:B:607:LEU:HD23 | 1:B:607:LEU:H    | 1.66                     | 0.61              |
| 1:D:607:LEU:HD23 | 1:D:607:LEU:H    | 1.66                     | 0.61              |
| 1:E:257:LEU:HD12 | 1:E:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:F:505:LEU:HD23 | 1:F:527:CYS:SG   | 2.40                     | 0.61              |
| 1:N:505:LEU:HD23 | 1:N:527:CYS:SG   | 2.40                     | 0.61              |
| 1:P:257:LEU:HD12 | 1:P:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:74:GLN:O     | 1:A:77:SER:OG    | 2.19                     | 0.61              |
| 1:B:74:GLN:O     | 1:B:77:SER:OG    | 2.19                     | 0.61              |
| 1:B:257:LEU:HD12 | 1:B:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:D:465:ARG:NH2  | 1:E:437:GLN:OE1  | 2.33                     | 0.61              |
| 1:E:77:SER:O     | 1:E:81:GLN:NE2   | 2.32                     | 0.61              |
| 1:F:239:GLN:HB2  | 1:G:478:ASN:ND2  | 2.16                     | 0.61              |
| 1:I:505:LEU:HD23 | 1:I:527:CYS:SG   | 2.40                     | 0.61              |
| 1:N:607:LEU:HD23 | 1:N:607:LEU:H    | 1.66                     | 0.61              |
| 1:A:607:LEU:HD23 | 1:A:607:LEU:H    | 1.66                     | 0.61              |
| 1:M:74:GLN:O     | 1:M:77:SER:OG    | 2.19                     | 0.61              |
| 1:M:257:LEU:HD12 | 1:M:266:LEU:HD21 | 1.82                     | 0.61              |
| 1:O:607:LEU:HD23 | 1:O:607:LEU:H    | 1.66                     | 0.61              |
| 1:P:77:SER:O     | 1:P:81:GLN:NE2   | 2.32                     | 0.61              |
| 1:L:74:GLN:O     | 1:L:77:SER:OG    | 2.19                     | 0.61              |
| 1:L:607:LEU:HD23 | 1:L:607:LEU:H    | 1.66                     | 0.61              |
| 1:P:105:LEU:HD12 | 1:P:106:PRO:HD2  | 1.82                     | 0.61              |
| 1:C:607:LEU:H    | 1:C:607:LEU:HD23 | 1.66                     | 0.60              |
| 1:D:257:LEU:HD12 | 1:D:266:LEU:HD21 | 1.82                     | 0.60              |
| 1:J:607:LEU:HD23 | 1:J:607:LEU:H    | 1.66                     | 0.60              |
| 1:O:257:LEU:HD12 | 1:O:266:LEU:HD21 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:105:LEU:HD12 | 1:E:106:PRO:HD2  | 1.82                     | 0.60              |
| 1:E:505:LEU:HD23 | 1:E:527:CYS:SG   | 2.40                     | 0.60              |
| 1:G:607:LEU:HD23 | 1:G:607:LEU:H    | 1.66                     | 0.60              |
| 1:M:596:GLU:HG2  | 1:M:598:LEU:H    | 1.66                     | 0.60              |
| 1:O:596:GLU:HG2  | 1:O:598:LEU:H    | 1.66                     | 0.60              |
| 1:D:596:GLU:HG2  | 1:D:598:LEU:H    | 1.66                     | 0.60              |
| 1:O:105:LEU:HD12 | 1:O:106:PRO:HD2  | 1.82                     | 0.60              |
| 1:P:505:LEU:HD23 | 1:P:527:CYS:SG   | 2.40                     | 0.60              |
| 1:B:596:GLU:HG2  | 1:B:598:LEU:H    | 1.66                     | 0.60              |
| 1:C:74:GLN:O     | 1:C:77:SER:OG    | 2.19                     | 0.60              |
| 1:C:257:LEU:HD12 | 1:C:266:LEU:HD21 | 1.82                     | 0.60              |
| 1:C:263:ASP:OD1  | 1:C:264:GLU:N    | 2.35                     | 0.60              |
| 1:D:263:ASP:OD1  | 1:D:264:GLU:N    | 2.35                     | 0.60              |
| 1:H:607:LEU:HD23 | 1:H:607:LEU:H    | 1.66                     | 0.60              |
| 1:N:257:LEU:HD12 | 1:N:266:LEU:HD21 | 1.82                     | 0.60              |
| 1:N:263:ASP:OD1  | 1:N:264:GLU:N    | 2.35                     | 0.60              |
| 1:D:304:ASP:OD1  | 1:D:392:ARG:NH1  | 2.29                     | 0.60              |
| 1:H:74:GLN:O     | 1:H:77:SER:OG    | 2.19                     | 0.60              |
| 1:O:263:ASP:OD1  | 1:O:264:GLU:N    | 2.35                     | 0.60              |
| 1:K:607:LEU:H    | 1:K:607:LEU:HD23 | 1.66                     | 0.60              |
| 1:N:74:GLN:O     | 1:N:77:SER:OG    | 2.19                     | 0.60              |
| 1:O:258:ALA:HA   | 1:O:267:ARG:HA   | 1.83                     | 0.60              |
| 1:A:596:GLU:HG2  | 1:A:598:LEU:H    | 1.66                     | 0.60              |
| 1:B:263:ASP:OD1  | 1:B:264:GLU:N    | 2.35                     | 0.60              |
| 1:D:105:LEU:HD12 | 1:D:106:PRO:HD2  | 1.82                     | 0.60              |
| 1:D:258:ALA:HA   | 1:D:267:ARG:HA   | 1.83                     | 0.60              |
| 1:G:74:GLN:O     | 1:G:77:SER:OG    | 2.19                     | 0.60              |
| 1:G:263:ASP:OD1  | 1:G:264:GLU:N    | 2.35                     | 0.60              |
| 1:H:88:VAL:O     | 1:H:92:LEU:HG    | 2.02                     | 0.60              |
| 1:H:105:LEU:HD12 | 1:H:106:PRO:HD2  | 1.81                     | 0.60              |
| 1:I:391:LYS:HA   | 1:I:394:LEU:HD12 | 1.84                     | 0.60              |
| 1:K:74:GLN:O     | 1:K:77:SER:OG    | 2.19                     | 0.60              |
| 1:L:239:GLN:HG3  | 1:M:480:SER:HB2  | 1.83                     | 0.60              |
| 1:N:258:ALA:HA   | 1:N:267:ARG:HA   | 1.83                     | 0.60              |
| 1:P:596:GLU:HG2  | 1:P:598:LEU:H    | 1.66                     | 0.60              |
| 1:A:263:ASP:OD1  | 1:A:264:GLU:N    | 2.35                     | 0.60              |
| 1:C:596:GLU:HG2  | 1:C:598:LEU:H    | 1.66                     | 0.60              |
| 1:E:217:ARG:NH1  | 1:F:685:HIS:HB3  | 2.15                     | 0.60              |
| 1:F:391:LYS:HA   | 1:F:394:LEU:HD12 | 1.84                     | 0.60              |
| 1:J:263:ASP:OD1  | 1:J:264:GLU:N    | 2.35                     | 0.60              |
| 1:K:105:LEU:HD12 | 1:K:106:PRO:HD2  | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:258:ALA:HA   | 1:K:267:ARG:HA   | 1.83                     | 0.60              |
| 1:K:328:GLN:NE2  | 1:L:416:GLU:OE2  | 2.35                     | 0.60              |
| 1:N:376:ARG:NH2  | 1:N:424:ILE:HA   | 2.17                     | 0.60              |
| 1:N:596:GLU:HG2  | 1:N:598:LEU:H    | 1.66                     | 0.60              |
| 1:A:239:GLN:HB2  | 1:B:478:ASN:HD21 | 1.66                     | 0.60              |
| 1:A:376:ARG:NH2  | 1:A:424:ILE:HA   | 2.17                     | 0.60              |
| 1:C:258:ALA:HA   | 1:C:267:ARG:HA   | 1.83                     | 0.60              |
| 1:D:391:LYS:HA   | 1:D:394:LEU:HD12 | 1.84                     | 0.60              |
| 1:K:88:VAL:O     | 1:K:92:LEU:HG    | 2.02                     | 0.60              |
| 1:L:376:ARG:NH2  | 1:L:424:ILE:HA   | 2.17                     | 0.60              |
| 1:M:263:ASP:OD1  | 1:M:264:GLU:N    | 2.35                     | 0.60              |
| 1:O:304:ASP:OD1  | 1:O:392:ARG:NH1  | 2.29                     | 0.60              |
| 1:P:391:LYS:HA   | 1:P:394:LEU:HD12 | 1.84                     | 0.60              |
| 1:C:376:ARG:NH2  | 1:C:424:ILE:HA   | 2.17                     | 0.60              |
| 1:F:376:ARG:NH2  | 1:F:424:ILE:HA   | 2.17                     | 0.60              |
| 1:G:391:LYS:HA   | 1:G:394:LEU:HD12 | 1.84                     | 0.60              |
| 1:H:258:ALA:HA   | 1:H:267:ARG:HA   | 1.83                     | 0.60              |
| 1:I:263:ASP:OD1  | 1:I:264:GLU:N    | 2.35                     | 0.60              |
| 1:I:376:ARG:NH2  | 1:I:424:ILE:HA   | 2.17                     | 0.60              |
| 1:J:74:GLN:O     | 1:J:77:SER:OG    | 2.19                     | 0.60              |
| 1:J:596:GLU:HG2  | 1:J:598:LEU:H    | 1.66                     | 0.60              |
| 1:L:263:ASP:OD1  | 1:L:264:GLU:N    | 2.35                     | 0.60              |
| 1:D:376:ARG:NH2  | 1:D:424:ILE:HA   | 2.17                     | 0.59              |
| 1:E:376:ARG:NH2  | 1:E:424:ILE:HA   | 2.17                     | 0.59              |
| 1:E:391:LYS:HA   | 1:E:394:LEU:HD12 | 1.84                     | 0.59              |
| 1:E:596:GLU:HG2  | 1:E:598:LEU:H    | 1.66                     | 0.59              |
| 1:F:263:ASP:OD1  | 1:F:264:GLU:N    | 2.35                     | 0.59              |
| 1:G:465:ARG:NH2  | 1:H:437:GLN:OE1  | 2.35                     | 0.59              |
| 1:H:263:ASP:OD1  | 1:H:264:GLU:N    | 2.35                     | 0.59              |
| 1:J:88:VAL:O     | 1:J:92:LEU:HG    | 2.02                     | 0.59              |
| 1:J:391:LYS:HA   | 1:J:394:LEU:HD12 | 1.84                     | 0.59              |
| 1:L:596:GLU:HG2  | 1:L:598:LEU:H    | 1.66                     | 0.59              |
| 1:O:340:GLU:OE1  | 1:O:340:GLU:N    | 2.30                     | 0.59              |
| 1:D:340:GLU:OE1  | 1:D:340:GLU:N    | 2.30                     | 0.59              |
| 1:F:88:VAL:O     | 1:F:92:LEU:HG    | 2.02                     | 0.59              |
| 1:G:88:VAL:O     | 1:G:92:LEU:HG    | 2.02                     | 0.59              |
| 1:K:263:ASP:OD1  | 1:K:264:GLU:N    | 2.35                     | 0.59              |
| 1:M:88:VAL:O     | 1:M:92:LEU:HG    | 2.02                     | 0.59              |
| 1:O:391:LYS:HA   | 1:O:394:LEU:HD12 | 1.84                     | 0.59              |
| 1:P:376:ARG:NH2  | 1:P:424:ILE:HA   | 2.17                     | 0.59              |
| 1:P:607:LEU:HD23 | 1:P:607:LEU:H    | 1.66                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:88:VAL:O     | 1:B:92:LEU:HG    | 2.02                     | 0.59              |
| 1:E:133:LEU:HD23 | 1:E:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:E:159:ARG:O    | 1:E:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:I:88:VAL:O     | 1:I:92:LEU:HG    | 2.02                     | 0.59              |
| 1:I:596:GLU:HG2  | 1:I:598:LEU:H    | 1.66                     | 0.59              |
| 1:O:376:ARG:NH2  | 1:O:424:ILE:HA   | 2.17                     | 0.59              |
| 1:P:159:ARG:O    | 1:P:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:C:133:LEU:HD23 | 1:C:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:C:391:LYS:HA   | 1:C:394:LEU:HD12 | 1.84                     | 0.59              |
| 1:D:88:VAL:O     | 1:D:92:LEU:HG    | 2.02                     | 0.59              |
| 1:F:258:ALA:HA   | 1:F:267:ARG:HA   | 1.83                     | 0.59              |
| 1:F:596:GLU:HG2  | 1:F:598:LEU:H    | 1.66                     | 0.59              |
| 1:G:596:GLU:HG2  | 1:G:598:LEU:H    | 1.66                     | 0.59              |
| 1:H:133:LEU:HD23 | 1:H:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:N:133:LEU:HD23 | 1:N:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:P:133:LEU:HD23 | 1:P:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:A:159:ARG:O    | 1:A:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:B:376:ARG:NH2  | 1:B:424:ILE:HA   | 2.17                     | 0.59              |
| 1:C:159:ARG:O    | 1:C:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:E:607:LEU:HD23 | 1:E:607:LEU:H    | 1.66                     | 0.59              |
| 1:I:258:ALA:HA   | 1:I:267:ARG:HA   | 1.83                     | 0.59              |
| 1:N:391:LYS:HA   | 1:N:394:LEU:HD12 | 1.84                     | 0.59              |
| 1:O:88:VAL:O     | 1:O:92:LEU:HG    | 2.02                     | 0.59              |
| 1:A:258:ALA:HA   | 1:A:267:ARG:HA   | 1.83                     | 0.59              |
| 1:I:74:GLN:O     | 1:I:77:SER:OG    | 2.19                     | 0.59              |
| 1:I:685:HIS:HB3  | 1:P:217:ARG:HH12 | 1.67                     | 0.59              |
| 1:J:376:ARG:NH2  | 1:J:424:ILE:HA   | 2.17                     | 0.59              |
| 1:K:133:LEU:HD23 | 1:K:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:N:159:ARG:O    | 1:N:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:C:88:VAL:O     | 1:C:92:LEU:HG    | 2.02                     | 0.59              |
| 1:D:74:GLN:O     | 1:D:77:SER:OG    | 2.19                     | 0.59              |
| 1:E:263:ASP:OD1  | 1:E:264:GLU:N    | 2.35                     | 0.59              |
| 1:G:159:ARG:O    | 1:G:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:G:304:ASP:OD1  | 1:G:392:ARG:NH1  | 2.29                     | 0.59              |
| 1:G:376:ARG:NH2  | 1:G:424:ILE:HA   | 2.17                     | 0.59              |
| 1:K:376:ARG:NH2  | 1:K:424:ILE:HA   | 2.17                     | 0.59              |
| 1:L:88:VAL:O     | 1:L:92:LEU:HG    | 2.02                     | 0.59              |
| 1:L:133:LEU:HD23 | 1:L:171:LEU:HD11 | 1.84                     | 0.59              |
| 1:L:159:ARG:O    | 1:L:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:L:258:ALA:HA   | 1:L:267:ARG:HA   | 1.83                     | 0.59              |
| 1:A:88:VAL:O     | 1:A:92:LEU:HG    | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:133:LEU:HD23 | 1:B:171:LEU:HD11 | 1.84                     | 0.59              |
| 1:E:258:ALA:HA   | 1:E:267:ARG:HA   | 1.83                     | 0.59              |
| 1:H:304:ASP:OD1  | 1:H:392:ARG:NH1  | 2.29                     | 0.59              |
| 1:I:437:GLN:HB2  | 1:P:465:ARG:NH2  | 2.17                     | 0.59              |
| 1:J:133:LEU:HD23 | 1:J:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:M:159:ARG:O    | 1:M:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:M:376:ARG:NH2  | 1:M:424:ILE:HA   | 2.17                     | 0.59              |
| 1:P:258:ALA:HA   | 1:P:267:ARG:HA   | 1.83                     | 0.59              |
| 1:P:263:ASP:OD1  | 1:P:264:GLU:N    | 2.35                     | 0.59              |
| 1:A:133:LEU:HD23 | 1:A:171:LEU:HD11 | 1.84                     | 0.59              |
| 1:G:602:LYS:HD2  | 1:G:606:LYS:HE3  | 1.85                     | 0.59              |
| 1:H:376:ARG:NH2  | 1:H:424:ILE:HA   | 2.17                     | 0.59              |
| 1:H:391:LYS:HA   | 1:H:394:LEU:HD12 | 1.84                     | 0.59              |
| 1:J:159:ARG:O    | 1:J:163:ILE:HG12 | 2.03                     | 0.59              |
| 1:N:88:VAL:O     | 1:N:92:LEU:HG    | 2.02                     | 0.59              |
| 1:O:74:GLN:O     | 1:O:77:SER:OG    | 2.19                     | 0.59              |
| 1:P:88:VAL:O     | 1:P:92:LEU:HG    | 2.02                     | 0.59              |
| 1:E:88:VAL:O     | 1:E:92:LEU:HG    | 2.02                     | 0.59              |
| 1:G:133:LEU:HD23 | 1:G:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:I:602:LYS:HD2  | 1:I:606:LYS:HE3  | 1.85                     | 0.59              |
| 1:J:602:LYS:HD2  | 1:J:606:LYS:HE3  | 1.85                     | 0.59              |
| 1:K:304:ASP:OD1  | 1:K:392:ARG:NH1  | 2.29                     | 0.59              |
| 1:M:133:LEU:HD23 | 1:M:171:LEU:HD11 | 1.85                     | 0.59              |
| 1:B:159:ARG:O    | 1:B:163:ILE:HG12 | 2.03                     | 0.58              |
| 1:F:602:LYS:HD2  | 1:F:606:LYS:HE3  | 1.85                     | 0.58              |
| 1:J:304:ASP:OD1  | 1:J:392:ARG:NH1  | 2.29                     | 0.58              |
| 1:K:391:LYS:HA   | 1:K:394:LEU:HD12 | 1.84                     | 0.58              |
| 1:O:409:VAL:HA   | 1:O:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:B:391:LYS:HA   | 1:B:394:LEU:HD12 | 1.84                     | 0.58              |
| 1:D:409:VAL:HA   | 1:D:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:F:397:LEU:HG   | 1:F:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:F:505:LEU:O    | 1:F:508:CYS:N    | 2.37                     | 0.58              |
| 1:G:258:ALA:HA   | 1:G:267:ARG:HA   | 1.83                     | 0.58              |
| 1:G:397:LEU:HG   | 1:G:399:GLU:HG2  | 1.86                     | 0.58              |
| 1:I:505:LEU:O    | 1:I:508:CYS:N    | 2.37                     | 0.58              |
| 1:J:258:ALA:HA   | 1:J:267:ARG:HA   | 1.83                     | 0.58              |
| 1:J:397:LEU:HG   | 1:J:399:GLU:HG2  | 1.86                     | 0.58              |
| 1:L:239:GLN:HB2  | 1:M:478:ASN:ND2  | 2.16                     | 0.58              |
| 1:B:258:ALA:HA   | 1:B:267:ARG:HA   | 1.83                     | 0.58              |
| 1:C:304:ASP:OD1  | 1:C:392:ARG:NH1  | 2.29                     | 0.58              |
| 1:C:409:VAL:HA   | 1:C:412:TRP:CD1  | 2.38                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:465:ARG:NH2  | 1:F:437:GLN:HB2  | 2.19                     | 0.58              |
| 1:H:397:LEU:HG   | 1:H:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:I:159:ARG:O    | 1:I:163:ILE:HG12 | 2.03                     | 0.58              |
| 1:I:397:LEU:HG   | 1:I:399:GLU:HG2  | 1.86                     | 0.58              |
| 1:M:391:LYS:HA   | 1:M:394:LEU:HD12 | 1.84                     | 0.58              |
| 1:O:159:ARG:O    | 1:O:163:ILE:HG12 | 2.03                     | 0.58              |
| 1:P:505:LEU:O    | 1:P:508:CYS:N    | 2.37                     | 0.58              |
| 1:F:378:VAL:HA   | 1:F:381:SER:HB3  | 1.85                     | 0.58              |
| 1:K:397:LEU:HG   | 1:K:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:L:397:LEU:HG   | 1:L:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:O:133:LEU:HD23 | 1:O:171:LEU:HD11 | 1.84                     | 0.58              |
| 1:E:505:LEU:O    | 1:E:508:CYS:N    | 2.37                     | 0.58              |
| 1:E:602:LYS:HD2  | 1:E:606:LYS:HE3  | 1.85                     | 0.58              |
| 1:F:159:ARG:O    | 1:F:163:ILE:HG12 | 2.03                     | 0.58              |
| 1:G:505:LEU:O    | 1:G:508:CYS:N    | 2.37                     | 0.58              |
| 1:I:378:VAL:HA   | 1:I:381:SER:HB3  | 1.85                     | 0.58              |
| 1:K:159:ARG:O    | 1:K:163:ILE:HG12 | 2.03                     | 0.58              |
| 1:K:409:VAL:HA   | 1:K:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:N:409:VAL:HA   | 1:N:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:P:602:LYS:HD2  | 1:P:606:LYS:HE3  | 1.85                     | 0.58              |
| 1:A:397:LEU:HG   | 1:A:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:D:159:ARG:O    | 1:D:163:ILE:HG12 | 2.03                     | 0.58              |
| 1:F:328:GLN:NE2  | 1:G:416:GLU:OE2  | 2.36                     | 0.58              |
| 1:J:505:LEU:O    | 1:J:508:CYS:N    | 2.37                     | 0.58              |
| 1:M:258:ALA:HA   | 1:M:267:ARG:HA   | 1.83                     | 0.58              |
| 1:B:378:VAL:HA   | 1:B:381:SER:HB3  | 1.85                     | 0.58              |
| 1:D:133:LEU:HD23 | 1:D:171:LEU:HD11 | 1.85                     | 0.58              |
| 1:E:397:LEU:HG   | 1:E:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:K:602:LYS:HD2  | 1:K:606:LYS:HE3  | 1.85                     | 0.58              |
| 1:L:391:LYS:HA   | 1:L:394:LEU:HD12 | 1.84                     | 0.58              |
| 1:M:397:LEU:HG   | 1:M:399:GLU:HG2  | 1.86                     | 0.58              |
| 1:M:505:LEU:O    | 1:M:508:CYS:N    | 2.37                     | 0.58              |
| 1:P:397:LEU:HG   | 1:P:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:A:391:LYS:HA   | 1:A:394:LEU:HD12 | 1.84                     | 0.58              |
| 1:B:75:ALA:O     | 1:B:79:LEU:HG    | 2.04                     | 0.58              |
| 1:B:397:LEU:HG   | 1:B:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:F:409:VAL:HA   | 1:F:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:H:159:ARG:O    | 1:H:163:ILE:HG12 | 2.03                     | 0.58              |
| 1:H:409:VAL:HA   | 1:H:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:N:304:ASP:OD1  | 1:N:392:ARG:NH1  | 2.29                     | 0.58              |
| 1:N:505:LEU:O    | 1:N:508:CYS:N    | 2.37                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:505:LEU:O    | 1:O:508:CYS:N    | 2.37                     | 0.58              |
| 1:A:75:ALA:O     | 1:A:79:LEU:HG    | 2.04                     | 0.58              |
| 1:A:431:GLU:HG2  | 1:A:432:SER:N    | 2.19                     | 0.58              |
| 1:C:397:LEU:HG   | 1:C:399:GLU:HG2  | 1.85                     | 0.58              |
| 1:C:505:LEU:O    | 1:C:508:CYS:N    | 2.37                     | 0.58              |
| 1:D:397:LEU:HG   | 1:D:399:GLU:HG2  | 1.86                     | 0.58              |
| 1:D:505:LEU:O    | 1:D:508:CYS:N    | 2.37                     | 0.58              |
| 1:E:378:VAL:HA   | 1:E:381:SER:HB3  | 1.85                     | 0.58              |
| 1:E:409:VAL:HA   | 1:E:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:E:431:GLU:HG2  | 1:E:432:SER:N    | 2.19                     | 0.58              |
| 1:G:461:ILE:HG22 | 1:H:442:LEU:HD13 | 1.85                     | 0.58              |
| 1:H:602:LYS:HD2  | 1:H:606:LYS:HE3  | 1.85                     | 0.58              |
| 1:I:409:VAL:HA   | 1:I:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:K:197:GLU:OE1  | 1:L:384:GLY:N    | 2.37                     | 0.58              |
| 1:K:431:GLU:HG2  | 1:K:432:SER:N    | 2.19                     | 0.58              |
| 1:L:431:GLU:HG2  | 1:L:432:SER:N    | 2.19                     | 0.58              |
| 1:M:304:ASP:OD1  | 1:M:392:ARG:NH1  | 2.29                     | 0.58              |
| 1:P:409:VAL:HA   | 1:P:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:B:505:LEU:O    | 1:B:508:CYS:N    | 2.37                     | 0.58              |
| 1:D:431:GLU:HG2  | 1:D:432:SER:N    | 2.19                     | 0.58              |
| 1:D:602:LYS:HD2  | 1:D:606:LYS:HE3  | 1.85                     | 0.58              |
| 1:F:133:LEU:HD23 | 1:F:171:LEU:HD11 | 1.84                     | 0.58              |
| 1:G:75:ALA:O     | 1:G:79:LEU:HG    | 2.04                     | 0.58              |
| 1:G:409:VAL:HA   | 1:G:412:TRP:CD1  | 2.38                     | 0.58              |
| 1:G:431:GLU:HG2  | 1:G:432:SER:N    | 2.19                     | 0.58              |
| 1:L:75:ALA:O     | 1:L:79:LEU:HG    | 2.04                     | 0.58              |
| 1:L:602:LYS:HD2  | 1:L:606:LYS:HE3  | 1.85                     | 0.58              |
| 1:M:75:ALA:O     | 1:M:79:LEU:HG    | 2.04                     | 0.58              |
| 1:M:378:VAL:HA   | 1:M:381:SER:HB3  | 1.85                     | 0.58              |
| 1:O:397:LEU:HG   | 1:O:399:GLU:HG2  | 1.86                     | 0.58              |
| 1:P:431:GLU:HG2  | 1:P:432:SER:N    | 2.19                     | 0.58              |
| 1:A:378:VAL:HA   | 1:A:381:SER:HB3  | 1.85                     | 0.57              |
| 1:F:431:GLU:HG2  | 1:F:432:SER:N    | 2.19                     | 0.57              |
| 1:H:75:ALA:O     | 1:H:79:LEU:HG    | 2.04                     | 0.57              |
| 1:H:431:GLU:HG2  | 1:H:432:SER:N    | 2.19                     | 0.57              |
| 1:I:431:GLU:HG2  | 1:I:432:SER:N    | 2.19                     | 0.57              |
| 1:J:75:ALA:O     | 1:J:79:LEU:HG    | 2.04                     | 0.57              |
| 1:J:409:VAL:HA   | 1:J:412:TRP:CD1  | 2.38                     | 0.57              |
| 1:J:431:GLU:HG2  | 1:J:432:SER:N    | 2.19                     | 0.57              |
| 1:K:75:ALA:O     | 1:K:79:LEU:HG    | 2.04                     | 0.57              |
| 1:L:378:VAL:HA   | 1:L:381:SER:HB3  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:409:VAL:HA   | 1:L:412:TRP:CD1  | 2.38                     | 0.57              |
| 1:L:580:LEU:O    | 1:L:584:LEU:HG   | 2.04                     | 0.57              |
| 1:L:692:ILE:HD13 | 1:L:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:M:409:VAL:HA   | 1:M:412:TRP:CD1  | 2.38                     | 0.57              |
| 1:N:692:ILE:HD13 | 1:N:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:O:431:GLU:HG2  | 1:O:432:SER:N    | 2.19                     | 0.57              |
| 1:O:602:LYS:HD2  | 1:O:606:LYS:HE3  | 1.85                     | 0.57              |
| 1:A:580:LEU:O    | 1:A:584:LEU:HG   | 2.04                     | 0.57              |
| 1:A:602:LYS:HD2  | 1:A:606:LYS:HE3  | 1.85                     | 0.57              |
| 1:A:692:ILE:HD13 | 1:A:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:B:304:ASP:OD1  | 1:B:392:ARG:NH1  | 2.29                     | 0.57              |
| 1:B:692:ILE:HD13 | 1:B:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:C:199:CYS:O    | 1:C:203:VAL:HG23 | 2.04                     | 0.57              |
| 1:C:692:ILE:HD13 | 1:C:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:D:199:CYS:O    | 1:D:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:D:565:PHE:HE2  | 1:D:610:SER:HB2  | 1.70                     | 0.57              |
| 1:E:199:CYS:O    | 1:E:203:VAL:HG23 | 2.04                     | 0.57              |
| 1:E:565:PHE:HE2  | 1:E:610:SER:HB2  | 1.70                     | 0.57              |
| 1:H:505:LEU:O    | 1:H:508:CYS:N    | 2.37                     | 0.57              |
| 1:I:133:LEU:HD23 | 1:I:171:LEU:HD11 | 1.84                     | 0.57              |
| 1:L:505:LEU:O    | 1:L:508:CYS:N    | 2.37                     | 0.57              |
| 1:M:199:CYS:O    | 1:M:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:N:397:LEU:HG   | 1:N:399:GLU:HG2  | 1.86                     | 0.57              |
| 1:O:565:PHE:HE2  | 1:O:610:SER:HB2  | 1.70                     | 0.57              |
| 1:A:409:VAL:HA   | 1:A:412:TRP:CD1  | 2.38                     | 0.57              |
| 1:B:199:CYS:O    | 1:B:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:B:409:VAL:HA   | 1:B:412:TRP:CD1  | 2.38                     | 0.57              |
| 1:G:580:LEU:O    | 1:G:584:LEU:HG   | 2.04                     | 0.57              |
| 1:J:378:VAL:HA   | 1:J:381:SER:HB3  | 1.85                     | 0.57              |
| 1:N:199:CYS:O    | 1:N:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:O:75:ALA:O     | 1:O:79:LEU:HG    | 2.04                     | 0.57              |
| 1:O:199:CYS:O    | 1:O:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:P:378:VAL:HA   | 1:P:381:SER:HB3  | 1.85                     | 0.57              |
| 1:P:565:PHE:HE2  | 1:P:610:SER:HB2  | 1.70                     | 0.57              |
| 1:A:199:CYS:O    | 1:A:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:B:431:GLU:HG2  | 1:B:432:SER:N    | 2.19                     | 0.57              |
| 1:D:75:ALA:O     | 1:D:79:LEU:HG    | 2.04                     | 0.57              |
| 1:D:692:ILE:HD13 | 1:D:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:E:74:GLN:O     | 1:E:77:SER:OG    | 2.19                     | 0.57              |
| 1:E:75:ALA:O     | 1:E:79:LEU:HG    | 2.04                     | 0.57              |
| 1:G:378:VAL:HA   | 1:G:381:SER:HB3  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:580:LEU:O    | 1:J:584:LEU:HG   | 2.04                     | 0.57              |
| 1:K:505:LEU:O    | 1:K:508:CYS:N    | 2.37                     | 0.57              |
| 1:M:692:ILE:HD13 | 1:M:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:N:378:VAL:HA   | 1:N:381:SER:HB3  | 1.85                     | 0.57              |
| 1:O:692:ILE:HD13 | 1:O:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:P:199:CYS:O    | 1:P:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:C:378:VAL:HA   | 1:C:381:SER:HB3  | 1.85                     | 0.57              |
| 1:D:378:VAL:HA   | 1:D:381:SER:HB3  | 1.85                     | 0.57              |
| 1:L:199:CYS:O    | 1:L:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:M:431:GLU:HG2  | 1:M:432:SER:N    | 2.19                     | 0.57              |
| 1:N:239:GLN:HB2  | 1:O:478:ASN:HD21 | 1.68                     | 0.57              |
| 1:F:199:CYS:O    | 1:F:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:F:565:PHE:HE2  | 1:F:610:SER:HB2  | 1.70                     | 0.57              |
| 1:I:199:CYS:O    | 1:I:203:VAL:HG23 | 2.04                     | 0.57              |
| 1:J:199:CYS:O    | 1:J:203:VAL:HG23 | 2.04                     | 0.57              |
| 1:M:616:ASN:HA   | 1:M:652:ASN:HB3  | 1.87                     | 0.57              |
| 1:P:75:ALA:O     | 1:P:79:LEU:HG    | 2.04                     | 0.57              |
| 1:B:602:LYS:HD2  | 1:B:606:LYS:HE3  | 1.85                     | 0.57              |
| 1:B:616:ASN:HA   | 1:B:652:ASN:HB3  | 1.87                     | 0.57              |
| 1:G:199:CYS:O    | 1:G:203:VAL:HG23 | 2.05                     | 0.57              |
| 1:H:244:ARG:NH1  | 1:H:247:GLU:OE1  | 2.38                     | 0.57              |
| 1:I:565:PHE:HE2  | 1:I:610:SER:HB2  | 1.70                     | 0.57              |
| 1:K:244:ARG:NH1  | 1:K:247:GLU:OE1  | 2.38                     | 0.57              |
| 1:K:692:ILE:HD13 | 1:K:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:M:602:LYS:HD2  | 1:M:606:LYS:HE3  | 1.85                     | 0.57              |
| 1:P:74:GLN:O     | 1:P:77:SER:OG    | 2.19                     | 0.57              |
| 1:F:580:LEU:O    | 1:F:584:LEU:HG   | 2.04                     | 0.57              |
| 1:F:666:GLN:OE1  | 1:F:666:GLN:N    | 2.37                     | 0.57              |
| 1:G:565:PHE:HE2  | 1:G:610:SER:HB2  | 1.70                     | 0.57              |
| 1:H:692:ILE:HD13 | 1:H:695:ILE:HD12 | 1.86                     | 0.57              |
| 1:I:75:ALA:O     | 1:I:79:LEU:HG    | 2.04                     | 0.57              |
| 1:I:666:GLN:OE1  | 1:I:666:GLN:N    | 2.37                     | 0.57              |
| 1:J:565:PHE:HE2  | 1:J:610:SER:HB2  | 1.70                     | 0.57              |
| 1:O:378:VAL:HA   | 1:O:381:SER:HB3  | 1.85                     | 0.57              |
| 1:A:505:LEU:O    | 1:A:508:CYS:N    | 2.37                     | 0.57              |
| 1:C:565:PHE:HE2  | 1:C:610:SER:HB2  | 1.70                     | 0.57              |
| 1:C:602:LYS:HD2  | 1:C:606:LYS:HE3  | 1.85                     | 0.57              |
| 1:D:286:GLU:OE1  | 1:D:286:GLU:N    | 2.38                     | 0.57              |
| 1:I:580:LEU:O    | 1:I:584:LEU:HG   | 2.04                     | 0.57              |
| 1:N:376:ARG:NH2  | 1:N:423:GLN:O    | 2.38                     | 0.57              |
| 1:O:286:GLU:OE1  | 1:O:286:GLU:N    | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:616:ASN:HA   | 1:A:652:ASN:HB3  | 1.87                     | 0.57              |
| 1:E:228:LEU:HD21 | 1:E:269:HIS:CD2  | 2.40                     | 0.57              |
| 1:E:256:PRO:HB3  | 1:F:578:SER:OG   | 2.04                     | 0.57              |
| 1:E:286:GLU:N    | 1:E:286:GLU:OE1  | 2.38                     | 0.57              |
| 1:H:580:LEU:O    | 1:H:584:LEU:HG   | 2.04                     | 0.57              |
| 1:N:75:ALA:O     | 1:N:79:LEU:HG    | 2.04                     | 0.57              |
| 1:N:565:PHE:HE2  | 1:N:610:SER:HB2  | 1.70                     | 0.57              |
| 1:N:602:LYS:HD2  | 1:N:606:LYS:HE3  | 1.85                     | 0.57              |
| 1:P:286:GLU:OE1  | 1:P:286:GLU:N    | 2.38                     | 0.57              |
| 1:C:75:ALA:O     | 1:C:79:LEU:HG    | 2.04                     | 0.56              |
| 1:C:129:LEU:H    | 1:C:129:LEU:HD12 | 1.70                     | 0.56              |
| 1:C:376:ARG:NH2  | 1:C:423:GLN:O    | 2.38                     | 0.56              |
| 1:E:692:ILE:HD13 | 1:E:695:ILE:HD12 | 1.86                     | 0.56              |
| 1:F:75:ALA:O     | 1:F:79:LEU:HG    | 2.04                     | 0.56              |
| 1:J:616:ASN:HA   | 1:J:652:ASN:HB3  | 1.87                     | 0.56              |
| 1:K:616:ASN:HA   | 1:K:652:ASN:HB3  | 1.87                     | 0.56              |
| 1:O:498:PHE:HE1  | 1:O:534:HIS:CG   | 2.23                     | 0.56              |
| 1:O:580:LEU:O    | 1:O:584:LEU:HG   | 2.04                     | 0.56              |
| 1:P:228:LEU:HD21 | 1:P:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:B:129:LEU:HD12 | 1:B:129:LEU:H    | 1.70                     | 0.56              |
| 1:D:129:LEU:H    | 1:D:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:D:376:ARG:NH2  | 1:D:423:GLN:O    | 2.38                     | 0.56              |
| 1:D:580:LEU:O    | 1:D:584:LEU:HG   | 2.04                     | 0.56              |
| 1:G:129:LEU:H    | 1:G:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:G:616:ASN:HA   | 1:G:652:ASN:HB3  | 1.87                     | 0.56              |
| 1:I:634:ASP:HB2  | 1:I:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:J:129:LEU:HD12 | 1:J:129:LEU:H    | 1.71                     | 0.56              |
| 1:L:616:ASN:HA   | 1:L:652:ASN:HB3  | 1.87                     | 0.56              |
| 1:M:376:ARG:NH2  | 1:M:423:GLN:O    | 2.38                     | 0.56              |
| 1:M:580:LEU:O    | 1:M:584:LEU:HG   | 2.04                     | 0.56              |
| 1:O:129:LEU:H    | 1:O:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:O:376:ARG:NH2  | 1:O:423:GLN:O    | 2.38                     | 0.56              |
| 1:A:244:ARG:NH1  | 1:A:247:GLU:OE1  | 2.38                     | 0.56              |
| 1:A:304:ASP:OD1  | 1:A:392:ARG:NH1  | 2.29                     | 0.56              |
| 1:B:228:LEU:HD21 | 1:B:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:B:376:ARG:NH2  | 1:B:423:GLN:O    | 2.38                     | 0.56              |
| 1:C:498:PHE:HE1  | 1:C:534:HIS:CG   | 2.23                     | 0.56              |
| 1:D:228:LEU:HD21 | 1:D:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:D:498:PHE:HE1  | 1:D:534:HIS:CG   | 2.23                     | 0.56              |
| 1:F:228:LEU:HD21 | 1:F:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:F:376:ARG:NH2  | 1:F:423:GLN:O    | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:634:ASP:HB2  | 1:F:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:G:483:ASP:OD2  | 1:G:487:LEU:N    | 2.36                     | 0.56              |
| 1:G:634:ASP:HB2  | 1:G:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:H:129:LEU:H    | 1:H:129:LEU:HD12 | 1.70                     | 0.56              |
| 1:H:199:CYS:O    | 1:H:203:VAL:HG23 | 2.04                     | 0.56              |
| 1:H:616:ASN:HA   | 1:H:652:ASN:HB3  | 1.87                     | 0.56              |
| 1:H:631:GLN:H    | 1:H:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:I:631:GLN:H    | 1:I:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:J:286:GLU:N    | 1:J:286:GLU:OE1  | 2.38                     | 0.56              |
| 1:J:483:ASP:OD2  | 1:J:487:LEU:N    | 2.36                     | 0.56              |
| 1:J:634:ASP:HB2  | 1:J:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:K:378:VAL:HA   | 1:K:381:SER:HB3  | 1.85                     | 0.56              |
| 1:K:580:LEU:O    | 1:K:584:LEU:HG   | 2.04                     | 0.56              |
| 1:M:129:LEU:HD12 | 1:M:129:LEU:H    | 1.71                     | 0.56              |
| 1:M:228:LEU:HD21 | 1:M:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:N:129:LEU:H    | 1:N:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:N:217:ARG:HH22 | 1:O:688:GLN:NE2  | 2.02                     | 0.56              |
| 1:P:634:ASP:HB2  | 1:P:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:P:692:ILE:HD13 | 1:P:695:ILE:HD12 | 1.86                     | 0.56              |
| 1:B:580:LEU:O    | 1:B:584:LEU:HG   | 2.04                     | 0.56              |
| 1:C:580:LEU:O    | 1:C:584:LEU:HG   | 2.04                     | 0.56              |
| 1:E:580:LEU:O    | 1:E:584:LEU:HG   | 2.04                     | 0.56              |
| 1:E:634:ASP:HB2  | 1:E:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:F:631:GLN:H    | 1:F:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:G:286:GLU:N    | 1:G:286:GLU:OE1  | 2.38                     | 0.56              |
| 1:G:328:GLN:NE2  | 1:H:416:GLU:OE2  | 2.38                     | 0.56              |
| 1:I:228:LEU:HD21 | 1:I:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:I:376:ARG:NH2  | 1:I:423:GLN:O    | 2.38                     | 0.56              |
| 1:L:244:ARG:NH1  | 1:L:247:GLU:OE1  | 2.38                     | 0.56              |
| 1:N:498:PHE:HE1  | 1:N:534:HIS:CG   | 2.23                     | 0.56              |
| 1:O:228:LEU:HD21 | 1:O:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:B:170:ASN:HA   | 1:B:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:B:565:PHE:HE2  | 1:B:610:SER:HB2  | 1.70                     | 0.56              |
| 1:B:631:GLN:H    | 1:B:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:E:129:LEU:HD12 | 1:E:129:LEU:H    | 1.71                     | 0.56              |
| 1:G:376:ARG:NH2  | 1:G:423:GLN:O    | 2.38                     | 0.56              |
| 1:H:378:VAL:HA   | 1:H:381:SER:HB3  | 1.85                     | 0.56              |
| 1:I:498:PHE:HE1  | 1:I:534:HIS:CG   | 2.23                     | 0.56              |
| 1:J:376:ARG:NH2  | 1:J:423:GLN:O    | 2.38                     | 0.56              |
| 1:J:692:ILE:HD13 | 1:J:695:ILE:HD12 | 1.86                     | 0.56              |
| 1:K:199:CYS:O    | 1:K:203:VAL:HG23 | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:631:GLN:H    | 1:K:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:N:580:LEU:O    | 1:N:584:LEU:HG   | 2.04                     | 0.56              |
| 1:N:631:GLN:H    | 1:N:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:P:129:LEU:H    | 1:P:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:P:498:PHE:HE1  | 1:P:534:HIS:CG   | 2.23                     | 0.56              |
| 1:A:129:LEU:H    | 1:A:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:C:170:ASN:HA   | 1:C:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:E:498:PHE:HE1  | 1:E:534:HIS:CG   | 2.23                     | 0.56              |
| 1:F:286:GLU:OE1  | 1:F:286:GLU:N    | 2.38                     | 0.56              |
| 1:H:634:ASP:HB2  | 1:H:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:J:430:CYS:HB3  | 1:J:434:ARG:NH2  | 2.10                     | 0.56              |
| 1:K:634:ASP:HB2  | 1:K:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:M:565:PHE:HE2  | 1:M:610:SER:HB2  | 1.70                     | 0.56              |
| 1:M:631:GLN:H    | 1:M:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:N:170:ASN:HA   | 1:N:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:N:431:GLU:HG2  | 1:N:432:SER:N    | 2.19                     | 0.56              |
| 1:N:465:ARG:NH2  | 1:O:437:GLN:HB2  | 2.20                     | 0.56              |
| 1:P:580:LEU:O    | 1:P:584:LEU:HG   | 2.04                     | 0.56              |
| 1:C:431:GLU:HG2  | 1:C:432:SER:N    | 2.19                     | 0.56              |
| 1:C:631:GLN:H    | 1:C:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:D:170:ASN:HA   | 1:D:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:D:256:PRO:HG3  | 1:E:582:VAL:HG21 | 1.88                     | 0.56              |
| 1:E:631:GLN:H    | 1:E:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:G:228:LEU:HD21 | 1:G:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:K:129:LEU:H    | 1:K:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:L:129:LEU:H    | 1:L:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:L:170:ASN:HA   | 1:L:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:L:304:ASP:OD1  | 1:L:392:ARG:NH1  | 2.29                     | 0.56              |
| 1:M:170:ASN:HA   | 1:M:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:O:170:ASN:HA   | 1:O:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:O:239:GLN:HB2  | 1:P:478:ASN:HD21 | 1.70                     | 0.56              |
| 1:P:631:GLN:H    | 1:P:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:A:170:ASN:HA   | 1:A:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:A:565:PHE:HE2  | 1:A:610:SER:HB2  | 1.70                     | 0.56              |
| 1:E:170:ASN:HA   | 1:E:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:E:376:ARG:NH2  | 1:E:423:GLN:O    | 2.38                     | 0.56              |
| 1:E:431:GLU:O    | 1:E:434:ARG:HG2  | 2.06                     | 0.56              |
| 1:F:498:PHE:HE1  | 1:F:534:HIS:CG   | 2.23                     | 0.56              |
| 1:G:692:ILE:HD13 | 1:G:695:ILE:HD12 | 1.86                     | 0.56              |
| 1:I:170:ASN:HA   | 1:I:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:I:286:GLU:OE1  | 1:I:286:GLU:N    | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:170:ASN:HA   | 1:J:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:J:228:LEU:HD21 | 1:J:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:J:498:PHE:HE1  | 1:J:534:HIS:CG   | 2.23                     | 0.56              |
| 1:K:498:PHE:HE1  | 1:K:534:HIS:CG   | 2.23                     | 0.56              |
| 1:L:565:PHE:HE2  | 1:L:610:SER:HB2  | 1.69                     | 0.56              |
| 1:M:498:PHE:HE1  | 1:M:534:HIS:CG   | 2.23                     | 0.56              |
| 1:P:170:ASN:HA   | 1:P:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:P:431:GLU:O    | 1:P:434:ARG:HG2  | 2.06                     | 0.56              |
| 1:B:498:PHE:HE1  | 1:B:534:HIS:CG   | 2.23                     | 0.56              |
| 1:D:634:ASP:HB2  | 1:D:636:LYS:HG2  | 1.87                     | 0.56              |
| 1:E:217:ARG:HH22 | 1:F:688:GLN:NE2  | 2.04                     | 0.56              |
| 1:F:74:GLN:O     | 1:F:77:SER:OG    | 2.19                     | 0.56              |
| 1:F:170:ASN:HA   | 1:F:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:F:692:ILE:HD13 | 1:F:695:ILE:HD12 | 1.86                     | 0.56              |
| 1:G:170:ASN:HA   | 1:G:173:LYS:HE3  | 1.88                     | 0.56              |
| 1:G:498:PHE:HE1  | 1:G:534:HIS:CG   | 2.23                     | 0.56              |
| 1:I:431:GLU:O    | 1:I:434:ARG:HG2  | 2.06                     | 0.56              |
| 1:I:548:SER:HB2  | 1:I:549:PRO:HD3  | 1.88                     | 0.56              |
| 1:K:228:LEU:HD21 | 1:K:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:L:376:ARG:NH2  | 1:L:423:GLN:O    | 2.38                     | 0.56              |
| 1:L:498:PHE:HE1  | 1:L:534:HIS:CG   | 2.23                     | 0.56              |
| 1:L:631:GLN:H    | 1:L:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:P:376:ARG:NH2  | 1:P:423:GLN:O    | 2.38                     | 0.56              |
| 1:A:228:LEU:HD21 | 1:A:269:HIS:CD2  | 2.40                     | 0.56              |
| 1:A:376:ARG:NH2  | 1:A:423:GLN:O    | 2.38                     | 0.56              |
| 1:E:616:ASN:HA   | 1:E:652:ASN:HB3  | 1.87                     | 0.56              |
| 1:F:431:GLU:O    | 1:F:434:ARG:HG2  | 2.06                     | 0.56              |
| 1:F:548:SER:HB2  | 1:F:549:PRO:HD3  | 1.88                     | 0.56              |
| 1:G:430:CYS:HB3  | 1:G:434:ARG:NH2  | 2.10                     | 0.56              |
| 1:G:631:GLN:H    | 1:G:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:I:129:LEU:H    | 1:I:129:LEU:HD12 | 1.71                     | 0.56              |
| 1:I:692:ILE:HD13 | 1:I:695:ILE:HD12 | 1.86                     | 0.56              |
| 1:J:631:GLN:H    | 1:J:669:PRO:HD3  | 1.71                     | 0.56              |
| 1:M:548:SER:HB2  | 1:M:549:PRO:HD3  | 1.88                     | 0.56              |
| 1:O:634:ASP:HB2  | 1:O:636:LYS:HG2  | 1.88                     | 0.56              |
| 1:P:616:ASN:HA   | 1:P:652:ASN:HB3  | 1.87                     | 0.56              |
| 1:A:498:PHE:HE1  | 1:A:534:HIS:CG   | 2.23                     | 0.55              |
| 1:E:548:SER:HB2  | 1:E:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:F:483:ASP:OD2  | 1:F:487:LEU:N    | 2.36                     | 0.55              |
| 1:H:498:PHE:HE1  | 1:H:534:HIS:CG   | 2.23                     | 0.55              |
| 1:H:548:SER:HB2  | 1:H:549:PRO:HD3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:184:VAL:HA   | 1:I:187:ILE:HD12 | 1.88                     | 0.55              |
| 1:I:239:GLN:HB2  | 1:J:478:ASN:HD21 | 1.70                     | 0.55              |
| 1:I:483:ASP:OD2  | 1:I:487:LEU:N    | 2.36                     | 0.55              |
| 1:K:170:ASN:HA   | 1:K:173:LYS:HE3  | 1.88                     | 0.55              |
| 1:K:548:SER:HB2  | 1:K:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:L:465:ARG:NH2  | 1:M:437:GLN:OE1  | 2.39                     | 0.55              |
| 1:P:548:SER:HB2  | 1:P:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:A:548:SER:HB2  | 1:A:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:D:616:ASN:HA   | 1:D:652:ASN:HB3  | 1.87                     | 0.55              |
| 1:E:666:GLN:OE1  | 1:E:666:GLN:N    | 2.37                     | 0.55              |
| 1:F:129:LEU:H    | 1:F:129:LEU:HD12 | 1.71                     | 0.55              |
| 1:F:184:VAL:HA   | 1:F:187:ILE:HD12 | 1.88                     | 0.55              |
| 1:H:170:ASN:HA   | 1:H:173:LYS:HE3  | 1.88                     | 0.55              |
| 1:K:376:ARG:NH2  | 1:K:423:GLN:O    | 2.38                     | 0.55              |
| 1:L:228:LEU:HD21 | 1:L:269:HIS:CD2  | 2.40                     | 0.55              |
| 1:N:548:SER:HB2  | 1:N:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:O:616:ASN:HA   | 1:O:652:ASN:HB3  | 1.87                     | 0.55              |
| 1:A:631:GLN:H    | 1:A:669:PRO:HD3  | 1.71                     | 0.55              |
| 1:B:548:SER:HB2  | 1:B:549:PRO:HD3  | 1.89                     | 0.55              |
| 1:C:548:SER:HB2  | 1:C:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:F:414:GLU:O    | 1:F:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:H:228:LEU:HD21 | 1:H:269:HIS:CD2  | 2.40                     | 0.55              |
| 1:H:414:GLU:O    | 1:H:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:M:217:ARG:HH12 | 1:N:685:HIS:HB3  | 1.72                     | 0.55              |
| 1:P:666:GLN:OE1  | 1:P:666:GLN:N    | 2.37                     | 0.55              |
| 1:B:219:ASP:HB3  | 1:B:222:LEU:HB3  | 1.89                     | 0.55              |
| 1:C:228:LEU:HD21 | 1:C:269:HIS:CD2  | 2.40                     | 0.55              |
| 1:G:548:SER:HB2  | 1:G:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:H:376:ARG:NH2  | 1:H:423:GLN:O    | 2.38                     | 0.55              |
| 1:H:431:GLU:O    | 1:H:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:H:483:ASP:OD2  | 1:H:487:LEU:N    | 2.36                     | 0.55              |
| 1:I:414:GLU:O    | 1:I:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:K:219:ASP:HB3  | 1:K:222:LEU:HB3  | 1.89                     | 0.55              |
| 1:L:197:GLU:CD   | 1:M:383:ASN:HA   | 2.31                     | 0.55              |
| 1:L:548:SER:HB2  | 1:L:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:N:228:LEU:HD21 | 1:N:269:HIS:CD2  | 2.40                     | 0.55              |
| 1:O:548:SER:HB2  | 1:O:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:A:634:ASP:HB2  | 1:A:636:LYS:HG2  | 1.88                     | 0.55              |
| 1:C:616:ASN:HA   | 1:C:652:ASN:HB3  | 1.87                     | 0.55              |
| 1:D:548:SER:HB2  | 1:D:549:PRO:HD3  | 1.88                     | 0.55              |
| 1:F:616:ASN:HA   | 1:F:652:ASN:HB3  | 1.87                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:184:VAL:HA  | 1:G:187:ILE:HD12 | 1.88                     | 0.55              |
| 1:J:414:GLU:O   | 1:J:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:K:414:GLU:O   | 1:K:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:K:431:GLU:O   | 1:K:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:M:219:ASP:HB3 | 1:M:222:LEU:HB3  | 1.89                     | 0.55              |
| 1:N:217:ARG:NH1 | 1:O:685:HIS:HB3  | 2.19                     | 0.55              |
| 1:O:431:GLU:O   | 1:O:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:P:414:GLU:O   | 1:P:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:D:631:GLN:H   | 1:D:669:PRO:HD3  | 1.71                     | 0.55              |
| 1:E:414:GLU:O   | 1:E:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:G:414:GLU:O   | 1:G:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:H:142:VAL:O   | 1:H:146:ARG:HG3  | 2.07                     | 0.55              |
| 1:I:616:ASN:HA  | 1:I:652:ASN:HB3  | 1.87                     | 0.55              |
| 1:J:184:VAL:HA  | 1:J:187:ILE:HD12 | 1.88                     | 0.55              |
| 1:K:142:VAL:O   | 1:K:146:ARG:HG3  | 2.07                     | 0.55              |
| 1:L:634:ASP:HB2 | 1:L:636:LYS:HG2  | 1.88                     | 0.55              |
| 1:N:616:ASN:HA  | 1:N:652:ASN:HB3  | 1.87                     | 0.55              |
| 1:A:219:ASP:HB3 | 1:A:222:LEU:HB3  | 1.89                     | 0.55              |
| 1:B:244:ARG:NH1 | 1:B:247:GLU:OE1  | 2.38                     | 0.55              |
| 1:C:414:GLU:O   | 1:C:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:C:431:GLU:O   | 1:C:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:C:634:ASP:HB2 | 1:C:636:LYS:HG2  | 1.88                     | 0.55              |
| 1:D:431:GLU:O   | 1:D:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:H:219:ASP:HB3 | 1:H:222:LEU:HB3  | 1.89                     | 0.55              |
| 1:H:565:PHE:HE2 | 1:H:610:SER:HB2  | 1.70                     | 0.55              |
| 1:J:548:SER:HB2 | 1:J:549:PRO:HD3  | 1.89                     | 0.55              |
| 1:M:244:ARG:NH1 | 1:M:247:GLU:OE1  | 2.38                     | 0.55              |
| 1:M:340:GLU:OE1 | 1:M:340:GLU:N    | 2.30                     | 0.55              |
| 1:O:631:GLN:H   | 1:O:669:PRO:HD3  | 1.71                     | 0.55              |
| 1:B:634:ASP:HB2 | 1:B:636:LYS:HG2  | 1.88                     | 0.55              |
| 1:C:627:ASP:N   | 1:C:627:ASP:OD1  | 2.40                     | 0.55              |
| 1:F:142:VAL:O   | 1:F:146:ARG:HG3  | 2.07                     | 0.55              |
| 1:I:142:VAL:O   | 1:I:146:ARG:HG3  | 2.07                     | 0.55              |
| 1:K:483:ASP:OD2 | 1:K:487:LEU:N    | 2.36                     | 0.55              |
| 1:N:414:GLU:O   | 1:N:418:GLN:HG2  | 2.07                     | 0.55              |
| 1:N:627:ASP:OD1 | 1:N:627:ASP:N    | 2.40                     | 0.55              |
| 1:G:219:ASP:HB3 | 1:G:222:LEU:HB3  | 1.89                     | 0.55              |
| 1:G:627:ASP:OD1 | 1:G:627:ASP:N    | 2.40                     | 0.55              |
| 1:M:634:ASP:HB2 | 1:M:636:LYS:HG2  | 1.88                     | 0.55              |
| 1:N:431:GLU:O   | 1:N:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:N:634:ASP:HB2 | 1:N:636:LYS:HG2  | 1.88                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:431:GLU:O   | 1:A:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:B:340:GLU:OE1 | 1:B:340:GLU:N    | 2.30                     | 0.55              |
| 1:K:565:PHE:HE2 | 1:K:610:SER:HB2  | 1.70                     | 0.55              |
| 1:L:219:ASP:HB3 | 1:L:222:LEU:HB3  | 1.89                     | 0.55              |
| 1:L:431:GLU:O   | 1:L:434:ARG:HG2  | 2.06                     | 0.55              |
| 1:P:430:CYS:HB3 | 1:P:434:ARG:NH2  | 2.10                     | 0.55              |
| 1:A:184:VAL:HA  | 1:A:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:A:340:GLU:OE1 | 1:A:340:GLU:N    | 2.30                     | 0.54              |
| 1:A:414:GLU:O   | 1:A:418:GLN:HG2  | 2.07                     | 0.54              |
| 1:B:414:GLU:O   | 1:B:418:GLN:HG2  | 2.07                     | 0.54              |
| 1:B:627:ASP:N   | 1:B:627:ASP:OD1  | 2.40                     | 0.54              |
| 1:J:219:ASP:HB3 | 1:J:222:LEU:HB3  | 1.89                     | 0.54              |
| 1:J:627:ASP:N   | 1:J:627:ASP:OD1  | 2.40                     | 0.54              |
| 1:K:184:VAL:HA  | 1:K:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:M:239:GLN:HB2 | 1:N:478:ASN:HD21 | 1.70                     | 0.54              |
| 1:M:627:ASP:N   | 1:M:627:ASP:OD1  | 2.40                     | 0.54              |
| 1:C:142:VAL:O   | 1:C:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:D:142:VAL:O   | 1:D:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:E:617:PHE:HB3 | 1:E:653:ILE:HA   | 1.90                     | 0.54              |
| 1:H:184:VAL:HA  | 1:H:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:L:414:GLU:O   | 1:L:418:GLN:HG2  | 2.07                     | 0.54              |
| 1:M:184:VAL:HA  | 1:M:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:M:414:GLU:O   | 1:M:418:GLN:HG2  | 2.07                     | 0.54              |
| 1:B:184:VAL:HA  | 1:B:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:C:617:PHE:HB3 | 1:C:653:ILE:HA   | 1.90                     | 0.54              |
| 1:F:617:PHE:HB3 | 1:F:653:ILE:HA   | 1.90                     | 0.54              |
| 1:I:617:PHE:HB3 | 1:I:653:ILE:HA   | 1.90                     | 0.54              |
| 1:K:375:LYS:O   | 1:K:376:ARG:NH1  | 2.41                     | 0.54              |
| 1:L:184:VAL:HA  | 1:L:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:L:340:GLU:OE1 | 1:L:340:GLU:N    | 2.30                     | 0.54              |
| 1:L:430:CYS:HB3 | 1:L:434:ARG:NH2  | 2.10                     | 0.54              |
| 1:N:142:VAL:O   | 1:N:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:O:617:PHE:HB3 | 1:O:653:ILE:HA   | 1.90                     | 0.54              |
| 1:P:142:VAL:O   | 1:P:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:A:375:LYS:O   | 1:A:376:ARG:NH1  | 2.41                     | 0.54              |
| 1:D:617:PHE:HB3 | 1:D:653:ILE:HA   | 1.90                     | 0.54              |
| 1:D:627:ASP:OD1 | 1:D:627:ASP:N    | 2.40                     | 0.54              |
| 1:E:430:CYS:HB3 | 1:E:434:ARG:NH2  | 2.10                     | 0.54              |
| 1:G:375:LYS:O   | 1:G:376:ARG:NH1  | 2.41                     | 0.54              |
| 1:G:431:GLU:O   | 1:G:434:ARG:HG2  | 2.06                     | 0.54              |
| 1:H:375:LYS:O   | 1:H:376:ARG:NH1  | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:375:LYS:O    | 1:J:376:ARG:NH1  | 2.41                     | 0.54              |
| 1:M:142:VAL:O    | 1:M:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:N:617:PHE:HB3  | 1:N:653:ILE:HA   | 1.90                     | 0.54              |
| 1:O:142:VAL:O    | 1:O:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:P:617:PHE:HB3  | 1:P:653:ILE:HA   | 1.90                     | 0.54              |
| 1:A:286:GLU:OE1  | 1:A:286:GLU:N    | 2.38                     | 0.54              |
| 1:B:375:LYS:O    | 1:B:376:ARG:NH1  | 2.41                     | 0.54              |
| 1:D:184:VAL:HA   | 1:D:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:E:142:VAL:O    | 1:E:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:G:617:PHE:HB3  | 1:G:653:ILE:HA   | 1.90                     | 0.54              |
| 1:B:431:GLU:O    | 1:B:434:ARG:HG2  | 2.06                     | 0.54              |
| 1:D:414:GLU:O    | 1:D:418:GLN:HG2  | 2.07                     | 0.54              |
| 1:J:142:VAL:O    | 1:J:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:J:431:GLU:O    | 1:J:434:ARG:HG2  | 2.06                     | 0.54              |
| 1:K:261:LYS:HG2  | 1:L:574:SER:OG   | 2.07                     | 0.54              |
| 1:L:286:GLU:OE1  | 1:L:286:GLU:N    | 2.38                     | 0.54              |
| 1:L:375:LYS:O    | 1:L:376:ARG:NH1  | 2.41                     | 0.54              |
| 1:M:375:LYS:O    | 1:M:376:ARG:NH1  | 2.41                     | 0.54              |
| 1:O:627:ASP:OD1  | 1:O:627:ASP:N    | 2.40                     | 0.54              |
| 1:P:184:VAL:HA   | 1:P:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:B:142:VAL:O    | 1:B:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:C:516:HIS:CD2  | 1:C:546:LEU:HD13 | 2.43                     | 0.54              |
| 1:F:138:LEU:O    | 1:F:142:VAL:HG23 | 2.08                     | 0.54              |
| 1:F:219:ASP:HB3  | 1:F:222:LEU:HB3  | 1.89                     | 0.54              |
| 1:H:640:HIS:O    | 1:H:644:VAL:HG23 | 2.08                     | 0.54              |
| 1:I:138:LEU:O    | 1:I:142:VAL:HG23 | 2.08                     | 0.54              |
| 1:I:219:ASP:HB3  | 1:I:222:LEU:HB3  | 1.89                     | 0.54              |
| 1:I:582:VAL:HG21 | 1:P:256:PRO:HG3  | 1.89                     | 0.54              |
| 1:J:617:PHE:HB3  | 1:J:653:ILE:HA   | 1.90                     | 0.54              |
| 1:K:640:HIS:O    | 1:K:644:VAL:HG23 | 2.08                     | 0.54              |
| 1:L:617:PHE:HB3  | 1:L:653:ILE:HA   | 1.90                     | 0.54              |
| 1:N:184:VAL:HA   | 1:N:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:O:414:GLU:O    | 1:O:418:GLN:HG2  | 2.07                     | 0.54              |
| 1:B:256:PRO:HG3  | 1:C:582:VAL:HG21 | 1.88                     | 0.54              |
| 1:C:184:VAL:HA   | 1:C:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:C:219:ASP:HB3  | 1:C:222:LEU:HB3  | 1.89                     | 0.54              |
| 1:D:128:LEU:O    | 1:D:132:LEU:HG   | 2.08                     | 0.54              |
| 1:E:184:VAL:HA   | 1:E:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:G:142:VAL:O    | 1:G:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:G:640:HIS:O    | 1:G:644:VAL:HG23 | 2.08                     | 0.54              |
| 1:I:128:LEU:O    | 1:I:132:LEU:HG   | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:128:LEU:O    | 1:J:132:LEU:HG   | 2.08                     | 0.54              |
| 1:J:640:HIS:O    | 1:J:644:VAL:HG23 | 2.08                     | 0.54              |
| 1:M:617:PHE:HB3  | 1:M:653:ILE:HA   | 1.90                     | 0.54              |
| 1:N:516:HIS:CD2  | 1:N:546:LEU:HD13 | 2.43                     | 0.54              |
| 1:P:516:HIS:CD2  | 1:P:546:LEU:HD13 | 2.43                     | 0.54              |
| 1:A:412:TRP:O    | 1:A:440:GLY:N    | 2.33                     | 0.54              |
| 1:A:617:PHE:HB3  | 1:A:653:ILE:HA   | 1.90                     | 0.54              |
| 1:B:617:PHE:HB3  | 1:B:653:ILE:HA   | 1.90                     | 0.54              |
| 1:E:516:HIS:CD2  | 1:E:546:LEU:HD13 | 2.43                     | 0.54              |
| 1:F:128:LEU:O    | 1:F:132:LEU:HG   | 2.08                     | 0.54              |
| 1:G:128:LEU:O    | 1:G:132:LEU:HG   | 2.08                     | 0.54              |
| 1:H:617:PHE:HB3  | 1:H:653:ILE:HA   | 1.90                     | 0.54              |
| 1:H:627:ASP:N    | 1:H:627:ASP:OD1  | 2.40                     | 0.54              |
| 1:K:617:PHE:HB3  | 1:K:653:ILE:HA   | 1.90                     | 0.54              |
| 1:M:431:GLU:O    | 1:M:434:ARG:HG2  | 2.06                     | 0.54              |
| 1:N:219:ASP:HB3  | 1:N:222:LEU:HB3  | 1.89                     | 0.54              |
| 1:O:128:LEU:O    | 1:O:132:LEU:HG   | 2.08                     | 0.54              |
| 1:O:184:VAL:HA   | 1:O:187:ILE:HD12 | 1.88                     | 0.54              |
| 1:O:244:ARG:NH1  | 1:O:247:GLU:OE1  | 2.38                     | 0.54              |
| 1:A:142:VAL:O    | 1:A:146:ARG:HG3  | 2.07                     | 0.54              |
| 1:D:244:ARG:NH1  | 1:D:247:GLU:OE1  | 2.38                     | 0.54              |
| 1:G:138:LEU:O    | 1:G:142:VAL:HG23 | 2.08                     | 0.54              |
| 1:L:640:HIS:O    | 1:L:644:VAL:HG23 | 2.08                     | 0.54              |
| 1:M:128:LEU:O    | 1:M:132:LEU:HG   | 2.08                     | 0.54              |
| 1:N:244:ARG:NH1  | 1:N:247:GLU:OE1  | 2.38                     | 0.54              |
| 1:N:286:GLU:OE1  | 1:N:286:GLU:N    | 2.38                     | 0.54              |
| 1:N:340:GLU:OE1  | 1:N:340:GLU:N    | 2.30                     | 0.54              |
| 1:O:219:ASP:HB3  | 1:O:222:LEU:HB3  | 1.89                     | 0.54              |
| 1:A:128:LEU:O    | 1:A:132:LEU:HG   | 2.08                     | 0.53              |
| 1:A:430:CYS:HB3  | 1:A:434:ARG:NH2  | 2.11                     | 0.53              |
| 1:B:128:LEU:O    | 1:B:132:LEU:HG   | 2.08                     | 0.53              |
| 1:B:286:GLU:N    | 1:B:286:GLU:OE1  | 2.38                     | 0.53              |
| 1:C:244:ARG:NH1  | 1:C:247:GLU:OE1  | 2.38                     | 0.53              |
| 1:E:159:ARG:HD2  | 1:E:162:ARG:HH21 | 1.73                     | 0.53              |
| 1:H:516:HIS:CD2  | 1:H:546:LEU:HD13 | 2.43                     | 0.53              |
| 1:I:375:LYS:O    | 1:I:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:J:138:LEU:O    | 1:J:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:K:340:GLU:OE1  | 1:K:340:GLU:N    | 2.30                     | 0.53              |
| 1:K:516:HIS:CD2  | 1:K:546:LEU:HD13 | 2.43                     | 0.53              |
| 1:L:142:VAL:O    | 1:L:146:ARG:HG3  | 2.07                     | 0.53              |
| 1:M:217:ARG:HH22 | 1:N:688:GLN:NE2  | 2.06                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:286:GLU:N    | 1:M:286:GLU:OE1  | 2.38                     | 0.53              |
| 1:D:219:ASP:HB3  | 1:D:222:LEU:HB3  | 1.89                     | 0.53              |
| 1:F:375:LYS:O    | 1:F:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:H:340:GLU:OE1  | 1:H:340:GLU:N    | 2.30                     | 0.53              |
| 1:K:627:ASP:N    | 1:K:627:ASP:OD1  | 2.40                     | 0.53              |
| 1:L:128:LEU:O    | 1:L:132:LEU:HG   | 2.08                     | 0.53              |
| 1:N:159:ARG:HD2  | 1:N:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:O:666:GLN:OE1  | 1:O:666:GLN:N    | 2.37                     | 0.53              |
| 1:P:128:LEU:O    | 1:P:132:LEU:HG   | 2.08                     | 0.53              |
| 1:P:159:ARG:HD2  | 1:P:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:A:640:HIS:O    | 1:A:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:B:121:ARG:NH1  | 1:B:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:C:286:GLU:OE1  | 1:C:286:GLU:N    | 2.38                     | 0.53              |
| 1:D:487:LEU:HD13 | 1:D:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:E:128:LEU:O    | 1:E:132:LEU:HG   | 2.08                     | 0.53              |
| 1:M:159:ARG:HD2  | 1:M:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:P:138:LEU:O    | 1:P:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:P:219:ASP:HB3  | 1:P:222:LEU:HB3  | 1.89                     | 0.53              |
| 1:P:487:LEU:HD13 | 1:P:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:A:516:HIS:CD2  | 1:A:546:LEU:HD13 | 2.43                     | 0.53              |
| 1:A:666:GLN:OE1  | 1:A:666:GLN:N    | 2.37                     | 0.53              |
| 1:C:128:LEU:O    | 1:C:132:LEU:HG   | 2.08                     | 0.53              |
| 1:C:159:ARG:HD2  | 1:C:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:C:340:GLU:OE1  | 1:C:340:GLU:N    | 2.30                     | 0.53              |
| 1:D:640:HIS:O    | 1:D:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:E:219:ASP:HB3  | 1:E:222:LEU:HB3  | 1.89                     | 0.53              |
| 1:E:244:ARG:NH1  | 1:E:247:GLU:OE1  | 2.38                     | 0.53              |
| 1:E:487:LEU:HD13 | 1:E:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:F:322:ARG:HH11 | 1:F:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:F:487:LEU:HD13 | 1:F:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:G:256:PRO:HB3  | 1:H:578:SER:OG   | 2.09                     | 0.53              |
| 1:G:516:HIS:CD2  | 1:G:546:LEU:HD13 | 2.43                     | 0.53              |
| 1:H:666:GLN:OE1  | 1:H:666:GLN:N    | 2.37                     | 0.53              |
| 1:K:666:GLN:OE1  | 1:K:666:GLN:N    | 2.37                     | 0.53              |
| 1:L:159:ARG:HD2  | 1:L:162:ARG:HH21 | 1.73                     | 0.53              |
| 1:L:412:TRP:O    | 1:L:440:GLY:N    | 2.33                     | 0.53              |
| 1:L:516:HIS:CD2  | 1:L:546:LEU:HD13 | 2.43                     | 0.53              |
| 1:M:121:ARG:NH1  | 1:M:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:O:640:HIS:O    | 1:O:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:A:322:ARG:HH11 | 1:A:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:B:159:ARG:HD2  | 1:B:162:ARG:HH21 | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:121:ARG:NH1  | 1:C:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:D:121:ARG:NH1  | 1:D:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:D:159:ARG:HD2  | 1:D:162:ARG:HH21 | 1.73                     | 0.53              |
| 1:D:666:GLN:OE1  | 1:D:666:GLN:N    | 2.37                     | 0.53              |
| 1:F:244:ARG:NH1  | 1:F:247:GLU:OE1  | 2.38                     | 0.53              |
| 1:F:640:HIS:O    | 1:F:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:G:685:HIS:O    | 1:G:688:GLN:NE2  | 2.38                     | 0.53              |
| 1:H:286:GLU:OE1  | 1:H:286:GLU:N    | 2.38                     | 0.53              |
| 1:I:322:ARG:HH11 | 1:I:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:J:516:HIS:CD2  | 1:J:546:LEU:HD13 | 2.43                     | 0.53              |
| 1:J:564:VAL:HG12 | 1:J:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:K:286:GLU:OE1  | 1:K:286:GLU:N    | 2.38                     | 0.53              |
| 1:L:322:ARG:HH11 | 1:L:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:L:666:GLN:OE1  | 1:L:666:GLN:N    | 2.37                     | 0.53              |
| 1:M:430:CYS:HB3  | 1:M:434:ARG:NH2  | 2.10                     | 0.53              |
| 1:N:121:ARG:NH1  | 1:N:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:N:375:LYS:O    | 1:N:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:O:487:LEU:HD13 | 1:O:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:P:244:ARG:NH1  | 1:P:247:GLU:OE1  | 2.38                     | 0.53              |
| 1:A:121:ARG:NH1  | 1:A:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:A:138:LEU:O    | 1:A:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:A:159:ARG:HD2  | 1:A:162:ARG:HH21 | 1.73                     | 0.53              |
| 1:C:375:LYS:O    | 1:C:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:E:138:LEU:O    | 1:E:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:G:487:LEU:HD13 | 1:G:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:G:564:VAL:HG12 | 1:G:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:H:564:VAL:HG12 | 1:H:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:I:478:ASN:HD21 | 1:P:239:GLN:HB2  | 1.74                     | 0.53              |
| 1:I:487:LEU:HD13 | 1:I:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:I:564:VAL:HG12 | 1:I:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:I:640:HIS:O    | 1:I:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:J:487:LEU:HD13 | 1:J:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:K:159:ARG:HD2  | 1:K:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:K:487:LEU:HD13 | 1:K:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:K:564:VAL:HG12 | 1:K:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:L:121:ARG:NH1  | 1:L:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:N:128:LEU:O    | 1:N:132:LEU:HG   | 2.08                     | 0.53              |
| 1:O:121:ARG:NH1  | 1:O:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:O:159:ARG:HD2  | 1:O:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:P:375:LYS:O    | 1:P:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:P:564:VAL:HG12 | 1:P:591:VAL:HG23 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:640:HIS:O    | 1:B:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:E:121:ARG:NH1  | 1:E:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:E:375:LYS:O    | 1:E:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:E:564:VAL:HG12 | 1:E:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:F:564:VAL:HG12 | 1:F:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:F:668:LEU:HD13 | 1:F:672:MET:HE2  | 1.91                     | 0.53              |
| 1:G:533:VAL:HG21 | 1:H:510:LEU:HD11 | 1.89                     | 0.53              |
| 1:H:159:ARG:HD2  | 1:H:162:ARG:HH21 | 1.73                     | 0.53              |
| 1:H:487:LEU:HD13 | 1:H:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:I:244:ARG:NH1  | 1:I:247:GLU:OE1  | 2.38                     | 0.53              |
| 1:J:159:ARG:HD2  | 1:J:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:K:322:ARG:HH11 | 1:K:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:L:138:LEU:O    | 1:L:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:L:564:VAL:HG12 | 1:L:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:M:94:GLU:HA    | 1:M:97:GLN:OE1   | 2.09                     | 0.53              |
| 1:M:640:HIS:O    | 1:M:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:P:121:ARG:NH1  | 1:P:155:GLU:OE1  | 2.42                     | 0.53              |
| 1:A:564:VAL:HG12 | 1:A:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:B:94:GLU:HA    | 1:B:97:GLN:OE1   | 2.09                     | 0.53              |
| 1:C:685:HIS:O    | 1:C:688:GLN:NE2  | 2.38                     | 0.53              |
| 1:E:627:ASP:N    | 1:E:627:ASP:OD1  | 2.40                     | 0.53              |
| 1:E:640:HIS:O    | 1:E:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:G:159:ARG:HD2  | 1:G:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:H:138:LEU:O    | 1:H:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:H:322:ARG:HH11 | 1:H:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:I:159:ARG:HD2  | 1:I:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:M:666:GLN:OE1  | 1:M:666:GLN:N    | 2.37                     | 0.53              |
| 1:N:94:GLU:HA    | 1:N:97:GLN:OE1   | 2.09                     | 0.53              |
| 1:O:88:VAL:HG23  | 1:O:89:GLY:H     | 1.74                     | 0.53              |
| 1:O:375:LYS:O    | 1:O:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:P:640:HIS:O    | 1:P:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:B:322:ARG:HH11 | 1:B:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:C:640:HIS:O    | 1:C:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:D:88:VAL:HG23  | 1:D:89:GLY:H     | 1.74                     | 0.53              |
| 1:D:138:LEU:O    | 1:D:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:D:375:LYS:O    | 1:D:376:ARG:NH1  | 2.41                     | 0.53              |
| 1:D:564:VAL:HG12 | 1:D:591:VAL:HG23 | 1.91                     | 0.53              |
| 1:D:668:LEU:HD13 | 1:D:672:MET:HE2  | 1.91                     | 0.53              |
| 1:I:668:LEU:HD13 | 1:I:672:MET:HE2  | 1.91                     | 0.53              |
| 1:J:685:HIS:O    | 1:J:688:GLN:NE2  | 2.38                     | 0.53              |
| 1:M:127:ASP:N    | 1:M:127:ASP:OD1  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:640:HIS:O    | 1:N:644:VAL:HG23 | 2.08                     | 0.53              |
| 1:O:138:LEU:O    | 1:O:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:P:627:ASP:N    | 1:P:627:ASP:OD1  | 2.40                     | 0.53              |
| 1:A:487:LEU:HD13 | 1:A:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:B:127:ASP:OD1  | 1:B:127:ASP:N    | 2.42                     | 0.53              |
| 1:C:94:GLU:HA    | 1:C:97:GLN:OE1   | 2.09                     | 0.53              |
| 1:C:487:LEU:HD13 | 1:C:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:D:94:GLU:HA    | 1:D:97:GLN:OE1   | 2.09                     | 0.53              |
| 1:E:216:ARG:HB2  | 1:F:688:GLN:OE1  | 2.09                     | 0.53              |
| 1:F:159:ARG:HD2  | 1:F:162:ARG:HH21 | 1.74                     | 0.53              |
| 1:I:516:HIS:CD2  | 1:I:546:LEU:HD13 | 2.43                     | 0.53              |
| 1:K:138:LEU:O    | 1:K:142:VAL:HG23 | 2.08                     | 0.53              |
| 1:L:88:VAL:HG23  | 1:L:89:GLY:H     | 1.74                     | 0.53              |
| 1:M:322:ARG:HH11 | 1:M:326:ASP:HB3  | 1.74                     | 0.53              |
| 1:N:487:LEU:HD13 | 1:N:505:LEU:HD13 | 1.91                     | 0.53              |
| 1:O:94:GLU:HA    | 1:O:97:GLN:OE1   | 2.09                     | 0.53              |
| 1:O:668:LEU:HD13 | 1:O:672:MET:HE2  | 1.91                     | 0.53              |
| 1:A:483:ASP:OD2  | 1:A:487:LEU:N    | 2.36                     | 0.52              |
| 1:A:627:ASP:OD1  | 1:A:627:ASP:N    | 2.40                     | 0.52              |
| 1:B:430:CYS:HB3  | 1:B:434:ARG:NH2  | 2.10                     | 0.52              |
| 1:C:483:ASP:OD1  | 1:C:485:SER:N    | 2.43                     | 0.52              |
| 1:E:127:ASP:N    | 1:E:127:ASP:OD1  | 2.42                     | 0.52              |
| 1:F:516:HIS:CD2  | 1:F:546:LEU:HD13 | 2.43                     | 0.52              |
| 1:G:127:ASP:OD1  | 1:G:127:ASP:N    | 2.42                     | 0.52              |
| 1:J:127:ASP:OD1  | 1:J:127:ASP:N    | 2.42                     | 0.52              |
| 1:L:487:LEU:HD13 | 1:L:505:LEU:HD13 | 1.91                     | 0.52              |
| 1:N:127:ASP:N    | 1:N:127:ASP:OD1  | 2.42                     | 0.52              |
| 1:N:430:CYS:HB3  | 1:N:434:ARG:NH2  | 2.11                     | 0.52              |
| 1:N:483:ASP:OD1  | 1:N:485:SER:N    | 2.43                     | 0.52              |
| 1:N:630:MET:HA   | 1:N:668:LEU:HD23 | 1.92                     | 0.52              |
| 1:O:564:VAL:HG12 | 1:O:591:VAL:HG23 | 1.91                     | 0.52              |
| 1:P:127:ASP:N    | 1:P:127:ASP:OD1  | 2.42                     | 0.52              |
| 1:B:630:MET:HA   | 1:B:668:LEU:HD23 | 1.91                     | 0.52              |
| 1:C:127:ASP:N    | 1:C:127:ASP:OD1  | 2.42                     | 0.52              |
| 1:C:564:VAL:HG12 | 1:C:591:VAL:HG23 | 1.91                     | 0.52              |
| 1:C:630:MET:HA   | 1:C:668:LEU:HD23 | 1.91                     | 0.52              |
| 1:H:88:VAL:HG23  | 1:H:89:GLY:H     | 1.74                     | 0.52              |
| 1:H:121:ARG:NH1  | 1:H:155:GLU:OE1  | 2.42                     | 0.52              |
| 1:J:322:ARG:HH11 | 1:J:326:ASP:HB3  | 1.74                     | 0.52              |
| 1:K:121:ARG:NH1  | 1:K:155:GLU:OE1  | 2.42                     | 0.52              |
| 1:K:128:LEU:O    | 1:K:132:LEU:HG   | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:197:GLU:OE2  | 1:M:383:ASN:HA   | 2.08                     | 0.52              |
| 1:N:564:VAL:HG12 | 1:N:591:VAL:HG23 | 1.91                     | 0.52              |
| 1:N:685:HIS:O    | 1:N:688:GLN:NE2  | 2.38                     | 0.52              |
| 1:O:516:HIS:CD2  | 1:O:546:LEU:HD13 | 2.43                     | 0.52              |
| 1:A:88:VAL:HG23  | 1:A:89:GLY:H     | 1.74                     | 0.52              |
| 1:B:138:LEU:O    | 1:B:142:VAL:HG23 | 2.08                     | 0.52              |
| 1:B:516:HIS:CD2  | 1:B:546:LEU:HD13 | 2.43                     | 0.52              |
| 1:B:666:GLN:OE1  | 1:B:666:GLN:N    | 2.37                     | 0.52              |
| 1:C:430:CYS:HB3  | 1:C:434:ARG:NH2  | 2.10                     | 0.52              |
| 1:F:121:ARG:NH1  | 1:F:155:GLU:OE1  | 2.42                     | 0.52              |
| 1:G:288:GLU:OE2  | 1:G:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:K:88:VAL:HG23  | 1:K:89:GLY:H     | 1.74                     | 0.52              |
| 1:O:288:GLU:OE2  | 1:O:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:127:ASP:OD1  | 1:A:127:ASP:N    | 2.42                     | 0.52              |
| 1:B:564:VAL:HG12 | 1:B:591:VAL:HG23 | 1.91                     | 0.52              |
| 1:D:288:GLU:OE2  | 1:D:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:D:516:HIS:CD2  | 1:D:546:LEU:HD13 | 2.43                     | 0.52              |
| 1:E:668:LEU:HD13 | 1:E:672:MET:HE2  | 1.91                     | 0.52              |
| 1:G:244:ARG:NH1  | 1:G:247:GLU:OE1  | 2.38                     | 0.52              |
| 1:G:322:ARG:HH11 | 1:G:326:ASP:HB3  | 1.74                     | 0.52              |
| 1:H:127:ASP:N    | 1:H:127:ASP:OD1  | 2.42                     | 0.52              |
| 1:H:128:LEU:O    | 1:H:132:LEU:HG   | 2.08                     | 0.52              |
| 1:H:412:TRP:O    | 1:H:440:GLY:N    | 2.33                     | 0.52              |
| 1:H:432:SER:HA   | 1:H:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:H:483:ASP:OD1  | 1:H:485:SER:N    | 2.43                     | 0.52              |
| 1:I:121:ARG:NH1  | 1:I:155:GLU:OE1  | 2.42                     | 0.52              |
| 1:J:288:GLU:OE2  | 1:J:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:J:432:SER:HA   | 1:J:435:GLU:OE1  | 2.09                     | 0.52              |
| 1:K:127:ASP:N    | 1:K:127:ASP:OD1  | 2.42                     | 0.52              |
| 1:K:483:ASP:OD1  | 1:K:485:SER:N    | 2.43                     | 0.52              |
| 1:M:138:LEU:O    | 1:M:142:VAL:HG23 | 2.08                     | 0.52              |
| 1:M:564:VAL:HG12 | 1:M:591:VAL:HG23 | 1.91                     | 0.52              |
| 1:O:322:ARG:HH11 | 1:O:326:ASP:HB3  | 1.74                     | 0.52              |
| 1:P:668:LEU:HD13 | 1:P:672:MET:HE2  | 1.91                     | 0.52              |
| 1:C:88:VAL:HG23  | 1:C:89:GLY:H     | 1.74                     | 0.52              |
| 1:C:138:LEU:O    | 1:C:142:VAL:HG23 | 2.08                     | 0.52              |
| 1:E:288:GLU:OE2  | 1:E:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:E:630:MET:HA   | 1:E:668:LEU:HD23 | 1.92                     | 0.52              |
| 1:K:432:SER:HA   | 1:K:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:L:127:ASP:OD1  | 1:L:127:ASP:N    | 2.42                     | 0.52              |
| 1:L:483:ASP:OD2  | 1:L:487:LEU:N    | 2.36                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:627:ASP:OD1  | 1:L:627:ASP:N    | 2.40                     | 0.52              |
| 1:M:630:MET:HA   | 1:M:668:LEU:HD23 | 1.91                     | 0.52              |
| 1:P:288:GLU:OE2  | 1:P:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:P:483:ASP:OD1  | 1:P:485:SER:N    | 2.43                     | 0.52              |
| 1:P:630:MET:HA   | 1:P:668:LEU:HD23 | 1.91                     | 0.52              |
| 1:A:432:SER:HA   | 1:A:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:C:288:GLU:OE2  | 1:C:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:D:322:ARG:HH11 | 1:D:326:ASP:HB3  | 1.74                     | 0.52              |
| 1:E:483:ASP:OD1  | 1:E:485:SER:N    | 2.43                     | 0.52              |
| 1:G:432:SER:HA   | 1:G:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:I:483:ASP:OD1  | 1:I:485:SER:N    | 2.43                     | 0.52              |
| 1:L:432:SER:HA   | 1:L:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:M:88:VAL:HG23  | 1:M:89:GLY:H     | 1.74                     | 0.52              |
| 1:M:422:GLN:HG2  | 1:M:427:SER:HB3  | 1.92                     | 0.52              |
| 1:M:516:HIS:CD2  | 1:M:546:LEU:HD13 | 2.43                     | 0.52              |
| 1:N:88:VAL:HG23  | 1:N:89:GLY:H     | 1.74                     | 0.52              |
| 1:N:138:LEU:O    | 1:N:142:VAL:HG23 | 2.08                     | 0.52              |
| 1:N:422:GLN:HG2  | 1:N:427:SER:HB3  | 1.92                     | 0.52              |
| 1:N:432:SER:HA   | 1:N:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:A:94:GLU:HA    | 1:A:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:D:127:ASP:OD1  | 1:D:127:ASP:N    | 2.42                     | 0.52              |
| 1:E:94:GLU:HA    | 1:E:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:F:483:ASP:OD1  | 1:F:485:SER:N    | 2.43                     | 0.52              |
| 1:G:483:ASP:OD1  | 1:G:485:SER:N    | 2.43                     | 0.52              |
| 1:H:94:GLU:HA    | 1:H:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:I:94:GLU:HA    | 1:I:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:J:244:ARG:NH1  | 1:J:247:GLU:OE1  | 2.38                     | 0.52              |
| 1:K:94:GLU:HA    | 1:K:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:K:288:GLU:OE2  | 1:K:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:M:483:ASP:OD1  | 1:M:485:SER:N    | 2.43                     | 0.52              |
| 1:M:685:HIS:O    | 1:M:688:GLN:NE2  | 2.38                     | 0.52              |
| 1:N:197:GLU:OE1  | 1:O:384:GLY:N    | 2.43                     | 0.52              |
| 1:O:127:ASP:OD1  | 1:O:127:ASP:N    | 2.42                     | 0.52              |
| 1:P:88:VAL:HG23  | 1:P:89:GLY:H     | 1.74                     | 0.52              |
| 1:P:94:GLU:HA    | 1:P:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:A:179:GLU:CD   | 1:A:179:GLU:H    | 2.18                     | 0.52              |
| 1:B:88:VAL:HG23  | 1:B:89:GLY:H     | 1.74                     | 0.52              |
| 1:B:422:GLN:HG2  | 1:B:427:SER:HB3  | 1.92                     | 0.52              |
| 1:B:483:ASP:OD1  | 1:B:485:SER:N    | 2.43                     | 0.52              |
| 1:B:487:LEU:HD13 | 1:B:505:LEU:HD13 | 1.91                     | 0.52              |
| 1:B:685:HIS:O    | 1:B:688:GLN:NE2  | 2.38                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:418:GLN:HA   | 1:C:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:C:422:GLN:HG2  | 1:C:427:SER:HB3  | 1.92                     | 0.52              |
| 1:C:432:SER:HA   | 1:C:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:C:668:LEU:HD13 | 1:C:672:MET:HE2  | 1.91                     | 0.52              |
| 1:E:88:VAL:HG23  | 1:E:89:GLY:H     | 1.74                     | 0.52              |
| 1:F:94:GLU:HA    | 1:F:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:H:288:GLU:OE2  | 1:H:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:J:483:ASP:OD1  | 1:J:485:SER:N    | 2.43                     | 0.52              |
| 1:K:179:GLU:CD   | 1:K:179:GLU:H    | 2.18                     | 0.52              |
| 1:K:418:GLN:HA   | 1:K:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:L:197:GLU:HB2  | 1:M:382:THR:O    | 2.10                     | 0.52              |
| 1:N:288:GLU:OE2  | 1:N:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:418:GLN:HA   | 1:A:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:B:418:GLN:HA   | 1:B:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:F:127:ASP:OD1  | 1:F:127:ASP:N    | 2.42                     | 0.52              |
| 1:F:630:MET:HA   | 1:F:668:LEU:HD23 | 1.91                     | 0.52              |
| 1:G:94:GLU:HA    | 1:G:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:I:432:SER:HA   | 1:I:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:L:94:GLU:HA    | 1:L:97:GLN:OE1   | 2.09                     | 0.52              |
| 1:L:179:GLU:CD   | 1:L:179:GLU:H    | 2.18                     | 0.52              |
| 1:L:288:GLU:OE2  | 1:L:338:ARG:NH1  | 2.43                     | 0.52              |
| 1:L:418:GLN:HA   | 1:L:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:N:418:GLN:HA   | 1:N:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:N:666:GLN:OE1  | 1:N:666:GLN:N    | 2.37                     | 0.52              |
| 1:N:668:LEU:HD13 | 1:N:672:MET:HE2  | 1.91                     | 0.52              |
| 1:O:94:GLU:O     | 1:O:98:LEU:HG    | 2.10                     | 0.52              |
| 1:B:432:SER:HA   | 1:B:435:GLU:OE1  | 2.10                     | 0.52              |
| 1:C:322:ARG:HH11 | 1:C:326:ASP:HB3  | 1.74                     | 0.52              |
| 1:D:94:GLU:O     | 1:D:98:LEU:HG    | 2.10                     | 0.52              |
| 1:E:94:GLU:O     | 1:E:98:LEU:HG    | 2.10                     | 0.52              |
| 1:G:94:GLU:O     | 1:G:98:LEU:HG    | 2.10                     | 0.52              |
| 1:G:422:GLN:HG2  | 1:G:427:SER:HB3  | 1.92                     | 0.52              |
| 1:H:179:GLU:H    | 1:H:179:GLU:CD   | 2.18                     | 0.52              |
| 1:H:418:GLN:HA   | 1:H:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:I:94:GLU:O     | 1:I:98:LEU:HG    | 2.10                     | 0.52              |
| 1:I:127:ASP:OD1  | 1:I:127:ASP:N    | 2.42                     | 0.52              |
| 1:I:422:GLN:HG2  | 1:I:427:SER:HB3  | 1.92                     | 0.52              |
| 1:I:630:MET:HA   | 1:I:668:LEU:HD23 | 1.92                     | 0.52              |
| 1:J:94:GLU:O     | 1:J:98:LEU:HG    | 2.10                     | 0.52              |
| 1:J:121:ARG:NH1  | 1:J:155:GLU:OE1  | 2.42                     | 0.52              |
| 1:J:666:GLN:OE1  | 1:J:666:GLN:N    | 2.37                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:418:GLN:HA   | 1:M:421:LEU:HD12 | 1.92                     | 0.52              |
| 1:M:448:GLU:OE2  | 1:M:463:ARG:NE   | 2.42                     | 0.52              |
| 1:M:487:LEU:HD13 | 1:M:505:LEU:HD13 | 1.91                     | 0.52              |
| 1:P:94:GLU:O     | 1:P:98:LEU:HG    | 2.10                     | 0.52              |
| 1:A:422:GLN:HG2  | 1:A:427:SER:HB3  | 1.91                     | 0.51              |
| 1:F:94:GLU:O     | 1:F:98:LEU:HG    | 2.10                     | 0.51              |
| 1:F:412:TRP:O    | 1:F:440:GLY:N    | 2.33                     | 0.51              |
| 1:F:418:GLN:HA   | 1:F:421:LEU:HD12 | 1.92                     | 0.51              |
| 1:F:432:SER:HA   | 1:F:435:GLU:OE1  | 2.10                     | 0.51              |
| 1:G:418:GLN:HA   | 1:G:421:LEU:HD12 | 1.92                     | 0.51              |
| 1:H:151:ILE:HG13 | 1:H:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:H:668:LEU:HD13 | 1:H:672:MET:HE2  | 1.91                     | 0.51              |
| 1:J:94:GLU:HA    | 1:J:97:GLN:OE1   | 2.09                     | 0.51              |
| 1:J:418:GLN:HA   | 1:J:421:LEU:HD12 | 1.92                     | 0.51              |
| 1:M:432:SER:HA   | 1:M:435:GLU:OE1  | 2.10                     | 0.51              |
| 1:A:288:GLU:OE2  | 1:A:338:ARG:NH1  | 2.43                     | 0.51              |
| 1:A:483:ASP:OD1  | 1:A:485:SER:N    | 2.43                     | 0.51              |
| 1:A:668:LEU:HD13 | 1:A:672:MET:HE2  | 1.91                     | 0.51              |
| 1:C:666:GLN:OE1  | 1:C:666:GLN:N    | 2.37                     | 0.51              |
| 1:D:483:ASP:OD1  | 1:D:485:SER:N    | 2.43                     | 0.51              |
| 1:E:322:ARG:HH11 | 1:E:326:ASP:HB3  | 1.74                     | 0.51              |
| 1:E:432:SER:HA   | 1:E:435:GLU:OE1  | 2.10                     | 0.51              |
| 1:F:88:VAL:HG23  | 1:F:89:GLY:H     | 1.74                     | 0.51              |
| 1:G:88:VAL:HG23  | 1:G:89:GLY:H     | 1.74                     | 0.51              |
| 1:G:121:ARG:NH1  | 1:G:155:GLU:OE1  | 2.42                     | 0.51              |
| 1:I:88:VAL:HG23  | 1:I:89:GLY:H     | 1.74                     | 0.51              |
| 1:J:88:VAL:HG23  | 1:J:89:GLY:H     | 1.74                     | 0.51              |
| 1:J:180:LEU:O    | 1:J:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:K:151:ILE:HG13 | 1:K:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:K:412:TRP:O    | 1:K:440:GLY:N    | 2.33                     | 0.51              |
| 1:L:94:GLU:O     | 1:L:98:LEU:HG    | 2.10                     | 0.51              |
| 1:L:668:LEU:HD13 | 1:L:672:MET:HE2  | 1.91                     | 0.51              |
| 1:M:179:GLU:H    | 1:M:179:GLU:CD   | 2.18                     | 0.51              |
| 1:M:197:GLU:OE1  | 1:N:384:GLY:N    | 2.43                     | 0.51              |
| 1:P:418:GLN:HA   | 1:P:421:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:94:GLU:O     | 1:A:98:LEU:HG    | 2.10                     | 0.51              |
| 1:A:151:ILE:HG13 | 1:A:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:B:179:GLU:H    | 1:B:179:GLU:CD   | 2.18                     | 0.51              |
| 1:D:418:GLN:HA   | 1:D:421:LEU:HD12 | 1.92                     | 0.51              |
| 1:E:179:GLU:H    | 1:E:179:GLU:CD   | 2.18                     | 0.51              |
| 1:E:418:GLN:HA   | 1:E:421:LEU:HD12 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:448:GLU:OE2  | 1:F:463:ARG:NE   | 2.42                     | 0.51              |
| 1:G:151:ILE:HG13 | 1:G:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:G:180:LEU:O    | 1:G:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:G:666:GLN:N    | 1:G:666:GLN:OE1  | 2.37                     | 0.51              |
| 1:I:288:GLU:OE2  | 1:I:338:ARG:NH1  | 2.43                     | 0.51              |
| 1:J:422:GLN:HG2  | 1:J:427:SER:HB3  | 1.92                     | 0.51              |
| 1:L:422:GLN:HG2  | 1:L:427:SER:HB3  | 1.92                     | 0.51              |
| 1:M:668:LEU:HD13 | 1:M:672:MET:HE2  | 1.91                     | 0.51              |
| 1:N:322:ARG:HH11 | 1:N:326:ASP:HB3  | 1.74                     | 0.51              |
| 1:O:180:LEU:O    | 1:O:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:P:203:VAL:HA   | 1:P:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:D:180:LEU:O    | 1:D:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:D:422:GLN:HG2  | 1:D:427:SER:HB3  | 1.91                     | 0.51              |
| 1:F:288:GLU:OE2  | 1:F:338:ARG:NH1  | 2.43                     | 0.51              |
| 1:F:422:GLN:HG2  | 1:F:427:SER:HB3  | 1.92                     | 0.51              |
| 1:G:412:TRP:O    | 1:G:440:GLY:N    | 2.33                     | 0.51              |
| 1:G:668:LEU:HD13 | 1:G:672:MET:HE2  | 1.91                     | 0.51              |
| 1:H:180:LEU:O    | 1:H:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:I:418:GLN:HA   | 1:I:421:LEU:HD12 | 1.92                     | 0.51              |
| 1:I:448:GLU:OE2  | 1:I:463:ARG:NE   | 2.42                     | 0.51              |
| 1:J:668:LEU:HD13 | 1:J:672:MET:HE2  | 1.91                     | 0.51              |
| 1:K:668:LEU:HD13 | 1:K:672:MET:HE2  | 1.91                     | 0.51              |
| 1:L:483:ASP:OD1  | 1:L:485:SER:N    | 2.43                     | 0.51              |
| 1:N:94:GLU:O     | 1:N:98:LEU:HG    | 2.10                     | 0.51              |
| 1:O:418:GLN:HA   | 1:O:421:LEU:HD12 | 1.92                     | 0.51              |
| 1:O:432:SER:HA   | 1:O:435:GLU:OE1  | 2.10                     | 0.51              |
| 1:O:483:ASP:OD1  | 1:O:485:SER:N    | 2.43                     | 0.51              |
| 1:P:179:GLU:H    | 1:P:179:GLU:CD   | 2.18                     | 0.51              |
| 1:P:322:ARG:HH11 | 1:P:326:ASP:HB3  | 1.74                     | 0.51              |
| 1:P:432:SER:HA   | 1:P:435:GLU:OE1  | 2.10                     | 0.51              |
| 1:B:668:LEU:HD13 | 1:B:672:MET:HE2  | 1.91                     | 0.51              |
| 1:D:60:GLU:OE2   | 1:L:310:ARG:NH2  | 2.44                     | 0.51              |
| 1:D:203:VAL:HA   | 1:D:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:D:630:MET:HA   | 1:D:668:LEU:HD23 | 1.92                     | 0.51              |
| 1:E:151:ILE:HG13 | 1:E:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:E:203:VAL:HA   | 1:E:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:J:151:ILE:HG13 | 1:J:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:J:179:GLU:H    | 1:J:179:GLU:CD   | 2.18                     | 0.51              |
| 1:K:180:LEU:O    | 1:K:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:L:151:ILE:HG13 | 1:L:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:O:422:GLN:HG2  | 1:O:427:SER:HB3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:94:GLU:O     | 1:B:98:LEU:HG    | 2.10                     | 0.51              |
| 1:B:101:GLU:HA   | 1:B:104:LEU:HB2  | 1.93                     | 0.51              |
| 1:B:151:ILE:HG13 | 1:B:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:B:235:LEU:HD13 | 1:B:276:VAL:HG21 | 1.93                     | 0.51              |
| 1:B:288:GLU:OE2  | 1:B:338:ARG:NH1  | 2.43                     | 0.51              |
| 1:D:432:SER:HA   | 1:D:435:GLU:OE1  | 2.10                     | 0.51              |
| 1:F:180:LEU:O    | 1:F:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:I:180:LEU:O    | 1:I:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:I:412:TRP:O    | 1:I:440:GLY:N    | 2.33                     | 0.51              |
| 1:J:340:GLU:OE1  | 1:J:340:GLU:N    | 2.30                     | 0.51              |
| 1:M:151:ILE:HG13 | 1:M:156:ASN:HD21 | 1.75                     | 0.51              |
| 1:M:235:LEU:HD13 | 1:M:276:VAL:HG21 | 1.93                     | 0.51              |
| 1:O:179:GLU:H    | 1:O:179:GLU:CD   | 2.18                     | 0.51              |
| 1:P:151:ILE:HG13 | 1:P:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:P:422:GLN:HG2  | 1:P:427:SER:HB3  | 1.91                     | 0.51              |
| 1:A:180:LEU:O    | 1:A:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:C:94:GLU:O     | 1:C:98:LEU:HG    | 2.10                     | 0.51              |
| 1:E:422:GLN:HG2  | 1:E:427:SER:HB3  | 1.92                     | 0.51              |
| 1:G:179:GLU:H    | 1:G:179:GLU:CD   | 2.18                     | 0.51              |
| 1:J:630:MET:HA   | 1:J:668:LEU:HD23 | 1.92                     | 0.51              |
| 1:K:422:GLN:HG2  | 1:K:427:SER:HB3  | 1.92                     | 0.51              |
| 1:K:630:MET:HA   | 1:K:668:LEU:HD23 | 1.91                     | 0.51              |
| 1:M:203:VAL:HA   | 1:M:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:N:235:LEU:HD13 | 1:N:276:VAL:HG21 | 1.93                     | 0.51              |
| 1:O:203:VAL:HA   | 1:O:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:O:583:HIS:ND1  | 1:O:692:ILE:HG13 | 2.26                     | 0.51              |
| 1:O:630:MET:HA   | 1:O:668:LEU:HD23 | 1.91                     | 0.51              |
| 1:P:180:LEU:O    | 1:P:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:630:MET:HA   | 1:A:668:LEU:HD23 | 1.91                     | 0.51              |
| 1:B:203:VAL:HA   | 1:B:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:C:175:ARG:HD3  | 1:C:213:TYR:CD1  | 2.46                     | 0.51              |
| 1:C:217:ARG:HH12 | 1:D:685:HIS:HB3  | 1.76                     | 0.51              |
| 1:C:235:LEU:HD13 | 1:C:276:VAL:HG21 | 1.93                     | 0.51              |
| 1:D:179:GLU:CD   | 1:D:179:GLU:H    | 2.18                     | 0.51              |
| 1:D:583:HIS:ND1  | 1:D:692:ILE:HG13 | 2.26                     | 0.51              |
| 1:E:180:LEU:O    | 1:E:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:F:627:ASP:OD1  | 1:F:627:ASP:N    | 2.40                     | 0.51              |
| 1:H:422:GLN:HG2  | 1:H:427:SER:HB3  | 1.92                     | 0.51              |
| 1:I:179:GLU:CD   | 1:I:179:GLU:H    | 2.18                     | 0.51              |
| 1:I:203:VAL:HA   | 1:I:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:M:94:GLU:O     | 1:M:98:LEU:HG    | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:101:GLU:HA   | 1:M:104:LEU:HB2  | 1.93                     | 0.51              |
| 1:M:288:GLU:OE2  | 1:M:338:ARG:NH1  | 2.43                     | 0.51              |
| 1:N:175:ARG:HD3  | 1:N:213:TYR:CD1  | 2.46                     | 0.51              |
| 1:A:483:ASP:OD1  | 1:A:484:ARG:N    | 2.44                     | 0.51              |
| 1:C:101:GLU:HA   | 1:C:104:LEU:HB2  | 1.93                     | 0.51              |
| 1:D:151:ILE:HG13 | 1:D:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:E:483:ASP:OD2  | 1:E:487:LEU:N    | 2.36                     | 0.51              |
| 1:F:179:GLU:CD   | 1:F:179:GLU:H    | 2.18                     | 0.51              |
| 1:G:630:MET:HA   | 1:G:668:LEU:HD23 | 1.92                     | 0.51              |
| 1:H:483:ASP:OD1  | 1:H:484:ARG:N    | 2.44                     | 0.51              |
| 1:J:412:TRP:O    | 1:J:440:GLY:N    | 2.33                     | 0.51              |
| 1:K:483:ASP:OD1  | 1:K:484:ARG:N    | 2.44                     | 0.51              |
| 1:L:180:LEU:O    | 1:L:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:L:203:VAL:HA   | 1:L:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:L:235:LEU:HD13 | 1:L:276:VAL:HG21 | 1.93                     | 0.51              |
| 1:L:483:ASP:OD1  | 1:L:484:ARG:N    | 2.44                     | 0.51              |
| 1:M:328:GLN:NE2  | 1:N:416:GLU:OE2  | 2.43                     | 0.51              |
| 1:N:101:GLU:HA   | 1:N:104:LEU:HB2  | 1.93                     | 0.51              |
| 1:A:203:VAL:HA   | 1:A:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:A:235:LEU:HD13 | 1:A:276:VAL:HG21 | 1.93                     | 0.51              |
| 1:A:310:ARG:NH2  | 1:O:60:GLU:OE2   | 2.43                     | 0.51              |
| 1:B:180:LEU:O    | 1:B:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:C:516:HIS:CG   | 1:C:546:LEU:HD13 | 2.47                     | 0.51              |
| 1:D:685:HIS:O    | 1:D:688:GLN:NE2  | 2.38                     | 0.51              |
| 1:E:464:LYS:HE2  | 1:F:445:ARG:NH2  | 2.25                     | 0.51              |
| 1:F:203:VAL:HA   | 1:F:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:G:340:GLU:OE1  | 1:G:340:GLU:N    | 2.30                     | 0.51              |
| 1:G:483:ASP:OD1  | 1:G:484:ARG:N    | 2.44                     | 0.51              |
| 1:H:630:MET:HA   | 1:H:668:LEU:HD23 | 1.92                     | 0.51              |
| 1:J:483:ASP:OD1  | 1:J:484:ARG:N    | 2.44                     | 0.51              |
| 1:M:175:ARG:HD3  | 1:M:213:TYR:CD1  | 2.46                     | 0.51              |
| 1:N:180:LEU:O    | 1:N:184:VAL:HG23 | 2.11                     | 0.51              |
| 1:N:516:HIS:CG   | 1:N:546:LEU:HD13 | 2.47                     | 0.51              |
| 1:A:151:ILE:O    | 1:A:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:B:151:ILE:O    | 1:B:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:B:175:ARG:HD3  | 1:B:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:C:151:ILE:HG13 | 1:C:156:ASN:HD21 | 1.76                     | 0.50              |
| 1:C:179:GLU:CD   | 1:C:179:GLU:H    | 2.18                     | 0.50              |
| 1:C:180:LEU:O    | 1:C:184:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:244:ARG:NH1  | 1:D:244:ARG:HA   | 2.26                     | 0.50              |
| 1:E:483:ASP:OD1  | 1:E:484:ARG:N    | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:244:ARG:NH1  | 1:F:244:ARG:HA   | 2.26                     | 0.50              |
| 1:H:448:GLU:OE2  | 1:H:463:ARG:NE   | 2.42                     | 0.50              |
| 1:I:627:ASP:OD1  | 1:I:627:ASP:N    | 2.40                     | 0.50              |
| 1:L:151:ILE:O    | 1:L:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:L:244:ARG:NH1  | 1:L:244:ARG:HA   | 2.26                     | 0.50              |
| 1:L:630:MET:HA   | 1:L:668:LEU:HD23 | 1.91                     | 0.50              |
| 1:M:151:ILE:O    | 1:M:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:N:151:ILE:HG13 | 1:N:156:ASN:HD21 | 1.76                     | 0.50              |
| 1:N:179:GLU:CD   | 1:N:179:GLU:H    | 2.18                     | 0.50              |
| 1:O:101:GLU:HA   | 1:O:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:O:256:PRO:HG3  | 1:P:582:VAL:HG21 | 1.92                     | 0.50              |
| 1:P:483:ASP:OD2  | 1:P:487:LEU:N    | 2.36                     | 0.50              |
| 1:P:516:HIS:CG   | 1:P:546:LEU:HD13 | 2.46                     | 0.50              |
| 1:A:244:ARG:NH1  | 1:A:244:ARG:HA   | 2.26                     | 0.50              |
| 1:C:151:ILE:O    | 1:C:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:E:516:HIS:CG   | 1:E:546:LEU:HD13 | 2.47                     | 0.50              |
| 1:H:151:ILE:O    | 1:H:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:I:151:ILE:HG13 | 1:I:156:ASN:HD21 | 1.76                     | 0.50              |
| 1:I:244:ARG:NH1  | 1:I:244:ARG:HA   | 2.27                     | 0.50              |
| 1:J:244:ARG:NH1  | 1:J:244:ARG:HA   | 2.26                     | 0.50              |
| 1:K:94:GLU:O     | 1:K:98:LEU:HG    | 2.10                     | 0.50              |
| 1:K:583:HIS:ND1  | 1:K:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:M:180:LEU:O    | 1:M:184:VAL:HG23 | 2.11                     | 0.50              |
| 1:N:483:ASP:OD2  | 1:N:487:LEU:N    | 2.36                     | 0.50              |
| 1:O:151:ILE:HG13 | 1:O:156:ASN:HD21 | 1.76                     | 0.50              |
| 1:O:235:LEU:HD13 | 1:O:276:VAL:HG21 | 1.93                     | 0.50              |
| 1:O:244:ARG:NH1  | 1:O:244:ARG:HA   | 2.27                     | 0.50              |
| 1:P:293:LEU:HB3  | 1:P:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:P:483:ASP:OD1  | 1:P:484:ARG:N    | 2.44                     | 0.50              |
| 1:C:448:GLU:OE2  | 1:C:463:ARG:NE   | 2.42                     | 0.50              |
| 1:D:101:GLU:HA   | 1:D:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:D:175:ARG:HD3  | 1:D:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:E:293:LEU:HB3  | 1:E:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:F:101:GLU:HA   | 1:F:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:F:151:ILE:HG13 | 1:F:156:ASN:HD21 | 1.76                     | 0.50              |
| 1:F:235:LEU:HD13 | 1:F:276:VAL:HG21 | 1.93                     | 0.50              |
| 1:F:516:HIS:CG   | 1:F:546:LEU:HD13 | 2.47                     | 0.50              |
| 1:G:180:LEU:O    | 1:G:183:SER:OG   | 2.24                     | 0.50              |
| 1:H:94:GLU:O     | 1:H:98:LEU:HG    | 2.10                     | 0.50              |
| 1:H:583:HIS:ND1  | 1:H:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:I:235:LEU:HD13 | 1:I:276:VAL:HG21 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:516:HIS:CG   | 1:I:546:LEU:HD13 | 2.47                     | 0.50              |
| 1:J:583:HIS:ND1  | 1:J:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:K:151:ILE:O    | 1:K:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:L:175:ARG:HD3  | 1:L:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:L:583:HIS:ND1  | 1:L:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:N:151:ILE:O    | 1:N:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:N:203:VAL:HA   | 1:N:208:LEU:HD23 | 1.92                     | 0.50              |
| 1:O:175:ARG:HD3  | 1:O:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:A:175:ARG:HD3  | 1:A:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:A:583:HIS:ND1  | 1:A:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:C:203:VAL:HA   | 1:C:208:LEU:HD23 | 1.92                     | 0.50              |
| 1:C:483:ASP:OD2  | 1:C:487:LEU:N    | 2.36                     | 0.50              |
| 1:D:235:LEU:HD13 | 1:D:276:VAL:HG21 | 1.93                     | 0.50              |
| 1:D:483:ASP:OD2  | 1:D:487:LEU:N    | 2.36                     | 0.50              |
| 1:F:293:LEU:HB3  | 1:F:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:G:244:ARG:NH1  | 1:G:244:ARG:HA   | 2.27                     | 0.50              |
| 1:I:101:GLU:HA   | 1:I:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:I:293:LEU:HB3  | 1:I:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:K:217:ARG:HH22 | 1:L:688:GLN:NE2  | 2.10                     | 0.50              |
| 1:K:448:GLU:OE2  | 1:K:463:ARG:NE   | 2.42                     | 0.50              |
| 1:O:483:ASP:OD2  | 1:O:487:LEU:N    | 2.36                     | 0.50              |
| 1:A:240:ALA:O    | 1:A:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:B:516:HIS:CG   | 1:B:546:LEU:HD13 | 2.47                     | 0.50              |
| 1:C:433:PHE:CE1  | 1:C:455:LEU:HD13 | 2.47                     | 0.50              |
| 1:C:501:TYR:CZ   | 1:C:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:D:501:TYR:CZ   | 1:D:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:G:583:HIS:ND1  | 1:G:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:H:101:GLU:HA   | 1:H:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:I:583:HIS:ND1  | 1:I:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:K:203:VAL:HA   | 1:K:208:LEU:HD23 | 1.92                     | 0.50              |
| 1:K:430:CYS:HB3  | 1:K:434:ARG:NH2  | 2.10                     | 0.50              |
| 1:L:240:ALA:O    | 1:L:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:N:464:LYS:HD3  | 1:O:442:LEU:CD2  | 2.41                     | 0.50              |
| 1:N:483:ASP:OD1  | 1:N:484:ARG:N    | 2.44                     | 0.50              |
| 1:N:501:TYR:CZ   | 1:N:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:O:293:LEU:HB3  | 1:O:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:O:501:TYR:CZ   | 1:O:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:O:685:HIS:O    | 1:O:688:GLN:NE2  | 2.38                     | 0.50              |
| 1:P:235:LEU:HD13 | 1:P:276:VAL:HG21 | 1.93                     | 0.50              |
| 1:C:483:ASP:OD1  | 1:C:484:ARG:N    | 2.44                     | 0.50              |
| 1:E:235:LEU:HD13 | 1:E:276:VAL:HG21 | 1.93                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:483:ASP:OD1 | 1:F:484:ARG:N    | 2.44                     | 0.50              |
| 1:I:175:ARG:HD3 | 1:I:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:I:384:GLY:N   | 1:P:197:GLU:OE1  | 2.44                     | 0.50              |
| 1:I:483:ASP:OD1 | 1:I:484:ARG:N    | 2.44                     | 0.50              |
| 1:J:180:LEU:O   | 1:J:183:SER:OG   | 2.24                     | 0.50              |
| 1:K:101:GLU:HA  | 1:K:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:K:252:GLU:OE1 | 1:K:252:GLU:N    | 2.45                     | 0.50              |
| 1:L:101:GLU:HA  | 1:L:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:M:583:HIS:ND1 | 1:M:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:N:433:PHE:CE1 | 1:N:455:LEU:HD13 | 2.47                     | 0.50              |
| 1:B:240:ALA:O   | 1:B:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:B:583:HIS:ND1 | 1:B:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:C:583:HIS:ND1 | 1:C:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:D:293:LEU:HB3 | 1:D:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:F:175:ARG:HD3 | 1:F:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:F:240:ALA:O   | 1:F:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:F:433:PHE:CE1 | 1:F:455:LEU:HD13 | 2.47                     | 0.50              |
| 1:F:583:HIS:ND1 | 1:F:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:H:252:GLU:OE1 | 1:H:252:GLU:N    | 2.45                     | 0.50              |
| 1:I:688:GLN:NE2 | 1:P:217:ARG:HH22 | 2.08                     | 0.50              |
| 1:K:240:ALA:O   | 1:K:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:M:240:ALA:O   | 1:M:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:M:501:TYR:CZ  | 1:M:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:M:516:HIS:CG  | 1:M:546:LEU:HD13 | 2.46                     | 0.50              |
| 1:N:448:GLU:OE2 | 1:N:463:ARG:NE   | 2.42                     | 0.50              |
| 1:A:101:GLU:HA  | 1:A:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:B:501:TYR:CZ  | 1:B:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:D:433:PHE:CE1 | 1:D:455:LEU:HD13 | 2.47                     | 0.50              |
| 1:E:151:ILE:O   | 1:E:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:F:501:TYR:CZ  | 1:F:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:G:151:ILE:O   | 1:G:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:G:293:LEU:HB3 | 1:G:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:H:203:VAL:HA  | 1:H:208:LEU:HD23 | 1.92                     | 0.50              |
| 1:H:240:ALA:O   | 1:H:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:H:244:ARG:NH1 | 1:H:244:ARG:HA   | 2.26                     | 0.50              |
| 1:H:685:HIS:O   | 1:H:688:GLN:NE2  | 2.38                     | 0.50              |
| 1:I:240:ALA:O   | 1:I:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:I:501:TYR:CZ  | 1:I:529:ILE:HG23 | 2.47                     | 0.50              |
| 1:J:151:ILE:O   | 1:J:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:J:293:LEU:HB3 | 1:J:340:GLU:HG2  | 1.94                     | 0.50              |
| 1:K:256:PRO:CG  | 1:L:582:VAL:HG21 | 2.41                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:244:ARG:NH1  | 1:N:244:ARG:HA   | 2.26                     | 0.50              |
| 1:N:583:HIS:ND1  | 1:N:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:O:433:PHE:CE1  | 1:O:455:LEU:HD13 | 2.47                     | 0.50              |
| 1:P:151:ILE:O    | 1:P:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:P:583:HIS:ND1  | 1:P:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:A:252:GLU:OE1  | 1:A:252:GLU:N    | 2.45                     | 0.50              |
| 1:B:483:ASP:OD1  | 1:B:484:ARG:N    | 2.44                     | 0.50              |
| 1:B:483:ASP:OD2  | 1:B:487:LEU:N    | 2.36                     | 0.50              |
| 1:E:101:GLU:HA   | 1:E:104:LEU:HB2  | 1.93                     | 0.50              |
| 1:E:240:ALA:O    | 1:E:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:E:583:HIS:ND1  | 1:E:692:ILE:HG13 | 2.26                     | 0.50              |
| 1:F:151:ILE:O    | 1:F:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:F:180:LEU:O    | 1:F:183:SER:OG   | 2.24                     | 0.50              |
| 1:G:175:ARG:HD3  | 1:G:213:TYR:CD1  | 2.46                     | 0.50              |
| 1:G:235:LEU:HD13 | 1:G:276:VAL:HG21 | 1.92                     | 0.50              |
| 1:H:430:CYS:HB3  | 1:H:434:ARG:NH2  | 2.10                     | 0.50              |
| 1:I:151:ILE:O    | 1:I:156:ASN:ND2  | 2.45                     | 0.50              |
| 1:I:180:LEU:O    | 1:I:183:SER:OG   | 2.24                     | 0.50              |
| 1:I:430:CYS:HB3  | 1:I:434:ARG:NH2  | 2.10                     | 0.50              |
| 1:I:433:PHE:CE1  | 1:I:455:LEU:HD13 | 2.47                     | 0.50              |
| 1:J:516:HIS:CG   | 1:J:546:LEU:HD13 | 2.46                     | 0.50              |
| 1:P:240:ALA:O    | 1:P:244:ARG:HG2  | 2.12                     | 0.50              |
| 1:B:244:ARG:NH1  | 1:B:244:ARG:HA   | 2.26                     | 0.49              |
| 1:C:293:LEU:HB3  | 1:C:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:D:151:ILE:O    | 1:D:156:ASN:ND2  | 2.45                     | 0.49              |
| 1:E:412:TRP:O    | 1:E:440:GLY:N    | 2.33                     | 0.49              |
| 1:E:433:PHE:CE1  | 1:E:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:G:433:PHE:CE1  | 1:G:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:K:235:LEU:HD13 | 1:K:276:VAL:HG21 | 1.93                     | 0.49              |
| 1:L:252:GLU:OE1  | 1:L:252:GLU:N    | 2.45                     | 0.49              |
| 1:M:433:PHE:CE1  | 1:M:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:M:483:ASP:OD1  | 1:M:484:ARG:N    | 2.44                     | 0.49              |
| 1:M:483:ASP:OD2  | 1:M:487:LEU:N    | 2.36                     | 0.49              |
| 1:N:240:ALA:O    | 1:N:244:ARG:HG2  | 2.12                     | 0.49              |
| 1:P:101:GLU:HA   | 1:P:104:LEU:HB2  | 1.93                     | 0.49              |
| 1:B:433:PHE:CE1  | 1:B:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:C:244:ARG:NH1  | 1:C:244:ARG:HA   | 2.27                     | 0.49              |
| 1:E:501:TYR:CZ   | 1:E:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:G:203:VAL:HA   | 1:G:208:LEU:HD23 | 1.92                     | 0.49              |
| 1:H:235:LEU:HD13 | 1:H:276:VAL:HG21 | 1.93                     | 0.49              |
| 1:J:175:ARG:HD3  | 1:J:213:TYR:CD1  | 2.46                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:235:LEU:HD13 | 1:J:276:VAL:HG21 | 1.92                     | 0.49              |
| 1:J:433:PHE:CE1  | 1:J:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:K:244:ARG:NH1  | 1:K:244:ARG:HA   | 2.26                     | 0.49              |
| 1:K:516:HIS:CG   | 1:K:546:LEU:HD13 | 2.46                     | 0.49              |
| 1:L:433:PHE:CE1  | 1:L:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:L:501:TYR:CZ   | 1:L:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:O:151:ILE:O    | 1:O:156:ASN:ND2  | 2.45                     | 0.49              |
| 1:O:516:HIS:CG   | 1:O:546:LEU:HD13 | 2.46                     | 0.49              |
| 1:P:175:ARG:HD3  | 1:P:213:TYR:CD1  | 2.46                     | 0.49              |
| 1:P:244:ARG:NH1  | 1:P:244:ARG:HA   | 2.27                     | 0.49              |
| 1:P:433:PHE:CE1  | 1:P:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:P:501:TYR:CZ   | 1:P:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:C:240:ALA:O    | 1:C:244:ARG:HG2  | 2.12                     | 0.49              |
| 1:D:128:LEU:HD12 | 1:D:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:E:61:VAL:HG13  | 1:E:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:E:175:ARG:HD3  | 1:E:213:TYR:CD1  | 2.46                     | 0.49              |
| 1:E:244:ARG:NH1  | 1:E:244:ARG:HA   | 2.26                     | 0.49              |
| 1:F:256:PRO:HG3  | 1:G:582:VAL:HG21 | 1.95                     | 0.49              |
| 1:F:533:VAL:HG23 | 1:G:526:ASP:OD2  | 2.13                     | 0.49              |
| 1:G:516:HIS:CG   | 1:G:546:LEU:HD13 | 2.47                     | 0.49              |
| 1:P:61:VAL:HG13  | 1:P:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:A:501:TYR:CZ   | 1:A:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:C:461:ILE:HD12 | 1:D:436:GLN:HG3  | 1.95                     | 0.49              |
| 1:D:61:VAL:HG13  | 1:D:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:E:456:GLY:HA2  | 1:E:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:F:61:VAL:HG13  | 1:F:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:F:430:CYS:HB3  | 1:F:434:ARG:NH2  | 2.11                     | 0.49              |
| 1:G:101:GLU:HA   | 1:G:104:LEU:HB2  | 1.93                     | 0.49              |
| 1:G:632:ASP:OD2  | 1:G:636:LYS:N    | 2.46                     | 0.49              |
| 1:H:433:PHE:CE1  | 1:H:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:I:456:GLY:HA2  | 1:I:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:J:632:ASP:OD2  | 1:J:636:LYS:N    | 2.46                     | 0.49              |
| 1:L:516:HIS:CG   | 1:L:546:LEU:HD13 | 2.47                     | 0.49              |
| 1:M:244:ARG:NH1  | 1:M:244:ARG:HA   | 2.27                     | 0.49              |
| 1:M:456:GLY:HA2  | 1:M:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:N:293:LEU:HB3  | 1:N:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:O:61:VAL:HG13  | 1:O:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:O:128:LEU:HD12 | 1:O:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:A:433:PHE:CE1  | 1:A:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:A:456:GLY:HA2  | 1:A:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:A:516:HIS:CG   | 1:A:546:LEU:HD13 | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:456:GLY:HA2  | 1:B:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:D:240:ALA:O    | 1:D:244:ARG:HG2  | 2.12                     | 0.49              |
| 1:D:516:HIS:CG   | 1:D:546:LEU:HD13 | 2.47                     | 0.49              |
| 1:E:328:GLN:NE2  | 1:F:416:GLU:OE2  | 2.45                     | 0.49              |
| 1:F:456:GLY:HA2  | 1:F:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:G:128:LEU:HD12 | 1:G:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:H:293:LEU:HB3  | 1:H:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:H:516:HIS:CG   | 1:H:546:LEU:HD13 | 2.47                     | 0.49              |
| 1:K:293:LEU:HB3  | 1:K:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:K:501:TYR:CZ   | 1:K:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:P:412:TRP:O    | 1:P:440:GLY:N    | 2.33                     | 0.49              |
| 1:P:456:GLY:HA2  | 1:P:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:A:293:LEU:HB3  | 1:A:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:A:478:ASN:ND2  | 1:H:239:GLN:HB2  | 2.27                     | 0.49              |
| 1:B:293:LEU:HB3  | 1:B:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:B:412:TRP:O    | 1:B:440:GLY:N    | 2.33                     | 0.49              |
| 1:C:632:ASP:OD2  | 1:C:636:LYS:N    | 2.46                     | 0.49              |
| 1:D:430:CYS:HB3  | 1:D:434:ARG:NH2  | 2.11                     | 0.49              |
| 1:D:483:ASP:OD1  | 1:D:484:ARG:N    | 2.44                     | 0.49              |
| 1:G:240:ALA:O    | 1:G:244:ARG:HG2  | 2.12                     | 0.49              |
| 1:H:531:LEU:HD12 | 1:H:534:HIS:CE1  | 2.48                     | 0.49              |
| 1:I:61:VAL:HG13  | 1:I:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:J:101:GLU:HA   | 1:J:104:LEU:HB2  | 1.93                     | 0.49              |
| 1:J:128:LEU:HD12 | 1:J:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:J:240:ALA:O    | 1:J:244:ARG:HG2  | 2.12                     | 0.49              |
| 1:K:433:PHE:CE1  | 1:K:455:LEU:HD13 | 2.47                     | 0.49              |
| 1:K:685:HIS:O    | 1:K:688:GLN:NE2  | 2.38                     | 0.49              |
| 1:L:219:ASP:OD1  | 1:L:222:LEU:N    | 2.31                     | 0.49              |
| 1:L:293:LEU:HB3  | 1:L:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:M:632:ASP:OD2  | 1:M:636:LYS:N    | 2.46                     | 0.49              |
| 1:N:252:GLU:OE1  | 1:N:252:GLU:N    | 2.45                     | 0.49              |
| 1:N:632:ASP:OD2  | 1:N:636:LYS:N    | 2.46                     | 0.49              |
| 1:B:431:GLU:HG2  | 1:B:432:SER:H    | 1.78                     | 0.49              |
| 1:B:632:ASP:OD2  | 1:B:636:LYS:N    | 2.46                     | 0.49              |
| 1:H:501:TYR:CZ   | 1:H:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:H:632:ASP:OD2  | 1:H:636:LYS:N    | 2.46                     | 0.49              |
| 1:I:128:LEU:HD12 | 1:I:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:J:61:VAL:HG13  | 1:J:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:J:203:VAL:HA   | 1:J:208:LEU:HD23 | 1.92                     | 0.49              |
| 1:J:501:TYR:CZ   | 1:J:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:K:531:LEU:HD12 | 1:K:534:HIS:CE1  | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:219:ASP:OD1  | 1:M:222:LEU:N    | 2.31                     | 0.49              |
| 1:M:293:LEU:HB3  | 1:M:340:GLU:HG2  | 1.94                     | 0.49              |
| 1:O:240:ALA:O    | 1:O:244:ARG:HG2  | 2.12                     | 0.49              |
| 1:A:582:VAL:HG21 | 1:H:256:PRO:HG3  | 1.94                     | 0.49              |
| 1:C:252:GLU:OE1  | 1:C:252:GLU:N    | 2.45                     | 0.49              |
| 1:C:431:GLU:HG2  | 1:C:432:SER:H    | 1.78                     | 0.49              |
| 1:E:531:LEU:HD12 | 1:E:534:HIS:CE1  | 2.48                     | 0.49              |
| 1:F:128:LEU:HD12 | 1:F:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:G:501:TYR:CZ   | 1:G:529:ILE:HG23 | 2.47                     | 0.49              |
| 1:K:175:ARG:HD3  | 1:K:213:TYR:CD1  | 2.46                     | 0.49              |
| 1:L:456:GLY:HA2  | 1:L:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:M:431:GLU:HG2  | 1:M:432:SER:H    | 1.78                     | 0.49              |
| 1:N:431:GLU:HG2  | 1:N:432:SER:H    | 1.78                     | 0.49              |
| 1:O:430:CYS:HB3  | 1:O:434:ARG:NH2  | 2.10                     | 0.49              |
| 1:O:483:ASP:OD1  | 1:O:484:ARG:N    | 2.44                     | 0.49              |
| 1:B:219:ASP:OD1  | 1:B:222:LEU:N    | 2.31                     | 0.49              |
| 1:D:197:GLU:CD   | 1:E:383:ASN:HA   | 2.38                     | 0.49              |
| 1:D:531:LEU:HD12 | 1:D:534:HIS:CE1  | 2.48                     | 0.49              |
| 1:F:443:LEU:HD12 | 1:F:446:LEU:HD12 | 1.95                     | 0.49              |
| 1:G:61:VAL:HG13  | 1:G:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:I:443:LEU:HD12 | 1:I:446:LEU:HD12 | 1.95                     | 0.49              |
| 1:K:632:ASP:OD2  | 1:K:636:LYS:N    | 2.46                     | 0.49              |
| 1:N:461:ILE:HD12 | 1:O:436:GLN:HG3  | 1.93                     | 0.49              |
| 1:P:531:LEU:HD12 | 1:P:534:HIS:CE1  | 2.48                     | 0.49              |
| 1:A:478:ASN:OD1  | 1:A:479:TYR:N    | 2.46                     | 0.49              |
| 1:C:61:VAL:HG13  | 1:C:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:128:LEU:HD12 | 1:C:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:E:219:ASP:O    | 1:E:223:LEU:HG   | 2.13                     | 0.49              |
| 1:F:185:ALA:HB2  | 1:F:214:TRP:CZ3  | 2.48                     | 0.49              |
| 1:G:456:GLY:HA2  | 1:G:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:H:175:ARG:HD3  | 1:H:213:TYR:CD1  | 2.46                     | 0.49              |
| 1:I:185:ALA:HB2  | 1:I:214:TRP:CZ3  | 2.48                     | 0.49              |
| 1:J:456:GLY:HA2  | 1:J:458:LYS:HE2  | 1.94                     | 0.49              |
| 1:K:180:LEU:O    | 1:K:183:SER:OG   | 2.24                     | 0.49              |
| 1:L:478:ASN:OD1  | 1:L:479:TYR:N    | 2.46                     | 0.49              |
| 1:M:128:LEU:HD12 | 1:M:131:ARG:NH2  | 2.28                     | 0.49              |
| 1:N:61:VAL:HG13  | 1:N:112:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:456:GLY:HA2  | 1:C:458:LYS:HE2  | 1.94                     | 0.48              |
| 1:C:531:LEU:HD12 | 1:C:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:D:239:GLN:HG3  | 1:E:480:SER:HB2  | 1.95                     | 0.48              |
| 1:E:128:LEU:HD12 | 1:E:131:ARG:NH2  | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:443:LEU:HD12 | 1:G:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:G:531:LEU:HD12 | 1:G:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:H:180:LEU:O    | 1:H:183:SER:OG   | 2.24                     | 0.48              |
| 1:L:128:LEU:HD12 | 1:L:131:ARG:NH2  | 2.28                     | 0.48              |
| 1:L:531:LEU:HD12 | 1:L:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:M:412:TRP:O    | 1:M:440:GLY:N    | 2.33                     | 0.48              |
| 1:N:128:LEU:HD12 | 1:N:131:ARG:NH2  | 2.28                     | 0.48              |
| 1:N:456:GLY:HA2  | 1:N:458:LYS:HE2  | 1.94                     | 0.48              |
| 1:O:531:LEU:HD12 | 1:O:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:P:443:LEU:HD12 | 1:P:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:128:LEU:HD12 | 1:A:131:ARG:NH2  | 2.28                     | 0.48              |
| 1:A:531:LEU:HD12 | 1:A:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:B:252:GLU:N    | 1:B:252:GLU:OE1  | 2.45                     | 0.48              |
| 1:E:185:ALA:HB2  | 1:E:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:E:443:LEU:HD12 | 1:E:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:I:632:ASP:OD2  | 1:I:636:LYS:N    | 2.46                     | 0.48              |
| 1:J:443:LEU:HD12 | 1:J:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:K:456:GLY:HA2  | 1:K:458:LYS:HE2  | 1.94                     | 0.48              |
| 1:N:216:ARG:HB2  | 1:O:688:GLN:OE1  | 2.13                     | 0.48              |
| 1:N:464:LYS:HD3  | 1:O:442:LEU:HD21 | 1.94                     | 0.48              |
| 1:N:531:LEU:HD12 | 1:N:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:P:128:LEU:HD12 | 1:P:131:ARG:NH2  | 2.28                     | 0.48              |
| 1:P:180:LEU:O    | 1:P:183:SER:OG   | 2.24                     | 0.48              |
| 1:P:185:ALA:HB2  | 1:P:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:P:219:ASP:O    | 1:P:223:LEU:HG   | 2.14                     | 0.48              |
| 1:B:128:LEU:HD12 | 1:B:131:ARG:NH2  | 2.28                     | 0.48              |
| 1:D:443:LEU:HD12 | 1:D:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:D:478:ASN:OD1  | 1:D:479:TYR:N    | 2.46                     | 0.48              |
| 1:E:461:ILE:HG22 | 1:F:442:LEU:HD13 | 1.94                     | 0.48              |
| 1:F:252:GLU:OE1  | 1:F:252:GLU:N    | 2.45                     | 0.48              |
| 1:F:478:ASN:OD1  | 1:F:479:TYR:N    | 2.46                     | 0.48              |
| 1:F:632:ASP:OD2  | 1:F:636:LYS:N    | 2.46                     | 0.48              |
| 1:H:61:VAL:HG13  | 1:H:112:VAL:HG22 | 1.94                     | 0.48              |
| 1:H:219:ASP:OD1  | 1:H:222:LEU:N    | 2.31                     | 0.48              |
| 1:H:456:GLY:HA2  | 1:H:458:LYS:HE2  | 1.94                     | 0.48              |
| 1:I:219:ASP:O    | 1:I:223:LEU:HG   | 2.13                     | 0.48              |
| 1:I:252:GLU:OE1  | 1:I:252:GLU:N    | 2.45                     | 0.48              |
| 1:I:437:GLN:HB2  | 1:P:465:ARG:CZ   | 2.44                     | 0.48              |
| 1:I:478:ASN:OD1  | 1:I:479:TYR:N    | 2.46                     | 0.48              |
| 1:J:531:LEU:HD12 | 1:J:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:K:217:ARG:NH1  | 1:L:685:HIS:HB3  | 2.26                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:219:ASP:O    | 1:K:223:LEU:HG   | 2.14                     | 0.48              |
| 1:O:443:LEU:HD12 | 1:O:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:O:478:ASN:OD1  | 1:O:479:TYR:N    | 2.46                     | 0.48              |
| 1:A:219:ASP:O    | 1:A:223:LEU:HG   | 2.13                     | 0.48              |
| 1:D:632:ASP:OD2  | 1:D:636:LYS:N    | 2.46                     | 0.48              |
| 1:E:180:LEU:O    | 1:E:183:SER:OG   | 2.24                     | 0.48              |
| 1:E:448:GLU:OE2  | 1:E:463:ARG:NE   | 2.42                     | 0.48              |
| 1:F:219:ASP:O    | 1:F:223:LEU:HG   | 2.13                     | 0.48              |
| 1:G:185:ALA:HB2  | 1:G:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:H:478:ASN:OD1  | 1:H:479:TYR:N    | 2.46                     | 0.48              |
| 1:J:185:ALA:HB2  | 1:J:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:K:61:VAL:HG13  | 1:K:112:VAL:HG22 | 1.95                     | 0.48              |
| 1:M:213:TYR:HA   | 1:M:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:M:252:GLU:N    | 1:M:252:GLU:OE1  | 2.45                     | 0.48              |
| 1:M:478:ASN:OD1  | 1:M:479:TYR:N    | 2.46                     | 0.48              |
| 1:M:696:ILE:HA   | 1:M:699:LEU:HG   | 1.96                     | 0.48              |
| 1:N:328:GLN:NE2  | 1:O:416:GLU:OE2  | 2.47                     | 0.48              |
| 1:O:456:GLY:HA2  | 1:O:458:LYS:HE2  | 1.94                     | 0.48              |
| 1:A:608:ILE:HG22 | 1:A:612:MET:HE3  | 1.96                     | 0.48              |
| 1:B:696:ILE:HA   | 1:B:699:LEU:HG   | 1.96                     | 0.48              |
| 1:D:219:ASP:O    | 1:D:223:LEU:HG   | 2.14                     | 0.48              |
| 1:D:412:TRP:O    | 1:D:440:GLY:N    | 2.33                     | 0.48              |
| 1:D:456:GLY:HA2  | 1:D:458:LYS:HE2  | 1.94                     | 0.48              |
| 1:F:696:ILE:HA   | 1:F:699:LEU:HG   | 1.96                     | 0.48              |
| 1:G:213:TYR:HA   | 1:G:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:G:249:ARG:CD   | 1:H:586:LEU:HD22 | 2.43                     | 0.48              |
| 1:G:431:GLU:HG2  | 1:G:432:SER:H    | 1.78                     | 0.48              |
| 1:H:219:ASP:O    | 1:H:223:LEU:HG   | 2.14                     | 0.48              |
| 1:I:447:THR:N    | 1:I:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:I:696:ILE:HA   | 1:I:699:LEU:HG   | 1.96                     | 0.48              |
| 1:K:128:LEU:HD12 | 1:K:131:ARG:NH2  | 2.28                     | 0.48              |
| 1:K:219:ASP:OD1  | 1:K:222:LEU:N    | 2.31                     | 0.48              |
| 1:K:252:GLU:HB3  | 1:L:586:LEU:HD21 | 1.95                     | 0.48              |
| 1:K:478:ASN:OD1  | 1:K:479:TYR:N    | 2.46                     | 0.48              |
| 1:K:669:PRO:O    | 1:K:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:L:219:ASP:O    | 1:L:223:LEU:HG   | 2.13                     | 0.48              |
| 1:L:608:ILE:HG22 | 1:L:612:MET:HE3  | 1.96                     | 0.48              |
| 1:O:219:ASP:O    | 1:O:223:LEU:HG   | 2.14                     | 0.48              |
| 1:A:213:TYR:HA   | 1:A:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:B:213:TYR:HA   | 1:B:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:B:478:ASN:OD1  | 1:B:479:TYR:N    | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:443:LEU:HD12 | 1:C:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:E:285:ARG:HD3  | 1:E:285:ARG:HA   | 1.75                     | 0.48              |
| 1:F:447:THR:N    | 1:F:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:G:249:ARG:HD2  | 1:H:586:LEU:HD22 | 1.96                     | 0.48              |
| 1:G:447:THR:N    | 1:G:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:H:669:PRO:O    | 1:H:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:I:669:PRO:O    | 1:I:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:J:213:TYR:HA   | 1:J:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:J:669:PRO:O    | 1:J:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:L:447:THR:N    | 1:L:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:N:478:ASN:OD1  | 1:N:479:TYR:N    | 2.46                     | 0.48              |
| 1:N:626:LEU:O    | 1:N:630:MET:HG3  | 2.14                     | 0.48              |
| 1:O:213:TYR:HA   | 1:O:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:O:632:ASP:OD2  | 1:O:636:LYS:N    | 2.46                     | 0.48              |
| 1:P:252:GLU:OE1  | 1:P:252:GLU:N    | 2.45                     | 0.48              |
| 1:A:129:LEU:O    | 1:A:133:LEU:HD13 | 2.14                     | 0.48              |
| 1:A:447:THR:N    | 1:A:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:A:632:ASP:OD2  | 1:A:636:LYS:N    | 2.46                     | 0.48              |
| 1:B:61:VAL:HG13  | 1:B:112:VAL:HG22 | 1.94                     | 0.48              |
| 1:C:219:ASP:O    | 1:C:223:LEU:HG   | 2.14                     | 0.48              |
| 1:C:478:ASN:OD1  | 1:C:479:TYR:N    | 2.46                     | 0.48              |
| 1:C:626:LEU:O    | 1:C:630:MET:HG3  | 2.14                     | 0.48              |
| 1:D:431:GLU:HG2  | 1:D:432:SER:H    | 1.78                     | 0.48              |
| 1:D:696:ILE:HA   | 1:D:699:LEU:HG   | 1.96                     | 0.48              |
| 1:E:252:GLU:OE1  | 1:E:252:GLU:N    | 2.45                     | 0.48              |
| 1:F:669:PRO:O    | 1:F:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:G:478:ASN:OD1  | 1:G:479:TYR:N    | 2.46                     | 0.48              |
| 1:G:669:PRO:O    | 1:G:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:H:128:LEU:HD12 | 1:H:131:ARG:NH2  | 2.28                     | 0.48              |
| 1:H:129:LEU:O    | 1:H:133:LEU:HD13 | 2.14                     | 0.48              |
| 1:H:443:LEU:HD12 | 1:H:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:K:129:LEU:O    | 1:K:133:LEU:HD13 | 2.14                     | 0.48              |
| 1:L:61:VAL:HG13  | 1:L:112:VAL:HG22 | 1.94                     | 0.48              |
| 1:L:129:LEU:O    | 1:L:133:LEU:HD13 | 2.14                     | 0.48              |
| 1:L:144:ALA:O    | 1:L:148:LEU:HG   | 2.14                     | 0.48              |
| 1:L:213:TYR:HA   | 1:L:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:M:256:PRO:HB3  | 1:N:578:SER:OG   | 2.13                     | 0.48              |
| 1:O:217:ARG:HH12 | 1:P:685:HIS:HB3  | 1.78                     | 0.48              |
| 1:O:431:GLU:HG2  | 1:O:432:SER:H    | 1.78                     | 0.48              |
| 1:O:696:ILE:HA   | 1:O:699:LEU:HG   | 1.96                     | 0.48              |
| 1:A:144:ALA:O    | 1:A:148:LEU:HG   | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:669:PRO:O    | 1:C:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:D:185:ALA:HB2  | 1:D:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:D:213:TYR:HA   | 1:D:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:D:239:GLN:HB2  | 1:E:478:ASN:ND2  | 2.28                     | 0.48              |
| 1:D:328:GLN:CD   | 1:E:416:GLU:OE2  | 2.57                     | 0.48              |
| 1:E:447:THR:N    | 1:E:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:F:213:TYR:HA   | 1:F:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:F:531:LEU:HD12 | 1:F:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:H:254:LEU:HD13 | 1:H:274:VAL:HG13 | 1.96                     | 0.48              |
| 1:H:696:ILE:HA   | 1:H:699:LEU:HG   | 1.96                     | 0.48              |
| 1:I:213:TYR:HA   | 1:I:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:J:431:GLU:HG2  | 1:J:432:SER:H    | 1.78                     | 0.48              |
| 1:J:447:THR:N    | 1:J:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:J:478:ASN:OD1  | 1:J:479:TYR:N    | 2.46                     | 0.48              |
| 1:L:305:PRO:HD2  | 1:L:392:ARG:NH1  | 2.29                     | 0.48              |
| 1:M:305:PRO:HD2  | 1:M:392:ARG:NH1  | 2.29                     | 0.48              |
| 1:M:562:PRO:HA   | 1:M:590:SER:OG   | 2.14                     | 0.48              |
| 1:N:443:LEU:HD12 | 1:N:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:N:447:THR:N    | 1:N:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:O:185:ALA:HB2  | 1:O:214:TRP:CZ3  | 2.49                     | 0.48              |
| 1:P:447:THR:N    | 1:P:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:P:448:GLU:OE2  | 1:P:463:ARG:NE   | 2.42                     | 0.48              |
| 1:A:61:VAL:HG13  | 1:A:112:VAL:HG22 | 1.94                     | 0.48              |
| 1:A:305:PRO:HD2  | 1:A:392:ARG:NH1  | 2.29                     | 0.48              |
| 1:B:531:LEU:HD12 | 1:B:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:C:447:THR:N    | 1:C:450:GLU:OE2  | 2.47                     | 0.48              |
| 1:E:213:TYR:HA   | 1:E:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:G:254:LEU:HD13 | 1:G:274:VAL:HG13 | 1.96                     | 0.48              |
| 1:I:531:LEU:HD12 | 1:I:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:J:254:LEU:HD13 | 1:J:274:VAL:HG13 | 1.96                     | 0.48              |
| 1:K:254:LEU:HD13 | 1:K:274:VAL:HG13 | 1.96                     | 0.48              |
| 1:L:185:ALA:HB2  | 1:L:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:L:562:PRO:HA   | 1:L:590:SER:OG   | 2.14                     | 0.48              |
| 1:L:669:PRO:O    | 1:L:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:M:61:VAL:HG13  | 1:M:112:VAL:HG22 | 1.94                     | 0.48              |
| 1:M:531:LEU:HD12 | 1:M:534:HIS:CE1  | 2.48                     | 0.48              |
| 1:M:626:LEU:O    | 1:M:630:MET:HG3  | 2.14                     | 0.48              |
| 1:N:185:ALA:HB2  | 1:N:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:N:213:TYR:HA   | 1:N:216:ARG:NH2  | 2.28                     | 0.48              |
| 1:N:219:ASP:O    | 1:N:223:LEU:HG   | 2.14                     | 0.48              |
| 1:N:669:PRO:O    | 1:N:673:GLN:HG3  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:412:TRP:O    | 1:O:440:GLY:N    | 2.33                     | 0.48              |
| 1:P:478:ASN:OD1  | 1:P:479:TYR:N    | 2.46                     | 0.48              |
| 1:A:185:ALA:HB2  | 1:A:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:A:256:PRO:HG3  | 1:B:582:VAL:HG21 | 1.96                     | 0.48              |
| 1:A:669:PRO:O    | 1:A:673:GLN:HG3  | 2.14                     | 0.48              |
| 1:B:144:ALA:O    | 1:B:148:LEU:HG   | 2.14                     | 0.48              |
| 1:B:305:PRO:HD2  | 1:B:392:ARG:NH1  | 2.29                     | 0.48              |
| 1:B:562:PRO:HA   | 1:B:590:SER:OG   | 2.14                     | 0.48              |
| 1:B:626:LEU:O    | 1:B:630:MET:HG3  | 2.14                     | 0.48              |
| 1:E:305:PRO:HD2  | 1:E:392:ARG:NH1  | 2.29                     | 0.48              |
| 1:E:478:ASN:OD1  | 1:E:479:TYR:N    | 2.46                     | 0.48              |
| 1:G:331:VAL:HG22 | 1:G:370:ALA:HB2  | 1.96                     | 0.48              |
| 1:G:464:LYS:HB3  | 1:H:442:LEU:HD21 | 1.96                     | 0.48              |
| 1:H:144:ALA:O    | 1:H:148:LEU:HG   | 2.14                     | 0.48              |
| 1:J:331:VAL:HG22 | 1:J:370:ALA:HB2  | 1.96                     | 0.48              |
| 1:K:144:ALA:O    | 1:K:148:LEU:HG   | 2.14                     | 0.48              |
| 1:K:443:LEU:HD12 | 1:K:446:LEU:HD12 | 1.95                     | 0.48              |
| 1:K:608:ILE:HG22 | 1:K:612:MET:HE3  | 1.96                     | 0.48              |
| 1:K:696:ILE:HA   | 1:K:699:LEU:HG   | 1.96                     | 0.48              |
| 1:L:632:ASP:OD2  | 1:L:636:LYS:N    | 2.46                     | 0.48              |
| 1:M:144:ALA:O    | 1:M:148:LEU:HG   | 2.14                     | 0.48              |
| 1:M:185:ALA:HB2  | 1:M:214:TRP:CZ3  | 2.48                     | 0.48              |
| 1:O:129:LEU:O    | 1:O:133:LEU:HD13 | 2.14                     | 0.48              |
| 1:O:305:PRO:HD2  | 1:O:392:ARG:NH1  | 2.29                     | 0.48              |
| 1:P:305:PRO:HD2  | 1:P:392:ARG:NH1  | 2.29                     | 0.48              |
| 1:A:448:GLU:OE2  | 1:A:463:ARG:NE   | 2.42                     | 0.47              |
| 1:A:562:PRO:HA   | 1:A:590:SER:OG   | 2.14                     | 0.47              |
| 1:B:129:LEU:O    | 1:B:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:B:185:ALA:HB2  | 1:B:214:TRP:CZ3  | 2.48                     | 0.47              |
| 1:C:185:ALA:HB2  | 1:C:214:TRP:CZ3  | 2.48                     | 0.47              |
| 1:C:213:TYR:HA   | 1:C:216:ARG:NH2  | 2.28                     | 0.47              |
| 1:D:129:LEU:O    | 1:D:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:D:252:GLU:OE1  | 1:D:252:GLU:N    | 2.45                     | 0.47              |
| 1:D:305:PRO:HD2  | 1:D:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:D:447:THR:N    | 1:D:450:GLU:OE2  | 2.47                     | 0.47              |
| 1:D:562:PRO:HA   | 1:D:590:SER:OG   | 2.14                     | 0.47              |
| 1:E:256:PRO:HG3  | 1:F:582:VAL:HG21 | 1.96                     | 0.47              |
| 1:E:685:HIS:O    | 1:E:688:GLN:NE2  | 2.38                     | 0.47              |
| 1:F:254:LEU:HD13 | 1:F:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:F:331:VAL:HG22 | 1:F:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:F:608:ILE:HG22 | 1:F:612:MET:HE3  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:331:VAL:HG22 | 1:H:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:I:254:LEU:HD13 | 1:I:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:I:331:VAL:HG22 | 1:I:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:I:608:ILE:HG22 | 1:I:612:MET:HE3  | 1.96                     | 0.47              |
| 1:M:129:LEU:O    | 1:M:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:N:129:LEU:O    | 1:N:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:P:213:TYR:HA   | 1:P:216:ARG:NH2  | 2.28                     | 0.47              |
| 1:B:447:THR:N    | 1:B:450:GLU:OE2  | 2.47                     | 0.47              |
| 1:C:129:LEU:O    | 1:C:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:C:412:TRP:O    | 1:C:440:GLY:N    | 2.33                     | 0.47              |
| 1:C:427:SER:HA   | 1:C:430:CYS:SG   | 2.54                     | 0.47              |
| 1:D:197:GLU:HB2  | 1:E:382:THR:O    | 2.14                     | 0.47              |
| 1:E:331:VAL:HG22 | 1:E:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:E:562:PRO:HA   | 1:E:590:SER:OG   | 2.14                     | 0.47              |
| 1:G:608:ILE:HG22 | 1:G:612:MET:HE3  | 1.96                     | 0.47              |
| 1:H:185:ALA:HB2  | 1:H:214:TRP:CZ3  | 2.48                     | 0.47              |
| 1:H:447:THR:N    | 1:H:450:GLU:OE2  | 2.47                     | 0.47              |
| 1:M:447:THR:N    | 1:M:450:GLU:OE2  | 2.47                     | 0.47              |
| 1:N:427:SER:HA   | 1:N:430:CYS:SG   | 2.54                     | 0.47              |
| 1:O:252:GLU:OE1  | 1:O:252:GLU:N    | 2.45                     | 0.47              |
| 1:O:447:THR:N    | 1:O:450:GLU:OE2  | 2.47                     | 0.47              |
| 1:O:562:PRO:HA   | 1:O:590:SER:OG   | 2.14                     | 0.47              |
| 1:O:626:LEU:O    | 1:O:630:MET:HG3  | 2.14                     | 0.47              |
| 1:P:562:PRO:HA   | 1:P:590:SER:OG   | 2.14                     | 0.47              |
| 1:P:685:HIS:O    | 1:P:688:GLN:NE2  | 2.38                     | 0.47              |
| 1:A:254:LEU:HD13 | 1:A:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:A:626:LEU:O    | 1:A:630:MET:HG3  | 2.14                     | 0.47              |
| 1:B:427:SER:HA   | 1:B:430:CYS:SG   | 2.55                     | 0.47              |
| 1:C:465:ARG:NH2  | 1:D:437:GLN:HB2  | 2.29                     | 0.47              |
| 1:D:626:LEU:O    | 1:D:630:MET:HG3  | 2.14                     | 0.47              |
| 1:F:175:ARG:HG2  | 1:F:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:G:144:ALA:O    | 1:G:148:LEU:HG   | 2.14                     | 0.47              |
| 1:G:427:SER:HA   | 1:G:430:CYS:SG   | 2.54                     | 0.47              |
| 1:H:608:ILE:HG22 | 1:H:612:MET:HE3  | 1.96                     | 0.47              |
| 1:I:175:ARG:HG2  | 1:I:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:J:427:SER:HA   | 1:J:430:CYS:SG   | 2.54                     | 0.47              |
| 1:K:185:ALA:HB2  | 1:K:214:TRP:CZ3  | 2.48                     | 0.47              |
| 1:L:626:LEU:O    | 1:L:630:MET:HG3  | 2.14                     | 0.47              |
| 1:P:331:VAL:HG22 | 1:P:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:B:443:LEU:HD12 | 1:B:446:LEU:HD12 | 1.95                     | 0.47              |
| 1:D:669:PRO:O    | 1:D:673:GLN:HG3  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:252:GLU:OE1  | 1:G:252:GLU:N    | 2.45                     | 0.47              |
| 1:I:305:PRO:HD2  | 1:I:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:I:626:LEU:O    | 1:I:630:MET:HG3  | 2.14                     | 0.47              |
| 1:J:144:ALA:O    | 1:J:148:LEU:HG   | 2.14                     | 0.47              |
| 1:J:219:ASP:O    | 1:J:223:LEU:HG   | 2.14                     | 0.47              |
| 1:J:608:ILE:HG22 | 1:J:612:MET:HE3  | 1.96                     | 0.47              |
| 1:K:331:VAL:HG22 | 1:K:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:L:448:GLU:OE2  | 1:L:463:ARG:NE   | 2.42                     | 0.47              |
| 1:M:239:GLN:HG3  | 1:N:480:SER:HB2  | 1.96                     | 0.47              |
| 1:M:427:SER:HA   | 1:M:430:CYS:SG   | 2.55                     | 0.47              |
| 1:N:608:ILE:HG22 | 1:N:612:MET:HE3  | 1.96                     | 0.47              |
| 1:P:669:PRO:O    | 1:P:673:GLN:HG3  | 2.14                     | 0.47              |
| 1:A:431:GLU:HG2  | 1:A:432:SER:H    | 1.78                     | 0.47              |
| 1:C:175:ARG:CG   | 1:C:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:C:608:ILE:HG22 | 1:C:612:MET:HE3  | 1.96                     | 0.47              |
| 1:E:254:LEU:HD13 | 1:E:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:E:427:SER:HA   | 1:E:430:CYS:SG   | 2.55                     | 0.47              |
| 1:E:632:ASP:OD2  | 1:E:636:LYS:N    | 2.46                     | 0.47              |
| 1:E:669:PRO:O    | 1:E:673:GLN:HG3  | 2.14                     | 0.47              |
| 1:E:696:ILE:HA   | 1:E:699:LEU:HG   | 1.96                     | 0.47              |
| 1:F:197:GLU:OE2  | 1:G:383:ASN:HA   | 2.15                     | 0.47              |
| 1:F:626:LEU:O    | 1:F:630:MET:HG3  | 2.14                     | 0.47              |
| 1:G:175:ARG:HG2  | 1:G:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:G:219:ASP:O    | 1:G:223:LEU:HG   | 2.13                     | 0.47              |
| 1:J:175:ARG:HG2  | 1:J:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:K:447:THR:N    | 1:K:450:GLU:OE2  | 2.47                     | 0.47              |
| 1:L:443:LEU:HD12 | 1:L:446:LEU:HD12 | 1.95                     | 0.47              |
| 1:M:219:ASP:O    | 1:M:223:LEU:HG   | 2.13                     | 0.47              |
| 1:M:443:LEU:HD12 | 1:M:446:LEU:HD12 | 1.95                     | 0.47              |
| 1:B:219:ASP:O    | 1:B:223:LEU:HG   | 2.13                     | 0.47              |
| 1:C:219:ASP:OD1  | 1:C:222:LEU:N    | 2.31                     | 0.47              |
| 1:D:175:ARG:CG   | 1:D:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:E:129:LEU:O    | 1:E:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:E:175:ARG:HG2  | 1:E:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:F:305:PRO:HD2  | 1:F:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:G:129:LEU:O    | 1:G:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:I:431:GLU:HG2  | 1:I:432:SER:H    | 1.78                     | 0.47              |
| 1:J:129:LEU:O    | 1:J:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:J:252:GLU:N    | 1:J:252:GLU:OE1  | 2.45                     | 0.47              |
| 1:J:305:PRO:HD2  | 1:J:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:K:213:TYR:HA   | 1:K:216:ARG:NH2  | 2.28                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:305:PRO:HD2  | 1:K:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:L:254:LEU:HD13 | 1:L:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:N:175:ARG:CG   | 1:N:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:N:219:ASP:OD1  | 1:N:222:LEU:N    | 2.31                     | 0.47              |
| 1:O:175:ARG:CG   | 1:O:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:O:669:PRO:O    | 1:O:673:GLN:HG3  | 2.14                     | 0.47              |
| 1:P:129:LEU:O    | 1:P:133:LEU:HD13 | 2.14                     | 0.47              |
| 1:P:175:ARG:HG2  | 1:P:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:P:427:SER:HA   | 1:P:430:CYS:SG   | 2.55                     | 0.47              |
| 1:P:632:ASP:OD2  | 1:P:636:LYS:N    | 2.46                     | 0.47              |
| 1:P:696:ILE:HA   | 1:P:699:LEU:HG   | 1.96                     | 0.47              |
| 1:A:175:ARG:HG2  | 1:A:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:A:443:LEU:HD12 | 1:A:446:LEU:HD12 | 1.95                     | 0.47              |
| 1:B:175:ARG:CG   | 1:B:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:B:669:PRO:O    | 1:B:673:GLN:HG3  | 2.14                     | 0.47              |
| 1:C:144:ALA:O    | 1:C:148:LEU:HG   | 2.14                     | 0.47              |
| 1:F:144:ALA:O    | 1:F:148:LEU:HG   | 2.14                     | 0.47              |
| 1:F:431:GLU:HG2  | 1:F:432:SER:H    | 1.78                     | 0.47              |
| 1:F:562:PRO:HA   | 1:F:590:SER:OG   | 2.14                     | 0.47              |
| 1:G:305:PRO:HD2  | 1:G:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:G:533:VAL:HG11 | 1:H:510:LEU:HG   | 1.96                     | 0.47              |
| 1:H:213:TYR:HA   | 1:H:216:ARG:NH2  | 2.28                     | 0.47              |
| 1:H:305:PRO:HD2  | 1:H:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:H:427:SER:HA   | 1:H:430:CYS:SG   | 2.55                     | 0.47              |
| 1:I:144:ALA:O    | 1:I:148:LEU:HG   | 2.14                     | 0.47              |
| 1:J:562:PRO:HA   | 1:J:590:SER:OG   | 2.14                     | 0.47              |
| 1:K:427:SER:HA   | 1:K:430:CYS:SG   | 2.55                     | 0.47              |
| 1:L:175:ARG:HG2  | 1:L:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:L:331:VAL:HG22 | 1:L:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:L:431:GLU:HG2  | 1:L:432:SER:H    | 1.78                     | 0.47              |
| 1:M:175:ARG:CG   | 1:M:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:M:669:PRO:O    | 1:M:673:GLN:HG3  | 2.14                     | 0.47              |
| 1:N:144:ALA:O    | 1:N:148:LEU:HG   | 2.14                     | 0.47              |
| 1:N:305:PRO:HD2  | 1:N:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:N:412:TRP:O    | 1:N:440:GLY:N    | 2.33                     | 0.47              |
| 1:P:254:LEU:HD13 | 1:P:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:B:608:ILE:HG22 | 1:B:612:MET:HE3  | 1.96                     | 0.47              |
| 1:C:305:PRO:HD2  | 1:C:392:ARG:NH1  | 2.29                     | 0.47              |
| 1:G:330:LEU:O    | 1:G:333:LEU:HB2  | 2.15                     | 0.47              |
| 1:G:562:PRO:HA   | 1:G:590:SER:OG   | 2.14                     | 0.47              |
| 1:K:562:PRO:HA   | 1:K:590:SER:OG   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:608:ILE:HG22 | 1:M:612:MET:HE3  | 1.96                     | 0.47              |
| 1:A:331:VAL:HG22 | 1:A:370:ALA:HB2  | 1.96                     | 0.47              |
| 1:A:696:ILE:HA   | 1:A:699:LEU:HG   | 1.96                     | 0.47              |
| 1:C:563:ASP:CG   | 1:C:590:SER:HB3  | 2.40                     | 0.47              |
| 1:D:254:LEU:HD13 | 1:D:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:D:285:ARG:HH21 | 1:E:484:ARG:NH1  | 2.13                     | 0.47              |
| 1:E:144:ALA:O    | 1:E:148:LEU:HG   | 2.14                     | 0.47              |
| 1:E:175:ARG:CG   | 1:E:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:E:626:LEU:O    | 1:E:630:MET:HG3  | 2.14                     | 0.47              |
| 1:F:143:GLN:O    | 1:F:147:LEU:HG   | 2.15                     | 0.47              |
| 1:F:197:GLU:CD   | 1:G:383:ASN:HA   | 2.40                     | 0.47              |
| 1:H:563:ASP:CG   | 1:H:590:SER:HB3  | 2.40                     | 0.47              |
| 1:I:143:GLN:O    | 1:I:147:LEU:HG   | 2.15                     | 0.47              |
| 1:I:562:PRO:HA   | 1:I:590:SER:OG   | 2.14                     | 0.47              |
| 1:J:330:LEU:O    | 1:J:333:LEU:HB2  | 2.15                     | 0.47              |
| 1:K:563:ASP:CG   | 1:K:590:SER:HB3  | 2.40                     | 0.47              |
| 1:N:562:PRO:HA   | 1:N:590:SER:OG   | 2.14                     | 0.47              |
| 1:N:563:ASP:CG   | 1:N:590:SER:HB3  | 2.40                     | 0.47              |
| 1:O:406:LEU:HD12 | 1:O:416:GLU:HG2  | 1.97                     | 0.47              |
| 1:P:144:ALA:O    | 1:P:148:LEU:HG   | 2.14                     | 0.47              |
| 1:P:406:LEU:HD12 | 1:P:416:GLU:HG2  | 1.97                     | 0.47              |
| 1:A:175:ARG:CG   | 1:A:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:C:562:PRO:HA   | 1:C:590:SER:OG   | 2.14                     | 0.47              |
| 1:C:575:GLN:O    | 1:C:579:LEU:HG   | 2.15                     | 0.47              |
| 1:D:175:ARG:HG2  | 1:D:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:E:406:LEU:HD12 | 1:E:416:GLU:HG2  | 1.97                     | 0.47              |
| 1:G:406:LEU:HD12 | 1:G:416:GLU:HG2  | 1.97                     | 0.47              |
| 1:H:119:ALA:O    | 1:H:123:ASP:N    | 2.49                     | 0.47              |
| 1:H:175:ARG:HG2  | 1:H:214:TRP:HE1  | 1.80                     | 0.47              |
| 1:H:562:PRO:HA   | 1:H:590:SER:OG   | 2.14                     | 0.47              |
| 1:H:575:GLN:O    | 1:H:579:LEU:HG   | 2.15                     | 0.47              |
| 1:I:406:LEU:HD12 | 1:I:416:GLU:HG2  | 1.97                     | 0.47              |
| 1:N:575:GLN:O    | 1:N:579:LEU:HG   | 2.16                     | 0.47              |
| 1:O:254:LEU:HD13 | 1:O:274:VAL:HG13 | 1.96                     | 0.47              |
| 1:P:175:ARG:CG   | 1:P:214:TRP:HE1  | 2.28                     | 0.47              |
| 1:P:626:LEU:O    | 1:P:630:MET:HG3  | 2.14                     | 0.47              |
| 1:A:685:HIS:O    | 1:A:688:GLN:NE2  | 2.38                     | 0.46              |
| 1:D:232:ASN:O    | 1:D:236:HIS:HB2  | 2.15                     | 0.46              |
| 1:D:406:LEU:HD12 | 1:D:416:GLU:HG2  | 1.98                     | 0.46              |
| 1:E:460:GLY:O    | 1:E:464:LYS:N    | 2.30                     | 0.46              |
| 1:E:563:ASP:CG   | 1:E:590:SER:HB3  | 2.40                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:608:ILE:HG22 | 1:E:612:MET:HE3  | 1.96                     | 0.46              |
| 1:F:232:ASN:O    | 1:F:236:HIS:HB2  | 2.16                     | 0.46              |
| 1:F:406:LEU:HD12 | 1:F:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:H:330:LEU:O    | 1:H:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:J:128:LEU:HD12 | 1:J:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:J:406:LEU:HD12 | 1:J:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:J:575:GLN:O    | 1:J:579:LEU:HG   | 2.15                     | 0.46              |
| 1:J:696:ILE:HA   | 1:J:699:LEU:HG   | 1.96                     | 0.46              |
| 1:K:119:ALA:O    | 1:K:123:ASP:N    | 2.49                     | 0.46              |
| 1:K:175:ARG:HG2  | 1:K:214:TRP:HE1  | 1.80                     | 0.46              |
| 1:K:252:GLU:CB   | 1:L:586:LEU:HD21 | 2.44                     | 0.46              |
| 1:K:330:LEU:O    | 1:K:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:K:575:GLN:O    | 1:K:579:LEU:HG   | 2.15                     | 0.46              |
| 1:L:128:LEU:HD12 | 1:L:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:L:143:GLN:O    | 1:L:147:LEU:HG   | 2.15                     | 0.46              |
| 1:L:175:ARG:CG   | 1:L:214:TRP:HE1  | 2.28                     | 0.46              |
| 1:L:696:ILE:HA   | 1:L:699:LEU:HG   | 1.96                     | 0.46              |
| 1:N:696:ILE:HA   | 1:N:699:LEU:HG   | 1.96                     | 0.46              |
| 1:O:175:ARG:HG2  | 1:O:214:TRP:HE1  | 1.80                     | 0.46              |
| 1:O:330:LEU:O    | 1:O:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:O:331:VAL:HG22 | 1:O:370:ALA:HB2  | 1.96                     | 0.46              |
| 1:P:563:ASP:CG   | 1:P:590:SER:HB3  | 2.40                     | 0.46              |
| 1:P:612:MET:O    | 1:P:651:LYS:NZ   | 2.33                     | 0.46              |
| 1:A:128:LEU:HD12 | 1:A:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:A:143:GLN:O    | 1:A:147:LEU:HG   | 2.15                     | 0.46              |
| 1:C:254:LEU:HD13 | 1:C:274:VAL:HG13 | 1.96                     | 0.46              |
| 1:C:696:ILE:HA   | 1:C:699:LEU:HG   | 1.96                     | 0.46              |
| 1:D:330:LEU:O    | 1:D:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:D:331:VAL:HG22 | 1:D:370:ALA:HB2  | 1.96                     | 0.46              |
| 1:D:427:SER:HA   | 1:D:430:CYS:SG   | 2.55                     | 0.46              |
| 1:D:448:GLU:OE2  | 1:D:463:ARG:NE   | 2.42                     | 0.46              |
| 1:D:516:HIS:HB2  | 1:D:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:E:143:GLN:O    | 1:E:147:LEU:HG   | 2.15                     | 0.46              |
| 1:E:562:PRO:HB2  | 1:E:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:G:128:LEU:HD12 | 1:G:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:G:575:GLN:O    | 1:G:579:LEU:HG   | 2.15                     | 0.46              |
| 1:G:696:ILE:HA   | 1:G:699:LEU:HG   | 1.96                     | 0.46              |
| 1:I:232:ASN:O    | 1:I:236:HIS:HB2  | 2.16                     | 0.46              |
| 1:I:427:SER:HA   | 1:I:430:CYS:SG   | 2.54                     | 0.46              |
| 1:J:119:ALA:O    | 1:J:123:ASP:N    | 2.49                     | 0.46              |
| 1:K:232:ASN:O    | 1:K:236:HIS:HB2  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:331:VAL:HG22 | 1:M:370:ALA:HB2  | 1.96                     | 0.46              |
| 1:O:232:ASN:O    | 1:O:236:HIS:HB2  | 2.16                     | 0.46              |
| 1:O:575:GLN:O    | 1:O:579:LEU:HG   | 2.15                     | 0.46              |
| 1:P:143:GLN:O    | 1:P:147:LEU:HG   | 2.15                     | 0.46              |
| 1:P:460:GLY:O    | 1:P:464:LYS:N    | 2.30                     | 0.46              |
| 1:A:575:GLN:O    | 1:A:579:LEU:HG   | 2.16                     | 0.46              |
| 1:B:331:VAL:HG22 | 1:B:370:ALA:HB2  | 1.96                     | 0.46              |
| 1:D:128:LEU:HD12 | 1:D:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:E:516:HIS:HB2  | 1:E:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:F:427:SER:HA   | 1:F:430:CYS:SG   | 2.54                     | 0.46              |
| 1:G:119:ALA:O    | 1:G:123:ASP:N    | 2.49                     | 0.46              |
| 1:G:143:GLN:O    | 1:G:147:LEU:HG   | 2.15                     | 0.46              |
| 1:G:175:ARG:CG   | 1:G:214:TRP:HE1  | 2.28                     | 0.46              |
| 1:H:232:ASN:O    | 1:H:236:HIS:HB2  | 2.16                     | 0.46              |
| 1:H:406:LEU:HD12 | 1:H:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:J:143:GLN:O    | 1:J:147:LEU:HG   | 2.15                     | 0.46              |
| 1:K:97:GLN:HA    | 1:K:100:GLU:HB2  | 1.97                     | 0.46              |
| 1:K:255:PHE:CE2  | 1:L:581:LYS:HD2  | 2.49                     | 0.46              |
| 1:L:427:SER:HA   | 1:L:430:CYS:SG   | 2.55                     | 0.46              |
| 1:N:254:LEU:HD13 | 1:N:274:VAL:HG13 | 1.96                     | 0.46              |
| 1:N:261:LYS:HG2  | 1:O:574:SER:OG   | 2.16                     | 0.46              |
| 1:O:427:SER:HA   | 1:O:430:CYS:SG   | 2.55                     | 0.46              |
| 1:O:562:PRO:HB2  | 1:O:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:P:562:PRO:HB2  | 1:P:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:P:608:ILE:HG22 | 1:P:612:MET:HE3  | 1.96                     | 0.46              |
| 1:A:180:LEU:O    | 1:A:183:SER:OG   | 2.24                     | 0.46              |
| 1:A:427:SER:HA   | 1:A:430:CYS:SG   | 2.55                     | 0.46              |
| 1:B:143:GLN:O    | 1:B:147:LEU:HG   | 2.15                     | 0.46              |
| 1:B:575:GLN:O    | 1:B:579:LEU:HG   | 2.16                     | 0.46              |
| 1:C:330:LEU:O    | 1:C:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:C:406:LEU:HD12 | 1:C:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:D:575:GLN:O    | 1:D:579:LEU:HG   | 2.16                     | 0.46              |
| 1:F:175:ARG:CG   | 1:F:214:TRP:HE1  | 2.28                     | 0.46              |
| 1:F:330:LEU:O    | 1:F:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:F:562:PRO:HB2  | 1:F:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:H:175:ARG:CG   | 1:H:214:TRP:HE1  | 2.28                     | 0.46              |
| 1:H:626:LEU:O    | 1:H:630:MET:HG3  | 2.14                     | 0.46              |
| 1:I:175:ARG:CG   | 1:I:214:TRP:HE1  | 2.28                     | 0.46              |
| 1:I:562:PRO:HB2  | 1:I:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:J:175:ARG:CG   | 1:J:214:TRP:HE1  | 2.28                     | 0.46              |
| 1:K:406:LEU:HD12 | 1:K:416:GLU:HG2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:575:GLN:O    | 1:L:579:LEU:HG   | 2.15                     | 0.46              |
| 1:M:143:GLN:O    | 1:M:147:LEU:HG   | 2.15                     | 0.46              |
| 1:M:418:GLN:OE1  | 1:M:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:O:448:GLU:OE2  | 1:O:463:ARG:NE   | 2.42                     | 0.46              |
| 1:O:516:HIS:HB2  | 1:O:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:C:516:HIS:HB2  | 1:C:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:D:562:PRO:HB2  | 1:D:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:F:129:LEU:O    | 1:F:133:LEU:HD13 | 2.14                     | 0.46              |
| 1:G:562:PRO:HB2  | 1:G:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:H:97:GLN:HA    | 1:H:100:GLU:HB2  | 1.97                     | 0.46              |
| 1:I:129:LEU:O    | 1:I:133:LEU:HD13 | 2.14                     | 0.46              |
| 1:I:330:LEU:O    | 1:I:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:J:76:LEU:HG    | 1:J:80:LYS:HE3   | 1.98                     | 0.46              |
| 1:K:175:ARG:CG   | 1:K:214:TRP:HE1  | 2.28                     | 0.46              |
| 1:K:626:LEU:O    | 1:K:630:MET:HG3  | 2.14                     | 0.46              |
| 1:L:180:LEU:O    | 1:L:183:SER:OG   | 2.24                     | 0.46              |
| 1:L:406:LEU:HD12 | 1:L:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:L:563:ASP:CG   | 1:L:590:SER:HB3  | 2.40                     | 0.46              |
| 1:N:330:LEU:O    | 1:N:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:N:406:LEU:HD12 | 1:N:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:N:516:HIS:HB2  | 1:N:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:O:128:LEU:HD12 | 1:O:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:P:516:HIS:HB2  | 1:P:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:A:139:GLU:H    | 1:A:139:GLU:CD   | 2.24                     | 0.46              |
| 1:A:216:ARG:O    | 1:A:217:ARG:NH2  | 2.49                     | 0.46              |
| 1:A:406:LEU:HD12 | 1:A:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:B:232:ASN:O    | 1:B:236:HIS:HB2  | 2.15                     | 0.46              |
| 1:B:254:LEU:HD13 | 1:B:274:VAL:HG13 | 1.96                     | 0.46              |
| 1:B:418:GLN:OE1  | 1:B:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:C:128:LEU:HD12 | 1:C:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:C:331:VAL:HG22 | 1:C:370:ALA:HB2  | 1.96                     | 0.46              |
| 1:D:144:ALA:O    | 1:D:148:LEU:HG   | 2.14                     | 0.46              |
| 1:E:418:GLN:OE1  | 1:E:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:F:216:ARG:O    | 1:F:217:ARG:NH2  | 2.49                     | 0.46              |
| 1:F:563:ASP:CG   | 1:F:590:SER:HB3  | 2.40                     | 0.46              |
| 1:G:76:LEU:HG    | 1:G:80:LYS:HE3   | 1.98                     | 0.46              |
| 1:G:97:GLN:HA    | 1:G:100:GLU:HB2  | 1.98                     | 0.46              |
| 1:G:216:ARG:O    | 1:G:217:ARG:NH2  | 2.49                     | 0.46              |
| 1:G:626:LEU:O    | 1:G:630:MET:HG3  | 2.14                     | 0.46              |
| 1:H:139:GLU:H    | 1:H:139:GLU:CD   | 2.24                     | 0.46              |
| 1:H:690:ALA:O    | 1:H:693:GLU:HG2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:562:PRO:HB2  | 1:J:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:K:139:GLU:H    | 1:K:139:GLU:CD   | 2.24                     | 0.46              |
| 1:K:216:ARG:HB2  | 1:L:688:GLN:OE1  | 2.16                     | 0.46              |
| 1:K:562:PRO:HB2  | 1:K:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:L:216:ARG:O    | 1:L:217:ARG:NH2  | 2.49                     | 0.46              |
| 1:L:330:LEU:O    | 1:L:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:L:418:GLN:OE1  | 1:L:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:M:254:LEU:HD13 | 1:M:274:VAL:HG13 | 1.96                     | 0.46              |
| 1:M:575:GLN:O    | 1:M:579:LEU:HG   | 2.16                     | 0.46              |
| 1:N:331:VAL:HG22 | 1:N:370:ALA:HB2  | 1.96                     | 0.46              |
| 1:N:418:GLN:OE1  | 1:N:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:O:144:ALA:O    | 1:O:148:LEU:HG   | 2.14                     | 0.46              |
| 1:O:608:ILE:HG22 | 1:O:612:MET:HE3  | 1.96                     | 0.46              |
| 1:A:330:LEU:O    | 1:A:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:A:690:ALA:O    | 1:A:693:GLU:HG2  | 2.16                     | 0.46              |
| 1:D:310:ARG:NH2  | 1:L:60:GLU:OE2   | 2.48                     | 0.46              |
| 1:E:431:GLU:HG2  | 1:E:432:SER:H    | 1.78                     | 0.46              |
| 1:F:431:GLU:OE1  | 1:F:431:GLU:N    | 2.43                     | 0.46              |
| 1:F:516:HIS:HB2  | 1:F:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:G:310:ARG:NH2  | 1:I:60:GLU:OE2   | 2.49                     | 0.46              |
| 1:H:562:PRO:HB2  | 1:H:614:ALA:HB2  | 1.98                     | 0.46              |
| 1:I:216:ARG:O    | 1:I:217:ARG:NH2  | 2.49                     | 0.46              |
| 1:I:516:HIS:HB2  | 1:I:546:LEU:HB2  | 1.97                     | 0.46              |
| 1:I:563:ASP:CG   | 1:I:590:SER:HB3  | 2.40                     | 0.46              |
| 1:J:97:GLN:HA    | 1:J:100:GLU:HB2  | 1.97                     | 0.46              |
| 1:J:626:LEU:O    | 1:J:630:MET:HG3  | 2.14                     | 0.46              |
| 1:K:143:GLN:O    | 1:K:147:LEU:HG   | 2.15                     | 0.46              |
| 1:K:431:GLU:HG2  | 1:K:432:SER:H    | 1.78                     | 0.46              |
| 1:L:690:ALA:O    | 1:L:693:GLU:HG2  | 2.16                     | 0.46              |
| 1:N:128:LEU:HD12 | 1:N:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:P:418:GLN:OE1  | 1:P:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:P:431:GLU:HG2  | 1:P:432:SER:H    | 1.78                     | 0.46              |
| 1:A:418:GLN:OE1  | 1:A:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:A:563:ASP:CG   | 1:A:590:SER:HB3  | 2.40                     | 0.46              |
| 1:B:330:LEU:O    | 1:B:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:B:563:ASP:CG   | 1:B:590:SER:HB3  | 2.40                     | 0.46              |
| 1:C:235:LEU:HG   | 1:C:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:C:418:GLN:OE1  | 1:C:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:D:235:LEU:HG   | 1:D:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:F:575:GLN:O    | 1:F:579:LEU:HG   | 2.15                     | 0.46              |
| 1:G:448:GLU:OE2  | 1:G:463:ARG:NE   | 2.42                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:143:GLN:O    | 1:H:147:LEU:HG   | 2.15                     | 0.46              |
| 1:I:119:ALA:O    | 1:I:123:ASP:N    | 2.49                     | 0.46              |
| 1:I:128:LEU:HD12 | 1:I:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:I:575:GLN:O    | 1:I:579:LEU:HG   | 2.16                     | 0.46              |
| 1:J:216:ARG:O    | 1:J:217:ARG:NH2  | 2.49                     | 0.46              |
| 1:L:139:GLU:H    | 1:L:139:GLU:CD   | 2.24                     | 0.46              |
| 1:L:685:HIS:O    | 1:L:688:GLN:NE2  | 2.38                     | 0.46              |
| 1:M:232:ASN:O    | 1:M:236:HIS:HB2  | 2.15                     | 0.46              |
| 1:P:330:LEU:O    | 1:P:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:A:151:ILE:HG13 | 1:A:156:ASN:ND2  | 2.31                     | 0.46              |
| 1:D:119:ALA:O    | 1:D:123:ASP:N    | 2.49                     | 0.46              |
| 1:D:180:LEU:O    | 1:D:183:SER:OG   | 2.24                     | 0.46              |
| 1:D:608:ILE:HG22 | 1:D:612:MET:HE3  | 1.96                     | 0.46              |
| 1:E:235:LEU:HG   | 1:E:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:E:330:LEU:O    | 1:E:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:F:119:ALA:O    | 1:F:123:ASP:N    | 2.49                     | 0.46              |
| 1:F:128:LEU:HD12 | 1:F:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:F:418:GLN:OE1  | 1:F:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:G:563:ASP:CG   | 1:G:590:SER:HB3  | 2.40                     | 0.46              |
| 1:G:690:ALA:O    | 1:G:693:GLU:HG2  | 2.16                     | 0.46              |
| 1:H:377:LEU:HD22 | 1:H:386:LYS:HZ2  | 1.81                     | 0.46              |
| 1:I:418:GLN:OE1  | 1:I:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:J:448:GLU:OE2  | 1:J:463:ARG:NE   | 2.42                     | 0.46              |
| 1:J:563:ASP:CG   | 1:J:590:SER:HB3  | 2.40                     | 0.46              |
| 1:K:239:GLN:HB2  | 1:L:478:ASN:HD21 | 1.81                     | 0.46              |
| 1:K:377:LEU:HD22 | 1:K:386:LYS:HZ2  | 1.81                     | 0.46              |
| 1:K:418:GLN:OE1  | 1:K:434:ARG:NH2  | 2.49                     | 0.46              |
| 1:K:690:ALA:O    | 1:K:693:GLU:HG2  | 2.16                     | 0.46              |
| 1:M:330:LEU:O    | 1:M:333:LEU:HB2  | 2.15                     | 0.46              |
| 1:M:406:LEU:HD12 | 1:M:416:GLU:HG2  | 1.97                     | 0.46              |
| 1:M:690:ALA:O    | 1:M:693:GLU:HG2  | 2.16                     | 0.46              |
| 1:O:235:LEU:HG   | 1:O:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:A:76:LEU:HG    | 1:A:80:LYS:HE3   | 1.98                     | 0.46              |
| 1:B:377:LEU:HD22 | 1:B:386:LYS:HZ2  | 1.81                     | 0.46              |
| 1:B:406:LEU:HD12 | 1:B:416:GLU:HG2  | 1.98                     | 0.46              |
| 1:B:516:HIS:HB2  | 1:B:546:LEU:HB2  | 1.98                     | 0.46              |
| 1:B:690:ALA:O    | 1:B:693:GLU:HG2  | 2.16                     | 0.46              |
| 1:C:377:LEU:HD22 | 1:C:386:LYS:HZ2  | 1.81                     | 0.46              |
| 1:D:143:GLN:O    | 1:D:147:LEU:HG   | 2.15                     | 0.46              |
| 1:E:128:LEU:HD12 | 1:E:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:E:216:ARG:O    | 1:E:217:ARG:NH2  | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:235:LEU:HG   | 1:F:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:F:685:HIS:O    | 1:F:688:GLN:NE2  | 2.38                     | 0.46              |
| 1:H:235:LEU:HG   | 1:H:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:I:97:GLN:HA    | 1:I:100:GLU:HB2  | 1.97                     | 0.46              |
| 1:K:235:LEU:HG   | 1:K:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:L:151:ILE:HG13 | 1:L:156:ASN:ND2  | 2.31                     | 0.46              |
| 1:N:235:LEU:HG   | 1:N:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:N:277:LEU:HD23 | 1:N:277:LEU:HA   | 1.81                     | 0.46              |
| 1:O:119:ALA:O    | 1:O:123:ASP:N    | 2.49                     | 0.46              |
| 1:O:180:LEU:O    | 1:O:183:SER:OG   | 2.24                     | 0.46              |
| 1:P:128:LEU:HD12 | 1:P:131:ARG:HH21 | 1.81                     | 0.46              |
| 1:P:216:ARG:O    | 1:P:217:ARG:NH2  | 2.49                     | 0.46              |
| 1:P:235:LEU:HG   | 1:P:329:ARG:HD3  | 1.98                     | 0.46              |
| 1:A:97:GLN:HA    | 1:A:100:GLU:HB2  | 1.97                     | 0.45              |
| 1:A:235:LEU:HG   | 1:A:329:ARG:HD3  | 1.98                     | 0.45              |
| 1:C:151:ILE:HG13 | 1:C:156:ASN:ND2  | 2.31                     | 0.45              |
| 1:C:562:PRO:HB2  | 1:C:614:ALA:HB2  | 1.98                     | 0.45              |
| 1:E:232:ASN:O    | 1:E:236:HIS:HB2  | 2.15                     | 0.45              |
| 1:E:690:ALA:O    | 1:E:693:GLU:HG2  | 2.16                     | 0.45              |
| 1:F:76:LEU:HG    | 1:F:80:LYS:HE3   | 1.98                     | 0.45              |
| 1:F:690:ALA:O    | 1:F:693:GLU:HG2  | 2.16                     | 0.45              |
| 1:G:139:GLU:H    | 1:G:139:GLU:CD   | 2.24                     | 0.45              |
| 1:G:235:LEU:HG   | 1:G:329:ARG:HD3  | 1.98                     | 0.45              |
| 1:H:418:GLN:OE1  | 1:H:434:ARG:NH2  | 2.49                     | 0.45              |
| 1:H:431:GLU:HG2  | 1:H:432:SER:H    | 1.78                     | 0.45              |
| 1:I:235:LEU:HG   | 1:I:329:ARG:HD3  | 1.98                     | 0.45              |
| 1:I:431:GLU:OE1  | 1:I:431:GLU:N    | 2.43                     | 0.45              |
| 1:J:139:GLU:H    | 1:J:139:GLU:CD   | 2.24                     | 0.45              |
| 1:L:76:LEU:HG    | 1:L:80:LYS:HE3   | 1.98                     | 0.45              |
| 1:L:235:LEU:HG   | 1:L:329:ARG:HD3  | 1.98                     | 0.45              |
| 1:L:562:PRO:HB2  | 1:L:614:ALA:HB2  | 1.98                     | 0.45              |
| 1:M:175:ARG:HG2  | 1:M:214:TRP:HE1  | 1.80                     | 0.45              |
| 1:M:563:ASP:CG   | 1:M:590:SER:HB3  | 2.40                     | 0.45              |
| 1:N:151:ILE:HG13 | 1:N:156:ASN:ND2  | 2.31                     | 0.45              |
| 1:N:377:LEU:HD22 | 1:N:386:LYS:HZ2  | 1.81                     | 0.45              |
| 1:N:562:PRO:HB2  | 1:N:614:ALA:HB2  | 1.98                     | 0.45              |
| 1:O:563:ASP:CG   | 1:O:590:SER:HB3  | 2.40                     | 0.45              |
| 1:P:690:ALA:O    | 1:P:693:GLU:HG2  | 2.16                     | 0.45              |
| 1:A:377:LEU:HD22 | 1:A:386:LYS:HZ2  | 1.81                     | 0.45              |
| 1:A:562:PRO:HB2  | 1:A:614:ALA:HB2  | 1.98                     | 0.45              |
| 1:C:97:GLN:HA    | 1:C:100:GLU:HB2  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:175:ARG:HG2  | 1:C:214:TRP:HE1 | 1.80                     | 0.45              |
| 1:C:232:ASN:O    | 1:C:236:HIS:HB2 | 2.15                     | 0.45              |
| 1:D:690:ALA:O    | 1:D:693:GLU:HG2 | 2.16                     | 0.45              |
| 1:E:76:LEU:HG    | 1:E:80:LYS:HE3  | 1.98                     | 0.45              |
| 1:F:97:GLN:HA    | 1:F:100:GLU:HB2 | 1.97                     | 0.45              |
| 1:G:151:ILE:HG13 | 1:G:156:ASN:ND2 | 2.31                     | 0.45              |
| 1:H:216:ARG:O    | 1:H:217:ARG:NH2 | 2.49                     | 0.45              |
| 1:I:76:LEU:HG    | 1:I:80:LYS:HE3  | 1.98                     | 0.45              |
| 1:J:151:ILE:HG13 | 1:J:156:ASN:ND2 | 2.31                     | 0.45              |
| 1:J:235:LEU:HG   | 1:J:329:ARG:HD3 | 1.98                     | 0.45              |
| 1:J:690:ALA:O    | 1:J:693:GLU:HG2 | 2.16                     | 0.45              |
| 1:L:277:LEU:HD23 | 1:L:277:LEU:HA  | 1.81                     | 0.45              |
| 1:M:516:HIS:HB2  | 1:M:546:LEU:HB2 | 1.97                     | 0.45              |
| 1:N:97:GLN:HA    | 1:N:100:GLU:HB2 | 1.97                     | 0.45              |
| 1:N:690:ALA:O    | 1:N:693:GLU:HG2 | 2.16                     | 0.45              |
| 1:O:143:GLN:O    | 1:O:147:LEU:HG  | 2.15                     | 0.45              |
| 1:P:76:LEU:HG    | 1:P:80:LYS:HE3  | 1.98                     | 0.45              |
| 1:P:232:ASN:O    | 1:P:236:HIS:HB2 | 2.16                     | 0.45              |
| 1:P:575:GLN:O    | 1:P:579:LEU:HG  | 2.15                     | 0.45              |
| 1:B:139:GLU:CD   | 1:B:139:GLU:H   | 2.24                     | 0.45              |
| 1:C:690:ALA:O    | 1:C:693:GLU:HG2 | 2.16                     | 0.45              |
| 1:D:97:GLN:HA    | 1:D:100:GLU:HB2 | 1.98                     | 0.45              |
| 1:D:219:ASP:OD1  | 1:D:222:LEU:N   | 2.31                     | 0.45              |
| 1:D:377:LEU:HD22 | 1:D:386:LYS:HZ2 | 1.81                     | 0.45              |
| 1:E:377:LEU:HD22 | 1:E:386:LYS:HZ2 | 1.81                     | 0.45              |
| 1:E:575:GLN:O    | 1:E:579:LEU:HG  | 2.15                     | 0.45              |
| 1:G:232:ASN:O    | 1:G:236:HIS:HB2 | 2.15                     | 0.45              |
| 1:G:516:HIS:HB2  | 1:G:546:LEU:HB2 | 1.97                     | 0.45              |
| 1:I:685:HIS:O    | 1:I:688:GLN:NE2 | 2.38                     | 0.45              |
| 1:J:516:HIS:HB2  | 1:J:546:LEU:HB2 | 1.97                     | 0.45              |
| 1:K:216:ARG:O    | 1:K:217:ARG:NH2 | 2.49                     | 0.45              |
| 1:L:377:LEU:HD22 | 1:L:386:LYS:HZ2 | 1.82                     | 0.45              |
| 1:N:143:GLN:O    | 1:N:147:LEU:HG  | 2.15                     | 0.45              |
| 1:N:175:ARG:HG2  | 1:N:214:TRP:HE1 | 1.80                     | 0.45              |
| 1:N:232:ASN:O    | 1:N:236:HIS:HB2 | 2.16                     | 0.45              |
| 1:O:97:GLN:HA    | 1:O:100:GLU:HB2 | 1.98                     | 0.45              |
| 1:P:119:ALA:O    | 1:P:123:ASP:N   | 2.49                     | 0.45              |
| 1:B:175:ARG:HG2  | 1:B:214:TRP:HE1 | 1.80                     | 0.45              |
| 1:C:216:ARG:O    | 1:C:217:ARG:NH2 | 2.49                     | 0.45              |
| 1:D:563:ASP:CG   | 1:D:590:SER:HB3 | 2.40                     | 0.45              |
| 1:E:119:ALA:O    | 1:E:123:ASP:N   | 2.49                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:460:GLY:O    | 1:F:464:LYS:N   | 2.30                     | 0.45              |
| 1:G:219:ASP:OD1  | 1:G:222:LEU:N   | 2.31                     | 0.45              |
| 1:I:690:ALA:O    | 1:I:693:GLU:HG2 | 2.16                     | 0.45              |
| 1:L:97:GLN:HA    | 1:L:100:GLU:HB2 | 1.97                     | 0.45              |
| 1:M:97:GLN:HA    | 1:M:100:GLU:HB2 | 1.97                     | 0.45              |
| 1:M:139:GLU:CD   | 1:M:139:GLU:H   | 2.24                     | 0.45              |
| 1:M:377:LEU:HD22 | 1:M:386:LYS:HZ2 | 1.82                     | 0.45              |
| 1:N:216:ARG:O    | 1:N:217:ARG:NH2 | 2.49                     | 0.45              |
| 1:N:694:LYS:HA   | 1:N:697:ARG:CZ  | 2.46                     | 0.45              |
| 1:O:219:ASP:OD1  | 1:O:222:LEU:N   | 2.31                     | 0.45              |
| 1:O:690:ALA:O    | 1:O:693:GLU:HG2 | 2.16                     | 0.45              |
| 1:B:235:LEU:HG   | 1:B:329:ARG:HD3 | 1.98                     | 0.45              |
| 1:B:562:PRO:HB2  | 1:B:614:ALA:HB2 | 1.98                     | 0.45              |
| 1:C:217:ARG:HH22 | 1:D:688:GLN:NE2 | 2.13                     | 0.45              |
| 1:C:694:LYS:HA   | 1:C:697:ARG:CZ  | 2.47                     | 0.45              |
| 1:H:76:LEU:HG    | 1:H:80:LYS:HE3  | 1.98                     | 0.45              |
| 1:J:219:ASP:OD1  | 1:J:222:LEU:N   | 2.31                     | 0.45              |
| 1:K:694:LYS:HA   | 1:K:697:ARG:CZ  | 2.46                     | 0.45              |
| 1:N:239:GLN:HG3  | 1:O:480:SER:HB2 | 1.98                     | 0.45              |
| 1:P:377:LEU:HD22 | 1:P:386:LYS:HZ2 | 1.81                     | 0.45              |
| 1:B:97:GLN:HA    | 1:B:100:GLU:HB2 | 1.97                     | 0.45              |
| 1:C:143:GLN:O    | 1:C:147:LEU:HG  | 2.15                     | 0.45              |
| 1:D:139:GLU:CD   | 1:D:139:GLU:H   | 2.24                     | 0.45              |
| 1:H:694:LYS:HA   | 1:H:697:ARG:CZ  | 2.47                     | 0.45              |
| 1:I:139:GLU:H    | 1:I:139:GLU:CD  | 2.24                     | 0.45              |
| 1:I:460:GLY:O    | 1:I:464:LYS:N   | 2.30                     | 0.45              |
| 1:J:232:ASN:O    | 1:J:236:HIS:HB2 | 2.16                     | 0.45              |
| 1:M:235:LEU:HG   | 1:M:329:ARG:HD3 | 1.98                     | 0.45              |
| 1:O:694:LYS:HA   | 1:O:697:ARG:CZ  | 2.46                     | 0.45              |
| 1:A:516:HIS:HB2  | 1:A:546:LEU:HB2 | 1.97                     | 0.45              |
| 1:B:216:ARG:O    | 1:B:217:ARG:NH2 | 2.49                     | 0.45              |
| 1:D:216:ARG:O    | 1:D:217:ARG:NH2 | 2.49                     | 0.45              |
| 1:F:139:GLU:H    | 1:F:139:GLU:CD  | 2.24                     | 0.45              |
| 1:G:431:GLU:OE1  | 1:G:431:GLU:N   | 2.43                     | 0.45              |
| 1:H:185:ALA:HB2  | 1:H:214:TRP:HZ3 | 1.82                     | 0.45              |
| 1:I:495:ASP:HB3  | 1:I:498:PHE:CD2 | 2.52                     | 0.45              |
| 1:I:685:HIS:HB3  | 1:P:217:ARG:NH1 | 2.29                     | 0.45              |
| 1:J:672:MET:HE3  | 1:J:672:MET:HB2 | 1.92                     | 0.45              |
| 1:K:76:LEU:HG    | 1:K:80:LYS:HE3  | 1.98                     | 0.45              |
| 1:L:516:HIS:HB2  | 1:L:546:LEU:HB2 | 1.97                     | 0.45              |
| 1:M:562:PRO:HB2  | 1:M:614:ALA:HB2 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:139:GLU:H    | 1:N:139:GLU:CD   | 2.24                     | 0.45              |
| 1:O:377:LEU:HD22 | 1:O:386:LYS:HZ2  | 1.82                     | 0.45              |
| 1:P:97:GLN:HA    | 1:P:100:GLU:HB2  | 1.98                     | 0.45              |
| 1:P:139:GLU:H    | 1:P:139:GLU:CD   | 2.24                     | 0.45              |
| 1:A:670:GLU:H    | 1:A:670:GLU:CD   | 2.25                     | 0.45              |
| 1:A:694:LYS:HA   | 1:A:697:ARG:CZ   | 2.47                     | 0.45              |
| 1:B:672:MET:HE3  | 1:B:672:MET:HB2  | 1.92                     | 0.45              |
| 1:D:694:LYS:HA   | 1:D:697:ARG:CZ   | 2.47                     | 0.45              |
| 1:E:97:GLN:HA    | 1:E:100:GLU:HB2  | 1.98                     | 0.45              |
| 1:E:151:ILE:HG13 | 1:E:156:ASN:ND2  | 2.31                     | 0.45              |
| 1:G:249:ARG:HD2  | 1:H:586:LEU:CD2  | 2.46                     | 0.45              |
| 1:G:694:LYS:HA   | 1:G:697:ARG:CZ   | 2.47                     | 0.45              |
| 1:H:151:ILE:HG13 | 1:H:156:ASN:ND2  | 2.31                     | 0.45              |
| 1:K:128:LEU:HD12 | 1:K:131:ARG:HH21 | 1.81                     | 0.45              |
| 1:L:694:LYS:HA   | 1:L:697:ARG:CZ   | 2.47                     | 0.45              |
| 1:M:217:ARG:NH1  | 1:N:685:HIS:HB3  | 2.31                     | 0.45              |
| 1:N:185:ALA:HB2  | 1:N:214:TRP:HZ3  | 1.82                     | 0.45              |
| 1:O:216:ARG:O    | 1:O:217:ARG:NH2  | 2.49                     | 0.45              |
| 1:O:418:GLN:OE1  | 1:O:434:ARG:NH2  | 2.49                     | 0.45              |
| 1:C:189:GLU:HG2  | 1:C:232:ASN:ND2  | 2.32                     | 0.45              |
| 1:D:189:GLU:HG2  | 1:D:232:ASN:ND2  | 2.32                     | 0.45              |
| 1:E:139:GLU:H    | 1:E:139:GLU:CD   | 2.24                     | 0.45              |
| 1:F:495:ASP:HB3  | 1:F:498:PHE:CD2  | 2.52                     | 0.45              |
| 1:G:418:GLN:OE1  | 1:G:434:ARG:NH2  | 2.49                     | 0.45              |
| 1:H:672:MET:HE3  | 1:H:672:MET:HB2  | 1.92                     | 0.45              |
| 1:J:418:GLN:OE1  | 1:J:434:ARG:NH2  | 2.49                     | 0.45              |
| 1:J:431:GLU:OE1  | 1:J:431:GLU:N    | 2.43                     | 0.45              |
| 1:J:694:LYS:HA   | 1:J:697:ARG:CZ   | 2.47                     | 0.45              |
| 1:K:185:ALA:HB2  | 1:K:214:TRP:HZ3  | 1.82                     | 0.45              |
| 1:N:189:GLU:HG2  | 1:N:232:ASN:ND2  | 2.32                     | 0.45              |
| 1:O:189:GLU:HG2  | 1:O:232:ASN:ND2  | 2.32                     | 0.45              |
| 1:B:495:ASP:HB3  | 1:B:498:PHE:CD2  | 2.52                     | 0.45              |
| 1:B:670:GLU:H    | 1:B:670:GLU:CD   | 2.25                     | 0.45              |
| 1:C:76:LEU:HG    | 1:C:80:LYS:HE3   | 1.98                     | 0.45              |
| 1:C:185:ALA:HB2  | 1:C:214:TRP:HZ3  | 1.82                     | 0.45              |
| 1:D:418:GLN:OE1  | 1:D:434:ARG:NH2  | 2.49                     | 0.45              |
| 1:F:151:ILE:HG13 | 1:F:156:ASN:ND2  | 2.31                     | 0.45              |
| 1:F:189:GLU:HG2  | 1:F:232:ASN:ND2  | 2.32                     | 0.45              |
| 1:H:378:VAL:CA   | 1:H:381:SER:HB3  | 2.47                     | 0.45              |
| 1:H:516:HIS:HB2  | 1:H:546:LEU:HB2  | 1.97                     | 0.45              |
| 1:H:670:GLU:H    | 1:H:670:GLU:CD   | 2.25                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:189:GLU:HG2  | 1:I:232:ASN:ND2  | 2.32                     | 0.45              |
| 1:K:151:ILE:HG13 | 1:K:156:ASN:ND2  | 2.31                     | 0.45              |
| 1:K:378:VAL:CA   | 1:K:381:SER:HB3  | 2.47                     | 0.45              |
| 1:L:232:ASN:O    | 1:L:236:HIS:HB2  | 2.16                     | 0.45              |
| 1:L:670:GLU:H    | 1:L:670:GLU:CD   | 2.25                     | 0.45              |
| 1:M:216:ARG:O    | 1:M:217:ARG:NH2  | 2.49                     | 0.45              |
| 1:M:293:LEU:HD22 | 1:M:340:GLU:HG2  | 1.99                     | 0.45              |
| 1:M:495:ASP:HB3  | 1:M:498:PHE:CD2  | 2.52                     | 0.45              |
| 1:N:76:LEU:HG    | 1:N:80:LYS:HE3   | 1.98                     | 0.45              |
| 1:O:236:HIS:HA   | 1:O:329:ARG:HH12 | 1.82                     | 0.45              |
| 1:P:151:ILE:HG13 | 1:P:156:ASN:ND2  | 2.32                     | 0.45              |
| 1:P:694:LYS:HA   | 1:P:697:ARG:CZ   | 2.46                     | 0.45              |
| 1:A:232:ASN:O    | 1:A:236:HIS:HB2  | 2.16                     | 0.44              |
| 1:A:672:MET:HE3  | 1:A:672:MET:HB2  | 1.92                     | 0.44              |
| 1:B:127:ASP:HB2  | 1:B:131:ARG:NH1  | 2.28                     | 0.44              |
| 1:B:185:ALA:HB2  | 1:B:214:TRP:HZ3  | 1.82                     | 0.44              |
| 1:B:293:LEU:HD22 | 1:B:340:GLU:HG2  | 1.99                     | 0.44              |
| 1:C:139:GLU:H    | 1:C:139:GLU:CD   | 2.24                     | 0.44              |
| 1:D:236:HIS:HA   | 1:D:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:E:189:GLU:HG2  | 1:E:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:E:694:LYS:HA   | 1:E:697:ARG:CZ   | 2.47                     | 0.44              |
| 1:H:495:ASP:HB3  | 1:H:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:H:603:PHE:HA   | 1:H:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:K:495:ASP:HB3  | 1:K:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:M:670:GLU:H    | 1:M:670:GLU:CD   | 2.25                     | 0.44              |
| 1:P:189:GLU:HG2  | 1:P:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:A:185:ALA:HB2  | 1:A:214:TRP:HZ3  | 1.82                     | 0.44              |
| 1:A:189:GLU:HG2  | 1:A:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:B:151:ILE:HG13 | 1:B:156:ASN:ND2  | 2.31                     | 0.44              |
| 1:C:69:LEU:O     | 1:C:73:GLN:HG2   | 2.17                     | 0.44              |
| 1:C:495:ASP:HB3  | 1:C:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:D:69:LEU:O     | 1:D:73:GLN:HG2   | 2.17                     | 0.44              |
| 1:D:495:ASP:HB3  | 1:D:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:E:260:SER:O    | 1:E:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:E:280:ASN:CG   | 1:E:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:E:378:VAL:CA   | 1:E:381:SER:HB3  | 2.47                     | 0.44              |
| 1:E:495:ASP:HB3  | 1:E:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:F:603:PHE:HA   | 1:F:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:F:694:LYS:HA   | 1:F:697:ARG:CZ   | 2.47                     | 0.44              |
| 1:G:670:GLU:H    | 1:G:670:GLU:CD   | 2.25                     | 0.44              |
| 1:H:128:LEU:HD12 | 1:H:131:ARG:HH21 | 1.81                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:151:ILE:HG13 | 1:I:156:ASN:ND2  | 2.31                     | 0.44              |
| 1:I:694:LYS:HA   | 1:I:697:ARG:CZ   | 2.47                     | 0.44              |
| 1:J:377:LEU:HD22 | 1:J:386:LYS:HZ2  | 1.81                     | 0.44              |
| 1:K:516:HIS:HB2  | 1:K:546:LEU:HB2  | 1.97                     | 0.44              |
| 1:K:603:PHE:HA   | 1:K:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:K:670:GLU:H    | 1:K:670:GLU:CD   | 2.25                     | 0.44              |
| 1:L:185:ALA:HB2  | 1:L:214:TRP:HZ3  | 1.82                     | 0.44              |
| 1:L:189:GLU:HG2  | 1:L:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:L:236:HIS:HA   | 1:L:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:N:69:LEU:O     | 1:N:73:GLN:HG2   | 2.18                     | 0.44              |
| 1:O:495:ASP:HB3  | 1:O:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:P:280:ASN:CG   | 1:P:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:P:495:ASP:HB3  | 1:P:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:A:236:HIS:HA   | 1:A:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:A:495:ASP:HB3  | 1:A:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:G:236:HIS:HA   | 1:G:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:G:260:SER:O    | 1:G:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:G:277:LEU:HA   | 1:G:277:LEU:HD23 | 1.81                     | 0.44              |
| 1:H:260:SER:O    | 1:H:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:I:442:LEU:CD2  | 1:P:464:LYS:HD3  | 2.48                     | 0.44              |
| 1:J:260:SER:O    | 1:J:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:J:670:GLU:H    | 1:J:670:GLU:CD   | 2.25                     | 0.44              |
| 1:K:260:SER:O    | 1:K:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:K:603:PHE:HD1  | 1:K:638:TRP:HZ2  | 1.65                     | 0.44              |
| 1:L:293:LEU:HD22 | 1:L:340:GLU:HG2  | 1.99                     | 0.44              |
| 1:L:603:PHE:HA   | 1:L:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:M:127:ASP:HB2  | 1:M:131:ARG:NH1  | 2.28                     | 0.44              |
| 1:M:151:ILE:HG13 | 1:M:156:ASN:ND2  | 2.31                     | 0.44              |
| 1:M:260:SER:O    | 1:M:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:N:356:LYS:O    | 1:N:361:LYS:N    | 2.51                     | 0.44              |
| 1:N:495:ASP:HB3  | 1:N:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:O:139:GLU:H    | 1:O:139:GLU:CD   | 2.24                     | 0.44              |
| 1:O:603:PHE:HA   | 1:O:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:P:260:SER:O    | 1:P:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:A:280:ASN:CG   | 1:A:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:A:603:PHE:HA   | 1:A:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:A:681:ILE:HD11 | 1:A:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:B:215:CYS:HB2  | 1:B:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:C:293:LEU:HD22 | 1:C:340:GLU:HG2  | 1.99                     | 0.44              |
| 1:C:356:LYS:O    | 1:C:361:LYS:N    | 2.51                     | 0.44              |
| 1:C:603:PHE:HA   | 1:C:638:TRP:CZ2  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:215:CYS:HB2  | 1:D:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:D:603:PHE:HA   | 1:D:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:F:670:GLU:H    | 1:F:670:GLU:CD   | 2.25                     | 0.44              |
| 1:G:377:LEU:HD22 | 1:G:386:LYS:HZ2  | 1.81                     | 0.44              |
| 1:H:681:ILE:HD11 | 1:H:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:I:603:PHE:HA   | 1:I:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:J:603:PHE:HA   | 1:J:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:K:280:ASN:CG   | 1:K:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:K:681:ILE:HD11 | 1:K:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:L:260:SER:O    | 1:L:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:L:280:ASN:CG   | 1:L:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:L:378:VAL:CA   | 1:L:381:SER:HB3  | 2.47                     | 0.44              |
| 1:L:603:PHE:HD1  | 1:L:638:TRP:HZ2  | 1.65                     | 0.44              |
| 1:M:189:GLU:HG2  | 1:M:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:M:215:CYS:HB2  | 1:M:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:O:69:LEU:O     | 1:O:73:GLN:HG2   | 2.18                     | 0.44              |
| 1:O:215:CYS:HB2  | 1:O:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:P:378:VAL:CA   | 1:P:381:SER:HB3  | 2.47                     | 0.44              |
| 1:A:69:LEU:O     | 1:A:73:GLN:HG2   | 2.18                     | 0.44              |
| 1:A:260:SER:O    | 1:A:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:A:293:LEU:HD22 | 1:A:340:GLU:HG2  | 1.99                     | 0.44              |
| 1:A:356:LYS:O    | 1:A:361:LYS:N    | 2.51                     | 0.44              |
| 1:B:76:LEU:HG    | 1:B:80:LYS:HE3   | 1.98                     | 0.44              |
| 1:B:189:GLU:HG2  | 1:B:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:B:260:SER:O    | 1:B:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:B:280:ASN:CG   | 1:B:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:B:681:ILE:HD11 | 1:B:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:B:694:LYS:HA   | 1:B:697:ARG:CZ   | 2.46                     | 0.44              |
| 1:C:670:GLU:H    | 1:C:670:GLU:CD   | 2.25                     | 0.44              |
| 1:D:76:LEU:HG    | 1:D:80:LYS:HE3   | 1.98                     | 0.44              |
| 1:E:494:LEU:HD12 | 1:E:494:LEU:HA   | 1.79                     | 0.44              |
| 1:F:236:HIS:HA   | 1:F:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:G:356:LYS:O    | 1:G:361:LYS:N    | 2.51                     | 0.44              |
| 1:H:236:HIS:HA   | 1:H:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:H:280:ASN:CG   | 1:H:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:H:431:GLU:OE1  | 1:H:431:GLU:N    | 2.43                     | 0.44              |
| 1:I:681:ILE:HD11 | 1:I:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:J:236:HIS:HA   | 1:J:329:ARG:HH12 | 1.83                     | 0.44              |
| 1:J:356:LYS:O    | 1:J:361:LYS:N    | 2.51                     | 0.44              |
| 1:J:681:ILE:HD11 | 1:J:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:K:236:HIS:HA   | 1:K:329:ARG:HH12 | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:356:LYS:O    | 1:L:361:LYS:N    | 2.51                     | 0.44              |
| 1:L:495:ASP:HB3  | 1:L:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:L:681:ILE:HD11 | 1:L:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:M:69:LEU:O     | 1:M:73:GLN:HG2   | 2.18                     | 0.44              |
| 1:M:76:LEU:HG    | 1:M:80:LYS:HE3   | 1.98                     | 0.44              |
| 1:M:180:LEU:O    | 1:M:183:SER:OG   | 2.24                     | 0.44              |
| 1:M:185:ALA:HB2  | 1:M:214:TRP:HZ3  | 1.82                     | 0.44              |
| 1:M:280:ASN:CG   | 1:M:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:A:378:VAL:CA   | 1:A:381:SER:HB3  | 2.47                     | 0.44              |
| 1:B:69:LEU:O     | 1:B:73:GLN:HG2   | 2.18                     | 0.44              |
| 1:B:180:LEU:O    | 1:B:183:SER:OG   | 2.24                     | 0.44              |
| 1:B:617:PHE:CD1  | 1:B:653:ILE:HG23 | 2.53                     | 0.44              |
| 1:C:236:HIS:HA   | 1:C:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:C:280:ASN:CG   | 1:C:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:C:681:ILE:HD11 | 1:C:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:D:151:ILE:HG13 | 1:D:156:ASN:ND2  | 2.32                     | 0.44              |
| 1:E:670:GLU:H    | 1:E:670:GLU:CD   | 2.25                     | 0.44              |
| 1:F:280:ASN:CG   | 1:F:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:F:681:ILE:HD11 | 1:F:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:G:189:GLU:HG2  | 1:G:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:G:495:ASP:HB3  | 1:G:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:G:603:PHE:HA   | 1:G:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:G:681:ILE:HD11 | 1:G:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:H:391:LYS:HD3  | 1:H:401:VAL:HG11 | 2.00                     | 0.44              |
| 1:I:236:HIS:HA   | 1:I:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:I:670:GLU:H    | 1:I:670:GLU:CD   | 2.25                     | 0.44              |
| 1:J:280:ASN:CG   | 1:J:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:J:495:ASP:HB3  | 1:J:498:PHE:CD2  | 2.52                     | 0.44              |
| 1:L:69:LEU:O     | 1:L:73:GLN:HG2   | 2.18                     | 0.44              |
| 1:L:672:MET:HE3  | 1:L:672:MET:HB2  | 1.92                     | 0.44              |
| 1:M:356:LYS:O    | 1:M:361:LYS:N    | 2.51                     | 0.44              |
| 1:M:672:MET:HE3  | 1:M:672:MET:HB2  | 1.92                     | 0.44              |
| 1:M:681:ILE:HD11 | 1:M:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:M:694:LYS:HA   | 1:M:697:ARG:CZ   | 2.47                     | 0.44              |
| 1:N:293:LEU:HD22 | 1:N:340:GLU:HG2  | 2.00                     | 0.44              |
| 1:N:603:PHE:HA   | 1:N:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:N:670:GLU:H    | 1:N:670:GLU:CD   | 2.25                     | 0.44              |
| 1:O:76:LEU:HG    | 1:O:80:LYS:HE3   | 1.98                     | 0.44              |
| 1:O:293:LEU:HD22 | 1:O:340:GLU:HG2  | 1.99                     | 0.44              |
| 1:P:494:LEU:HD12 | 1:P:494:LEU:HA   | 1.79                     | 0.44              |
| 1:P:670:GLU:H    | 1:P:670:GLU:CD   | 2.25                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:480:SER:HB2  | 1:H:239:GLN:HG3  | 1.99                     | 0.44              |
| 1:A:603:PHE:HD1  | 1:A:638:TRP:HZ2  | 1.65                     | 0.44              |
| 1:B:356:LYS:O    | 1:B:361:LYS:N    | 2.51                     | 0.44              |
| 1:C:215:CYS:HB2  | 1:C:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:C:617:PHE:CD1  | 1:C:653:ILE:HG23 | 2.53                     | 0.44              |
| 1:D:185:ALA:HB2  | 1:D:214:TRP:HZ3  | 1.82                     | 0.44              |
| 1:D:293:LEU:HD22 | 1:D:340:GLU:HG2  | 1.99                     | 0.44              |
| 1:D:670:GLU:H    | 1:D:670:GLU:CD   | 2.25                     | 0.44              |
| 1:E:603:PHE:HA   | 1:E:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:F:60:GLU:OE2   | 1:J:310:ARG:NH2  | 2.50                     | 0.44              |
| 1:F:215:CYS:HB2  | 1:F:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:F:356:LYS:O    | 1:F:361:LYS:N    | 2.51                     | 0.44              |
| 1:G:221:ALA:HA   | 1:G:224:ARG:HD3  | 2.00                     | 0.44              |
| 1:I:215:CYS:HB2  | 1:I:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:I:280:ASN:CG   | 1:I:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:I:356:LYS:O    | 1:I:361:LYS:N    | 2.51                     | 0.44              |
| 1:J:189:GLU:HG2  | 1:J:232:ASN:ND2  | 2.32                     | 0.44              |
| 1:K:391:LYS:HD3  | 1:K:401:VAL:HG11 | 2.00                     | 0.44              |
| 1:K:672:MET:HE3  | 1:K:672:MET:HB2  | 1.92                     | 0.44              |
| 1:L:328:GLN:CD   | 1:M:416:GLU:OE2  | 2.60                     | 0.44              |
| 1:M:128:LEU:HD12 | 1:M:131:ARG:HH21 | 1.81                     | 0.44              |
| 1:M:460:GLY:O    | 1:M:464:LYS:N    | 2.30                     | 0.44              |
| 1:M:603:PHE:HA   | 1:M:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:M:603:PHE:HD1  | 1:M:638:TRP:HZ2  | 1.65                     | 0.44              |
| 1:M:617:PHE:CD1  | 1:M:653:ILE:HG23 | 2.53                     | 0.44              |
| 1:N:260:SER:O    | 1:N:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:N:280:ASN:CG   | 1:N:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:N:617:PHE:CD1  | 1:N:653:ILE:HG23 | 2.53                     | 0.44              |
| 1:A:95:VAL:O     | 1:A:99:VAL:HG22  | 2.18                     | 0.44              |
| 1:A:391:LYS:HD3  | 1:A:401:VAL:HG11 | 2.00                     | 0.44              |
| 1:B:603:PHE:HA   | 1:B:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:D:124:GLY:O    | 1:D:128:LEU:HD13 | 2.18                     | 0.44              |
| 1:D:280:ASN:CG   | 1:D:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:D:356:LYS:O    | 1:D:361:LYS:N    | 2.51                     | 0.44              |
| 1:D:681:ILE:HD11 | 1:D:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:G:280:ASN:CG   | 1:G:283:VAL:HG22 | 2.42                     | 0.44              |
| 1:H:603:PHE:HD1  | 1:H:638:TRP:HZ2  | 1.65                     | 0.44              |
| 1:I:260:SER:O    | 1:I:267:ARG:HD2  | 2.18                     | 0.44              |
| 1:J:221:ALA:HA   | 1:J:224:ARG:HD3  | 2.00                     | 0.44              |
| 1:J:603:PHE:HD1  | 1:J:638:TRP:HZ2  | 1.65                     | 0.44              |
| 1:M:285:ARG:HD3  | 1:M:285:ARG:HA   | 1.75                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:215:CYS:HB2  | 1:N:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:N:681:ILE:HD11 | 1:N:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:O:124:GLY:O    | 1:O:128:LEU:HD13 | 2.18                     | 0.44              |
| 1:O:681:ILE:HD11 | 1:O:698:PHE:CD2  | 2.53                     | 0.44              |
| 1:P:617:PHE:CD1  | 1:P:653:ILE:HG23 | 2.53                     | 0.44              |
| 1:B:124:GLY:O    | 1:B:128:LEU:HD13 | 2.18                     | 0.44              |
| 1:B:128:LEU:HD12 | 1:B:131:ARG:HH21 | 1.81                     | 0.44              |
| 1:B:236:HIS:HA   | 1:B:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:B:448:GLU:OE2  | 1:B:463:ARG:NE   | 2.42                     | 0.44              |
| 1:E:215:CYS:HB2  | 1:E:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:E:356:LYS:O    | 1:E:361:LYS:N    | 2.51                     | 0.44              |
| 1:E:617:PHE:CD1  | 1:E:653:ILE:HG23 | 2.53                     | 0.44              |
| 1:G:185:ALA:HB2  | 1:G:214:TRP:HZ3  | 1.82                     | 0.44              |
| 1:H:69:LEU:O     | 1:H:73:GLN:HG2   | 2.17                     | 0.44              |
| 1:K:95:VAL:O     | 1:K:99:VAL:HG22  | 2.18                     | 0.44              |
| 1:K:285:ARG:HA   | 1:K:285:ARG:HD3  | 1.75                     | 0.44              |
| 1:L:95:VAL:O     | 1:L:99:VAL:HG22  | 2.18                     | 0.44              |
| 1:L:215:CYS:HB2  | 1:L:253:TRP:CE3  | 2.53                     | 0.44              |
| 1:M:119:ALA:O    | 1:M:123:ASP:N    | 2.49                     | 0.44              |
| 1:M:236:HIS:HA   | 1:M:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:N:236:HIS:HA   | 1:N:329:ARG:HH12 | 1.82                     | 0.44              |
| 1:O:151:ILE:HG13 | 1:O:156:ASN:ND2  | 2.31                     | 0.44              |
| 1:O:670:GLU:H    | 1:O:670:GLU:CD   | 2.25                     | 0.44              |
| 1:P:356:LYS:O    | 1:P:361:LYS:N    | 2.51                     | 0.44              |
| 1:P:603:PHE:HA   | 1:P:638:TRP:CZ2  | 2.53                     | 0.44              |
| 1:A:215:CYS:HB2  | 1:A:253:TRP:CE3  | 2.53                     | 0.43              |
| 1:B:119:ALA:O    | 1:B:123:ASP:N    | 2.49                     | 0.43              |
| 1:B:378:VAL:CA   | 1:B:381:SER:HB3  | 2.47                     | 0.43              |
| 1:C:260:SER:O    | 1:C:267:ARG:HD2  | 2.18                     | 0.43              |
| 1:E:464:LYS:HD3  | 1:F:442:LEU:CD2  | 2.48                     | 0.43              |
| 1:F:260:SER:O    | 1:F:267:ARG:HD2  | 2.18                     | 0.43              |
| 1:F:377:LEU:HD22 | 1:F:386:LYS:HZ2  | 1.82                     | 0.43              |
| 1:G:603:PHE:HD1  | 1:G:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:H:95:VAL:O     | 1:H:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:H:221:ALA:HA   | 1:H:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:I:377:LEU:HD22 | 1:I:386:LYS:HZ2  | 1.82                     | 0.43              |
| 1:J:116:LEU:O    | 1:J:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:K:69:LEU:O     | 1:K:73:GLN:HG2   | 2.17                     | 0.43              |
| 1:K:116:LEU:O    | 1:K:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:K:189:GLU:HG2  | 1:K:232:ASN:ND2  | 2.32                     | 0.43              |
| 1:K:221:ALA:HA   | 1:K:224:ARG:HD3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:285:ARG:HH21 | 1:M:484:ARG:NH1  | 2.16                     | 0.43              |
| 1:L:391:LYS:HD3  | 1:L:401:VAL:HG11 | 2.00                     | 0.43              |
| 1:M:124:GLY:O    | 1:M:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:M:378:VAL:CA   | 1:M:381:SER:HB3  | 2.47                     | 0.43              |
| 1:M:391:LYS:HD3  | 1:M:401:VAL:HG11 | 2.00                     | 0.43              |
| 1:O:185:ALA:HB2  | 1:O:214:TRP:HZ3  | 1.82                     | 0.43              |
| 1:O:280:ASN:CG   | 1:O:283:VAL:HG22 | 2.42                     | 0.43              |
| 1:O:356:LYS:O    | 1:O:361:LYS:N    | 2.51                     | 0.43              |
| 1:P:215:CYS:HB2  | 1:P:253:TRP:CE3  | 2.53                     | 0.43              |
| 1:B:391:LYS:HD3  | 1:B:401:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:143:GLN:HA   | 1:C:146:ARG:HE   | 1.83                     | 0.43              |
| 1:C:239:GLN:HG3  | 1:D:480:SER:HB2  | 1.99                     | 0.43              |
| 1:D:460:GLY:O    | 1:D:464:LYS:N    | 2.30                     | 0.43              |
| 1:D:669:PRO:HB2  | 1:D:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:F:95:VAL:O     | 1:F:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:F:143:GLN:HA   | 1:F:146:ARG:HE   | 1.84                     | 0.43              |
| 1:G:95:VAL:O     | 1:G:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:G:116:LEU:O    | 1:G:120:ILE:HG13 | 2.19                     | 0.43              |
| 1:I:143:GLN:HA   | 1:I:146:ARG:HE   | 1.84                     | 0.43              |
| 1:I:669:PRO:HB2  | 1:I:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:J:95:VAL:O     | 1:J:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:J:185:ALA:HB2  | 1:J:214:TRP:HZ3  | 1.82                     | 0.43              |
| 1:K:669:PRO:HB2  | 1:K:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:M:143:GLN:HA   | 1:M:146:ARG:HE   | 1.83                     | 0.43              |
| 1:N:256:PRO:HB3  | 1:O:578:SER:OG   | 2.18                     | 0.43              |
| 1:O:669:PRO:HB2  | 1:O:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:A:143:GLN:HA   | 1:A:146:ARG:HE   | 1.83                     | 0.43              |
| 1:A:672:MET:O    | 1:A:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:B:143:GLN:HA   | 1:B:146:ARG:HE   | 1.84                     | 0.43              |
| 1:B:603:PHE:HD1  | 1:B:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:C:127:ASP:HB2  | 1:C:131:ARG:NH1  | 2.28                     | 0.43              |
| 1:C:180:LEU:O    | 1:C:183:SER:OG   | 2.24                     | 0.43              |
| 1:E:669:PRO:HB2  | 1:E:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:G:460:GLY:O    | 1:G:464:LYS:N    | 2.30                     | 0.43              |
| 1:G:564:VAL:HG22 | 1:G:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:G:672:MET:O    | 1:G:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:H:669:PRO:HB2  | 1:H:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:I:95:VAL:O     | 1:I:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:I:221:ALA:HA   | 1:I:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:J:564:VAL:HG22 | 1:J:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:K:293:LEU:HD22 | 1:K:340:GLU:HG2  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:356:LYS:O    | 1:K:361:LYS:N    | 2.51                     | 0.43              |
| 1:K:431:GLU:OE1  | 1:K:431:GLU:N    | 2.43                     | 0.43              |
| 1:L:617:PHE:CD1  | 1:L:653:ILE:HG23 | 2.53                     | 0.43              |
| 1:M:127:ASP:HA   | 1:M:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:O:116:LEU:O    | 1:O:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:127:ASP:HA   | 1:A:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:A:669:PRO:HB2  | 1:A:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:B:127:ASP:HA   | 1:B:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:C:124:GLY:O    | 1:C:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:C:127:ASP:HA   | 1:C:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:D:116:LEU:O    | 1:D:120:ILE:HG13 | 2.19                     | 0.43              |
| 1:D:260:SER:O    | 1:D:267:ARG:HD2  | 2.18                     | 0.43              |
| 1:D:431:GLU:OE1  | 1:D:431:GLU:N    | 2.43                     | 0.43              |
| 1:F:603:PHE:HD1  | 1:F:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:F:669:PRO:HB2  | 1:F:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:G:124:GLY:O    | 1:G:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:H:116:LEU:O    | 1:H:120:ILE:HG13 | 2.19                     | 0.43              |
| 1:H:124:GLY:O    | 1:H:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:H:189:GLU:HG2  | 1:H:232:ASN:ND2  | 2.32                     | 0.43              |
| 1:H:293:LEU:HD22 | 1:H:340:GLU:HG2  | 2.00                     | 0.43              |
| 1:H:356:LYS:O    | 1:H:361:LYS:N    | 2.51                     | 0.43              |
| 1:H:513:SER:C    | 1:H:514:LEU:HD23 | 2.44                     | 0.43              |
| 1:I:603:PHE:HD1  | 1:I:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:J:124:GLY:O    | 1:J:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:J:173:LYS:H    | 1:J:173:LYS:HG3  | 1.66                     | 0.43              |
| 1:J:277:LEU:HD23 | 1:J:277:LEU:HA   | 1.81                     | 0.43              |
| 1:K:124:GLY:O    | 1:K:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:K:464:LYS:HE2  | 1:L:445:ARG:NH2  | 2.34                     | 0.43              |
| 1:K:564:VAL:HG22 | 1:K:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:L:127:ASP:HA   | 1:L:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:L:143:GLN:HA   | 1:L:146:ARG:HE   | 1.83                     | 0.43              |
| 1:L:221:ALA:HA   | 1:L:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:L:672:MET:O    | 1:L:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:M:593:ILE:HG23 | 1:M:595:VAL:HG22 | 2.00                     | 0.43              |
| 1:N:124:GLY:O    | 1:N:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:N:143:GLN:HA   | 1:N:146:ARG:HE   | 1.84                     | 0.43              |
| 1:N:180:LEU:O    | 1:N:183:SER:OG   | 2.24                     | 0.43              |
| 1:N:391:LYS:HD3  | 1:N:401:VAL:HG11 | 2.00                     | 0.43              |
| 1:P:236:HIS:HA   | 1:P:329:ARG:HH12 | 1.82                     | 0.43              |
| 1:P:293:LEU:HD22 | 1:P:340:GLU:HG2  | 1.99                     | 0.43              |
| 1:P:669:PRO:HB2  | 1:P:671:ASP:OD1  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:221:ALA:HA   | 1:A:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:A:617:PHE:CD1  | 1:A:653:ILE:HG23 | 2.53                     | 0.43              |
| 1:B:593:ILE:HG23 | 1:B:595:VAL:HG22 | 2.00                     | 0.43              |
| 1:C:239:GLN:HB2  | 1:D:478:ASN:ND2  | 2.30                     | 0.43              |
| 1:C:391:LYS:HD3  | 1:C:401:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:431:GLU:OE1  | 1:C:431:GLU:N    | 2.43                     | 0.43              |
| 1:C:669:PRO:HB2  | 1:C:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:C:672:MET:HE3  | 1:C:672:MET:HB2  | 1.92                     | 0.43              |
| 1:D:155:GLU:HA   | 1:D:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:E:116:LEU:O    | 1:E:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:E:221:ALA:HA   | 1:E:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:E:293:LEU:HD22 | 1:E:340:GLU:HG2  | 2.00                     | 0.43              |
| 1:F:116:LEU:O    | 1:F:120:ILE:HG13 | 2.19                     | 0.43              |
| 1:G:69:LEU:O     | 1:G:73:GLN:HG2   | 2.17                     | 0.43              |
| 1:G:143:GLN:HA   | 1:G:146:ARG:HE   | 1.83                     | 0.43              |
| 1:G:617:PHE:CD1  | 1:G:653:ILE:HG23 | 2.53                     | 0.43              |
| 1:H:215:CYS:HB2  | 1:H:253:TRP:CE3  | 2.53                     | 0.43              |
| 1:H:564:VAL:HG22 | 1:H:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:H:672:MET:O    | 1:H:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:I:116:LEU:O    | 1:I:120:ILE:HG13 | 2.19                     | 0.43              |
| 1:I:442:LEU:HD21 | 1:P:464:LYS:HB3  | 1.99                     | 0.43              |
| 1:I:513:SER:C    | 1:I:514:LEU:HD23 | 2.44                     | 0.43              |
| 1:J:285:ARG:HH21 | 1:K:484:ARG:NH1  | 2.15                     | 0.43              |
| 1:J:391:LYS:HD3  | 1:J:401:VAL:HG11 | 2.00                     | 0.43              |
| 1:J:672:MET:O    | 1:J:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:K:215:CYS:HB2  | 1:K:253:TRP:CE3  | 2.53                     | 0.43              |
| 1:K:513:SER:C    | 1:K:514:LEU:HD23 | 2.44                     | 0.43              |
| 1:K:672:MET:O    | 1:K:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:L:116:LEU:O    | 1:L:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:N:127:ASP:HA   | 1:N:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:N:491:LEU:HD23 | 1:N:491:LEU:HA   | 1.83                     | 0.43              |
| 1:N:603:PHE:HD1  | 1:N:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:N:669:PRO:HB2  | 1:N:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:O:155:GLU:HA   | 1:O:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:P:116:LEU:O    | 1:P:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:P:143:GLN:HA   | 1:P:146:ARG:HE   | 1.83                     | 0.43              |
| 1:P:221:ALA:HA   | 1:P:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:P:672:MET:O    | 1:P:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:A:60:GLU:OE2   | 1:O:310:ARG:NH2  | 2.50                     | 0.43              |
| 1:A:155:GLU:HA   | 1:A:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:A:513:SER:C    | 1:A:514:LEU:HD23 | 2.44                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:564:VAL:HG22 | 1:A:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:C:119:ALA:O    | 1:C:123:ASP:N    | 2.49                     | 0.43              |
| 1:D:95:VAL:O     | 1:D:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:D:143:GLN:HA   | 1:D:146:ARG:HE   | 1.84                     | 0.43              |
| 1:D:452:GLN:HB2  | 1:D:463:ARG:HD3  | 2.01                     | 0.43              |
| 1:D:540:THR:HG22 | 1:D:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:D:617:PHE:CD1  | 1:D:653:ILE:HG23 | 2.53                     | 0.43              |
| 1:E:69:LEU:O     | 1:E:73:GLN:HG2   | 2.17                     | 0.43              |
| 1:E:155:GLU:HA   | 1:E:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:E:431:GLU:OE1  | 1:E:431:GLU:N    | 2.43                     | 0.43              |
| 1:F:124:GLY:O    | 1:F:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:F:221:ALA:HA   | 1:F:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:F:513:SER:C    | 1:F:514:LEU:HD23 | 2.44                     | 0.43              |
| 1:F:564:VAL:HG22 | 1:F:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:G:293:LEU:HD22 | 1:G:340:GLU:HG2  | 2.00                     | 0.43              |
| 1:H:127:ASP:HA   | 1:H:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:I:124:GLY:O    | 1:I:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:I:452:GLN:HB2  | 1:I:463:ARG:HD3  | 2.01                     | 0.43              |
| 1:I:564:VAL:HG22 | 1:I:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:J:143:GLN:HA   | 1:J:146:ARG:HE   | 1.84                     | 0.43              |
| 1:J:192:PHE:CD2  | 1:J:233:CYS:HB2  | 2.54                     | 0.43              |
| 1:J:617:PHE:CD1  | 1:J:653:ILE:HG23 | 2.53                     | 0.43              |
| 1:L:513:SER:C    | 1:L:514:LEU:HD23 | 2.44                     | 0.43              |
| 1:L:669:PRO:HB2  | 1:L:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:N:119:ALA:O    | 1:N:123:ASP:N    | 2.49                     | 0.43              |
| 1:N:256:PRO:CG   | 1:O:582:VAL:HG21 | 2.47                     | 0.43              |
| 1:N:378:VAL:CA   | 1:N:381:SER:HB3  | 2.47                     | 0.43              |
| 1:N:540:THR:HG22 | 1:N:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:N:593:ILE:HG23 | 1:N:595:VAL:HG22 | 2.00                     | 0.43              |
| 1:O:143:GLN:HA   | 1:O:146:ARG:HE   | 1.84                     | 0.43              |
| 1:O:260:SER:O    | 1:O:267:ARG:HD2  | 2.18                     | 0.43              |
| 1:P:155:GLU:HA   | 1:P:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:P:603:PHE:HD1  | 1:P:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:B:672:MET:O    | 1:B:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:C:378:VAL:CA   | 1:C:381:SER:HB3  | 2.47                     | 0.43              |
| 1:C:540:THR:HG22 | 1:C:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:C:593:ILE:HG23 | 1:C:595:VAL:HG22 | 2.00                     | 0.43              |
| 1:C:603:PHE:HD1  | 1:C:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:D:623:PRO:HD3  | 1:D:658:ASP:O    | 2.19                     | 0.43              |
| 1:E:95:VAL:O     | 1:E:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:E:143:GLN:HA   | 1:E:146:ARG:HE   | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:236:HIS:HA   | 1:E:329:ARG:HH12 | 1.83                     | 0.43              |
| 1:E:540:THR:HG22 | 1:E:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:E:672:MET:O    | 1:E:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:F:540:THR:HG22 | 1:F:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:F:561:THR:HA   | 1:F:562:PRO:HD3  | 1.89                     | 0.43              |
| 1:G:192:PHE:CD2  | 1:G:233:CYS:HB2  | 2.54                     | 0.43              |
| 1:G:391:LYS:HD3  | 1:G:401:VAL:HG11 | 2.00                     | 0.43              |
| 1:G:540:THR:HG22 | 1:G:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:J:197:GLU:CD   | 1:K:384:GLY:H    | 2.23                     | 0.43              |
| 1:L:155:GLU:HA   | 1:L:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:M:672:MET:O    | 1:M:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:O:95:VAL:O     | 1:O:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:O:431:GLU:OE1  | 1:O:431:GLU:N    | 2.43                     | 0.43              |
| 1:O:460:GLY:O    | 1:O:464:LYS:N    | 2.30                     | 0.43              |
| 1:O:540:THR:HG22 | 1:O:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:O:603:PHE:HD1  | 1:O:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:O:617:PHE:CD1  | 1:O:653:ILE:HG23 | 2.53                     | 0.43              |
| 1:P:452:GLN:HB2  | 1:P:463:ARG:HD3  | 2.01                     | 0.43              |
| 1:A:116:LEU:O    | 1:A:120:ILE:HG13 | 2.19                     | 0.43              |
| 1:B:155:GLU:HA   | 1:B:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:B:447:THR:O    | 1:B:451:LEU:HD23 | 2.19                     | 0.43              |
| 1:C:116:LEU:O    | 1:C:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:447:THR:O    | 1:C:451:LEU:HD23 | 2.19                     | 0.43              |
| 1:D:406:LEU:O    | 1:D:412:TRP:NE1  | 2.52                     | 0.43              |
| 1:E:452:GLN:HB2  | 1:E:463:ARG:HD3  | 2.01                     | 0.43              |
| 1:E:603:PHE:HD1  | 1:E:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:F:452:GLN:HB2  | 1:F:463:ARG:HD3  | 2.01                     | 0.43              |
| 1:G:173:LYS:H    | 1:G:173:LYS:HG3  | 1.66                     | 0.43              |
| 1:H:155:GLU:HA   | 1:H:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:I:612:MET:O    | 1:I:651:LYS:NZ   | 2.33                     | 0.43              |
| 1:J:69:LEU:O     | 1:J:73:GLN:HG2   | 2.18                     | 0.43              |
| 1:J:293:LEU:HD22 | 1:J:340:GLU:HG2  | 2.00                     | 0.43              |
| 1:J:540:THR:HG22 | 1:J:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:J:593:ILE:HG23 | 1:J:595:VAL:HG22 | 2.00                     | 0.43              |
| 1:K:127:ASP:HA   | 1:K:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:K:143:GLN:HA   | 1:K:146:ARG:HE   | 1.83                     | 0.43              |
| 1:K:447:THR:O    | 1:K:451:LEU:HD23 | 2.19                     | 0.43              |
| 1:L:564:VAL:HG22 | 1:L:616:ASN:HB2  | 2.01                     | 0.43              |
| 1:M:95:VAL:O     | 1:M:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:M:155:GLU:HA   | 1:M:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:M:221:ALA:HA   | 1:M:224:ARG:HD3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:447:THR:O    | 1:M:451:LEU:HD23 | 2.19                     | 0.43              |
| 1:N:431:GLU:OE1  | 1:N:431:GLU:N    | 2.43                     | 0.43              |
| 1:N:447:THR:O    | 1:N:451:LEU:HD23 | 2.19                     | 0.43              |
| 1:P:69:LEU:O     | 1:P:73:GLN:HG2   | 2.18                     | 0.43              |
| 1:P:95:VAL:O     | 1:P:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:P:540:THR:HG22 | 1:P:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:A:124:GLY:O    | 1:A:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:A:447:THR:O    | 1:A:451:LEU:HD23 | 2.19                     | 0.43              |
| 1:A:593:ILE:HG23 | 1:A:595:VAL:HG22 | 2.00                     | 0.43              |
| 1:B:95:VAL:O     | 1:B:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:B:192:PHE:CD2  | 1:B:233:CYS:HB2  | 2.54                     | 0.43              |
| 1:D:127:ASP:HB2  | 1:D:131:ARG:NH1  | 2.28                     | 0.43              |
| 1:D:127:ASP:HA   | 1:D:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:D:241:VAL:O    | 1:D:245:MET:HG3  | 2.19                     | 0.43              |
| 1:D:603:PHE:HD1  | 1:D:638:TRP:HZ2  | 1.65                     | 0.43              |
| 1:E:239:GLN:HB2  | 1:F:478:ASN:HD21 | 1.83                     | 0.43              |
| 1:E:241:VAL:O    | 1:E:245:MET:HG3  | 2.19                     | 0.43              |
| 1:E:681:ILE:HD11 | 1:E:698:PHE:CD2  | 2.53                     | 0.43              |
| 1:F:69:LEU:O     | 1:F:73:GLN:HG2   | 2.18                     | 0.43              |
| 1:F:185:ALA:HB2  | 1:F:214:TRP:HZ3  | 1.82                     | 0.43              |
| 1:F:672:MET:O    | 1:F:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:H:487:LEU:HD23 | 1:H:487:LEU:HA   | 1.82                     | 0.43              |
| 1:H:617:PHE:CD1  | 1:H:653:ILE:HG23 | 2.53                     | 0.43              |
| 1:I:540:THR:HG22 | 1:I:544:GLU:OE2  | 2.19                     | 0.43              |
| 1:I:672:MET:O    | 1:I:675:VAL:HG22 | 2.19                     | 0.43              |
| 1:J:623:PRO:HD3  | 1:J:658:ASP:O    | 2.19                     | 0.43              |
| 1:K:465:ARG:NH2  | 1:L:437:GLN:HB2  | 2.33                     | 0.43              |
| 1:L:688:GLN:O    | 1:L:692:ILE:HG12 | 2.19                     | 0.43              |
| 1:N:127:ASP:HB2  | 1:N:131:ARG:NH1  | 2.28                     | 0.43              |
| 1:O:127:ASP:HA   | 1:O:130:LEU:HB2  | 2.01                     | 0.43              |
| 1:O:452:GLN:HB2  | 1:O:463:ARG:HD3  | 2.01                     | 0.43              |
| 1:O:623:PRO:HD3  | 1:O:658:ASP:O    | 2.19                     | 0.43              |
| 1:P:241:VAL:O    | 1:P:245:MET:HG3  | 2.19                     | 0.43              |
| 1:P:431:GLU:OE1  | 1:P:431:GLU:N    | 2.43                     | 0.43              |
| 1:P:513:SER:C    | 1:P:514:LEU:HD23 | 2.44                     | 0.43              |
| 1:P:681:ILE:HD11 | 1:P:698:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:688:GLN:O    | 1:A:692:ILE:HG12 | 2.19                     | 0.43              |
| 1:B:116:LEU:O    | 1:B:120:ILE:HG13 | 2.18                     | 0.43              |
| 1:B:221:ALA:HA   | 1:B:224:ARG:HD3  | 2.00                     | 0.43              |
| 1:C:95:VAL:O     | 1:C:99:VAL:HG22  | 2.18                     | 0.43              |
| 1:D:221:ALA:HA   | 1:D:224:ARG:HD3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:192:PHE:CD2  | 1:E:233:CYS:HB2  | 2.54                     | 0.43              |
| 1:E:486:ASN:HD21 | 1:E:489:ASP:CG   | 2.26                     | 0.43              |
| 1:F:241:VAL:O    | 1:F:245:MET:HG3  | 2.19                     | 0.43              |
| 1:G:167:VAL:O    | 1:G:171:LEU:HG   | 2.19                     | 0.43              |
| 1:G:593:ILE:HG23 | 1:G:595:VAL:HG22 | 2.00                     | 0.43              |
| 1:G:623:PRO:HD3  | 1:G:658:ASP:O    | 2.19                     | 0.43              |
| 1:G:669:PRO:HB2  | 1:G:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:I:69:LEU:O     | 1:I:73:GLN:HG2   | 2.18                     | 0.43              |
| 1:I:241:VAL:O    | 1:I:245:MET:HG3  | 2.19                     | 0.43              |
| 1:I:378:VAL:CA   | 1:I:381:SER:HB3  | 2.47                     | 0.43              |
| 1:J:669:PRO:HB2  | 1:J:671:ASP:OD1  | 2.18                     | 0.43              |
| 1:K:155:GLU:HA   | 1:K:158:ASP:OD2  | 2.19                     | 0.43              |
| 1:L:119:ALA:O    | 1:L:123:ASP:N    | 2.49                     | 0.43              |
| 1:L:124:GLY:O    | 1:L:128:LEU:HD13 | 2.18                     | 0.43              |
| 1:L:447:THR:O    | 1:L:451:LEU:HD23 | 2.19                     | 0.43              |
| 1:M:192:PHE:CD2  | 1:M:233:CYS:HB2  | 2.54                     | 0.43              |
| 1:O:406:LEU:O    | 1:O:412:TRP:NE1  | 2.52                     | 0.43              |
| 1:O:688:GLN:O    | 1:O:692:ILE:HG12 | 2.19                     | 0.43              |
| 1:P:185:ALA:HB2  | 1:P:214:TRP:HZ3  | 1.82                     | 0.43              |
| 1:P:192:PHE:CD2  | 1:P:233:CYS:HB2  | 2.54                     | 0.43              |
| 1:A:119:ALA:O    | 1:A:123:ASP:N    | 2.49                     | 0.42              |
| 1:B:458:LYS:HD3  | 1:B:458:LYS:HA   | 1.77                     | 0.42              |
| 1:B:513:SER:C    | 1:B:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:C:452:GLN:HB2  | 1:C:463:ARG:HD3  | 2.01                     | 0.42              |
| 1:C:491:LEU:HD23 | 1:C:491:LEU:HA   | 1.83                     | 0.42              |
| 1:D:71:GLU:HA    | 1:D:74:GLN:CD    | 2.44                     | 0.42              |
| 1:D:391:LYS:HD3  | 1:D:401:VAL:HG11 | 2.00                     | 0.42              |
| 1:E:513:SER:C    | 1:E:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:E:623:PRO:HD3  | 1:E:658:ASP:O    | 2.19                     | 0.42              |
| 1:F:155:GLU:HA   | 1:F:158:ASP:OD2  | 2.19                     | 0.42              |
| 1:F:167:VAL:O    | 1:F:171:LEU:HG   | 2.19                     | 0.42              |
| 1:F:378:VAL:CA   | 1:F:381:SER:HB3  | 2.47                     | 0.42              |
| 1:F:617:PHE:CD1  | 1:F:653:ILE:HG23 | 2.53                     | 0.42              |
| 1:G:127:ASP:HA   | 1:G:130:LEU:HB2  | 2.01                     | 0.42              |
| 1:G:285:ARG:HD3  | 1:G:285:ARG:HA   | 1.75                     | 0.42              |
| 1:H:143:GLN:HA   | 1:H:146:ARG:HE   | 1.84                     | 0.42              |
| 1:H:447:THR:O    | 1:H:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:H:623:PRO:HD3  | 1:H:658:ASP:O    | 2.19                     | 0.42              |
| 1:H:688:GLN:O    | 1:H:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:I:155:GLU:HA   | 1:I:158:ASP:OD2  | 2.19                     | 0.42              |
| 1:I:167:VAL:O    | 1:I:171:LEU:HG   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:185:ALA:HB2  | 1:I:214:TRP:HZ3  | 1.82                     | 0.42              |
| 1:J:127:ASP:HA   | 1:J:130:LEU:HB2  | 2.01                     | 0.42              |
| 1:J:460:GLY:O    | 1:J:464:LYS:N    | 2.30                     | 0.42              |
| 1:K:617:PHE:CD1  | 1:K:653:ILE:HG23 | 2.53                     | 0.42              |
| 1:L:593:ILE:HG23 | 1:L:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:N:95:VAL:O     | 1:N:99:VAL:HG22  | 2.18                     | 0.42              |
| 1:N:116:LEU:O    | 1:N:120:ILE:HG13 | 2.19                     | 0.42              |
| 1:N:155:GLU:HA   | 1:N:158:ASP:OD2  | 2.19                     | 0.42              |
| 1:N:672:MET:HE3  | 1:N:672:MET:HB2  | 1.92                     | 0.42              |
| 1:O:71:GLU:HA    | 1:O:74:GLN:CD    | 2.44                     | 0.42              |
| 1:O:221:ALA:HA   | 1:O:224:ARG:HD3  | 2.00                     | 0.42              |
| 1:O:241:VAL:O    | 1:O:245:MET:HG3  | 2.19                     | 0.42              |
| 1:O:391:LYS:HD3  | 1:O:401:VAL:HG11 | 2.00                     | 0.42              |
| 1:O:513:SER:C    | 1:O:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:P:564:VAL:HG22 | 1:P:616:ASN:HB2  | 2.01                     | 0.42              |
| 1:P:623:PRO:HD3  | 1:P:658:ASP:O    | 2.19                     | 0.42              |
| 1:A:192:PHE:CD2  | 1:A:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:A:431:GLU:OE1  | 1:A:431:GLU:N    | 2.43                     | 0.42              |
| 1:C:155:GLU:HA   | 1:C:158:ASP:OD2  | 2.19                     | 0.42              |
| 1:C:331:VAL:N    | 1:C:332:PRO:HD2  | 2.34                     | 0.42              |
| 1:D:688:GLN:O    | 1:D:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:E:127:ASP:HA   | 1:E:130:LEU:HB2  | 2.01                     | 0.42              |
| 1:E:185:ALA:HB2  | 1:E:214:TRP:HZ3  | 1.82                     | 0.42              |
| 1:E:564:VAL:HG22 | 1:E:616:ASN:HB2  | 2.01                     | 0.42              |
| 1:F:152:LEU:HD11 | 1:F:187:ILE:HG23 | 2.02                     | 0.42              |
| 1:F:293:LEU:HD22 | 1:F:340:GLU:HG2  | 2.00                     | 0.42              |
| 1:F:593:ILE:HG23 | 1:F:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:F:612:MET:O    | 1:F:651:LYS:NZ   | 2.33                     | 0.42              |
| 1:G:155:GLU:HA   | 1:G:158:ASP:OD2  | 2.19                     | 0.42              |
| 1:G:331:VAL:N    | 1:G:332:PRO:HD2  | 2.34                     | 0.42              |
| 1:H:486:ASN:HD21 | 1:H:489:ASP:CG   | 2.27                     | 0.42              |
| 1:I:152:LEU:HD11 | 1:I:187:ILE:HG23 | 2.02                     | 0.42              |
| 1:I:293:LEU:HD22 | 1:I:340:GLU:HG2  | 2.00                     | 0.42              |
| 1:I:486:ASN:HD21 | 1:I:489:ASP:CG   | 2.26                     | 0.42              |
| 1:I:593:ILE:HG23 | 1:I:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:J:167:VAL:O    | 1:J:171:LEU:HG   | 2.19                     | 0.42              |
| 1:K:623:PRO:HD3  | 1:K:658:ASP:O    | 2.19                     | 0.42              |
| 1:K:688:GLN:O    | 1:K:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:L:331:VAL:N    | 1:L:332:PRO:HD2  | 2.34                     | 0.42              |
| 1:L:486:ASN:HD21 | 1:L:489:ASP:CG   | 2.26                     | 0.42              |
| 1:N:452:GLN:HB2  | 1:N:463:ARG:HD3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:513:SER:C    | 1:N:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:O:127:ASP:HB2  | 1:O:131:ARG:NH1  | 2.28                     | 0.42              |
| 1:P:167:VAL:O    | 1:P:171:LEU:HG   | 2.19                     | 0.42              |
| 1:B:540:THR:HG22 | 1:B:544:GLU:OE2  | 2.19                     | 0.42              |
| 1:B:669:PRO:HB2  | 1:B:671:ASP:OD1  | 2.18                     | 0.42              |
| 1:C:192:PHE:CD2  | 1:C:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:C:513:SER:C    | 1:C:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:C:688:GLN:O    | 1:C:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:D:152:LEU:HD11 | 1:D:187:ILE:HG23 | 2.01                     | 0.42              |
| 1:D:165:LEU:HD12 | 1:D:166:GLY:N    | 2.35                     | 0.42              |
| 1:D:447:THR:O    | 1:D:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:E:124:GLY:O    | 1:E:128:LEU:HD13 | 2.18                     | 0.42              |
| 1:E:167:VAL:O    | 1:E:171:LEU:HG   | 2.19                     | 0.42              |
| 1:F:127:ASP:HA   | 1:F:130:LEU:HB2  | 2.01                     | 0.42              |
| 1:F:486:ASN:HD21 | 1:F:489:ASP:CG   | 2.27                     | 0.42              |
| 1:G:215:CYS:HB2  | 1:G:253:TRP:CE3  | 2.53                     | 0.42              |
| 1:G:452:GLN:HB2  | 1:G:463:ARG:HD3  | 2.01                     | 0.42              |
| 1:G:486:ASN:HD21 | 1:G:489:ASP:CG   | 2.26                     | 0.42              |
| 1:G:688:GLN:O    | 1:G:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:H:285:ARG:HD3  | 1:H:285:ARG:HA   | 1.75                     | 0.42              |
| 1:H:540:THR:HG22 | 1:H:544:GLU:OE2  | 2.19                     | 0.42              |
| 1:I:617:PHE:CD1  | 1:I:653:ILE:HG23 | 2.53                     | 0.42              |
| 1:J:155:GLU:HA   | 1:J:158:ASP:OD2  | 2.19                     | 0.42              |
| 1:J:215:CYS:HB2  | 1:J:253:TRP:CE3  | 2.53                     | 0.42              |
| 1:J:331:VAL:N    | 1:J:332:PRO:HD2  | 2.34                     | 0.42              |
| 1:J:452:GLN:HB2  | 1:J:463:ARG:HD3  | 2.01                     | 0.42              |
| 1:J:486:ASN:HD21 | 1:J:489:ASP:CG   | 2.26                     | 0.42              |
| 1:J:688:GLN:O    | 1:J:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:K:192:PHE:CD2  | 1:K:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:L:71:GLU:HA    | 1:L:74:GLN:CD    | 2.44                     | 0.42              |
| 1:L:192:PHE:CD2  | 1:L:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:M:116:LEU:O    | 1:M:120:ILE:HG13 | 2.19                     | 0.42              |
| 1:N:331:VAL:N    | 1:N:332:PRO:HD2  | 2.35                     | 0.42              |
| 1:O:152:LEU:HD11 | 1:O:187:ILE:HG23 | 2.01                     | 0.42              |
| 1:O:167:VAL:O    | 1:O:171:LEU:HG   | 2.19                     | 0.42              |
| 1:P:92:LEU:HB3   | 1:P:147:LEU:HD11 | 2.01                     | 0.42              |
| 1:P:124:GLY:O    | 1:P:128:LEU:HD13 | 2.18                     | 0.42              |
| 1:P:422:GLN:HA   | 1:P:427:SER:HB3  | 2.01                     | 0.42              |
| 1:P:486:ASN:HD21 | 1:P:489:ASP:CG   | 2.27                     | 0.42              |
| 1:P:688:GLN:O    | 1:P:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:A:71:GLU:HA    | 1:A:74:GLN:CD    | 2.44                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:152:LEU:HD11 | 1:A:187:ILE:HG23 | 2.01                     | 0.42              |
| 1:A:331:VAL:N    | 1:A:332:PRO:HD2  | 2.35                     | 0.42              |
| 1:A:486:ASN:HD21 | 1:A:489:ASP:CG   | 2.27                     | 0.42              |
| 1:B:331:VAL:N    | 1:B:332:PRO:HD2  | 2.35                     | 0.42              |
| 1:B:431:GLU:OE1  | 1:B:431:GLU:N    | 2.43                     | 0.42              |
| 1:C:221:ALA:HA   | 1:C:224:ARG:HD3  | 2.00                     | 0.42              |
| 1:C:422:GLN:HA   | 1:C:427:SER:HB3  | 2.01                     | 0.42              |
| 1:D:192:PHE:CD2  | 1:D:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:D:378:VAL:CA   | 1:D:381:SER:HB3  | 2.47                     | 0.42              |
| 1:D:486:ASN:HD21 | 1:D:489:ASP:CG   | 2.27                     | 0.42              |
| 1:D:672:MET:O    | 1:D:675:VAL:HG22 | 2.19                     | 0.42              |
| 1:E:111:GLU:HA   | 1:E:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:E:127:ASP:HB2  | 1:E:131:ARG:NH1  | 2.28                     | 0.42              |
| 1:E:331:VAL:N    | 1:E:332:PRO:HD2  | 2.35                     | 0.42              |
| 1:F:165:LEU:HD12 | 1:F:166:GLY:N    | 2.35                     | 0.42              |
| 1:F:285:ARG:HA   | 1:F:285:ARG:HD3  | 1.75                     | 0.42              |
| 1:F:391:LYS:HD3  | 1:F:401:VAL:HG11 | 2.00                     | 0.42              |
| 1:H:192:PHE:CD2  | 1:H:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:H:422:GLN:HA   | 1:H:427:SER:HB3  | 2.01                     | 0.42              |
| 1:I:111:GLU:HA   | 1:I:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:I:127:ASP:HA   | 1:I:130:LEU:HB2  | 2.01                     | 0.42              |
| 1:I:165:LEU:HD12 | 1:I:166:GLY:N    | 2.35                     | 0.42              |
| 1:I:285:ARG:HA   | 1:I:285:ARG:HD3  | 1.75                     | 0.42              |
| 1:I:391:LYS:HD3  | 1:I:401:VAL:HG11 | 2.00                     | 0.42              |
| 1:I:422:GLN:HA   | 1:I:427:SER:HB3  | 2.01                     | 0.42              |
| 1:J:152:LEU:HD11 | 1:J:187:ILE:HG23 | 2.01                     | 0.42              |
| 1:K:486:ASN:HD21 | 1:K:489:ASP:CG   | 2.27                     | 0.42              |
| 1:K:593:ILE:HG23 | 1:K:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:L:152:LEU:HD11 | 1:L:187:ILE:HG23 | 2.01                     | 0.42              |
| 1:L:422:GLN:HA   | 1:L:427:SER:HB3  | 2.01                     | 0.42              |
| 1:L:623:PRO:HD3  | 1:L:658:ASP:O    | 2.19                     | 0.42              |
| 1:M:331:VAL:N    | 1:M:332:PRO:HD2  | 2.35                     | 0.42              |
| 1:M:540:THR:HG22 | 1:M:544:GLU:OE2  | 2.19                     | 0.42              |
| 1:M:669:PRO:HB2  | 1:M:671:ASP:OD1  | 2.18                     | 0.42              |
| 1:N:192:PHE:CD2  | 1:N:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:N:221:ALA:HA   | 1:N:224:ARG:HD3  | 2.00                     | 0.42              |
| 1:O:92:LEU:HB3   | 1:O:147:LEU:HD11 | 2.01                     | 0.42              |
| 1:O:165:LEU:HD12 | 1:O:166:GLY:N    | 2.35                     | 0.42              |
| 1:O:378:VAL:CA   | 1:O:381:SER:HB3  | 2.47                     | 0.42              |
| 1:O:447:THR:O    | 1:O:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:O:672:MET:O    | 1:O:675:VAL:HG22 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:127:ASP:HA   | 1:P:130:LEU:HB2  | 2.01                     | 0.42              |
| 1:P:331:VAL:N    | 1:P:332:PRO:HD2  | 2.34                     | 0.42              |
| 1:A:165:LEU:HD12 | 1:A:166:GLY:N    | 2.35                     | 0.42              |
| 1:A:422:GLN:HA   | 1:A:427:SER:HB3  | 2.01                     | 0.42              |
| 1:A:460:GLY:O    | 1:A:464:LYS:N    | 2.30                     | 0.42              |
| 1:A:623:PRO:HD3  | 1:A:658:ASP:O    | 2.19                     | 0.42              |
| 1:D:92:LEU:HB3   | 1:D:147:LEU:HD11 | 2.01                     | 0.42              |
| 1:D:167:VAL:O    | 1:D:171:LEU:HG   | 2.19                     | 0.42              |
| 1:E:92:LEU:HB3   | 1:E:147:LEU:HD11 | 2.01                     | 0.42              |
| 1:E:688:GLN:O    | 1:E:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:F:111:GLU:HA   | 1:F:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:F:192:PHE:CD2  | 1:F:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:F:422:GLN:HA   | 1:F:427:SER:HB3  | 2.01                     | 0.42              |
| 1:G:71:GLU:HA    | 1:G:74:GLN:CD    | 2.44                     | 0.42              |
| 1:G:241:VAL:O    | 1:G:245:MET:HG3  | 2.19                     | 0.42              |
| 1:H:165:LEU:HD12 | 1:H:166:GLY:N    | 2.35                     | 0.42              |
| 1:J:71:GLU:HA    | 1:J:74:GLN:CD    | 2.44                     | 0.42              |
| 1:J:447:THR:O    | 1:J:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:J:513:SER:C    | 1:J:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:K:165:LEU:HD12 | 1:K:166:GLY:N    | 2.35                     | 0.42              |
| 1:K:422:GLN:HA   | 1:K:427:SER:HB3  | 2.01                     | 0.42              |
| 1:K:540:THR:HG22 | 1:K:544:GLU:OE2  | 2.19                     | 0.42              |
| 1:M:165:LEU:HD12 | 1:M:166:GLY:N    | 2.35                     | 0.42              |
| 1:M:486:ASN:HD21 | 1:M:489:ASP:CG   | 2.27                     | 0.42              |
| 1:M:513:SER:C    | 1:M:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:M:596:GLU:OE2  | 1:M:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:M:688:GLN:O    | 1:M:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:N:422:GLN:HA   | 1:N:427:SER:HB3  | 2.01                     | 0.42              |
| 1:N:688:GLN:O    | 1:N:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:O:192:PHE:CD2  | 1:O:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:O:486:ASN:HD21 | 1:O:489:ASP:CG   | 2.27                     | 0.42              |
| 1:P:111:GLU:HA   | 1:P:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:P:127:ASP:HB2  | 1:P:131:ARG:NH1  | 2.28                     | 0.42              |
| 1:B:215:CYS:HB2  | 1:B:253:TRP:HE3  | 1.85                     | 0.42              |
| 1:B:486:ASN:HD21 | 1:B:489:ASP:CG   | 2.27                     | 0.42              |
| 1:B:596:GLU:OE2  | 1:B:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:B:634:ASP:HB3  | 1:B:636:LYS:HE2  | 2.02                     | 0.42              |
| 1:C:165:LEU:HD12 | 1:C:166:GLY:N    | 2.35                     | 0.42              |
| 1:C:241:VAL:O    | 1:C:245:MET:HG3  | 2.19                     | 0.42              |
| 1:C:623:PRO:HD3  | 1:C:658:ASP:O    | 2.19                     | 0.42              |
| 1:D:513:SER:C    | 1:D:514:LEU:HD23 | 2.44                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:422:GLN:HA   | 1:E:427:SER:HB3  | 2.01                     | 0.42              |
| 1:E:447:THR:O    | 1:E:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:G:165:LEU:HD12 | 1:G:166:GLY:N    | 2.35                     | 0.42              |
| 1:G:378:VAL:CA   | 1:G:381:SER:HB3  | 2.47                     | 0.42              |
| 1:G:513:SER:C    | 1:G:514:LEU:HD23 | 2.44                     | 0.42              |
| 1:H:593:ILE:HG23 | 1:H:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:H:596:GLU:OE2  | 1:H:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:I:688:GLN:O    | 1:I:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:J:165:LEU:HD12 | 1:J:166:GLY:N    | 2.35                     | 0.42              |
| 1:J:241:VAL:O    | 1:J:245:MET:HG3  | 2.19                     | 0.42              |
| 1:K:596:GLU:OE2  | 1:K:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:L:165:LEU:HD12 | 1:L:166:GLY:N    | 2.35                     | 0.42              |
| 1:M:215:CYS:HB2  | 1:M:253:TRP:HE3  | 1.85                     | 0.42              |
| 1:M:564:VAL:HG22 | 1:M:616:ASN:HB2  | 2.01                     | 0.42              |
| 1:M:623:PRO:HD3  | 1:M:658:ASP:O    | 2.19                     | 0.42              |
| 1:N:241:VAL:O    | 1:N:245:MET:HG3  | 2.19                     | 0.42              |
| 1:A:452:GLN:HB2  | 1:A:463:ARG:HD3  | 2.01                     | 0.42              |
| 1:B:60:GLU:HA    | 1:B:63:ASP:OD2   | 2.20                     | 0.42              |
| 1:B:165:LEU:HD12 | 1:B:166:GLY:N    | 2.35                     | 0.42              |
| 1:B:494:LEU:HD12 | 1:B:494:LEU:HA   | 1.79                     | 0.42              |
| 1:B:564:VAL:HG22 | 1:B:616:ASN:HB2  | 2.01                     | 0.42              |
| 1:B:688:GLN:O    | 1:B:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:138:LEU:N    | 1:C:141:ARG:HH21 | 2.18                     | 0.42              |
| 1:C:383:ASN:HB3  | 1:C:386:LYS:HB3  | 2.02                     | 0.42              |
| 1:C:486:ASN:HD21 | 1:C:489:ASP:CG   | 2.27                     | 0.42              |
| 1:F:688:GLN:O    | 1:F:692:ILE:HG12 | 2.19                     | 0.42              |
| 1:G:152:LEU:HD11 | 1:G:187:ILE:HG23 | 2.02                     | 0.42              |
| 1:G:447:THR:O    | 1:G:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:H:71:GLU:HA    | 1:H:74:GLN:CD    | 2.44                     | 0.42              |
| 1:H:331:VAL:N    | 1:H:332:PRO:HD2  | 2.34                     | 0.42              |
| 1:I:192:PHE:CD2  | 1:I:233:CYS:HB2  | 2.54                     | 0.42              |
| 1:I:447:THR:O    | 1:I:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:I:623:PRO:HD3  | 1:I:658:ASP:O    | 2.19                     | 0.42              |
| 1:J:378:VAL:CA   | 1:J:381:SER:HB3  | 2.47                     | 0.42              |
| 1:K:449:GLU:O    | 1:K:453:THR:OG1  | 2.31                     | 0.42              |
| 1:K:461:ILE:H    | 1:K:461:ILE:HG13 | 1.63                     | 0.42              |
| 1:L:215:CYS:HB2  | 1:L:253:TRP:HE3  | 1.85                     | 0.42              |
| 1:L:452:GLN:HB2  | 1:L:463:ARG:HD3  | 2.01                     | 0.42              |
| 1:L:460:GLY:O    | 1:L:464:LYS:N    | 2.30                     | 0.42              |
| 1:M:60:GLU:HA    | 1:M:63:ASP:OD2   | 2.20                     | 0.42              |
| 1:M:431:GLU:OE1  | 1:M:431:GLU:N    | 2.43                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:502:THR:O    | 1:M:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:N:165:LEU:HD12 | 1:N:166:GLY:N    | 2.35                     | 0.42              |
| 1:N:486:ASN:HD21 | 1:N:489:ASP:CG   | 2.27                     | 0.42              |
| 1:P:447:THR:O    | 1:P:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:A:215:CYS:HB2  | 1:A:253:TRP:HE3  | 1.85                     | 0.42              |
| 1:A:406:LEU:O    | 1:A:412:TRP:NE1  | 2.52                     | 0.42              |
| 1:B:67:ARG:O     | 1:B:71:GLU:HG2   | 2.20                     | 0.42              |
| 1:B:71:GLU:HA    | 1:B:74:GLN:CD    | 2.44                     | 0.42              |
| 1:B:165:LEU:HA   | 1:B:168:ILE:HD12 | 2.02                     | 0.42              |
| 1:B:452:GLN:HB2  | 1:B:463:ARG:HD3  | 2.01                     | 0.42              |
| 1:B:502:THR:O    | 1:B:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:D:111:GLU:HA   | 1:D:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:D:502:THR:O    | 1:D:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:D:568:TYR:HE1  | 1:D:594:ASP:HB2  | 1.85                     | 0.42              |
| 1:E:391:LYS:HD3  | 1:E:401:VAL:HG11 | 2.00                     | 0.42              |
| 1:F:71:GLU:HA    | 1:F:74:GLN:CD    | 2.44                     | 0.42              |
| 1:F:596:GLU:OE2  | 1:F:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:F:623:PRO:HD3  | 1:F:658:ASP:O    | 2.19                     | 0.42              |
| 1:G:111:GLU:HA   | 1:G:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:H:152:LEU:HD11 | 1:H:187:ILE:HG23 | 2.01                     | 0.42              |
| 1:H:167:VAL:O    | 1:H:171:LEU:HG   | 2.19                     | 0.42              |
| 1:J:111:GLU:HA   | 1:J:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:J:138:LEU:N    | 1:J:141:ARG:HH21 | 2.18                     | 0.42              |
| 1:J:285:ARG:HD3  | 1:J:285:ARG:HA   | 1.75                     | 0.42              |
| 1:K:331:VAL:N    | 1:K:332:PRO:HD2  | 2.35                     | 0.42              |
| 1:M:165:LEU:HA   | 1:M:168:ILE:HD12 | 2.02                     | 0.42              |
| 1:N:138:LEU:N    | 1:N:141:ARG:HH21 | 2.18                     | 0.42              |
| 1:N:383:ASN:HB3  | 1:N:386:LYS:HB3  | 2.02                     | 0.42              |
| 1:N:623:PRO:HD3  | 1:N:658:ASP:O    | 2.19                     | 0.42              |
| 1:O:502:THR:O    | 1:O:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:O:596:GLU:OE2  | 1:O:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:O:692:ILE:HD13 | 1:O:692:ILE:HA   | 1.90                     | 0.42              |
| 1:P:67:ARG:O     | 1:P:71:GLU:HG2   | 2.20                     | 0.42              |
| 1:P:285:ARG:HD3  | 1:P:285:ARG:HA   | 1.75                     | 0.42              |
| 1:B:623:PRO:HD3  | 1:B:658:ASP:O    | 2.19                     | 0.42              |
| 1:C:256:PRO:CG   | 1:D:582:VAL:HG21 | 2.49                     | 0.42              |
| 1:D:60:GLU:HA    | 1:D:63:ASP:OD2   | 2.20                     | 0.42              |
| 1:D:422:GLN:HA   | 1:D:427:SER:HB3  | 2.01                     | 0.42              |
| 1:D:593:ILE:HG23 | 1:D:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:D:596:GLU:OE2  | 1:D:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:E:67:ARG:O     | 1:E:71:GLU:HG2   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:165:LEU:HD12 | 1:E:166:GLY:N    | 2.35                     | 0.42              |
| 1:F:92:LEU:HB3   | 1:F:147:LEU:HD11 | 2.01                     | 0.42              |
| 1:F:197:GLU:HB2  | 1:G:382:THR:O    | 2.19                     | 0.42              |
| 1:F:338:ARG:HE   | 1:F:338:ARG:HB3  | 1.74                     | 0.42              |
| 1:F:447:THR:O    | 1:F:451:LEU:HD23 | 2.19                     | 0.42              |
| 1:G:138:LEU:N    | 1:G:141:ARG:HH21 | 2.18                     | 0.42              |
| 1:H:241:VAL:O    | 1:H:245:MET:HG3  | 2.19                     | 0.42              |
| 1:I:71:GLU:HA    | 1:I:74:GLN:CD    | 2.44                     | 0.42              |
| 1:I:92:LEU:HB3   | 1:I:147:LEU:HD11 | 2.01                     | 0.42              |
| 1:I:578:SER:OG   | 1:P:256:PRO:HB3  | 2.19                     | 0.42              |
| 1:I:596:GLU:OE2  | 1:I:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:J:596:GLU:OE2  | 1:J:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:K:446:LEU:HD23 | 1:K:446:LEU:HA   | 1.92                     | 0.42              |
| 1:L:256:PRO:HG3  | 1:M:582:VAL:HG21 | 2.02                     | 0.42              |
| 1:L:406:LEU:O    | 1:L:412:TRP:NE1  | 2.52                     | 0.42              |
| 1:L:431:GLU:OE1  | 1:L:431:GLU:N    | 2.43                     | 0.42              |
| 1:M:67:ARG:O     | 1:M:71:GLU:HG2   | 2.20                     | 0.42              |
| 1:M:71:GLU:HA    | 1:M:74:GLN:CD    | 2.44                     | 0.42              |
| 1:M:452:GLN:HB2  | 1:M:463:ARG:HD3  | 2.01                     | 0.42              |
| 1:M:634:ASP:HB3  | 1:M:636:LYS:HE2  | 2.02                     | 0.42              |
| 1:N:173:LYS:H    | 1:N:173:LYS:HG3  | 1.66                     | 0.42              |
| 1:O:60:GLU:HA    | 1:O:63:ASP:OD2   | 2.20                     | 0.42              |
| 1:O:111:GLU:HA   | 1:O:114:GLN:HG2  | 2.02                     | 0.42              |
| 1:P:502:THR:O    | 1:P:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:148:LEU:O    | 1:A:152:LEU:HG   | 2.20                     | 0.42              |
| 1:A:502:THR:O    | 1:A:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:C:71:GLU:HA    | 1:C:74:GLN:CD    | 2.44                     | 0.42              |
| 1:C:672:MET:O    | 1:C:675:VAL:HG22 | 2.19                     | 0.42              |
| 1:D:121:ARG:HA   | 1:D:125:GLY:HA2  | 2.02                     | 0.42              |
| 1:E:502:THR:O    | 1:E:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:E:593:ILE:HG23 | 1:E:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:F:215:CYS:HB2  | 1:F:253:TRP:HE3  | 1.85                     | 0.42              |
| 1:F:494:LEU:HD12 | 1:F:494:LEU:HA   | 1.79                     | 0.42              |
| 1:F:568:TYR:HE1  | 1:F:594:ASP:HB2  | 1.85                     | 0.42              |
| 1:G:67:ARG:O     | 1:G:71:GLU:HG2   | 2.20                     | 0.42              |
| 1:G:596:GLU:OE2  | 1:G:598:LEU:HB2  | 2.20                     | 0.42              |
| 1:H:215:CYS:HB2  | 1:H:253:TRP:HE3  | 1.85                     | 0.42              |
| 1:H:502:THR:O    | 1:H:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:I:436:GLN:HG3  | 1:P:461:ILE:HD12 | 2.02                     | 0.42              |
| 1:I:494:LEU:HD12 | 1:I:494:LEU:HA   | 1.79                     | 0.42              |
| 1:I:568:TYR:HE1  | 1:I:594:ASP:HB2  | 1.85                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:60:GLU:HA    | 1:J:63:ASP:OD2   | 2.20                     | 0.42              |
| 1:K:71:GLU:HA    | 1:K:74:GLN:CD    | 2.44                     | 0.42              |
| 1:K:167:VAL:O    | 1:K:171:LEU:HG   | 2.19                     | 0.42              |
| 1:K:168:ILE:H    | 1:K:168:ILE:HG13 | 1.64                     | 0.42              |
| 1:K:215:CYS:HB2  | 1:K:253:TRP:HE3  | 1.85                     | 0.42              |
| 1:K:241:VAL:O    | 1:K:245:MET:HG3  | 2.19                     | 0.42              |
| 1:K:502:THR:O    | 1:K:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:L:148:LEU:O    | 1:L:152:LEU:HG   | 2.20                     | 0.42              |
| 1:M:121:ARG:HA   | 1:M:125:GLY:HA2  | 2.02                     | 0.42              |
| 1:N:121:ARG:HA   | 1:N:125:GLY:HA2  | 2.02                     | 0.42              |
| 1:N:502:THR:O    | 1:N:506:VAL:HG22 | 2.20                     | 0.42              |
| 1:N:634:ASP:HB3  | 1:N:636:LYS:HE2  | 2.02                     | 0.42              |
| 1:N:672:MET:O    | 1:N:675:VAL:HG22 | 2.19                     | 0.42              |
| 1:O:67:ARG:O     | 1:O:71:GLU:HG2   | 2.20                     | 0.42              |
| 1:O:422:GLN:HA   | 1:O:427:SER:HB3  | 2.01                     | 0.42              |
| 1:O:564:VAL:HG22 | 1:O:616:ASN:HB2  | 2.01                     | 0.42              |
| 1:O:568:TYR:HE1  | 1:O:594:ASP:HB2  | 1.85                     | 0.42              |
| 1:O:593:ILE:HG23 | 1:O:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:P:165:LEU:HD12 | 1:P:166:GLY:N    | 2.35                     | 0.42              |
| 1:P:391:LYS:HD3  | 1:P:401:VAL:HG11 | 2.00                     | 0.42              |
| 1:P:593:ILE:HG23 | 1:P:595:VAL:HG22 | 2.00                     | 0.42              |
| 1:A:92:LEU:HB3   | 1:A:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:127:ASP:HB2  | 1:A:131:ARG:NH1  | 2.28                     | 0.41              |
| 1:B:121:ARG:HA   | 1:B:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:B:152:LEU:HD11 | 1:B:187:ILE:HG23 | 2.02                     | 0.41              |
| 1:C:564:VAL:HG22 | 1:C:616:ASN:HB2  | 2.01                     | 0.41              |
| 1:C:596:GLU:OE2  | 1:C:598:LEU:HB2  | 2.20                     | 0.41              |
| 1:D:564:VAL:HG22 | 1:D:616:ASN:HB2  | 2.01                     | 0.41              |
| 1:E:138:LEU:N    | 1:E:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:F:138:LEU:N    | 1:F:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:G:60:GLU:HA    | 1:G:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:G:148:LEU:O    | 1:G:152:LEU:HG   | 2.20                     | 0.41              |
| 1:G:261:LYS:N    | 1:G:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:G:494:LEU:HD12 | 1:G:494:LEU:HA   | 1.79                     | 0.41              |
| 1:H:111:GLU:HA   | 1:H:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:H:138:LEU:N    | 1:H:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:I:215:CYS:HB2  | 1:I:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:J:148:LEU:O    | 1:J:152:LEU:HG   | 2.20                     | 0.41              |
| 1:J:261:LYS:N    | 1:J:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:J:405:ILE:H    | 1:J:405:ILE:HG13 | 1.69                     | 0.41              |
| 1:K:152:LEU:HD11 | 1:K:187:ILE:HG23 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:165:LEU:HA   | 1:L:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:L:502:THR:O    | 1:L:506:VAL:HG22 | 2.20                     | 0.41              |
| 1:N:215:CYS:HB2  | 1:N:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:N:564:VAL:HG22 | 1:N:616:ASN:HB2  | 2.01                     | 0.41              |
| 1:N:596:GLU:OE2  | 1:N:598:LEU:HB2  | 2.20                     | 0.41              |
| 1:O:121:ARG:HA   | 1:O:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:P:138:LEU:N    | 1:P:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:A:165:LEU:HA   | 1:A:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:634:ASP:HB3  | 1:A:636:LYS:HE2  | 2.02                     | 0.41              |
| 1:C:121:ARG:HA   | 1:C:125:GLY:HA2  | 2.03                     | 0.41              |
| 1:C:215:CYS:HB2  | 1:C:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:C:406:LEU:O    | 1:C:412:TRP:NE1  | 2.52                     | 0.41              |
| 1:C:502:THR:O    | 1:C:506:VAL:HG22 | 2.20                     | 0.41              |
| 1:C:634:ASP:HB3  | 1:C:636:LYS:HE2  | 2.02                     | 0.41              |
| 1:E:173:LYS:H    | 1:E:173:LYS:HG3  | 1.66                     | 0.41              |
| 1:E:608:ILE:HG23 | 1:E:645:THR:HG21 | 2.02                     | 0.41              |
| 1:F:60:GLU:HA    | 1:F:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:F:331:VAL:N    | 1:F:332:PRO:HD2  | 2.34                     | 0.41              |
| 1:G:215:CYS:HB2  | 1:G:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:G:383:ASN:HB3  | 1:G:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:I:60:GLU:HA    | 1:I:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:I:331:VAL:N    | 1:I:332:PRO:HD2  | 2.35                     | 0.41              |
| 1:J:67:ARG:O     | 1:J:71:GLU:HG2   | 2.20                     | 0.41              |
| 1:J:148:LEU:HA   | 1:J:151:ILE:HG12 | 2.02                     | 0.41              |
| 1:J:215:CYS:HB2  | 1:J:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:K:259:PHE:HD2  | 1:L:578:SER:HB3  | 1.84                     | 0.41              |
| 1:L:634:ASP:HB3  | 1:L:636:LYS:HE2  | 2.02                     | 0.41              |
| 1:M:152:LEU:HD11 | 1:M:187:ILE:HG23 | 2.01                     | 0.41              |
| 1:N:71:GLU:HA    | 1:N:74:GLN:CD    | 2.44                     | 0.41              |
| 1:N:111:GLU:HA   | 1:N:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:O:331:VAL:N    | 1:O:332:PRO:HD2  | 2.34                     | 0.41              |
| 1:O:608:ILE:HG23 | 1:O:645:THR:HG21 | 2.02                     | 0.41              |
| 1:P:568:TYR:HE1  | 1:P:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:P:608:ILE:HG23 | 1:P:645:THR:HG21 | 2.02                     | 0.41              |
| 1:A:110:ARG:O    | 1:A:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:A:121:ARG:HA   | 1:A:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:A:148:LEU:HA   | 1:A:151:ILE:HG12 | 2.02                     | 0.41              |
| 1:A:540:THR:HG22 | 1:A:544:GLU:OE2  | 2.19                     | 0.41              |
| 1:B:241:VAL:O    | 1:B:245:MET:HG3  | 2.19                     | 0.41              |
| 1:D:67:ARG:O     | 1:D:71:GLU:HG2   | 2.20                     | 0.41              |
| 1:D:608:ILE:HG23 | 1:D:645:THR:HG21 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:121:ARG:HA   | 1:E:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:E:168:ILE:H    | 1:E:168:ILE:HG13 | 1.64                     | 0.41              |
| 1:E:568:TYR:HE1  | 1:E:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:G:79:LEU:HD22  | 1:G:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:H:92:LEU:HB3   | 1:H:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:H:383:ASN:HB3  | 1:H:386:LYS:HB3  | 2.01                     | 0.41              |
| 1:H:461:ILE:H    | 1:H:461:ILE:HG13 | 1.63                     | 0.41              |
| 1:I:79:LEU:HD22  | 1:I:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:I:138:LEU:N    | 1:I:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:I:165:LEU:HA   | 1:I:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:I:261:LYS:N    | 1:I:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:I:406:LEU:O    | 1:I:412:TRP:NE1  | 2.52                     | 0.41              |
| 1:J:79:LEU:HD22  | 1:J:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:J:197:GLU:CD   | 1:K:383:ASN:HA   | 2.45                     | 0.41              |
| 1:J:383:ASN:HB3  | 1:J:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:K:92:LEU:HB3   | 1:K:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:K:111:GLU:HA   | 1:K:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:K:138:LEU:N    | 1:K:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:L:92:LEU:HB3   | 1:L:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:L:121:ARG:HA   | 1:L:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:L:148:LEU:HA   | 1:L:151:ILE:HG12 | 2.02                     | 0.41              |
| 1:L:203:VAL:HG21 | 1:L:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:M:110:ARG:O    | 1:M:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:M:422:GLN:HA   | 1:M:427:SER:HB3  | 2.01                     | 0.41              |
| 1:N:165:LEU:HA   | 1:N:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:N:338:ARG:HE   | 1:N:338:ARG:HB3  | 1.75                     | 0.41              |
| 1:O:406:LEU:HD23 | 1:O:406:LEU:HA   | 1.94                     | 0.41              |
| 1:O:561:THR:HA   | 1:O:562:PRO:HD3  | 1.89                     | 0.41              |
| 1:P:71:GLU:HA    | 1:P:74:GLN:CD    | 2.44                     | 0.41              |
| 1:P:215:CYS:HB2  | 1:P:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:A:203:VAL:HG21 | 1:A:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:241:VAL:O    | 1:A:245:MET:HG3  | 2.19                     | 0.41              |
| 1:C:92:LEU:HB3   | 1:C:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:C:111:GLU:HA   | 1:C:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:C:165:LEU:HA   | 1:C:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:C:464:LYS:HD3  | 1:D:442:LEU:CD2  | 2.50                     | 0.41              |
| 1:D:215:CYS:HB2  | 1:D:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:D:331:VAL:N    | 1:D:332:PRO:HD2  | 2.34                     | 0.41              |
| 1:E:71:GLU:HA    | 1:E:74:GLN:CD    | 2.44                     | 0.41              |
| 1:F:79:LEU:HD22  | 1:F:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:F:127:ASP:HB2  | 1:F:131:ARG:NH1  | 2.28                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:165:LEU:HA   | 1:F:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:F:261:LYS:N    | 1:F:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:G:148:LEU:HA   | 1:G:151:ILE:HG12 | 2.02                     | 0.41              |
| 1:G:406:LEU:O    | 1:G:412:TRP:NE1  | 2.52                     | 0.41              |
| 1:G:617:PHE:N    | 1:G:652:ASN:O    | 2.36                     | 0.41              |
| 1:H:60:GLU:HA    | 1:H:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:H:452:GLN:HB2  | 1:H:463:ARG:HD3  | 2.01                     | 0.41              |
| 1:H:669:PRO:HD2  | 1:H:672:MET:SD   | 2.61                     | 0.41              |
| 1:I:383:ASN:HB3  | 1:I:386:LYS:HB3  | 2.01                     | 0.41              |
| 1:J:458:LYS:HD3  | 1:J:458:LYS:HA   | 1.77                     | 0.41              |
| 1:K:235:LEU:HD21 | 1:K:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:K:458:LYS:HA   | 1:K:458:LYS:HD3  | 1.77                     | 0.41              |
| 1:L:110:ARG:O    | 1:L:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:L:111:GLU:HA   | 1:L:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:L:127:ASP:HB2  | 1:L:131:ARG:NH1  | 2.28                     | 0.41              |
| 1:L:167:VAL:O    | 1:L:171:LEU:HG   | 2.19                     | 0.41              |
| 1:L:241:VAL:O    | 1:L:245:MET:HG3  | 2.19                     | 0.41              |
| 1:L:540:THR:HG22 | 1:L:544:GLU:OE2  | 2.19                     | 0.41              |
| 1:M:92:LEU:HB3   | 1:M:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:M:148:LEU:O    | 1:M:152:LEU:HG   | 2.20                     | 0.41              |
| 1:M:241:VAL:O    | 1:M:245:MET:HG3  | 2.19                     | 0.41              |
| 1:N:79:LEU:HD22  | 1:N:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:N:92:LEU:HB3   | 1:N:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:N:406:LEU:O    | 1:N:412:TRP:NE1  | 2.52                     | 0.41              |
| 1:P:165:LEU:HA   | 1:P:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:P:634:ASP:HB3  | 1:P:636:LYS:HE2  | 2.02                     | 0.41              |
| 1:A:235:LEU:HD21 | 1:A:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:A:261:LYS:N    | 1:A:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:B:79:LEU:HD22  | 1:B:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:B:110:ARG:O    | 1:B:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:B:111:GLU:HA   | 1:B:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:B:148:LEU:O    | 1:B:152:LEU:HG   | 2.20                     | 0.41              |
| 1:B:167:VAL:O    | 1:B:171:LEU:HG   | 2.19                     | 0.41              |
| 1:B:683:TRP:HE1  | 1:B:685:HIS:CG   | 2.39                     | 0.41              |
| 1:E:60:GLU:HA    | 1:E:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:E:165:LEU:HA   | 1:E:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:E:215:CYS:HB2  | 1:E:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:E:406:LEU:HD23 | 1:E:406:LEU:HA   | 1.94                     | 0.41              |
| 1:F:383:ASN:HB3  | 1:F:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:F:608:ILE:HG23 | 1:F:645:THR:HG21 | 2.02                     | 0.41              |
| 1:G:165:LEU:HA   | 1:G:168:ILE:HD12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:683:TRP:HE1  | 1:G:685:HIS:CG   | 2.39                     | 0.41              |
| 1:H:127:ASP:HB2  | 1:H:131:ARG:NH1  | 2.28                     | 0.41              |
| 1:H:235:LEU:HD21 | 1:H:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:H:505:LEU:O    | 1:H:507:SER:N    | 2.54                     | 0.41              |
| 1:I:608:ILE:HG23 | 1:I:645:THR:HG21 | 2.02                     | 0.41              |
| 1:J:197:GLU:OE2  | 1:K:383:ASN:HA   | 2.21                     | 0.41              |
| 1:J:406:LEU:O    | 1:J:412:TRP:NE1  | 2.52                     | 0.41              |
| 1:J:568:TYR:HE1  | 1:J:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:J:683:TRP:HE1  | 1:J:685:HIS:CG   | 2.39                     | 0.41              |
| 1:K:383:ASN:HB3  | 1:K:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:K:505:LEU:O    | 1:K:507:SER:N    | 2.54                     | 0.41              |
| 1:K:669:PRO:HD2  | 1:K:672:MET:SD   | 2.61                     | 0.41              |
| 1:K:683:TRP:HE1  | 1:K:685:HIS:CG   | 2.39                     | 0.41              |
| 1:M:79:LEU:HD22  | 1:M:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:N:167:VAL:O    | 1:N:171:LEU:HG   | 2.19                     | 0.41              |
| 1:N:235:LEU:HD21 | 1:N:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:O:215:CYS:HB2  | 1:O:253:TRP:HE3  | 1.85                     | 0.41              |
| 1:P:60:GLU:HA    | 1:P:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:P:121:ARG:HA   | 1:P:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:P:152:LEU:HD11 | 1:P:187:ILE:HG23 | 2.01                     | 0.41              |
| 1:P:203:VAL:HG21 | 1:P:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:P:349:LEU:HD13 | 1:P:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:111:GLU:HA   | 1:A:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:A:167:VAL:O    | 1:A:171:LEU:HG   | 2.19                     | 0.41              |
| 1:B:153:VAL:HG22 | 1:B:154:ALA:H    | 1.86                     | 0.41              |
| 1:B:168:ILE:H    | 1:B:168:ILE:HG13 | 1.64                     | 0.41              |
| 1:B:422:GLN:HA   | 1:B:427:SER:HB3  | 2.01                     | 0.41              |
| 1:C:79:LEU:HD22  | 1:C:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:C:167:VAL:O    | 1:C:171:LEU:HG   | 2.19                     | 0.41              |
| 1:C:173:LYS:H    | 1:C:173:LYS:HG3  | 1.66                     | 0.41              |
| 1:C:235:LEU:HD21 | 1:C:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:C:406:LEU:HD23 | 1:C:406:LEU:HA   | 1.95                     | 0.41              |
| 1:D:356:LYS:HB3  | 1:D:361:LYS:O    | 2.21                     | 0.41              |
| 1:D:442:LEU:HD23 | 1:D:442:LEU:HA   | 1.92                     | 0.41              |
| 1:E:79:LEU:HD22  | 1:E:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:E:203:VAL:HG21 | 1:E:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:E:349:LEU:HD13 | 1:E:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:E:634:ASP:HB3  | 1:E:636:LYS:HE2  | 2.02                     | 0.41              |
| 1:F:349:LEU:HD13 | 1:F:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:F:634:ASP:HB3  | 1:F:636:LYS:HE2  | 2.02                     | 0.41              |
| 1:G:110:ARG:O    | 1:G:114:GLN:HG2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:203:VAL:HG21 | 1:G:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:G:568:TYR:HE1  | 1:G:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:H:110:ARG:O    | 1:H:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:H:121:ARG:HA   | 1:H:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:H:683:TRP:HE1  | 1:H:685:HIS:CG   | 2.39                     | 0.41              |
| 1:I:127:ASP:HB2  | 1:I:131:ARG:NH1  | 2.28                     | 0.41              |
| 1:I:349:LEU:HD13 | 1:I:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:I:634:ASP:HB3  | 1:I:636:LYS:HE2  | 2.02                     | 0.41              |
| 1:J:165:LEU:HA   | 1:J:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:J:203:VAL:HG21 | 1:J:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:K:60:GLU:HA    | 1:K:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:K:79:LEU:HD22  | 1:K:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:L:60:GLU:HA    | 1:L:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:L:235:LEU:HD21 | 1:L:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:L:261:LYS:N    | 1:L:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:L:285:ARG:HA   | 1:L:285:ARG:HD3  | 1.75                     | 0.41              |
| 1:L:349:LEU:HD13 | 1:L:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:L:505:LEU:O    | 1:L:507:SER:N    | 2.54                     | 0.41              |
| 1:M:111:GLU:HA   | 1:M:114:GLN:HG2  | 2.02                     | 0.41              |
| 1:M:235:LEU:HD21 | 1:M:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:M:683:TRP:HE1  | 1:M:685:HIS:CG   | 2.39                     | 0.41              |
| 1:N:152:LEU:HD11 | 1:N:187:ILE:HG23 | 2.02                     | 0.41              |
| 1:O:464:LYS:HE2  | 1:P:445:ARG:NH2  | 2.35                     | 0.41              |
| 1:P:79:LEU:HD22  | 1:P:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:P:596:GLU:OE2  | 1:P:598:LEU:HB2  | 2.20                     | 0.41              |
| 1:P:669:PRO:HD2  | 1:P:672:MET:SD   | 2.61                     | 0.41              |
| 1:A:349:LEU:HD13 | 1:A:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:449:GLU:O    | 1:A:453:THR:OG1  | 2.31                     | 0.41              |
| 1:A:505:LEU:O    | 1:A:507:SER:N    | 2.54                     | 0.41              |
| 1:B:92:LEU:HB3   | 1:B:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:B:235:LEU:HD21 | 1:B:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:B:277:LEU:HA   | 1:B:277:LEU:HD23 | 1.81                     | 0.41              |
| 1:B:349:LEU:HD13 | 1:B:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:669:PRO:HD2  | 1:B:672:MET:SD   | 2.61                     | 0.41              |
| 1:C:152:LEU:HD11 | 1:C:187:ILE:HG23 | 2.02                     | 0.41              |
| 1:C:203:VAL:HG21 | 1:C:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:C:460:GLY:O    | 1:C:464:LYS:N    | 2.30                     | 0.41              |
| 1:C:607:LEU:HD12 | 1:C:642:GLN:HE21 | 1.86                     | 0.41              |
| 1:C:608:ILE:HG23 | 1:C:645:THR:HG21 | 2.02                     | 0.41              |
| 1:C:683:TRP:HE1  | 1:C:685:HIS:CG   | 2.39                     | 0.41              |
| 1:E:152:LEU:HD11 | 1:E:187:ILE:HG23 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:356:LYS:HB3  | 1:E:361:LYS:O    | 2.21                     | 0.41              |
| 1:F:442:LEU:HD23 | 1:F:442:LEU:HA   | 1.93                     | 0.41              |
| 1:F:669:PRO:HD2  | 1:F:672:MET:SD   | 2.61                     | 0.41              |
| 1:G:502:THR:O    | 1:G:506:VAL:HG22 | 2.20                     | 0.41              |
| 1:I:356:LYS:HB3  | 1:I:361:LYS:O    | 2.21                     | 0.41              |
| 1:I:669:PRO:HD2  | 1:I:672:MET:SD   | 2.61                     | 0.41              |
| 1:J:110:ARG:O    | 1:J:114:GLN:HG2  | 2.21                     | 0.41              |
| 1:J:502:THR:O    | 1:J:506:VAL:HG22 | 2.20                     | 0.41              |
| 1:K:110:ARG:O    | 1:K:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:K:452:GLN:HB2  | 1:K:463:ARG:HD3  | 2.01                     | 0.41              |
| 1:M:153:VAL:HG22 | 1:M:154:ALA:H    | 1.86                     | 0.41              |
| 1:M:167:VAL:O    | 1:M:171:LEU:HG   | 2.19                     | 0.41              |
| 1:M:349:LEU:HD13 | 1:M:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:N:356:LYS:HB3  | 1:N:361:LYS:O    | 2.21                     | 0.41              |
| 1:O:356:LYS:HB3  | 1:O:361:LYS:O    | 2.21                     | 0.41              |
| 1:O:442:LEU:HD23 | 1:O:442:LEU:HA   | 1.92                     | 0.41              |
| 1:P:168:ILE:H    | 1:P:168:ILE:HG13 | 1.64                     | 0.41              |
| 1:P:228:LEU:HD23 | 1:P:228:LEU:HA   | 1.89                     | 0.41              |
| 1:P:356:LYS:HB3  | 1:P:361:LYS:O    | 2.21                     | 0.41              |
| 1:A:60:GLU:HA    | 1:A:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:A:161:ALA:HA   | 1:A:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:B:383:ASN:HB3  | 1:B:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:B:568:TYR:HE1  | 1:B:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:C:67:ARG:O     | 1:C:71:GLU:HG2   | 2.20                     | 0.41              |
| 1:C:356:LYS:HB3  | 1:C:361:LYS:O    | 2.21                     | 0.41              |
| 1:D:138:LEU:N    | 1:D:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:D:153:VAL:HG22 | 1:D:154:ALA:H    | 1.86                     | 0.41              |
| 1:D:505:LEU:O    | 1:D:507:SER:N    | 2.54                     | 0.41              |
| 1:E:505:LEU:O    | 1:E:507:SER:N    | 2.54                     | 0.41              |
| 1:E:596:GLU:OE2  | 1:E:598:LEU:HB2  | 2.20                     | 0.41              |
| 1:E:669:PRO:HD2  | 1:E:672:MET:SD   | 2.61                     | 0.41              |
| 1:F:148:LEU:O    | 1:F:152:LEU:HG   | 2.20                     | 0.41              |
| 1:F:356:LYS:HB3  | 1:F:361:LYS:O    | 2.21                     | 0.41              |
| 1:F:683:TRP:HE1  | 1:F:685:HIS:CG   | 2.39                     | 0.41              |
| 1:G:92:LEU:HB3   | 1:G:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:G:356:LYS:HB3  | 1:G:361:LYS:O    | 2.21                     | 0.41              |
| 1:G:422:GLN:HA   | 1:G:427:SER:HB3  | 2.01                     | 0.41              |
| 1:G:505:LEU:O    | 1:G:507:SER:N    | 2.54                     | 0.41              |
| 1:H:79:LEU:HD22  | 1:H:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:H:161:ALA:HA   | 1:H:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:H:446:LEU:HD23 | 1:H:446:LEU:HA   | 1.92                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:442:LEU:HD23 | 1:I:442:LEU:HA   | 1.92                     | 0.41              |
| 1:J:92:LEU:HB3   | 1:J:147:LEU:HD11 | 2.01                     | 0.41              |
| 1:J:494:LEU:HA   | 1:J:494:LEU:HD12 | 1.79                     | 0.41              |
| 1:J:505:LEU:O    | 1:J:507:SER:N    | 2.54                     | 0.41              |
| 1:K:121:ARG:HA   | 1:K:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:K:127:ASP:HB2  | 1:K:131:ARG:NH1  | 2.28                     | 0.41              |
| 1:K:165:LEU:HA   | 1:K:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:L:383:ASN:HB3  | 1:L:386:LYS:HB3  | 2.01                     | 0.41              |
| 1:M:138:LEU:N    | 1:M:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:M:277:LEU:HA   | 1:M:277:LEU:HD23 | 1.81                     | 0.41              |
| 1:M:406:LEU:HD23 | 1:M:406:LEU:HA   | 1.94                     | 0.41              |
| 1:M:561:THR:HA   | 1:M:562:PRO:HD3  | 1.89                     | 0.41              |
| 1:M:669:PRO:HD2  | 1:M:672:MET:SD   | 2.61                     | 0.41              |
| 1:N:203:VAL:HG21 | 1:N:241:VAL:HG13 | 2.03                     | 0.41              |
| 1:N:608:ILE:HG23 | 1:N:645:THR:HG21 | 2.02                     | 0.41              |
| 1:N:683:TRP:HE1  | 1:N:685:HIS:CG   | 2.39                     | 0.41              |
| 1:O:138:LEU:N    | 1:O:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:O:505:LEU:O    | 1:O:507:SER:N    | 2.54                     | 0.41              |
| 1:O:607:LEU:HD12 | 1:O:642:GLN:HE21 | 1.86                     | 0.41              |
| 1:P:110:ARG:O    | 1:P:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:P:153:VAL:HG22 | 1:P:154:ALA:H    | 1.86                     | 0.41              |
| 1:P:173:LYS:H    | 1:P:173:LYS:HG3  | 1.66                     | 0.41              |
| 1:P:406:LEU:HD23 | 1:P:406:LEU:HA   | 1.95                     | 0.41              |
| 1:P:505:LEU:O    | 1:P:507:SER:N    | 2.54                     | 0.41              |
| 1:A:285:ARG:HA   | 1:A:285:ARG:HD3  | 1.75                     | 0.41              |
| 1:A:383:ASN:HB3  | 1:A:386:LYS:HB3  | 2.01                     | 0.41              |
| 1:A:596:GLU:OE2  | 1:A:598:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:608:ILE:HG23 | 1:A:645:THR:HG21 | 2.02                     | 0.41              |
| 1:B:138:LEU:N    | 1:B:141:ARG:HH21 | 2.18                     | 0.41              |
| 1:B:161:ALA:HA   | 1:B:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:B:285:ARG:HA   | 1:B:285:ARG:HD3  | 1.75                     | 0.41              |
| 1:B:505:LEU:O    | 1:B:507:SER:N    | 2.54                     | 0.41              |
| 1:B:607:LEU:HD12 | 1:B:642:GLN:HE21 | 1.86                     | 0.41              |
| 1:C:60:GLU:HA    | 1:C:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:C:338:ARG:HE   | 1:C:338:ARG:HB3  | 1.75                     | 0.41              |
| 1:D:110:ARG:O    | 1:D:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:D:205:ALA:C    | 1:D:207:GLY:H    | 2.29                     | 0.41              |
| 1:D:607:LEU:HD12 | 1:D:642:GLN:HE21 | 1.86                     | 0.41              |
| 1:E:110:ARG:O    | 1:E:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:E:153:VAL:HG22 | 1:E:154:ALA:H    | 1.86                     | 0.41              |
| 1:E:383:ASN:HB3  | 1:E:386:LYS:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:148:LEU:HA   | 1:F:151:ILE:HG12 | 2.02                     | 0.41              |
| 1:F:219:ASP:OD1  | 1:F:222:LEU:N    | 2.31                     | 0.41              |
| 1:F:505:LEU:O    | 1:F:507:SER:N    | 2.54                     | 0.41              |
| 1:G:121:ARG:HA   | 1:G:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:G:161:ALA:HA   | 1:G:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:G:235:LEU:HD21 | 1:G:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:G:349:LEU:HD13 | 1:G:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:G:576:LEU:HA   | 1:G:579:LEU:HG   | 2.03                     | 0.41              |
| 1:H:67:ARG:O     | 1:H:71:GLU:HG2   | 2.20                     | 0.41              |
| 1:H:165:LEU:HA   | 1:H:168:ILE:HD12 | 2.02                     | 0.41              |
| 1:H:631:GLN:N    | 1:H:669:PRO:HD3  | 2.36                     | 0.41              |
| 1:I:148:LEU:O    | 1:I:152:LEU:HG   | 2.20                     | 0.41              |
| 1:I:505:LEU:O    | 1:I:507:SER:N    | 2.54                     | 0.41              |
| 1:I:683:TRP:HE1  | 1:I:685:HIS:CG   | 2.39                     | 0.41              |
| 1:J:121:ARG:HA   | 1:J:125:GLY:HA2  | 2.03                     | 0.41              |
| 1:J:161:ALA:HA   | 1:J:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:J:235:LEU:HD21 | 1:J:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:J:338:ARG:HE   | 1:J:338:ARG:HB3  | 1.74                     | 0.41              |
| 1:J:349:LEU:HD13 | 1:J:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:J:356:LYS:HB3  | 1:J:361:LYS:O    | 2.21                     | 0.41              |
| 1:J:422:GLN:HA   | 1:J:427:SER:HB3  | 2.01                     | 0.41              |
| 1:K:67:ARG:O     | 1:K:71:GLU:HG2   | 2.20                     | 0.41              |
| 1:K:148:LEU:O    | 1:K:152:LEU:HG   | 2.20                     | 0.41              |
| 1:K:349:LEU:HD13 | 1:K:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:K:631:GLN:N    | 1:K:669:PRO:HD3  | 2.36                     | 0.41              |
| 1:L:161:ALA:HA   | 1:L:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:L:596:GLU:OE2  | 1:L:598:LEU:HB2  | 2.20                     | 0.41              |
| 1:L:608:ILE:HG23 | 1:L:645:THR:HG21 | 2.02                     | 0.41              |
| 1:M:161:ALA:HA   | 1:M:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:M:253:TRP:HE1  | 1:N:586:LEU:HD11 | 1.85                     | 0.41              |
| 1:M:383:ASN:HB3  | 1:M:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:M:568:TYR:HE1  | 1:M:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:M:607:LEU:HD12 | 1:M:642:GLN:HE21 | 1.86                     | 0.41              |
| 1:N:67:ARG:O     | 1:N:71:GLU:HG2   | 2.20                     | 0.41              |
| 1:N:110:ARG:O    | 1:N:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:N:182:ARG:HD2  | 1:N:221:ALA:HB3  | 2.03                     | 0.41              |
| 1:N:568:TYR:HE1  | 1:N:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:N:607:LEU:HD12 | 1:N:642:GLN:HE21 | 1.86                     | 0.41              |
| 1:O:182:ARG:HD2  | 1:O:221:ALA:HB3  | 2.03                     | 0.41              |
| 1:O:235:LEU:HD21 | 1:O:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:O:349:LEU:HD13 | 1:O:374:LEU:HD21 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:383:ASN:HB3  | 1:O:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:O:494:LEU:HD12 | 1:O:494:LEU:HA   | 1.79                     | 0.41              |
| 1:P:383:ASN:HB3  | 1:P:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:A:205:ALA:C    | 1:A:207:GLY:H    | 2.29                     | 0.41              |
| 1:A:669:PRO:HD2  | 1:A:672:MET:SD   | 2.61                     | 0.41              |
| 1:A:683:TRP:HE1  | 1:A:685:HIS:CG   | 2.39                     | 0.41              |
| 1:C:182:ARG:HD2  | 1:C:221:ALA:HB3  | 2.03                     | 0.41              |
| 1:C:205:ALA:C    | 1:C:207:GLY:H    | 2.29                     | 0.41              |
| 1:C:349:LEU:HD13 | 1:C:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:D:182:ARG:HD2  | 1:D:221:ALA:HB3  | 2.03                     | 0.41              |
| 1:D:235:LEU:HD21 | 1:D:329:ARG:HB3  | 2.03                     | 0.41              |
| 1:D:261:LYS:N    | 1:D:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:D:349:LEU:HD13 | 1:D:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:D:383:ASN:HB3  | 1:D:386:LYS:HB3  | 2.02                     | 0.41              |
| 1:D:561:THR:HA   | 1:D:562:PRO:HD3  | 1.89                     | 0.41              |
| 1:E:576:LEU:HA   | 1:E:579:LEU:HG   | 2.03                     | 0.41              |
| 1:F:121:ARG:HA   | 1:F:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:F:285:ARG:HH21 | 1:G:484:ARG:NH1  | 2.18                     | 0.41              |
| 1:F:420:TRP:CE2  | 1:F:473:LEU:HD22 | 2.56                     | 0.41              |
| 1:F:617:PHE:N    | 1:F:652:ASN:O    | 2.36                     | 0.41              |
| 1:G:153:VAL:HG12 | 1:G:156:ASN:HB2  | 2.03                     | 0.41              |
| 1:G:420:TRP:CE2  | 1:G:473:LEU:HD22 | 2.56                     | 0.41              |
| 1:G:458:LYS:HD3  | 1:G:458:LYS:HA   | 1.77                     | 0.41              |
| 1:H:153:VAL:HG22 | 1:H:154:ALA:H    | 1.86                     | 0.41              |
| 1:H:284:GLU:OE1  | 1:H:285:ARG:NH2  | 2.54                     | 0.41              |
| 1:H:349:LEU:HD13 | 1:H:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:H:568:TYR:HE1  | 1:H:594:ASP:HB2  | 1.85                     | 0.41              |
| 1:I:67:ARG:O     | 1:I:71:GLU:HG2   | 2.20                     | 0.41              |
| 1:I:121:ARG:HA   | 1:I:125:GLY:HA2  | 2.02                     | 0.41              |
| 1:I:148:LEU:HA   | 1:I:151:ILE:HG12 | 2.02                     | 0.41              |
| 1:I:161:ALA:HA   | 1:I:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:I:420:TRP:CE2  | 1:I:473:LEU:HD22 | 2.56                     | 0.41              |
| 1:I:491:LEU:HD23 | 1:I:491:LEU:HA   | 1.83                     | 0.41              |
| 1:J:420:TRP:CE2  | 1:J:473:LEU:HD22 | 2.56                     | 0.41              |
| 1:K:161:ALA:HA   | 1:K:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:K:284:GLU:OE1  | 1:K:285:ARG:NH2  | 2.54                     | 0.41              |
| 1:L:205:ALA:C    | 1:L:207:GLY:H    | 2.29                     | 0.41              |
| 1:L:420:TRP:CE2  | 1:L:473:LEU:HD22 | 2.56                     | 0.41              |
| 1:L:669:PRO:HD2  | 1:L:672:MET:SD   | 2.61                     | 0.41              |
| 1:M:261:LYS:N    | 1:M:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:M:505:LEU:O    | 1:M:507:SER:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:60:GLU:HA    | 1:N:63:ASP:OD2   | 2.20                     | 0.41              |
| 1:N:349:LEU:HD13 | 1:N:374:LEU:HD21 | 2.03                     | 0.41              |
| 1:N:406:LEU:HD23 | 1:N:406:LEU:HA   | 1.94                     | 0.41              |
| 1:N:515:LEU:HD12 | 1:N:515:LEU:HA   | 1.84                     | 0.41              |
| 1:O:110:ARG:O    | 1:O:114:GLN:HG2  | 2.20                     | 0.41              |
| 1:O:153:VAL:HG22 | 1:O:154:ALA:H    | 1.86                     | 0.41              |
| 1:O:205:ALA:C    | 1:O:207:GLY:H    | 2.29                     | 0.41              |
| 1:P:261:LYS:N    | 1:P:262:GLU:OE1  | 2.53                     | 0.41              |
| 1:P:576:LEU:HA   | 1:P:579:LEU:HG   | 2.03                     | 0.41              |
| 1:A:414:GLU:CD   | 1:A:437:GLN:HA   | 2.47                     | 0.40              |
| 1:A:420:TRP:CE2  | 1:A:473:LEU:HD22 | 2.56                     | 0.40              |
| 1:B:182:ARG:HD2  | 1:B:221:ALA:HB3  | 2.03                     | 0.40              |
| 1:B:261:LYS:N    | 1:B:262:GLU:OE1  | 2.53                     | 0.40              |
| 1:B:608:ILE:HG23 | 1:B:645:THR:HG21 | 2.02                     | 0.40              |
| 1:B:692:ILE:HD13 | 1:B:692:ILE:HA   | 1.90                     | 0.40              |
| 1:C:110:ARG:O    | 1:C:114:GLN:HG2  | 2.20                     | 0.40              |
| 1:C:339:LEU:HA   | 1:C:342:GLN:OE1  | 2.22                     | 0.40              |
| 1:C:568:TYR:HE1  | 1:C:594:ASP:HB2  | 1.85                     | 0.40              |
| 1:D:165:LEU:HA   | 1:D:168:ILE:HD12 | 2.02                     | 0.40              |
| 1:D:631:GLN:N    | 1:D:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:D:634:ASP:HB3  | 1:D:636:LYS:HE2  | 2.02                     | 0.40              |
| 1:D:669:PRO:HD2  | 1:D:672:MET:SD   | 2.61                     | 0.40              |
| 1:E:235:LEU:HD21 | 1:E:329:ARG:HB3  | 2.03                     | 0.40              |
| 1:E:261:LYS:N    | 1:E:262:GLU:OE1  | 2.53                     | 0.40              |
| 1:E:442:LEU:HD23 | 1:E:442:LEU:HA   | 1.92                     | 0.40              |
| 1:F:235:LEU:HD21 | 1:F:329:ARG:HB3  | 2.03                     | 0.40              |
| 1:G:634:ASP:HB3  | 1:G:636:LYS:HE2  | 2.02                     | 0.40              |
| 1:G:669:PRO:HD2  | 1:G:672:MET:SD   | 2.61                     | 0.40              |
| 1:H:148:LEU:O    | 1:H:152:LEU:HG   | 2.20                     | 0.40              |
| 1:H:205:ALA:C    | 1:H:207:GLY:H    | 2.29                     | 0.40              |
| 1:H:458:LYS:HA   | 1:H:458:LYS:HD3  | 1.77                     | 0.40              |
| 1:J:258:ALA:HB1  | 1:J:271:CYS:SG   | 2.62                     | 0.40              |
| 1:J:284:GLU:OE1  | 1:J:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:J:561:THR:HA   | 1:J:562:PRO:HD3  | 1.89                     | 0.40              |
| 1:J:576:LEU:HA   | 1:J:579:LEU:HG   | 2.04                     | 0.40              |
| 1:J:669:PRO:HD2  | 1:J:672:MET:SD   | 2.61                     | 0.40              |
| 1:K:261:LYS:N    | 1:K:262:GLU:OE1  | 2.53                     | 0.40              |
| 1:K:414:GLU:CD   | 1:K:437:GLN:HA   | 2.47                     | 0.40              |
| 1:K:568:TYR:HE1  | 1:K:594:ASP:HB2  | 1.85                     | 0.40              |
| 1:L:414:GLU:CD   | 1:L:437:GLN:HA   | 2.47                     | 0.40              |
| 1:M:356:LYS:HB3  | 1:M:361:LYS:O    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:205:ALA:C    | 1:N:207:GLY:H    | 2.29                     | 0.40              |
| 1:N:617:PHE:N    | 1:N:652:ASN:O    | 2.36                     | 0.40              |
| 1:O:165:LEU:HA   | 1:O:168:ILE:HD12 | 2.02                     | 0.40              |
| 1:O:261:LYS:N    | 1:O:262:GLU:OE1  | 2.53                     | 0.40              |
| 1:O:631:GLN:N    | 1:O:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:O:634:ASP:HB3  | 1:O:636:LYS:HE2  | 2.02                     | 0.40              |
| 1:O:669:PRO:HD2  | 1:O:672:MET:SD   | 2.61                     | 0.40              |
| 1:P:569:ARG:HE   | 1:P:625:ALA:HA   | 1.86                     | 0.40              |
| 1:A:67:ARG:O     | 1:A:71:GLU:HG2   | 2.20                     | 0.40              |
| 1:A:138:LEU:N    | 1:A:141:ARG:HH21 | 2.18                     | 0.40              |
| 1:A:568:TYR:HE1  | 1:A:594:ASP:HB2  | 1.85                     | 0.40              |
| 1:B:460:GLY:O    | 1:B:464:LYS:N    | 2.30                     | 0.40              |
| 1:C:148:LEU:O    | 1:C:152:LEU:HG   | 2.20                     | 0.40              |
| 1:C:494:LEU:HA   | 1:C:494:LEU:HD12 | 1.79                     | 0.40              |
| 1:C:617:PHE:N    | 1:C:652:ASN:O    | 2.36                     | 0.40              |
| 1:C:669:PRO:HD2  | 1:C:672:MET:SD   | 2.61                     | 0.40              |
| 1:D:79:LEU:HD22  | 1:D:92:LEU:HD23  | 2.02                     | 0.40              |
| 1:D:148:LEU:O    | 1:D:152:LEU:HG   | 2.20                     | 0.40              |
| 1:D:284:GLU:OE1  | 1:D:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:D:420:TRP:CE2  | 1:D:473:LEU:HD22 | 2.56                     | 0.40              |
| 1:D:497:ARG:NH2  | 1:E:509:GLY:H    | 2.18                     | 0.40              |
| 1:E:228:LEU:HD23 | 1:E:228:LEU:HA   | 1.89                     | 0.40              |
| 1:E:569:ARG:HE   | 1:E:625:ALA:HA   | 1.86                     | 0.40              |
| 1:F:67:ARG:O     | 1:F:71:GLU:HG2   | 2.20                     | 0.40              |
| 1:F:161:ALA:HA   | 1:F:165:LEU:HD23 | 2.03                     | 0.40              |
| 1:F:203:VAL:HG21 | 1:F:241:VAL:HG13 | 2.03                     | 0.40              |
| 1:G:205:ALA:C    | 1:G:207:GLY:H    | 2.29                     | 0.40              |
| 1:G:258:ALA:HB1  | 1:G:271:CYS:SG   | 2.62                     | 0.40              |
| 1:G:582:VAL:O    | 1:G:586:LEU:HG   | 2.21                     | 0.40              |
| 1:G:608:ILE:HG23 | 1:G:645:THR:HG21 | 2.02                     | 0.40              |
| 1:H:420:TRP:CE2  | 1:H:473:LEU:HD22 | 2.56                     | 0.40              |
| 1:H:634:ASP:HB3  | 1:H:636:LYS:HE2  | 2.02                     | 0.40              |
| 1:I:203:VAL:HG21 | 1:I:241:VAL:HG13 | 2.03                     | 0.40              |
| 1:I:487:LEU:HD23 | 1:I:487:LEU:HA   | 1.82                     | 0.40              |
| 1:J:153:VAL:HG12 | 1:J:156:ASN:HB2  | 2.04                     | 0.40              |
| 1:J:205:ALA:C    | 1:J:207:GLY:H    | 2.29                     | 0.40              |
| 1:J:634:ASP:HB3  | 1:J:636:LYS:HE2  | 2.02                     | 0.40              |
| 1:K:205:ALA:C    | 1:K:207:GLY:H    | 2.29                     | 0.40              |
| 1:K:420:TRP:CE2  | 1:K:473:LEU:HD22 | 2.56                     | 0.40              |
| 1:L:280:ASN:OD1  | 1:L:280:ASN:C    | 2.65                     | 0.40              |
| 1:L:683:TRP:HE1  | 1:L:685:HIS:CG   | 2.39                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:168:ILE:H    | 1:M:168:ILE:HG13 | 1.64                     | 0.40              |
| 1:N:284:GLU:OE1  | 1:N:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:N:339:LEU:HA   | 1:N:342:GLN:OE1  | 2.22                     | 0.40              |
| 1:N:669:PRO:HD2  | 1:N:672:MET:SD   | 2.61                     | 0.40              |
| 1:O:148:LEU:O    | 1:O:152:LEU:HG   | 2.20                     | 0.40              |
| 1:O:339:LEU:HA   | 1:O:342:GLN:OE1  | 2.22                     | 0.40              |
| 1:O:420:TRP:CE2  | 1:O:473:LEU:HD22 | 2.56                     | 0.40              |
| 1:P:235:LEU:HD21 | 1:P:329:ARG:HB3  | 2.03                     | 0.40              |
| 1:P:414:GLU:CD   | 1:P:437:GLN:HA   | 2.47                     | 0.40              |
| 1:A:79:LEU:HD22  | 1:A:92:LEU:HD23  | 2.02                     | 0.40              |
| 1:A:280:ASN:OD1  | 1:A:280:ASN:C    | 2.65                     | 0.40              |
| 1:A:631:GLN:N    | 1:A:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:B:284:GLU:OE1  | 1:B:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:B:356:LYS:HB3  | 1:B:361:LYS:O    | 2.21                     | 0.40              |
| 1:B:414:GLU:CD   | 1:B:437:GLN:HA   | 2.47                     | 0.40              |
| 1:C:261:LYS:N    | 1:C:262:GLU:OE1  | 2.53                     | 0.40              |
| 1:C:284:GLU:OE1  | 1:C:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:D:339:LEU:HA   | 1:D:342:GLN:OE1  | 2.22                     | 0.40              |
| 1:E:205:ALA:C    | 1:E:207:GLY:H    | 2.29                     | 0.40              |
| 1:E:414:GLU:CD   | 1:E:437:GLN:HA   | 2.47                     | 0.40              |
| 1:F:153:VAL:HG22 | 1:F:154:ALA:H    | 1.86                     | 0.40              |
| 1:F:286:GLU:CD   | 1:F:289:ARG:HH22 | 2.29                     | 0.40              |
| 1:G:284:GLU:OE1  | 1:G:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:H:258:ALA:HB1  | 1:H:271:CYS:SG   | 2.62                     | 0.40              |
| 1:H:280:ASN:OD1  | 1:H:280:ASN:C    | 2.65                     | 0.40              |
| 1:H:356:LYS:HB3  | 1:H:361:LYS:O    | 2.21                     | 0.40              |
| 1:H:607:LEU:HD12 | 1:H:642:GLN:HE21 | 1.86                     | 0.40              |
| 1:I:173:LYS:H    | 1:I:173:LYS:HG3  | 1.66                     | 0.40              |
| 1:I:219:ASP:OD1  | 1:I:222:LEU:N    | 2.31                     | 0.40              |
| 1:I:286:GLU:CD   | 1:I:289:ARG:HH22 | 2.29                     | 0.40              |
| 1:I:502:THR:O    | 1:I:506:VAL:HG22 | 2.20                     | 0.40              |
| 1:J:582:VAL:O    | 1:J:586:LEU:HG   | 2.22                     | 0.40              |
| 1:K:258:ALA:HB1  | 1:K:271:CYS:SG   | 2.62                     | 0.40              |
| 1:K:280:ASN:OD1  | 1:K:280:ASN:C    | 2.65                     | 0.40              |
| 1:K:607:LEU:HD12 | 1:K:642:GLN:HE21 | 1.86                     | 0.40              |
| 1:L:67:ARG:O     | 1:L:71:GLU:HG2   | 2.20                     | 0.40              |
| 1:L:79:LEU:HD22  | 1:L:92:LEU:HD23  | 2.02                     | 0.40              |
| 1:L:491:LEU:HD23 | 1:L:491:LEU:HA   | 1.83                     | 0.40              |
| 1:L:568:TYR:HE1  | 1:L:594:ASP:HB2  | 1.85                     | 0.40              |
| 1:L:631:GLN:N    | 1:L:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:M:256:PRO:CG   | 1:N:582:VAL:HG21 | 2.49                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:284:GLU:OE1  | 1:M:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:M:608:ILE:HG23 | 1:M:645:THR:HG21 | 2.02                     | 0.40              |
| 1:N:148:LEU:O    | 1:N:152:LEU:HG   | 2.20                     | 0.40              |
| 1:N:161:ALA:HA   | 1:N:165:LEU:HD23 | 2.03                     | 0.40              |
| 1:N:460:GLY:O    | 1:N:464:LYS:N    | 2.30                     | 0.40              |
| 1:O:79:LEU:HD22  | 1:O:92:LEU:HD23  | 2.02                     | 0.40              |
| 1:O:148:LEU:HA   | 1:O:151:ILE:HG12 | 2.02                     | 0.40              |
| 1:A:182:ARG:HD2  | 1:A:221:ALA:HB3  | 2.03                     | 0.40              |
| 1:A:284:GLU:OE1  | 1:A:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:A:498:PHE:HD1  | 1:A:498:PHE:HA   | 1.76                     | 0.40              |
| 1:A:662:TRP:CZ3  | 1:A:676:LEU:HA   | 2.57                     | 0.40              |
| 1:B:497:ARG:O    | 1:B:500:GLN:NE2  | 2.52                     | 0.40              |
| 1:C:161:ALA:HA   | 1:C:165:LEU:HD23 | 2.03                     | 0.40              |
| 1:E:284:GLU:OE1  | 1:E:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:E:607:LEU:HD12 | 1:E:642:GLN:HE21 | 1.86                     | 0.40              |
| 1:E:631:GLN:N    | 1:E:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:F:173:LYS:H    | 1:F:173:LYS:HG3  | 1.66                     | 0.40              |
| 1:F:487:LEU:HD23 | 1:F:487:LEU:HA   | 1.82                     | 0.40              |
| 1:F:491:LEU:HD23 | 1:F:491:LEU:HA   | 1.83                     | 0.40              |
| 1:F:502:THR:O    | 1:F:506:VAL:HG22 | 2.20                     | 0.40              |
| 1:G:153:VAL:HG22 | 1:G:154:ALA:H    | 1.86                     | 0.40              |
| 1:G:414:GLU:CD   | 1:G:437:GLN:HA   | 2.47                     | 0.40              |
| 1:H:148:LEU:HA   | 1:H:151:ILE:HG12 | 2.02                     | 0.40              |
| 1:H:261:LYS:N    | 1:H:262:GLU:OE1  | 2.53                     | 0.40              |
| 1:H:286:GLU:CD   | 1:H:289:ARG:HH22 | 2.29                     | 0.40              |
| 1:H:414:GLU:CD   | 1:H:437:GLN:HA   | 2.47                     | 0.40              |
| 1:I:110:ARG:O    | 1:I:114:GLN:HG2  | 2.20                     | 0.40              |
| 1:I:153:VAL:HG22 | 1:I:154:ALA:H    | 1.86                     | 0.40              |
| 1:I:235:LEU:HD21 | 1:I:329:ARG:HB3  | 2.03                     | 0.40              |
| 1:J:153:VAL:HG22 | 1:J:154:ALA:H    | 1.86                     | 0.40              |
| 1:K:153:VAL:HG12 | 1:K:156:ASN:HB2  | 2.04                     | 0.40              |
| 1:K:153:VAL:HG22 | 1:K:154:ALA:H    | 1.86                     | 0.40              |
| 1:K:356:LYS:HB3  | 1:K:361:LYS:O    | 2.21                     | 0.40              |
| 1:L:284:GLU:OE1  | 1:L:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:M:182:ARG:HD2  | 1:M:221:ALA:HB3  | 2.03                     | 0.40              |
| 1:M:414:GLU:CD   | 1:M:437:GLN:HA   | 2.47                     | 0.40              |
| 1:N:148:LEU:HA   | 1:N:151:ILE:HG12 | 2.02                     | 0.40              |
| 1:O:284:GLU:OE1  | 1:O:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:O:520:GLU:OE2  | 1:O:535:ARG:NH1  | 2.55                     | 0.40              |
| 1:P:148:LEU:HA   | 1:P:151:ILE:HG12 | 2.02                     | 0.40              |
| 1:P:205:ALA:C    | 1:P:207:GLY:H    | 2.29                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:442:LEU:HD23 | 1:P:442:LEU:HA   | 1.93                     | 0.40              |
| 1:A:153:VAL:HG12 | 1:A:156:ASN:HB2  | 2.04                     | 0.40              |
| 1:A:395:ARG:C    | 1:A:398:GLY:H    | 2.30                     | 0.40              |
| 1:B:239:GLN:HG3  | 1:C:480:SER:HB2  | 2.02                     | 0.40              |
| 1:B:280:ASN:OD1  | 1:B:280:ASN:C    | 2.65                     | 0.40              |
| 1:B:339:LEU:HA   | 1:B:342:GLN:OE1  | 2.21                     | 0.40              |
| 1:B:561:THR:HA   | 1:B:562:PRO:HD3  | 1.89                     | 0.40              |
| 1:C:631:GLN:N    | 1:C:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:D:414:GLU:CD   | 1:D:437:GLN:HA   | 2.47                     | 0.40              |
| 1:D:520:GLU:OE2  | 1:D:535:ARG:NH1  | 2.55                     | 0.40              |
| 1:E:662:TRP:CZ3  | 1:E:676:LEU:HA   | 2.57                     | 0.40              |
| 1:E:683:TRP:HE1  | 1:E:685:HIS:CG   | 2.39                     | 0.40              |
| 1:F:110:ARG:O    | 1:F:114:GLN:HG2  | 2.20                     | 0.40              |
| 1:F:664:GLU:CD   | 1:F:664:GLU:H    | 2.30                     | 0.40              |
| 1:G:88:VAL:HG23  | 1:G:89:GLY:N     | 2.37                     | 0.40              |
| 1:G:338:ARG:HE   | 1:G:338:ARG:HB3  | 1.74                     | 0.40              |
| 1:G:662:TRP:CZ3  | 1:G:676:LEU:HA   | 2.57                     | 0.40              |
| 1:I:607:LEU:HD12 | 1:I:642:GLN:HE21 | 1.86                     | 0.40              |
| 1:I:664:GLU:CD   | 1:I:664:GLU:H    | 2.30                     | 0.40              |
| 1:J:520:GLU:OE2  | 1:J:535:ARG:NH1  | 2.55                     | 0.40              |
| 1:J:608:ILE:HG23 | 1:J:645:THR:HG21 | 2.02                     | 0.40              |
| 1:K:286:GLU:CD   | 1:K:289:ARG:HH22 | 2.30                     | 0.40              |
| 1:K:634:ASP:HB3  | 1:K:636:LYS:HE2  | 2.02                     | 0.40              |
| 1:L:153:VAL:HG12 | 1:L:156:ASN:HB2  | 2.03                     | 0.40              |
| 1:L:182:ARG:HD2  | 1:L:221:ALA:HB3  | 2.03                     | 0.40              |
| 1:L:395:ARG:C    | 1:L:398:GLY:H    | 2.30                     | 0.40              |
| 1:L:607:LEU:HD12 | 1:L:642:GLN:HE21 | 1.86                     | 0.40              |
| 1:L:662:TRP:CZ3  | 1:L:676:LEU:HA   | 2.57                     | 0.40              |
| 1:M:497:ARG:O    | 1:M:500:GLN:NE2  | 2.52                     | 0.40              |
| 1:M:520:GLU:OE2  | 1:M:535:ARG:NH1  | 2.55                     | 0.40              |
| 1:M:523:LEU:HD23 | 1:M:523:LEU:HA   | 1.81                     | 0.40              |
| 1:M:692:ILE:HD13 | 1:M:692:ILE:HA   | 1.90                     | 0.40              |
| 1:N:261:LYS:N    | 1:N:262:GLU:OE1  | 2.53                     | 0.40              |
| 1:N:631:GLN:N    | 1:N:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:O:414:GLU:CD   | 1:O:437:GLN:HA   | 2.46                     | 0.40              |
| 1:P:284:GLU:OE1  | 1:P:285:ARG:NH2  | 2.54                     | 0.40              |
| 1:P:631:GLN:N    | 1:P:669:PRO:HD3  | 2.36                     | 0.40              |
| 1:P:662:TRP:CZ3  | 1:P:676:LEU:HA   | 2.57                     | 0.40              |
| 1:P:683:TRP:HE1  | 1:P:685:HIS:CG   | 2.39                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 1   | A     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | B     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | C     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | D     | 625/726 (86%)     | 563 (90%)  | 62 (10%)   | 0        | 100         | 100 |
| 1   | E     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | F     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | G     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | H     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | I     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | J     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | K     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | L     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | M     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | N     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | O     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| 1   | P     | 625/726 (86%)     | 562 (90%)  | 63 (10%)   | 0        | 100         | 100 |
| All | All   | 10000/11616 (86%) | 8993 (90%) | 1007 (10%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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



| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | B     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | C     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | D     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | E     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | F     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | G     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | H     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | I     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | J     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | K     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | L     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | M     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | N     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | O     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| 1   | P     | 525/594 (88%)   | 516 (98%)  | 9 (2%)   | 53          | 68 |
| All | All   | 8400/9504 (88%) | 8256 (98%) | 144 (2%) | 52          | 68 |

All (144) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 123 | ASP  |
| 1   | A     | 313 | VAL  |
| 1   | A     | 325 | ASP  |
| 1   | A     | 381 | SER  |
| 1   | A     | 594 | ASP  |
| 1   | A     | 607 | LEU  |
| 1   | A     | 627 | ASP  |
| 1   | A     | 667 | VAL  |
| 1   | A     | 684 | SER  |
| 1   | B     | 123 | ASP  |
| 1   | B     | 313 | VAL  |
| 1   | B     | 325 | ASP  |
| 1   | B     | 381 | SER  |
| 1   | B     | 594 | ASP  |
| 1   | B     | 607 | LEU  |
| 1   | B     | 627 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 667 | VAL  |
| 1   | B     | 684 | SER  |
| 1   | C     | 123 | ASP  |
| 1   | C     | 313 | VAL  |
| 1   | C     | 325 | ASP  |
| 1   | C     | 381 | SER  |
| 1   | C     | 594 | ASP  |
| 1   | C     | 607 | LEU  |
| 1   | C     | 627 | ASP  |
| 1   | C     | 667 | VAL  |
| 1   | C     | 684 | SER  |
| 1   | D     | 123 | ASP  |
| 1   | D     | 313 | VAL  |
| 1   | D     | 325 | ASP  |
| 1   | D     | 381 | SER  |
| 1   | D     | 594 | ASP  |
| 1   | D     | 607 | LEU  |
| 1   | D     | 627 | ASP  |
| 1   | D     | 667 | VAL  |
| 1   | D     | 684 | SER  |
| 1   | E     | 123 | ASP  |
| 1   | E     | 313 | VAL  |
| 1   | E     | 325 | ASP  |
| 1   | E     | 381 | SER  |
| 1   | E     | 594 | ASP  |
| 1   | E     | 607 | LEU  |
| 1   | E     | 627 | ASP  |
| 1   | E     | 667 | VAL  |
| 1   | E     | 684 | SER  |
| 1   | F     | 123 | ASP  |
| 1   | F     | 313 | VAL  |
| 1   | F     | 325 | ASP  |
| 1   | F     | 381 | SER  |
| 1   | F     | 594 | ASP  |
| 1   | F     | 607 | LEU  |
| 1   | F     | 627 | ASP  |
| 1   | F     | 667 | VAL  |
| 1   | F     | 684 | SER  |
| 1   | G     | 123 | ASP  |
| 1   | G     | 313 | VAL  |
| 1   | G     | 325 | ASP  |
| 1   | G     | 381 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 594 | ASP  |
| 1   | G     | 607 | LEU  |
| 1   | G     | 627 | ASP  |
| 1   | G     | 667 | VAL  |
| 1   | G     | 684 | SER  |
| 1   | H     | 123 | ASP  |
| 1   | H     | 313 | VAL  |
| 1   | H     | 325 | ASP  |
| 1   | H     | 381 | SER  |
| 1   | H     | 594 | ASP  |
| 1   | H     | 607 | LEU  |
| 1   | H     | 627 | ASP  |
| 1   | H     | 667 | VAL  |
| 1   | H     | 684 | SER  |
| 1   | I     | 123 | ASP  |
| 1   | I     | 313 | VAL  |
| 1   | I     | 325 | ASP  |
| 1   | I     | 381 | SER  |
| 1   | I     | 594 | ASP  |
| 1   | I     | 607 | LEU  |
| 1   | I     | 627 | ASP  |
| 1   | I     | 667 | VAL  |
| 1   | I     | 684 | SER  |
| 1   | J     | 123 | ASP  |
| 1   | J     | 313 | VAL  |
| 1   | J     | 325 | ASP  |
| 1   | J     | 381 | SER  |
| 1   | J     | 594 | ASP  |
| 1   | J     | 607 | LEU  |
| 1   | J     | 627 | ASP  |
| 1   | J     | 667 | VAL  |
| 1   | J     | 684 | SER  |
| 1   | K     | 123 | ASP  |
| 1   | K     | 313 | VAL  |
| 1   | K     | 325 | ASP  |
| 1   | K     | 381 | SER  |
| 1   | K     | 594 | ASP  |
| 1   | K     | 607 | LEU  |
| 1   | K     | 627 | ASP  |
| 1   | K     | 667 | VAL  |
| 1   | K     | 684 | SER  |
| 1   | L     | 123 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 313 | VAL  |
| 1   | L     | 325 | ASP  |
| 1   | L     | 381 | SER  |
| 1   | L     | 594 | ASP  |
| 1   | L     | 607 | LEU  |
| 1   | L     | 627 | ASP  |
| 1   | L     | 667 | VAL  |
| 1   | L     | 684 | SER  |
| 1   | M     | 123 | ASP  |
| 1   | M     | 313 | VAL  |
| 1   | M     | 325 | ASP  |
| 1   | M     | 381 | SER  |
| 1   | M     | 594 | ASP  |
| 1   | M     | 607 | LEU  |
| 1   | M     | 627 | ASP  |
| 1   | M     | 667 | VAL  |
| 1   | M     | 684 | SER  |
| 1   | N     | 123 | ASP  |
| 1   | N     | 313 | VAL  |
| 1   | N     | 325 | ASP  |
| 1   | N     | 381 | SER  |
| 1   | N     | 594 | ASP  |
| 1   | N     | 607 | LEU  |
| 1   | N     | 627 | ASP  |
| 1   | N     | 667 | VAL  |
| 1   | N     | 684 | SER  |
| 1   | O     | 123 | ASP  |
| 1   | O     | 313 | VAL  |
| 1   | O     | 325 | ASP  |
| 1   | O     | 381 | SER  |
| 1   | O     | 594 | ASP  |
| 1   | O     | 607 | LEU  |
| 1   | O     | 627 | ASP  |
| 1   | O     | 667 | VAL  |
| 1   | O     | 684 | SER  |
| 1   | P     | 123 | ASP  |
| 1   | P     | 313 | VAL  |
| 1   | P     | 325 | ASP  |
| 1   | P     | 381 | SER  |
| 1   | P     | 594 | ASP  |
| 1   | P     | 607 | LEU  |
| 1   | P     | 627 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 667 | VAL  |
| 1   | P     | 684 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 114 | GLN  |
| 1   | A     | 150 | GLN  |
| 1   | A     | 232 | ASN  |
| 1   | A     | 422 | GLN  |
| 1   | A     | 534 | HIS  |
| 1   | A     | 547 | HIS  |
| 1   | A     | 642 | GLN  |
| 1   | B     | 114 | GLN  |
| 1   | B     | 232 | ASN  |
| 1   | B     | 337 | ASN  |
| 1   | B     | 422 | GLN  |
| 1   | B     | 436 | GLN  |
| 1   | B     | 534 | HIS  |
| 1   | B     | 547 | HIS  |
| 1   | B     | 587 | HIS  |
| 1   | B     | 642 | GLN  |
| 1   | C     | 114 | GLN  |
| 1   | C     | 150 | GLN  |
| 1   | C     | 232 | ASN  |
| 1   | C     | 337 | ASN  |
| 1   | C     | 422 | GLN  |
| 1   | C     | 436 | GLN  |
| 1   | C     | 534 | HIS  |
| 1   | C     | 547 | HIS  |
| 1   | C     | 587 | HIS  |
| 1   | C     | 642 | GLN  |
| 1   | D     | 114 | GLN  |
| 1   | D     | 232 | ASN  |
| 1   | D     | 337 | ASN  |
| 1   | D     | 422 | GLN  |
| 1   | D     | 436 | GLN  |
| 1   | D     | 534 | HIS  |
| 1   | D     | 547 | HIS  |
| 1   | D     | 587 | HIS  |
| 1   | D     | 642 | GLN  |
| 1   | E     | 114 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 150 | GLN  |
| 1   | E     | 232 | ASN  |
| 1   | E     | 328 | GLN  |
| 1   | E     | 337 | ASN  |
| 1   | E     | 422 | GLN  |
| 1   | E     | 436 | GLN  |
| 1   | E     | 534 | HIS  |
| 1   | E     | 547 | HIS  |
| 1   | E     | 587 | HIS  |
| 1   | E     | 642 | GLN  |
| 1   | F     | 114 | GLN  |
| 1   | F     | 150 | GLN  |
| 1   | F     | 232 | ASN  |
| 1   | F     | 422 | GLN  |
| 1   | F     | 436 | GLN  |
| 1   | F     | 534 | HIS  |
| 1   | F     | 547 | HIS  |
| 1   | F     | 587 | HIS  |
| 1   | F     | 642 | GLN  |
| 1   | G     | 114 | GLN  |
| 1   | G     | 150 | GLN  |
| 1   | G     | 232 | ASN  |
| 1   | G     | 337 | ASN  |
| 1   | G     | 422 | GLN  |
| 1   | G     | 436 | GLN  |
| 1   | G     | 534 | HIS  |
| 1   | G     | 547 | HIS  |
| 1   | G     | 587 | HIS  |
| 1   | G     | 642 | GLN  |
| 1   | H     | 114 | GLN  |
| 1   | H     | 150 | GLN  |
| 1   | H     | 232 | ASN  |
| 1   | H     | 236 | HIS  |
| 1   | H     | 337 | ASN  |
| 1   | H     | 422 | GLN  |
| 1   | H     | 436 | GLN  |
| 1   | H     | 534 | HIS  |
| 1   | H     | 547 | HIS  |
| 1   | H     | 587 | HIS  |
| 1   | H     | 642 | GLN  |
| 1   | I     | 114 | GLN  |
| 1   | I     | 150 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 232 | ASN  |
| 1   | I     | 422 | GLN  |
| 1   | I     | 534 | HIS  |
| 1   | I     | 547 | HIS  |
| 1   | I     | 587 | HIS  |
| 1   | I     | 642 | GLN  |
| 1   | J     | 114 | GLN  |
| 1   | J     | 150 | GLN  |
| 1   | J     | 232 | ASN  |
| 1   | J     | 236 | HIS  |
| 1   | J     | 337 | ASN  |
| 1   | J     | 422 | GLN  |
| 1   | J     | 436 | GLN  |
| 1   | J     | 534 | HIS  |
| 1   | J     | 547 | HIS  |
| 1   | J     | 587 | HIS  |
| 1   | J     | 642 | GLN  |
| 1   | K     | 114 | GLN  |
| 1   | K     | 232 | ASN  |
| 1   | K     | 236 | HIS  |
| 1   | K     | 337 | ASN  |
| 1   | K     | 422 | GLN  |
| 1   | K     | 436 | GLN  |
| 1   | K     | 534 | HIS  |
| 1   | K     | 547 | HIS  |
| 1   | K     | 587 | HIS  |
| 1   | K     | 642 | GLN  |
| 1   | L     | 114 | GLN  |
| 1   | L     | 150 | GLN  |
| 1   | L     | 232 | ASN  |
| 1   | L     | 337 | ASN  |
| 1   | L     | 422 | GLN  |
| 1   | L     | 436 | GLN  |
| 1   | L     | 534 | HIS  |
| 1   | L     | 547 | HIS  |
| 1   | L     | 642 | GLN  |
| 1   | M     | 114 | GLN  |
| 1   | M     | 150 | GLN  |
| 1   | M     | 156 | ASN  |
| 1   | M     | 232 | ASN  |
| 1   | M     | 422 | GLN  |
| 1   | M     | 534 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 547 | HIS  |
| 1   | M     | 587 | HIS  |
| 1   | M     | 642 | GLN  |
| 1   | N     | 114 | GLN  |
| 1   | N     | 150 | GLN  |
| 1   | N     | 232 | ASN  |
| 1   | N     | 337 | ASN  |
| 1   | N     | 422 | GLN  |
| 1   | N     | 436 | GLN  |
| 1   | N     | 534 | HIS  |
| 1   | N     | 547 | HIS  |
| 1   | N     | 587 | HIS  |
| 1   | N     | 642 | GLN  |
| 1   | O     | 114 | GLN  |
| 1   | O     | 232 | ASN  |
| 1   | O     | 337 | ASN  |
| 1   | O     | 422 | GLN  |
| 1   | O     | 436 | GLN  |
| 1   | O     | 534 | HIS  |
| 1   | O     | 547 | HIS  |
| 1   | O     | 587 | HIS  |
| 1   | O     | 642 | GLN  |
| 1   | P     | 114 | GLN  |
| 1   | P     | 150 | GLN  |
| 1   | P     | 232 | ASN  |
| 1   | P     | 337 | ASN  |
| 1   | P     | 422 | GLN  |
| 1   | P     | 436 | GLN  |
| 1   | P     | 534 | HIS  |
| 1   | P     | 547 | HIS  |
| 1   | P     | 587 | HIS  |
| 1   | P     | 642 | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

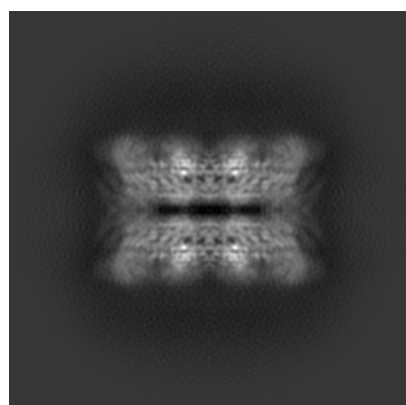
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13951. These allow visual inspection of the internal detail of the map and identification of artifacts.

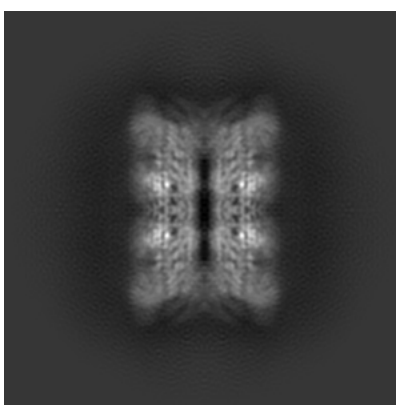
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

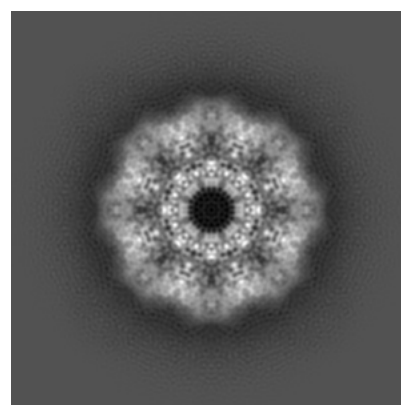
#### 6.1.1 Primary map



X



Y

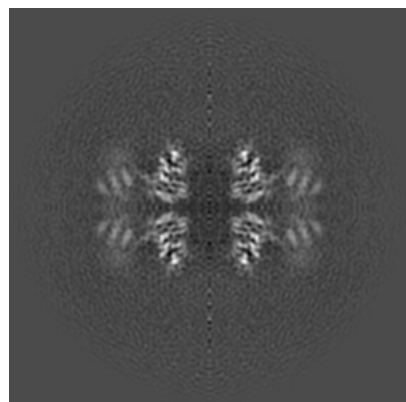


Z

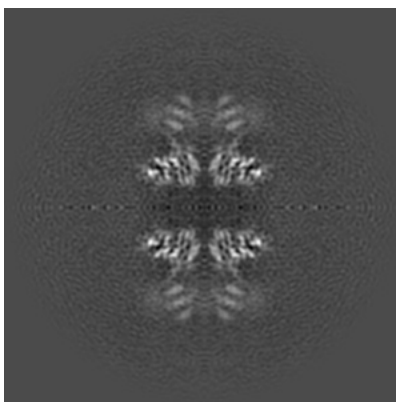
The images above show the map projected in three orthogonal directions.

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

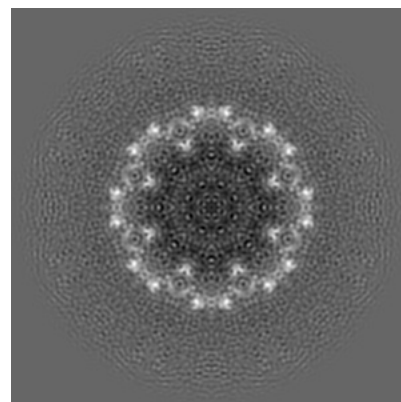
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

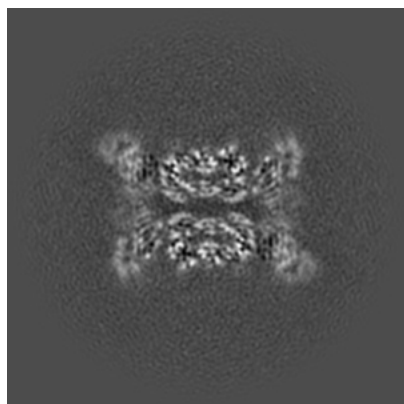


Z Index: 200

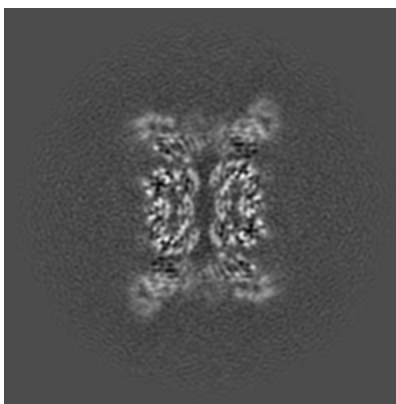
The images above show central slices of the map in three orthogonal directions.

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

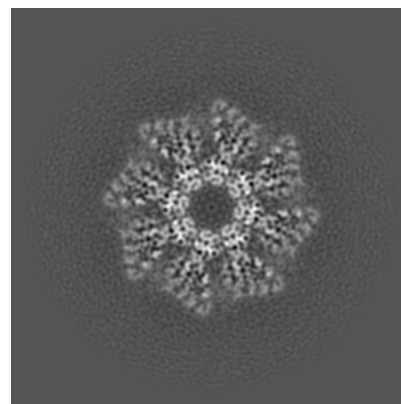
### 6.3.1 Primary map



X Index: 170



Y Index: 170

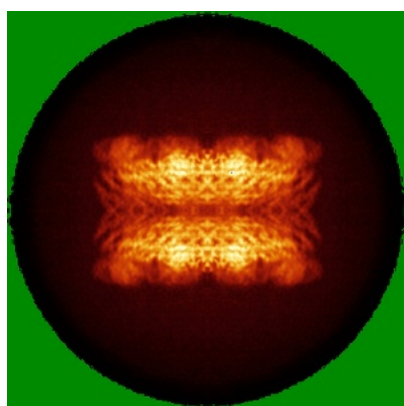


Z Index: 162

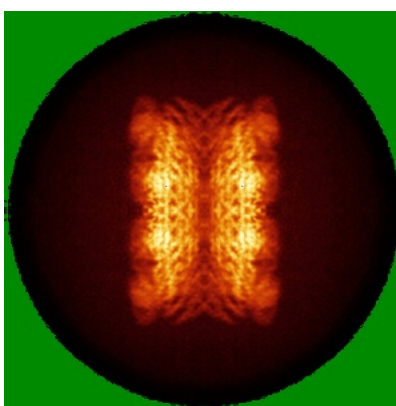
The images above show the largest variance slices of the map in three orthogonal directions.

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

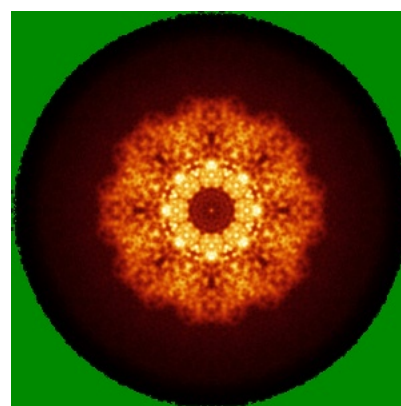
### 6.4.1 Primary map



X



Y

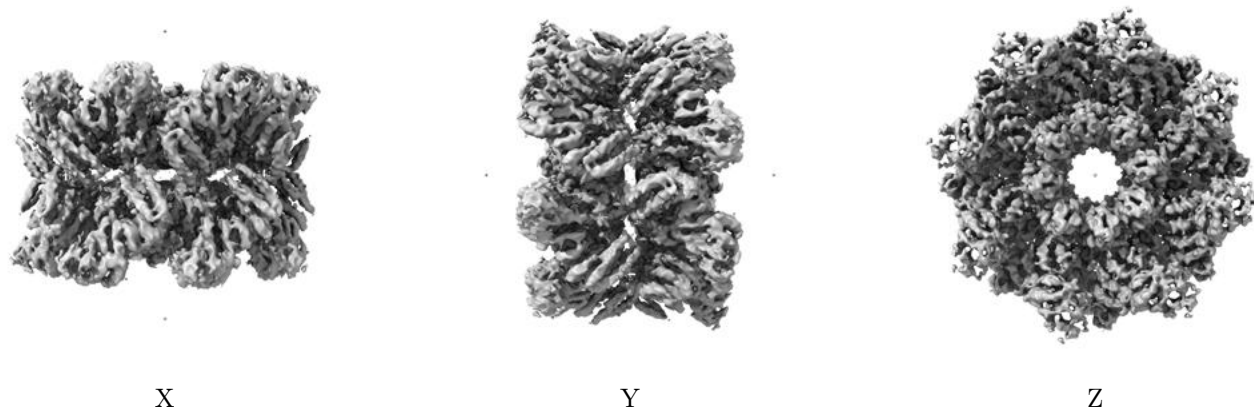


Z

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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

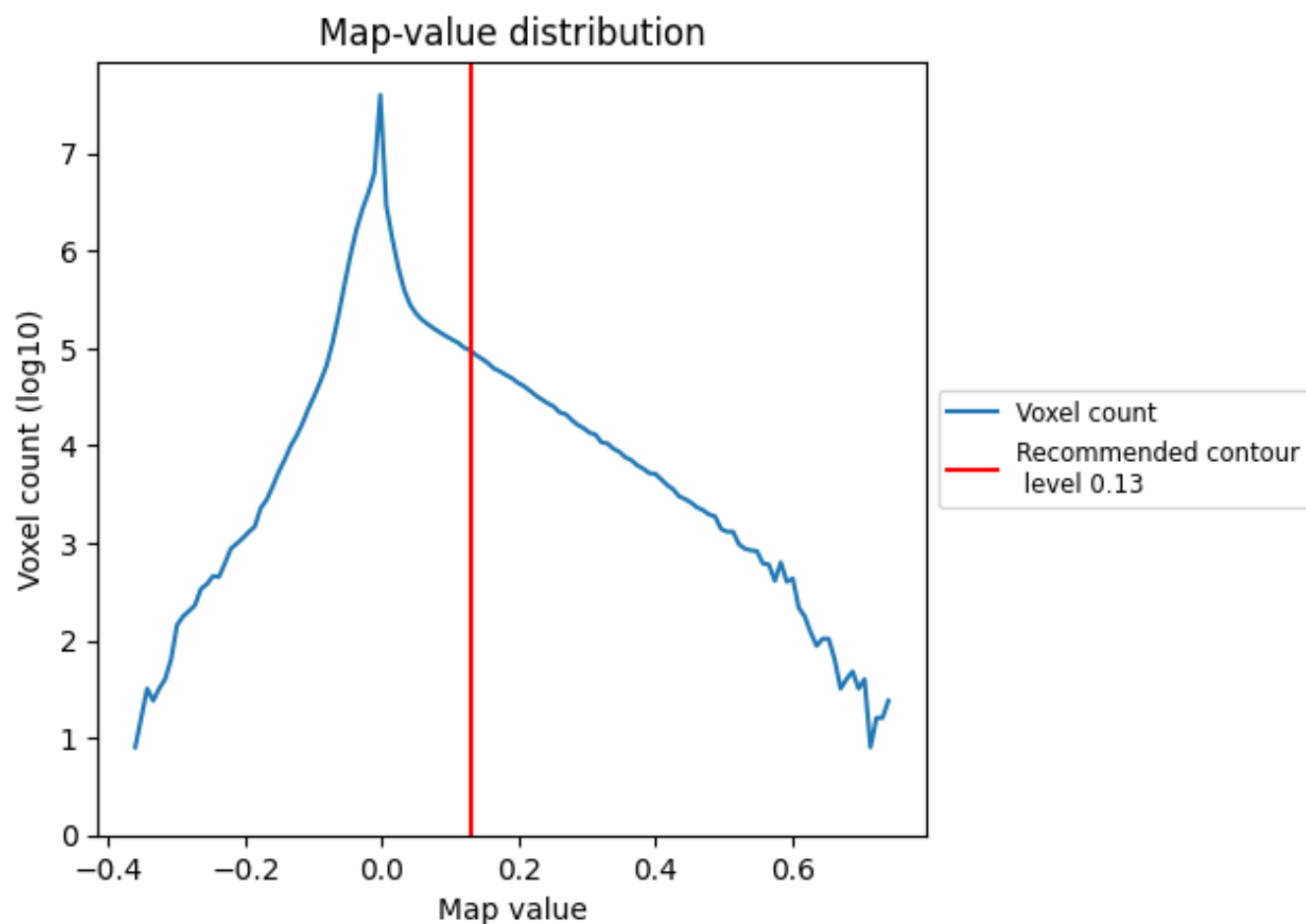
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

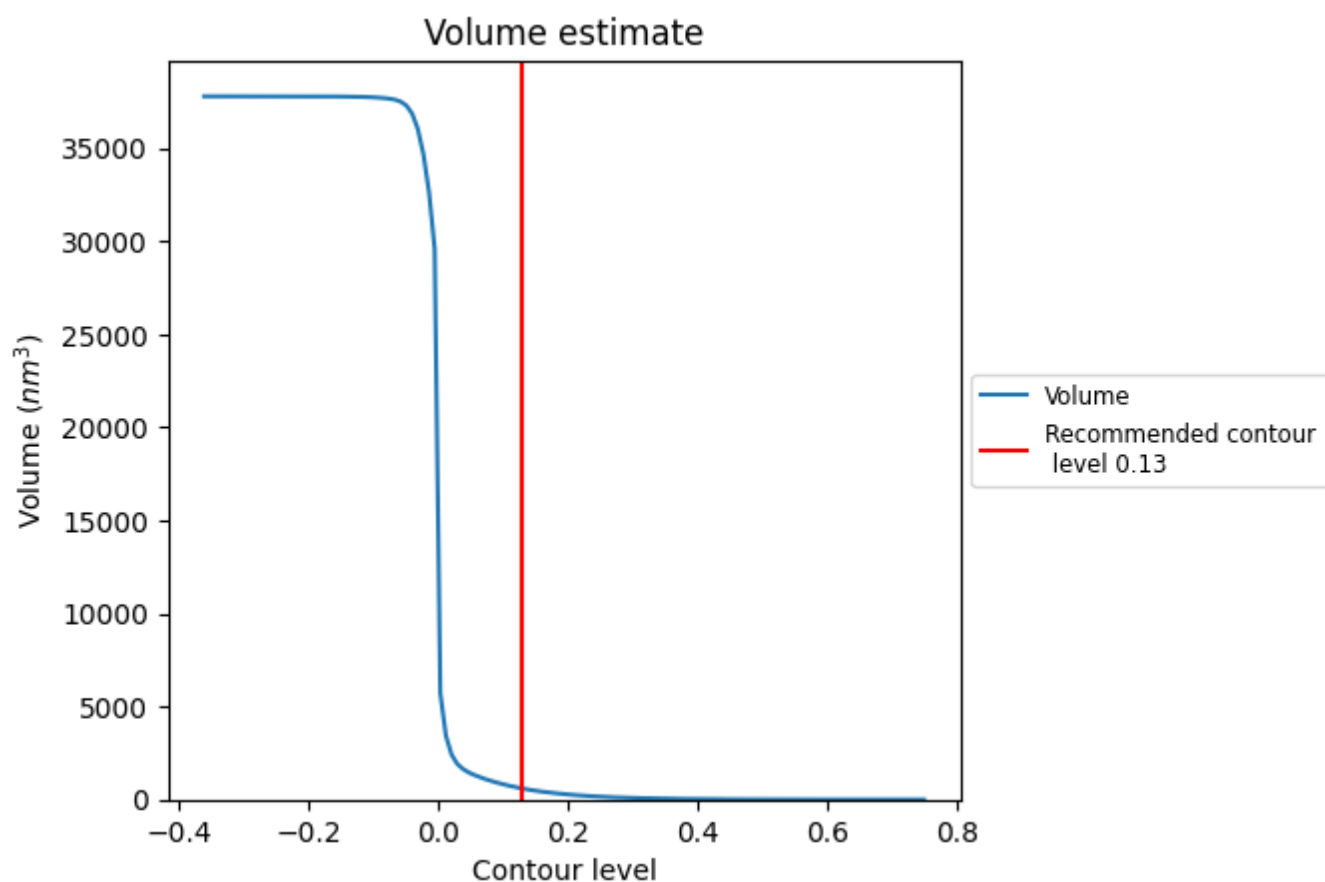
This section contains the results of statistical analysis of the map.

### 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](#)

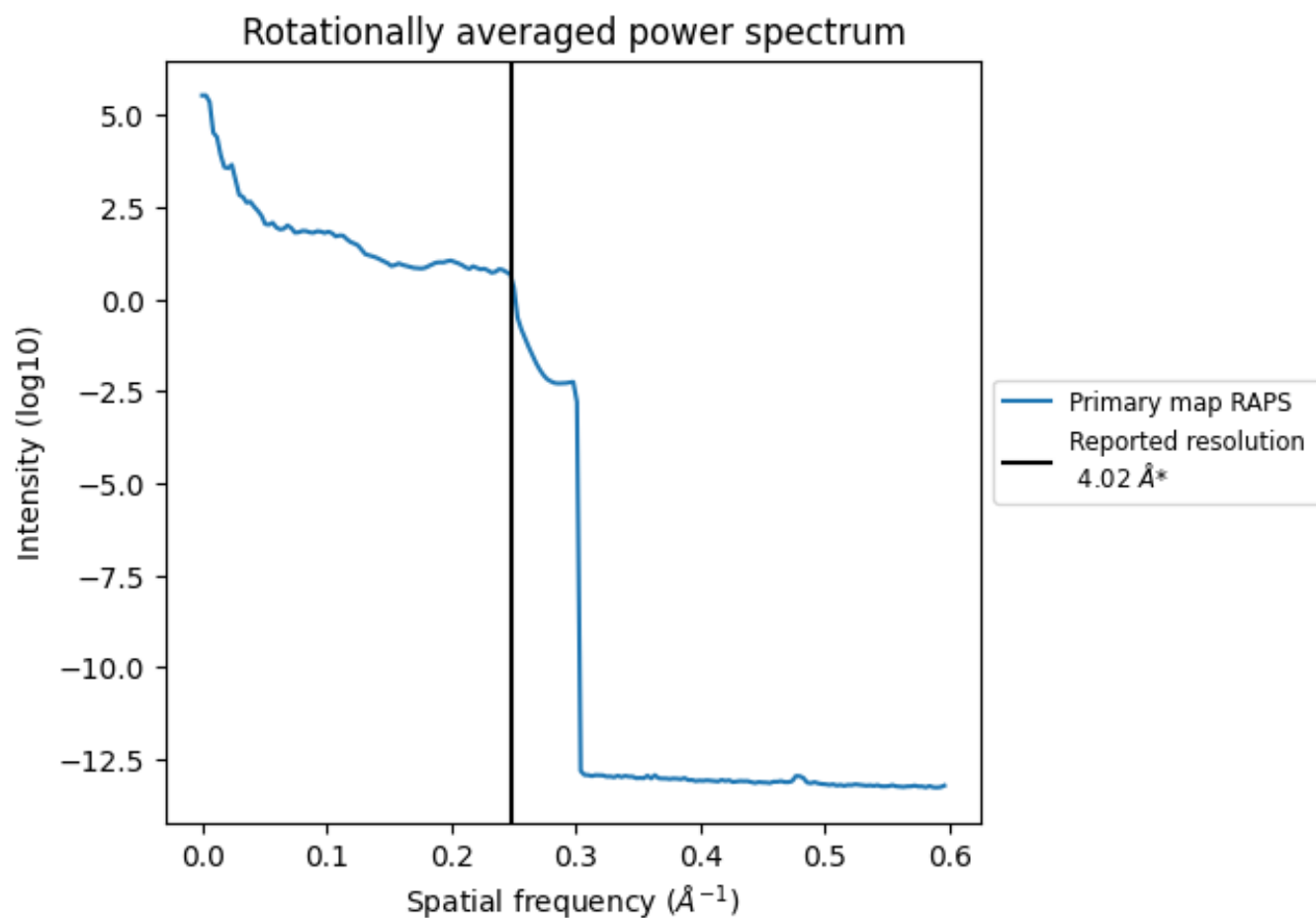


The volume at the recommended contour level is 596  $\text{nm}^3$ ; this corresponds to an approximate mass of 538 kDa.

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 0.249 Å<sup>-1</sup>

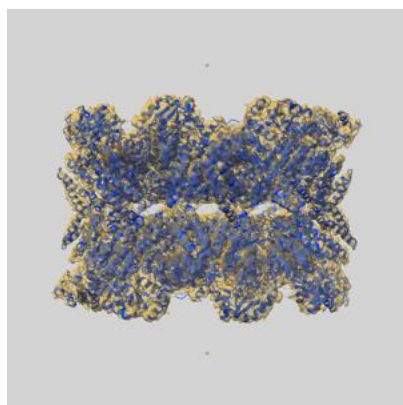
## 8 Fourier-Shell correlation

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

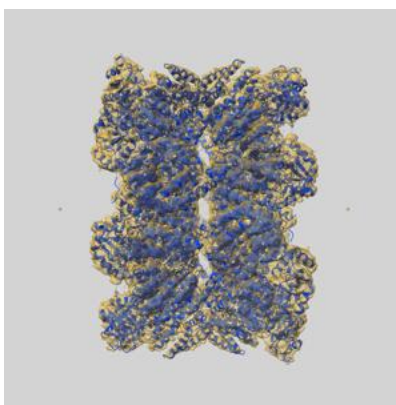
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13951 and PDB model 7QG0. Per-residue inclusion information can be found in section [3](#) on page [16](#).

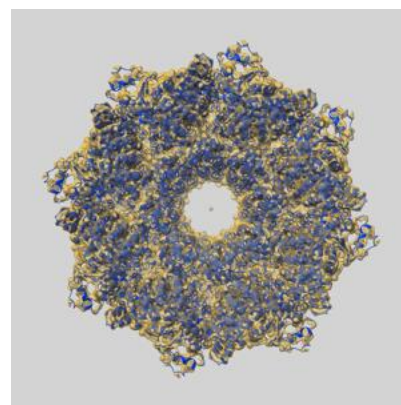
### 9.1 Map-model overlay [i](#)



X



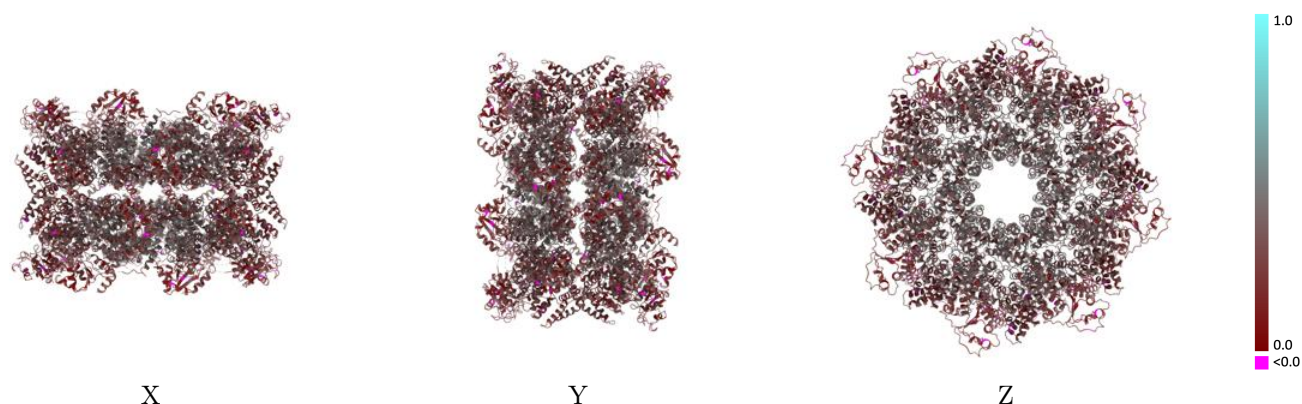
Y



Z

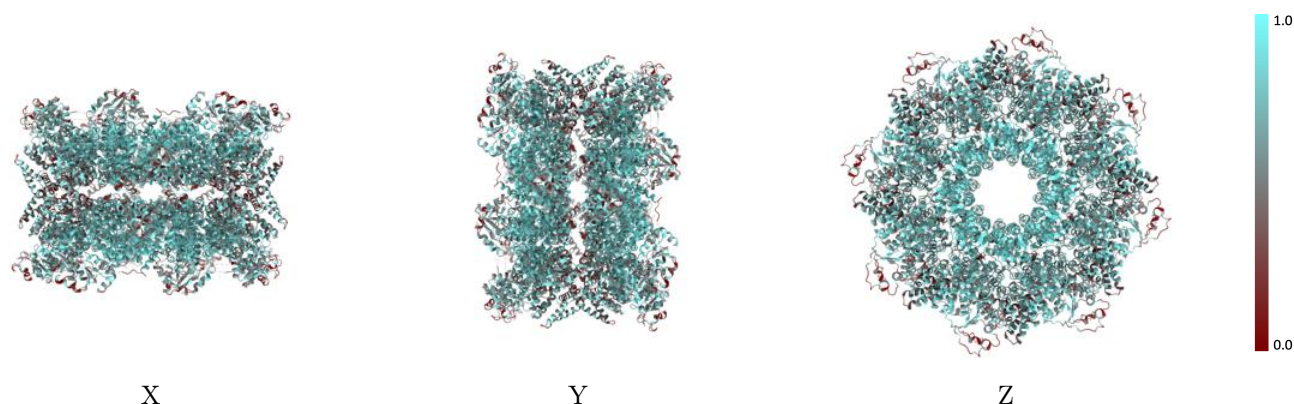
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



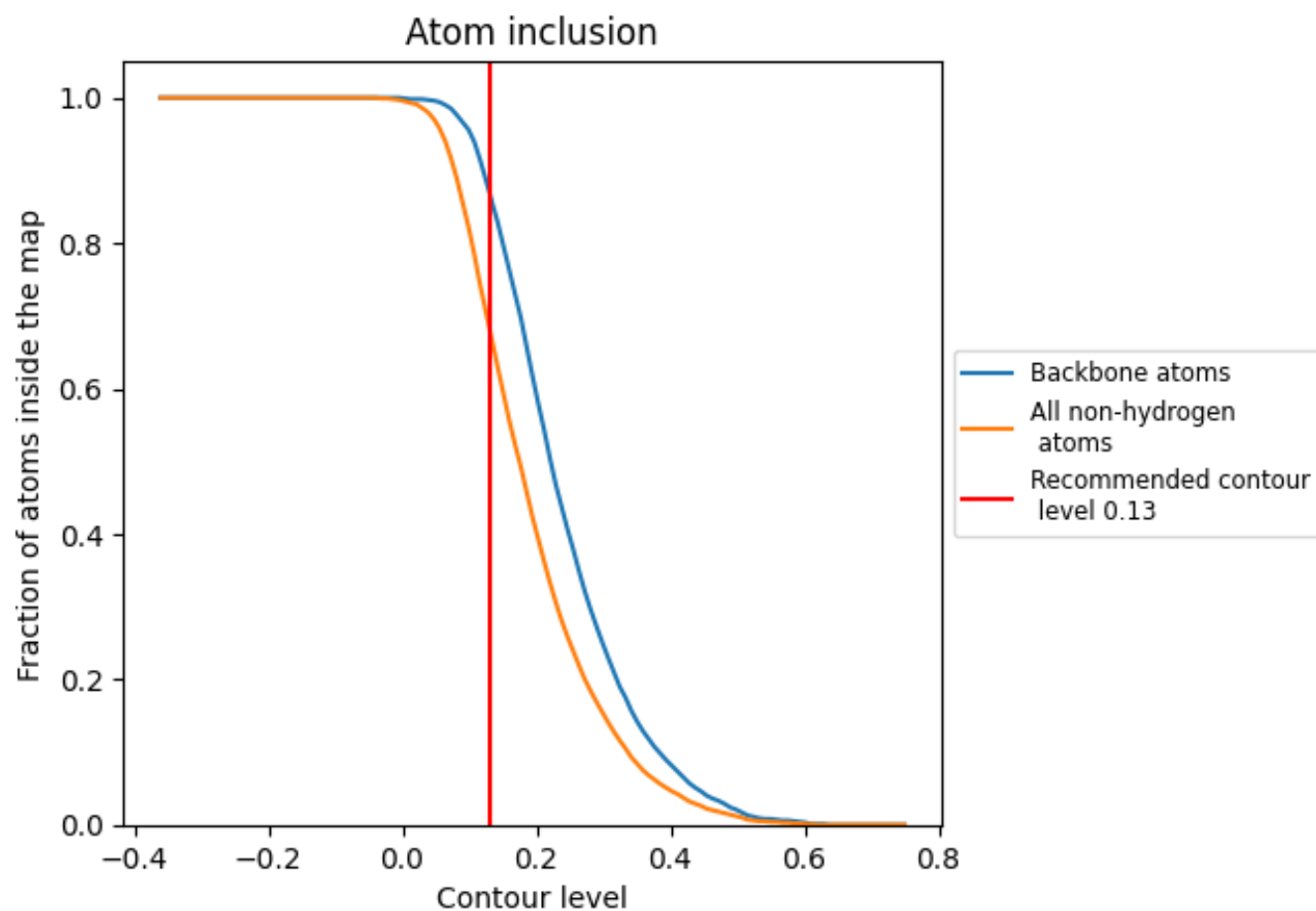
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.13).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 68% 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 (0.13) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6820 | <div></div> 0.3080 |
| A     | <div></div> 0.6840 | <div></div> 0.3070 |
| B     | <div></div> 0.6800 | <div></div> 0.3080 |
| C     | <div></div> 0.6840 | <div></div> 0.3070 |
| D     | <div></div> 0.6790 | <div></div> 0.3080 |
| E     | <div></div> 0.6850 | <div></div> 0.3100 |
| F     | <div></div> 0.6790 | <div></div> 0.3100 |
| G     | <div></div> 0.6830 | <div></div> 0.3070 |
| H     | <div></div> 0.6790 | <div></div> 0.3090 |
| I     | <div></div> 0.6780 | <div></div> 0.3070 |
| J     | <div></div> 0.6830 | <div></div> 0.3080 |
| K     | <div></div> 0.6820 | <div></div> 0.3080 |
| L     | <div></div> 0.6840 | <div></div> 0.3090 |
| M     | <div></div> 0.6850 | <div></div> 0.3090 |
| N     | <div></div> 0.6840 | <div></div> 0.3090 |
| O     | <div></div> 0.6790 | <div></div> 0.3090 |
| P     | <div></div> 0.6830 | <div></div> 0.3070 |

