



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:46 AM UTC

PDB ID : 7L0X / pdb\_00007l0x  
EMDB ID : EMD-23107  
Title : Human Bocavirus 2 (pH 2.6)  
Authors : Luo, M.; Mietzsch, M.; Agbandje-McKenna, M.  
Deposited on : 2020-12-13  
Resolution : 2.51 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

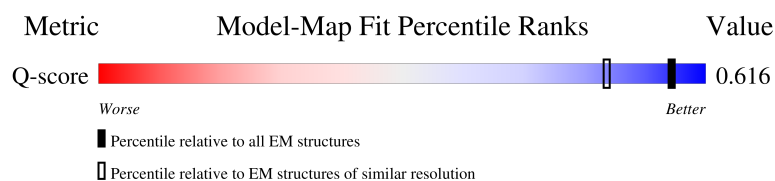
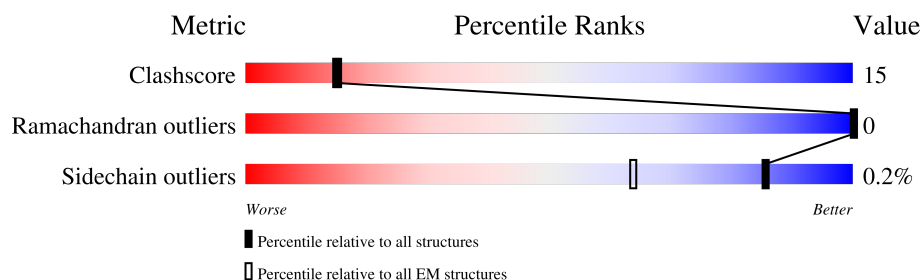
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.51 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                       | 7159 ( 2.01 - 3.01 )                                     |

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   | 1     | 516    | <div> <div>8%</div> <div>71%</div> <div>29%</div> </div> |
| 1   | 2     | 516    | <div> <div>8%</div> <div>69%</div> <div>30%</div> </div> |
| 1   | 3     | 516    | <div> <div>8%</div> <div>70%</div> <div>30%</div> </div> |
| 1   | 4     | 516    | <div> <div>8%</div> <div>69%</div> <div>31%</div> </div> |

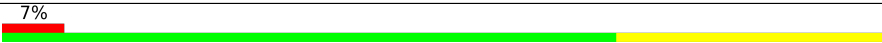
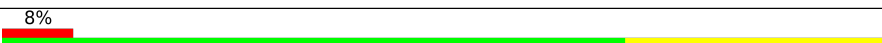
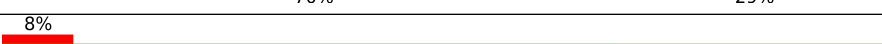
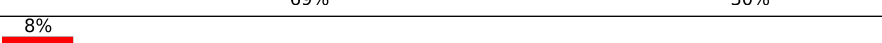
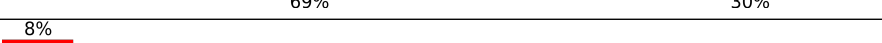
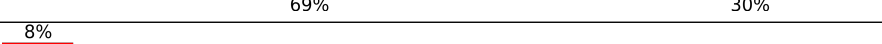
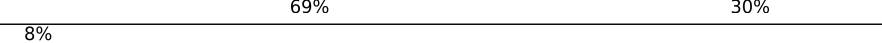
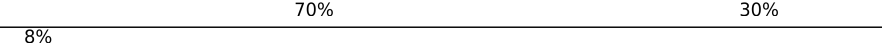
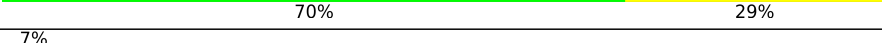
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| Mol | Chain | Length | Quality of chain |         |
|-----|-------|--------|------------------|---------|
| 1   | 5     | 516    | 7%               | 69% 30% |
| 1   | 6     | 516    | 7%               | 69% 30% |
| 1   | 7     | 516    | 7%               | 69% 31% |
| 1   | 8     | 516    | 8%               | 70% 30% |
| 1   | A     | 516    | 8%               | 70% 30% |
| 1   | B     | 516    | 8%               | 70% 30% |
| 1   | C     | 516    | 8%               | 70% 30% |
| 1   | D     | 516    | 7%               | 69% 30% |
| 1   | E     | 516    | 8%               | 70% 29% |
| 1   | F     | 516    | 8%               | 70% 30% |
| 1   | G     | 516    | 8%               | 69% 31% |
| 1   | H     | 516    | 7%               | 69% 30% |
| 1   | I     | 516    | 8%               | 69% 30% |
| 1   | J     | 516    | 7%               | 69% 31% |
| 1   | K     | 516    | 8%               | 69% 31% |
| 1   | L     | 516    | 8%               | 70% 30% |
| 1   | M     | 516    | 8%               | 70% 29% |
| 1   | N     | 516    | 7%               | 70% 30% |
| 1   | O     | 516    | 8%               | 69% 31% |
| 1   | P     | 516    | 7%               | 70% 30% |
| 1   | Q     | 516    | 8%               | 70% 30% |
| 1   | R     | 516    | 8%               | 69% 30% |
| 1   | S     | 516    | 8%               | 69% 30% |
| 1   | T     | 516    | 8%               | 69% 30% |
| 1   | U     | 516    | 8%               | 70% 29% |

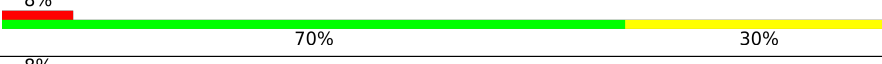
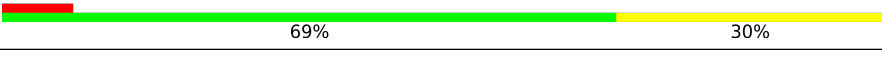
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| Mol | Chain | Length | Quality of chain                                                                           |     |
|-----|-------|--------|--------------------------------------------------------------------------------------------|-----|
| 1   | V     | 516    | 8%<br>   | 29% |
| 1   | W     | 516    | 7%<br>   | 30% |
| 1   | X     | 516    | 8%<br>   | 30% |
| 1   | Y     | 516    | 7%<br>   | 30% |
| 1   | Z     | 516    | 8%<br>   | 30% |
| 1   | a     | 516    | 8%<br>   | 30% |
| 1   | b     | 516    | 8%<br>   | 29% |
| 1   | c     | 516    | 8%<br>   | 30% |
| 1   | d     | 516    | 8%<br>   | 30% |
| 1   | e     | 516    | 8%<br>   | 30% |
| 1   | f     | 516    | 8%<br>   | 30% |
| 1   | g     | 516    | 8%<br>   | 30% |
| 1   | h     | 516    | 8%<br>  | 29% |
| 1   | i     | 516    | 7%<br> | 30% |
| 1   | j     | 516    | 7%<br> | 30% |
| 1   | k     | 516    | 7%<br> | 30% |
| 1   | l     | 516    | 8%<br> | 30% |
| 1   | m     | 516    | 8%<br> | 30% |
| 1   | n     | 516    | 8%<br> | 31% |
| 1   | o     | 516    | 8%<br> | 30% |
| 1   | p     | 516    | 8%<br> | 30% |
| 1   | q     | 516    | 8%<br> | 30% |
| 1   | r     | 516    | 8%<br> | 30% |
| 1   | s     | 516    | 8%<br> | 30% |
| 1   | t     | 516    | 8%<br> | 31% |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | u     | 516    |  |
| 1   | v     | 516    |  |
| 1   | w     | 516    |  |
| 1   | x     | 516    |  |
| 1   | y     | 516    |  |
| 1   | z     | 516    |  |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 246480 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 VP2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | B     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | C     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | D     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | E     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | F     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | G     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | H     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | I     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | J     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | K     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | L     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | M     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | N     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | O     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | P     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |
| 1   | Q     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1   | R     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | S     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | T     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | U     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | V     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | W     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | X     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | Y     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | Z     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | a     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | b     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | c     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | d     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | e     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | f     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | g     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | h     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | i     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | j     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | k     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | l     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1   | m     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | n     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | o     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | p     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | q     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | r     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | s     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | t     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | u     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | v     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | w     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | x     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | y     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | z     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | 1     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | 2     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | 3     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | 4     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | 5     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | 6     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |
| 1   | 7     | 516      | Total<br>4108 | C<br>2602 | N<br>708 | O<br>777 | S<br>21 | 0       | 0     |

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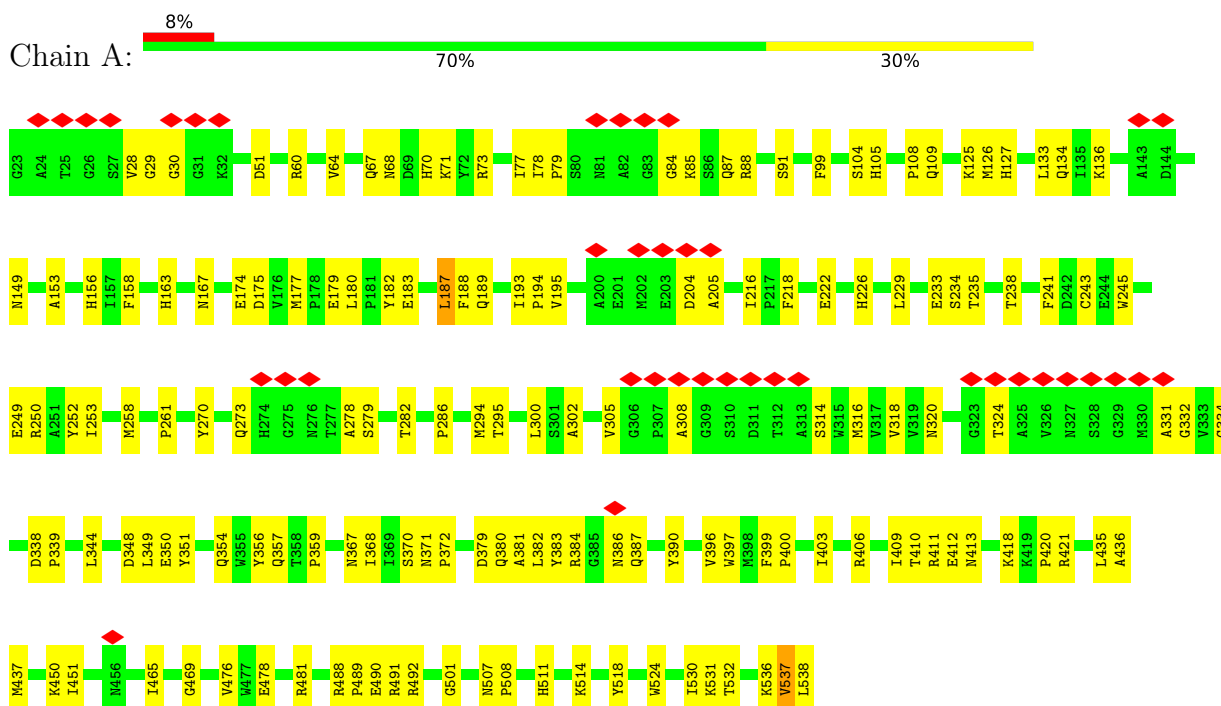
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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 8     | 516      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4108  | 2602 | 708 | 777 | 21 |         |       |

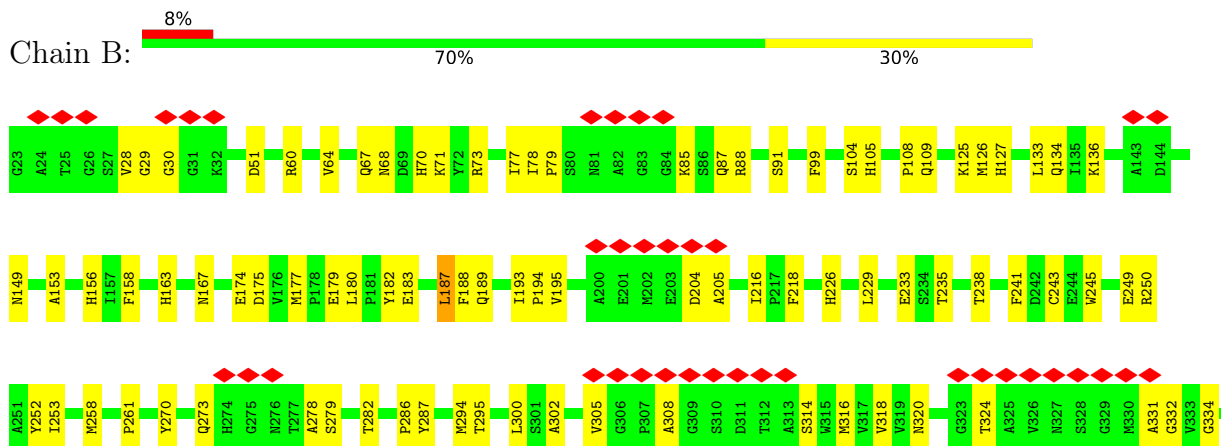
### 3 Residue-property plots

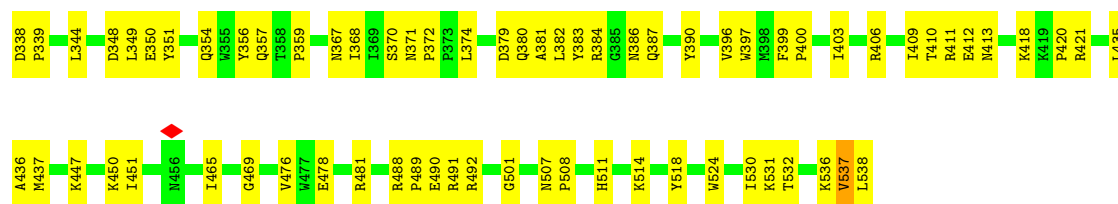
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: VP2

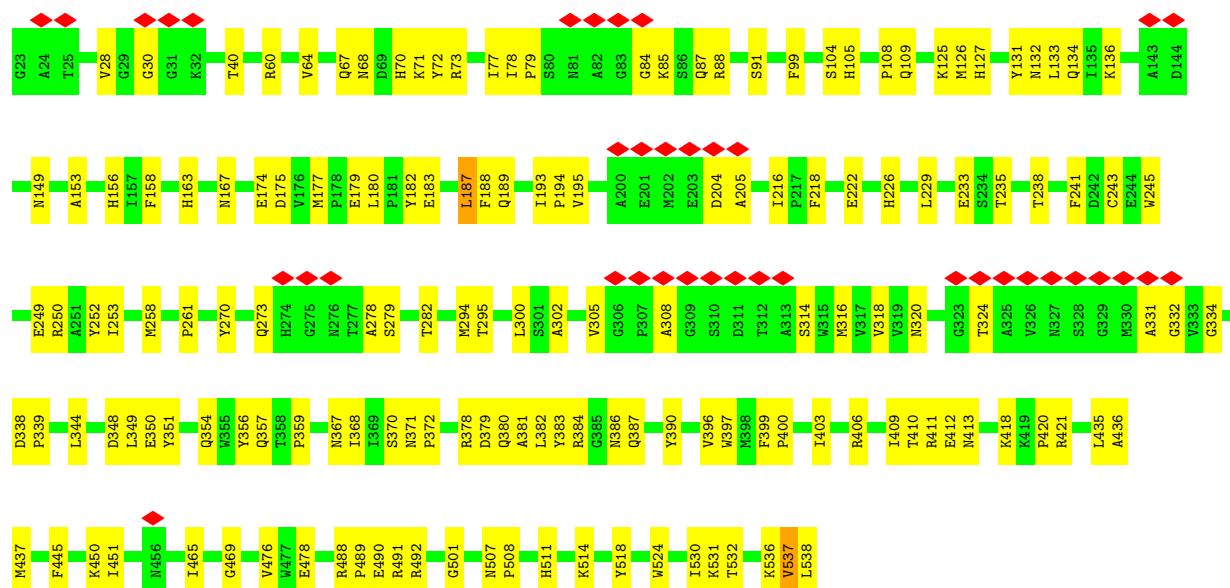


#### • Molecule 1: VP2

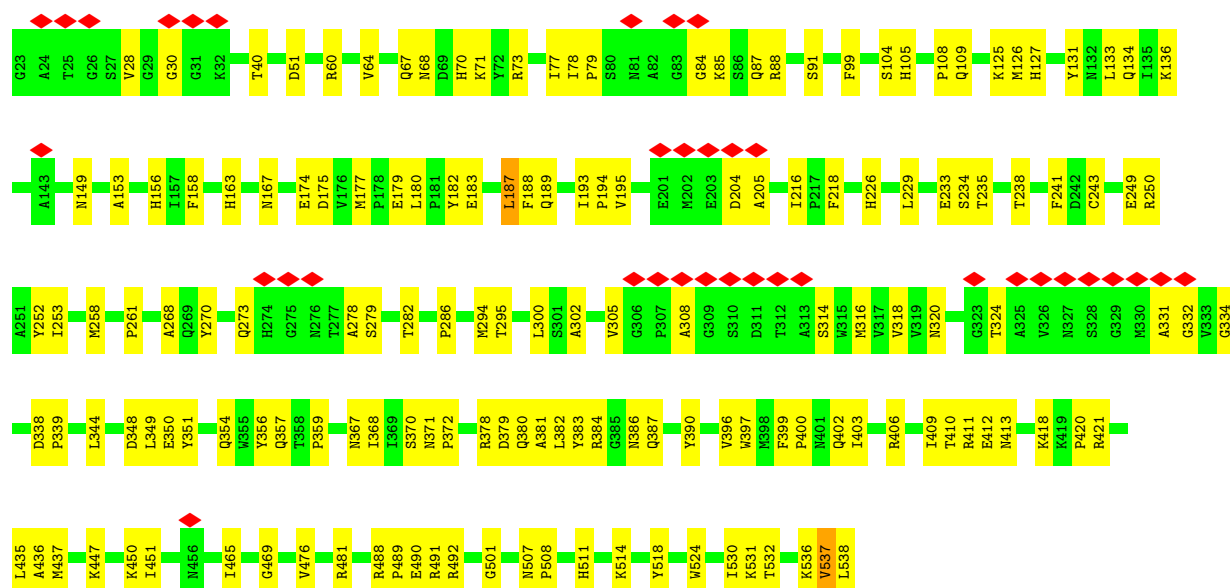




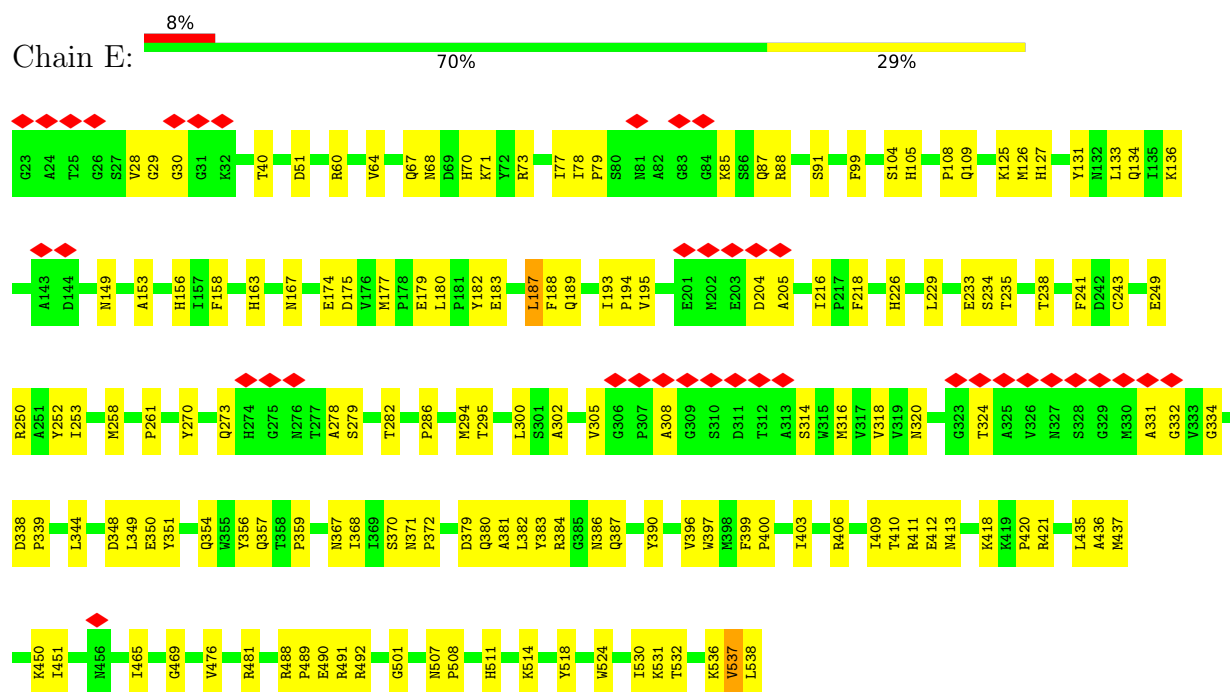
• Molecule 1: VP2



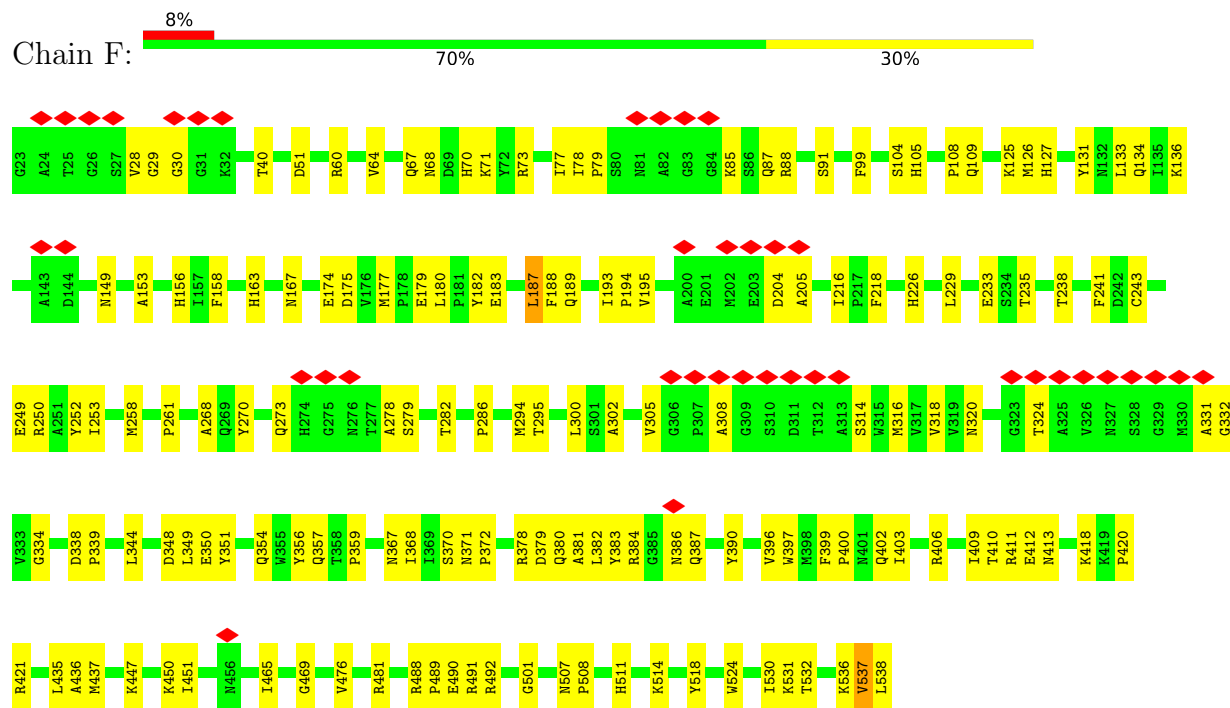
• Molecule 1: VP2



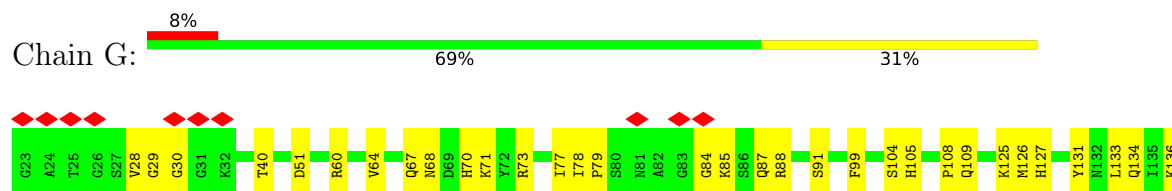
• Molecule 1: VP2

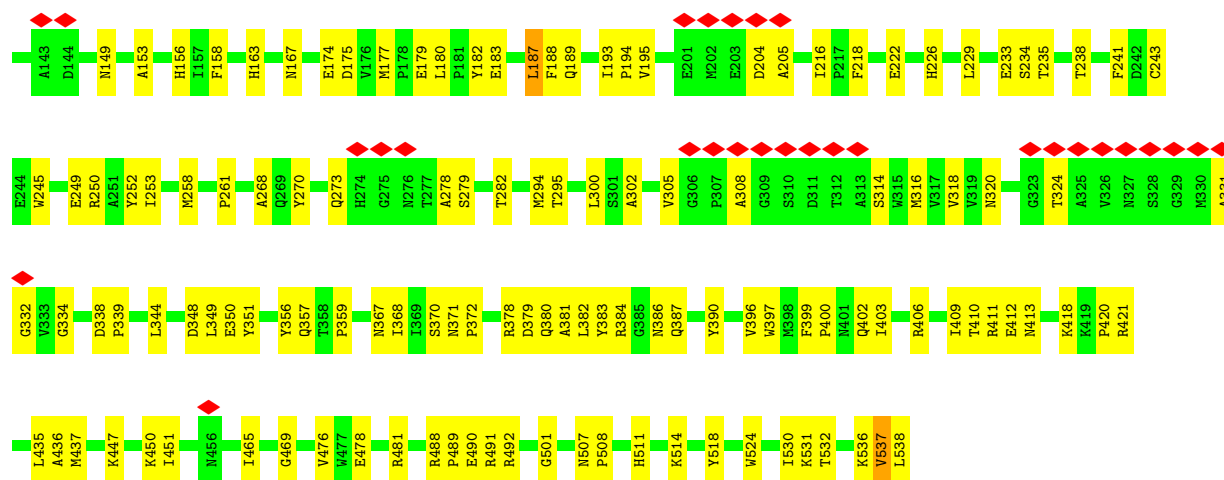


• Molecule 1: VP2

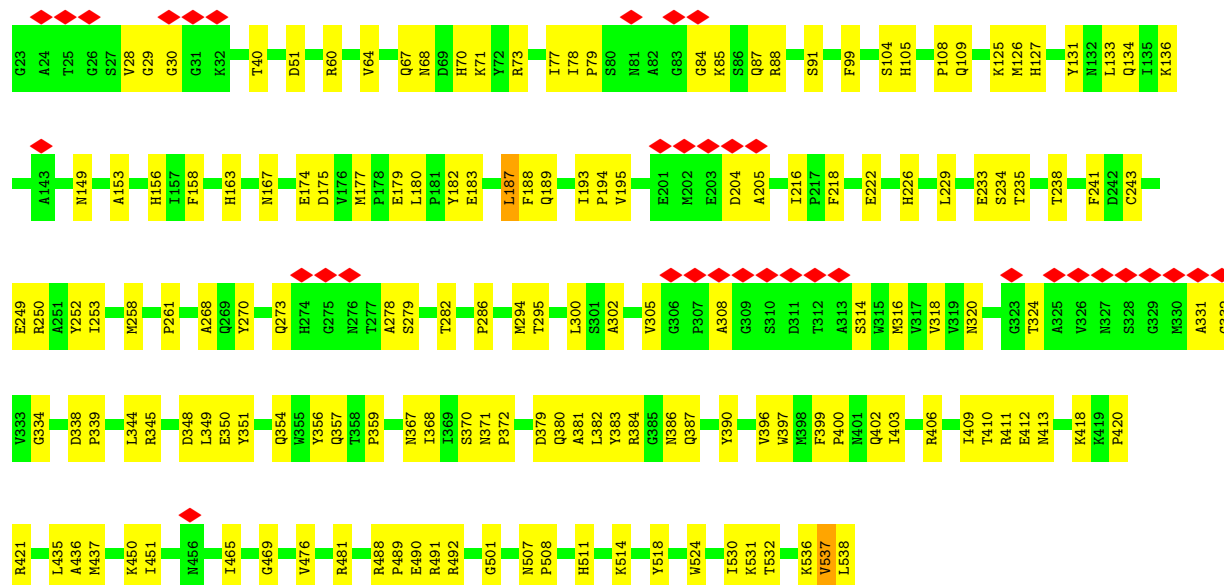


• Molecule 1: VP2

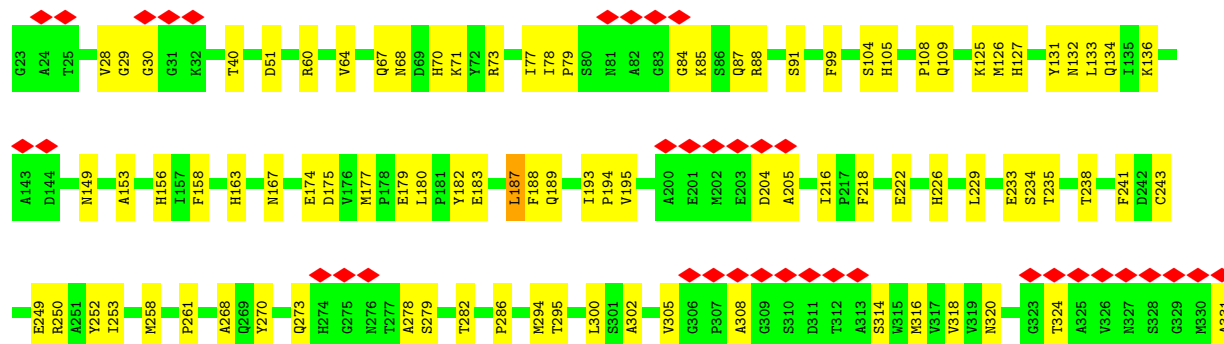


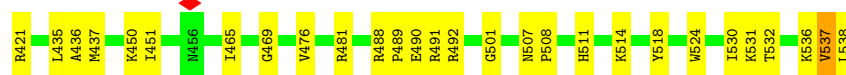
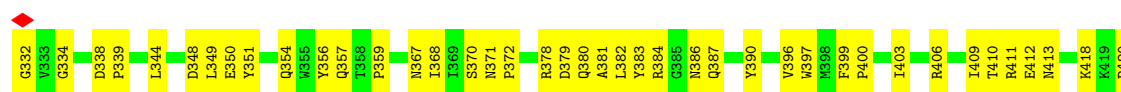


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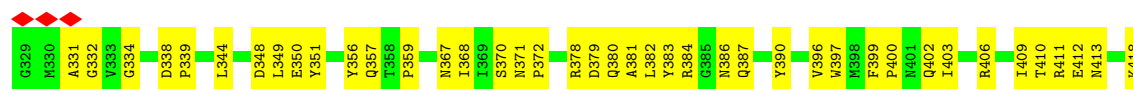
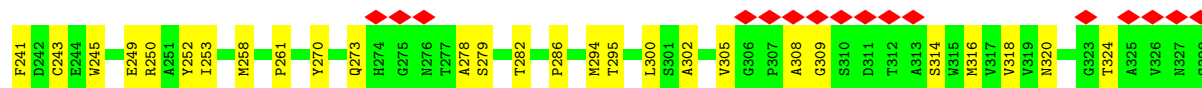


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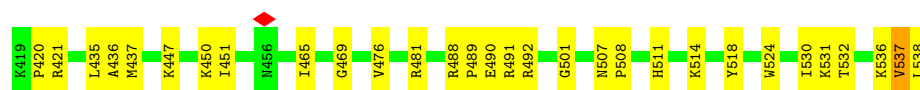
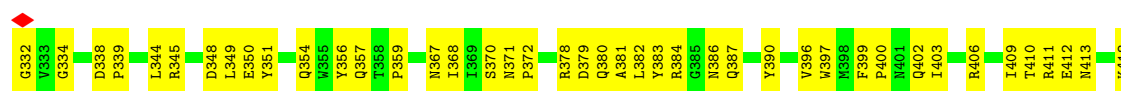
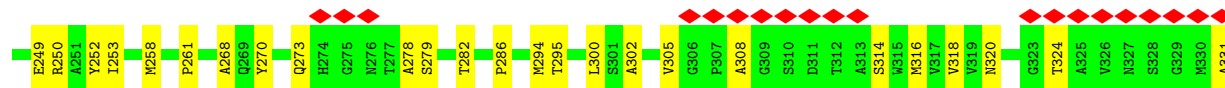
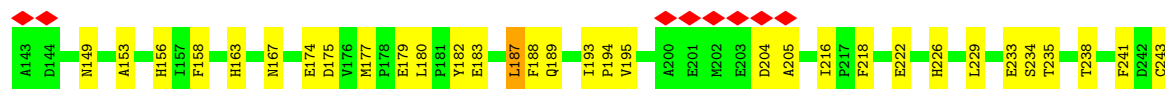




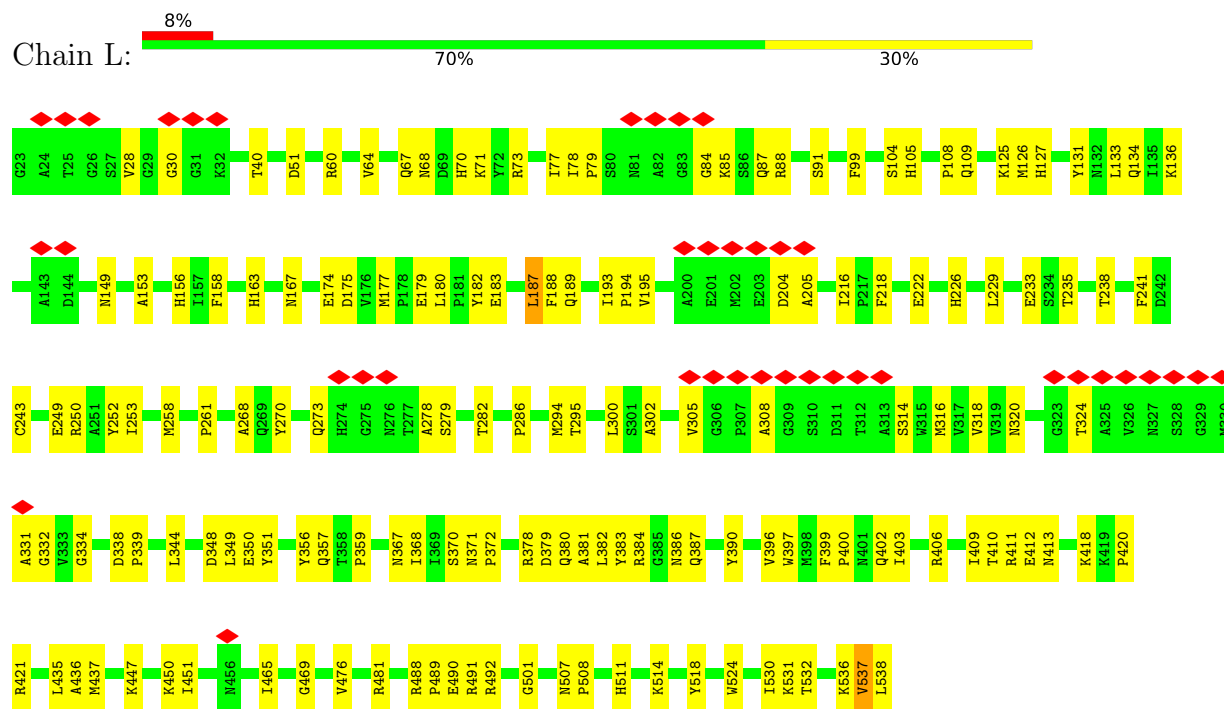
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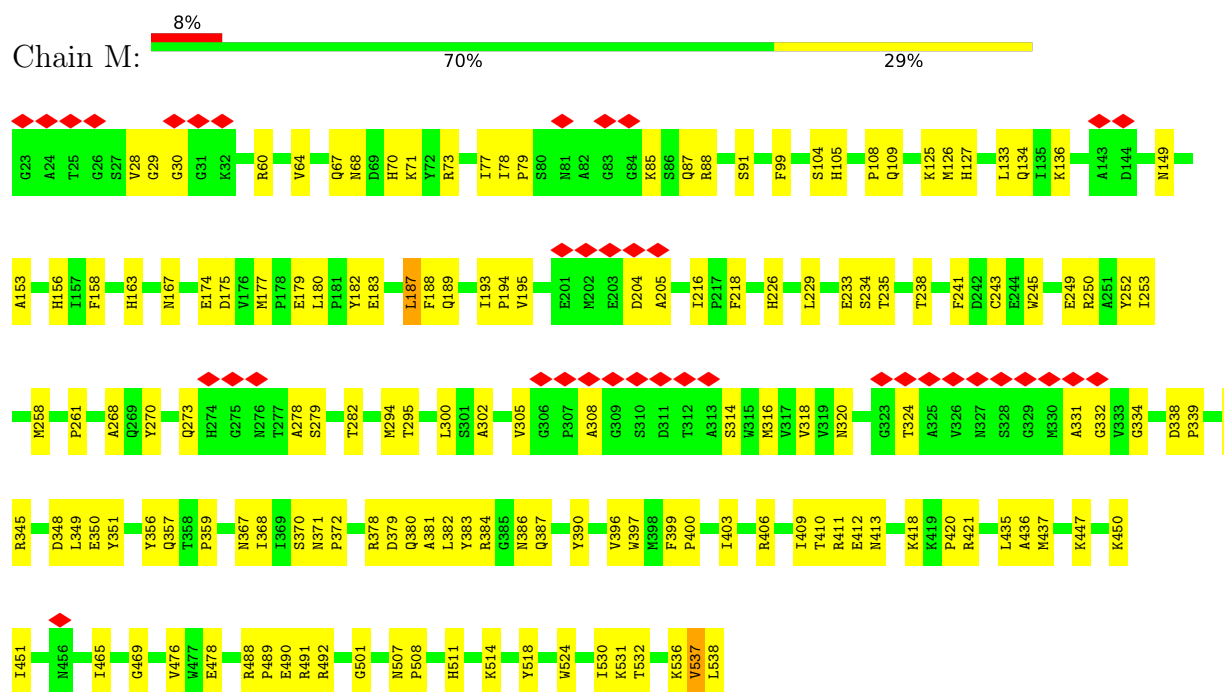
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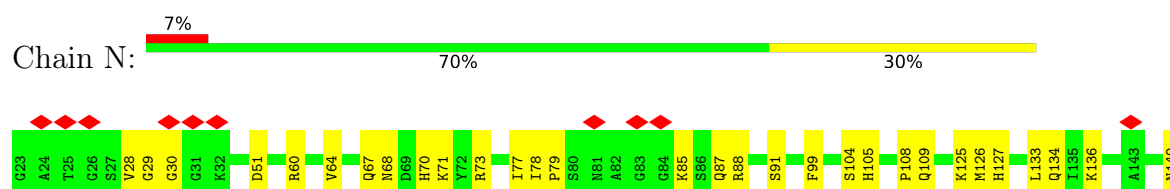
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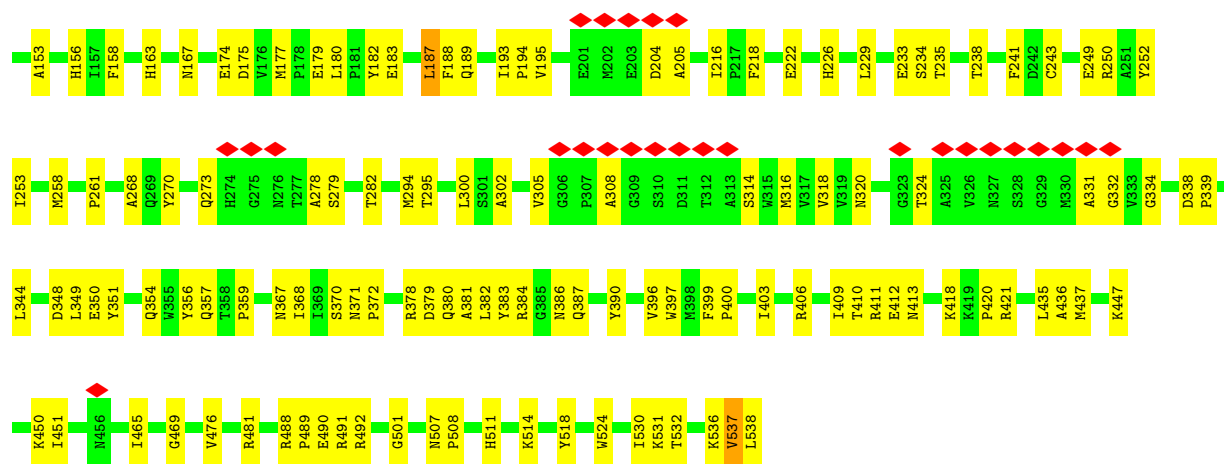


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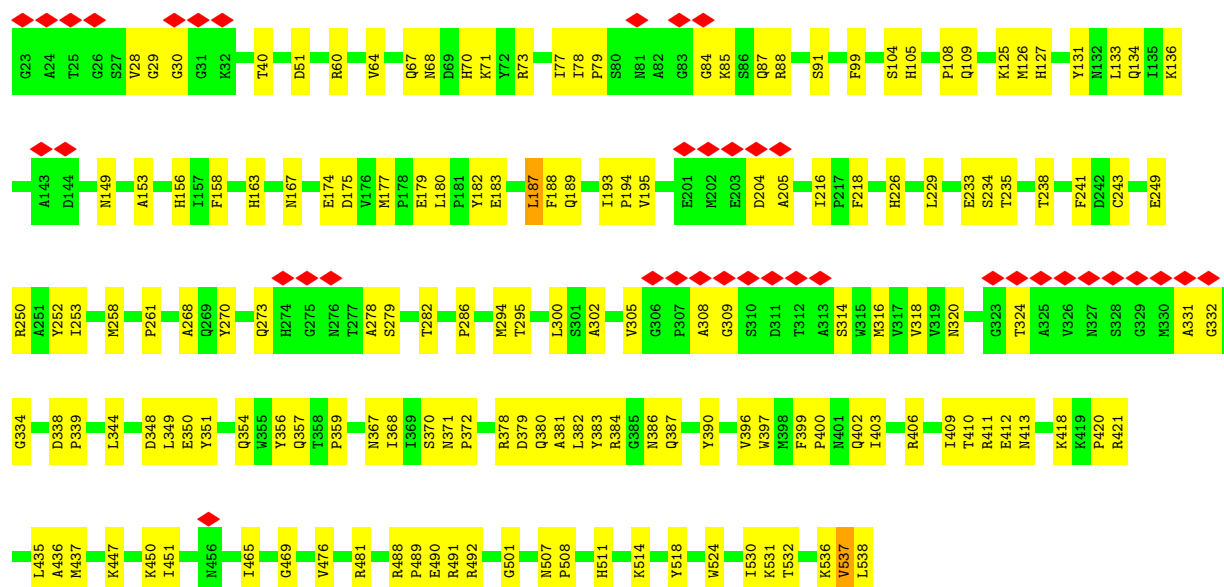


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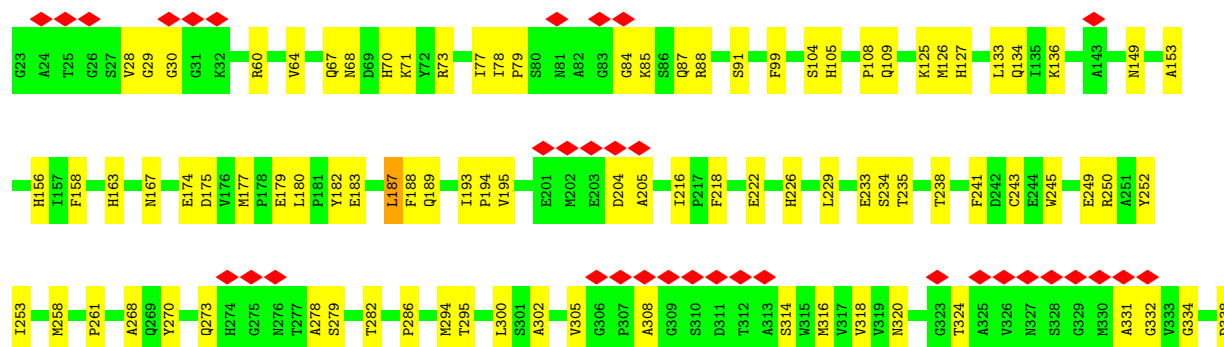


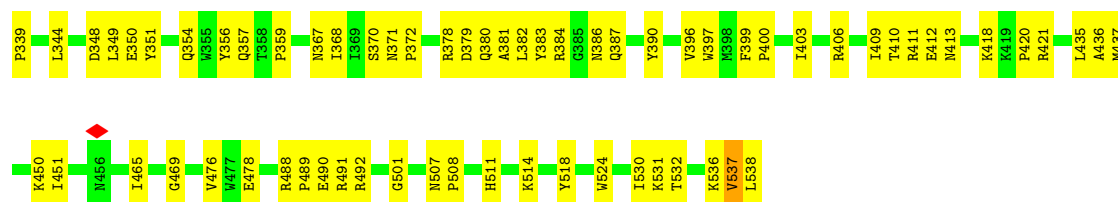


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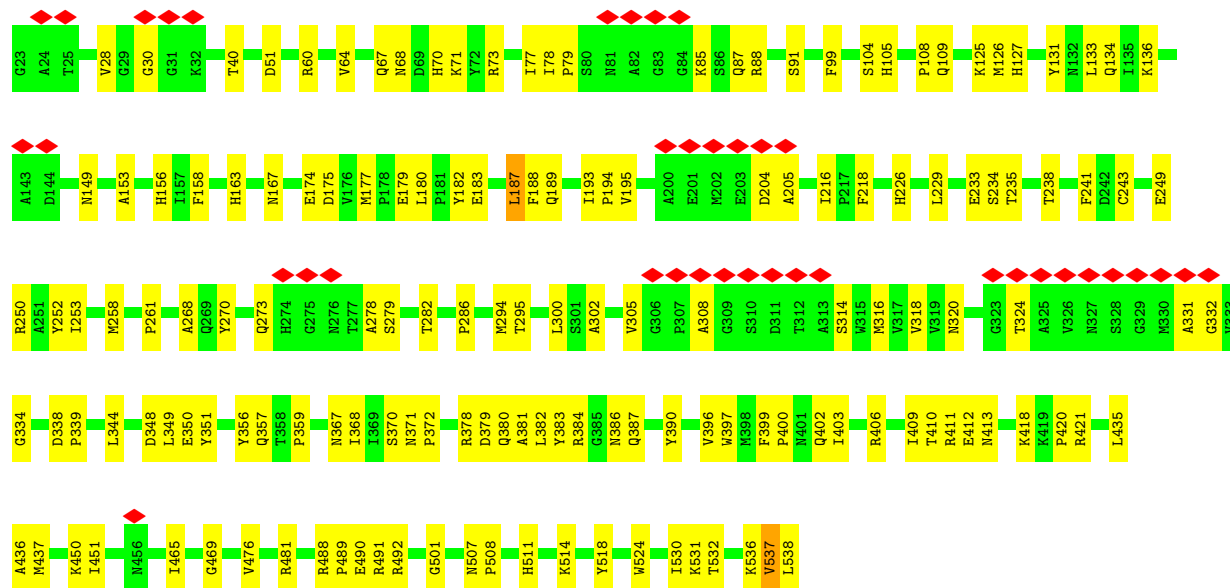


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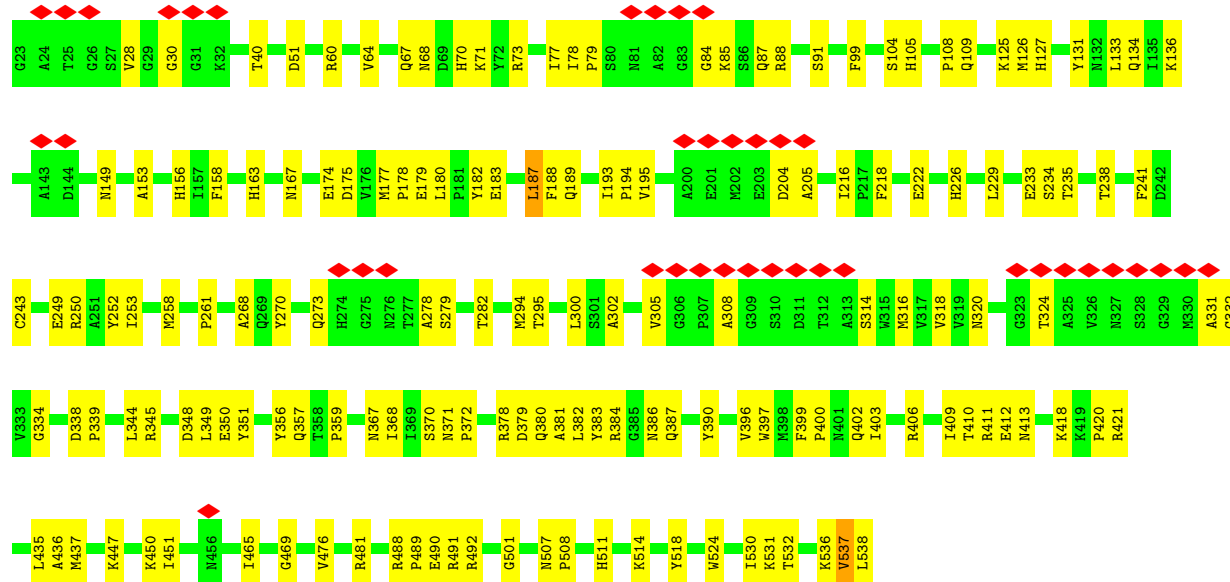


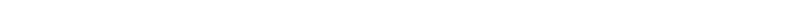


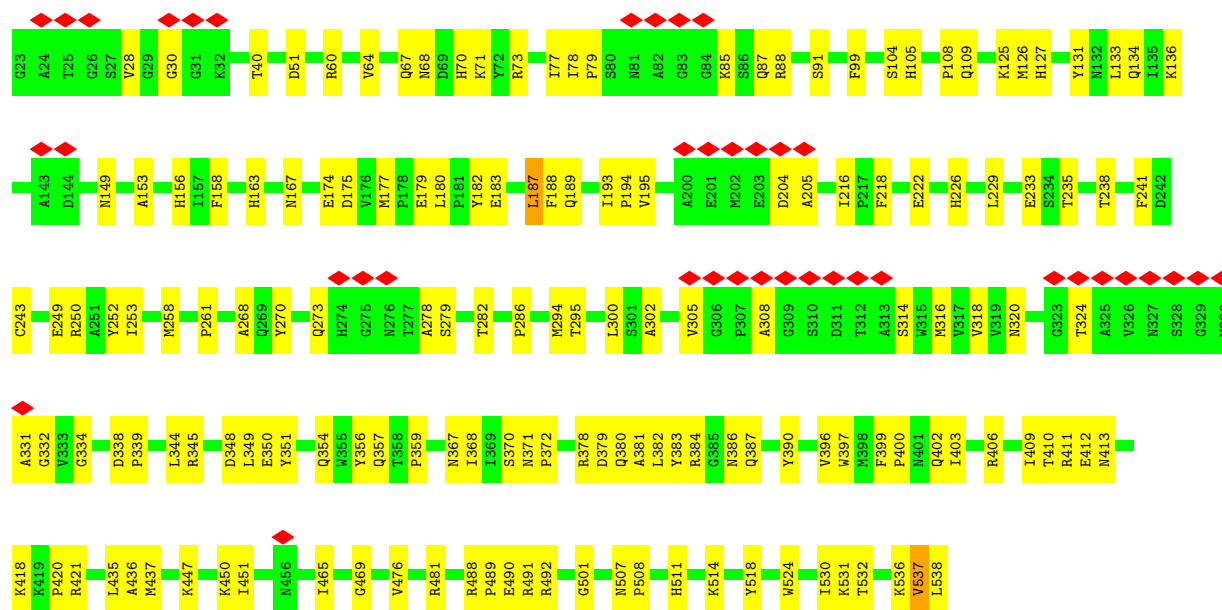
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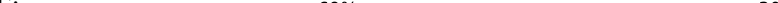


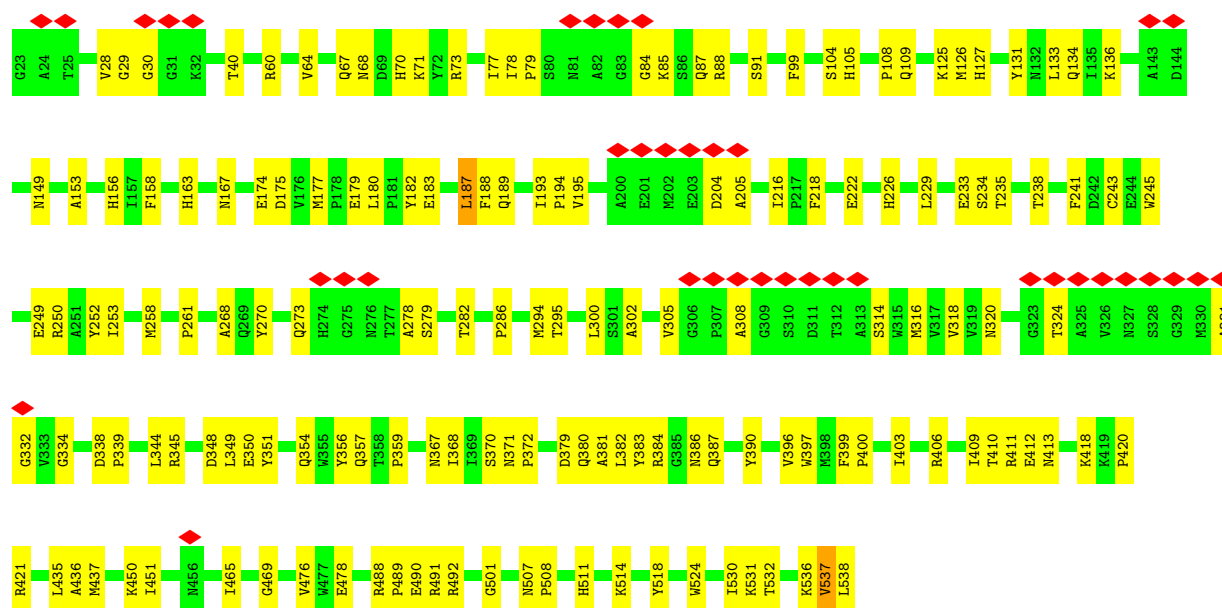
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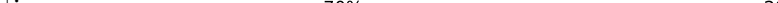


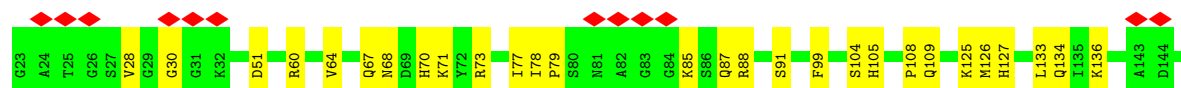
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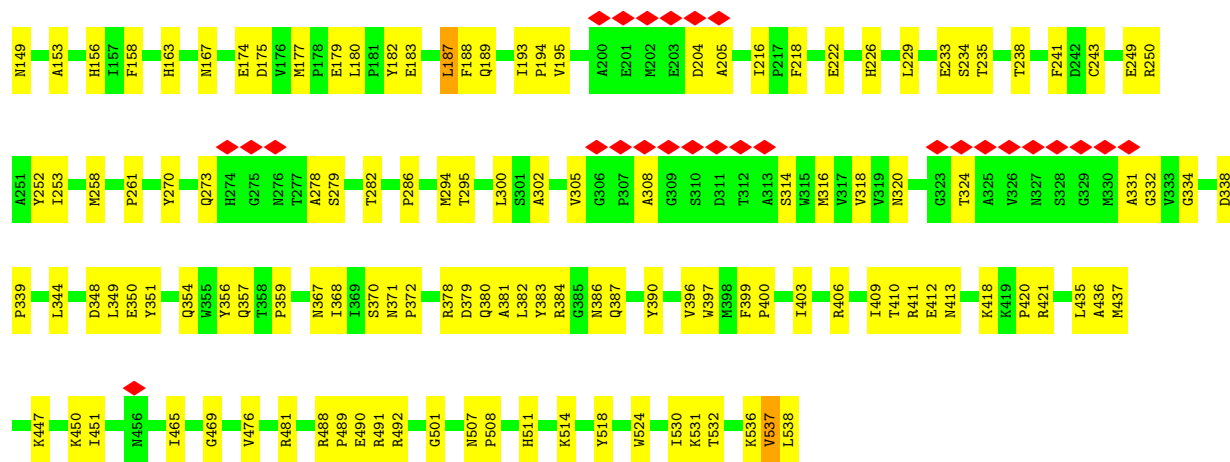


Chain T:  8% 69% 30%

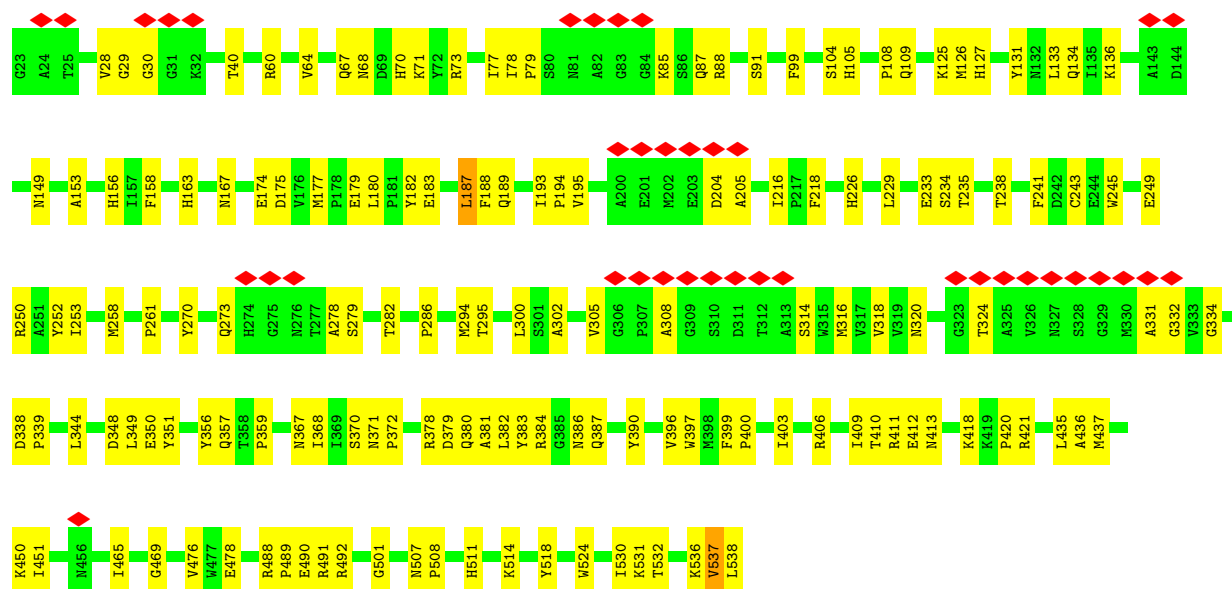


Chain U: 

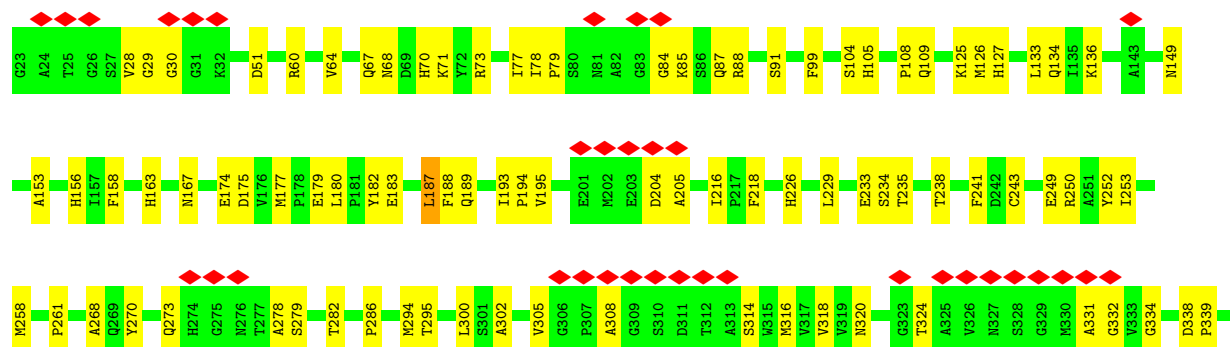


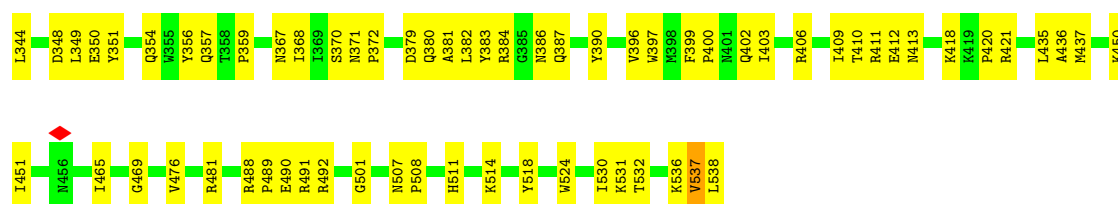


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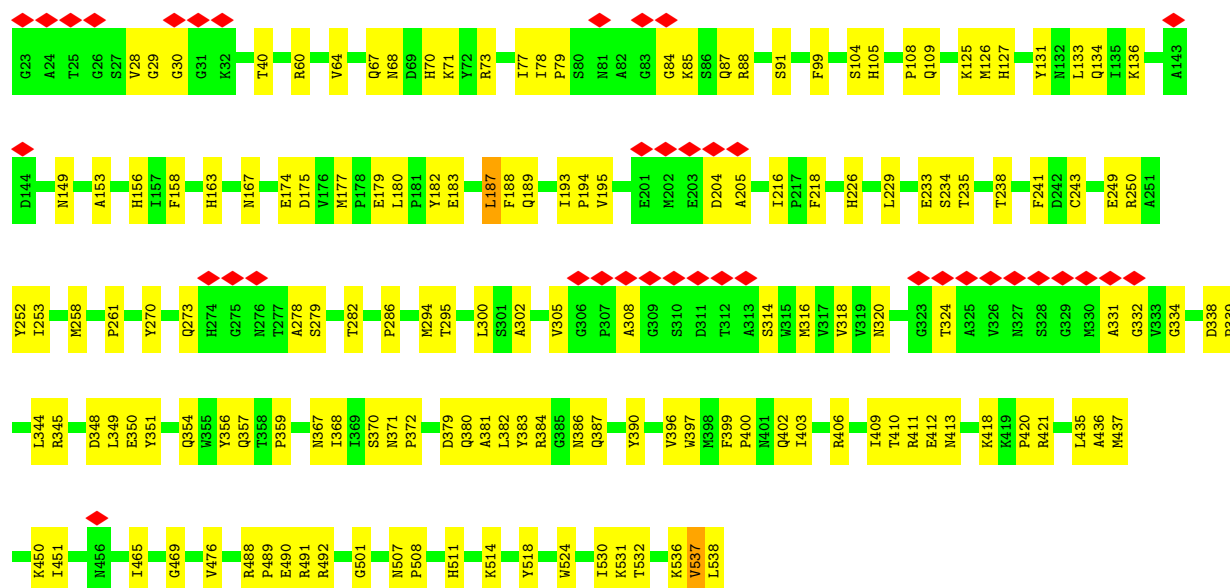


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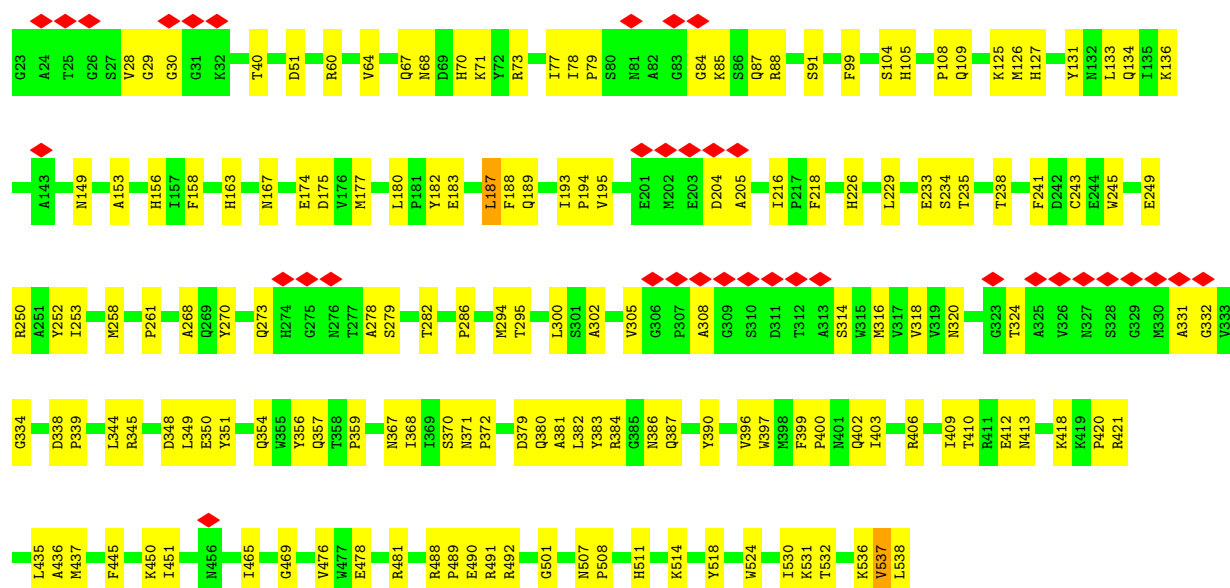




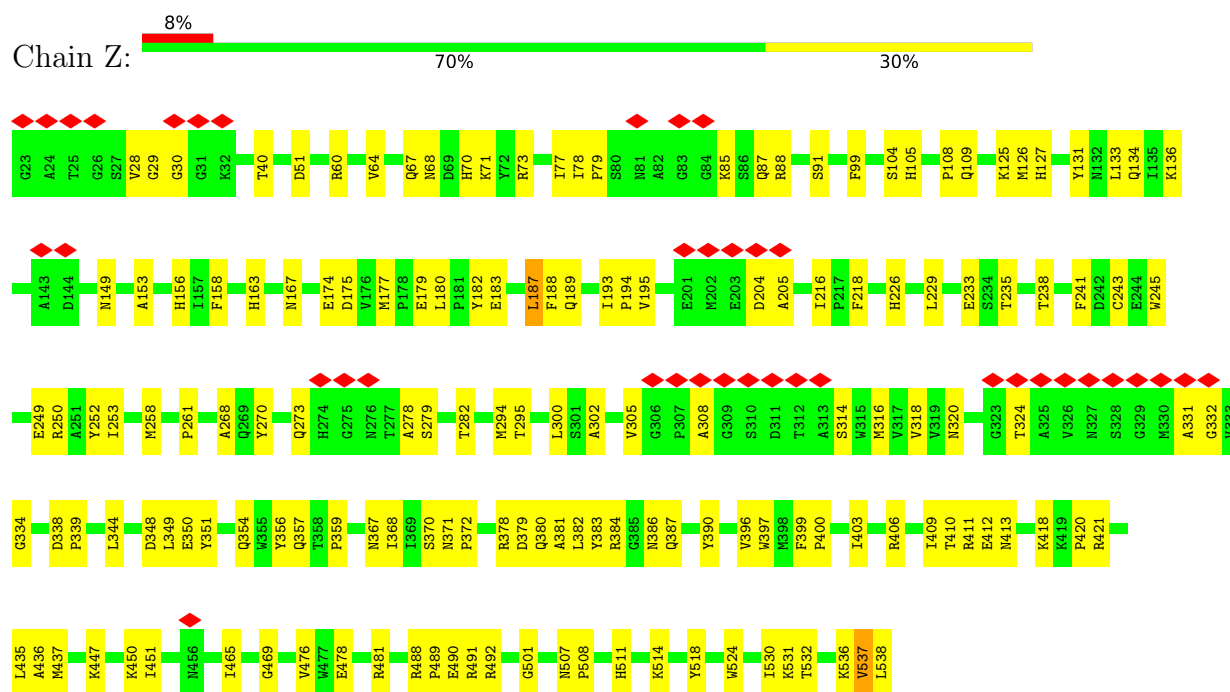
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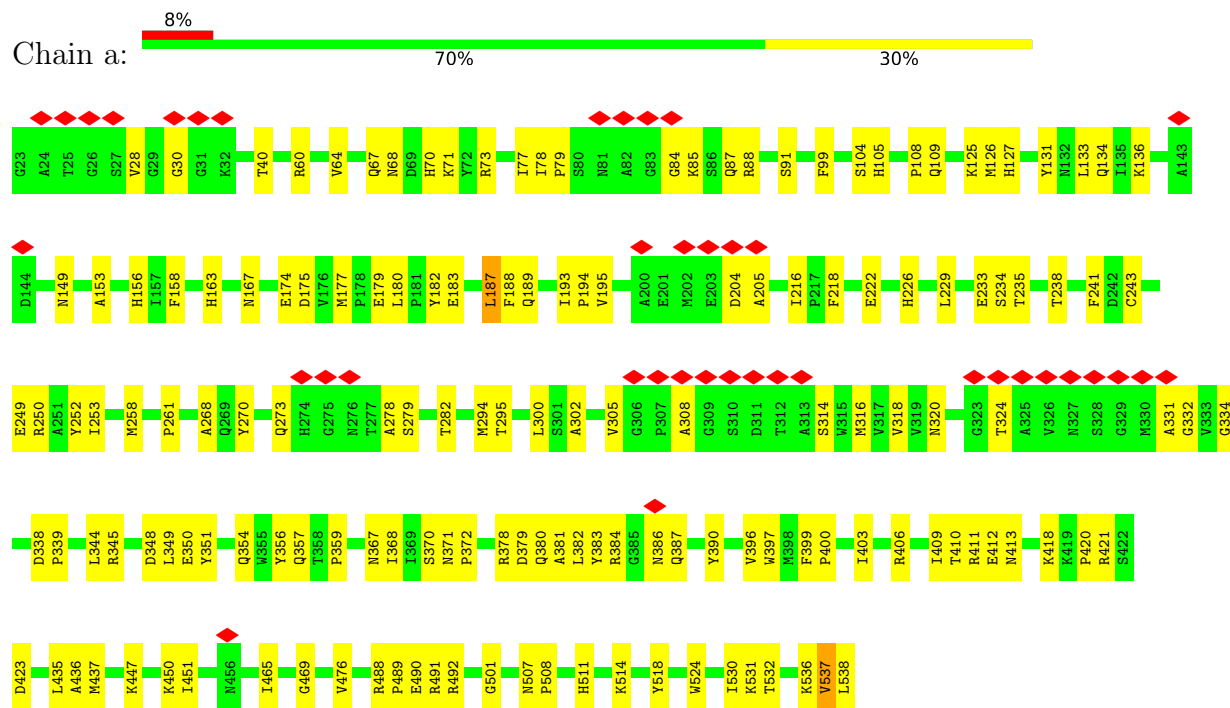
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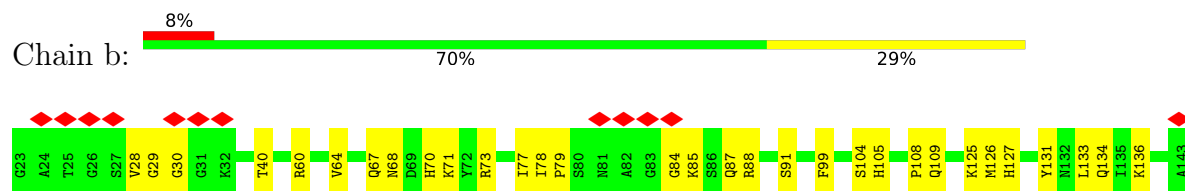
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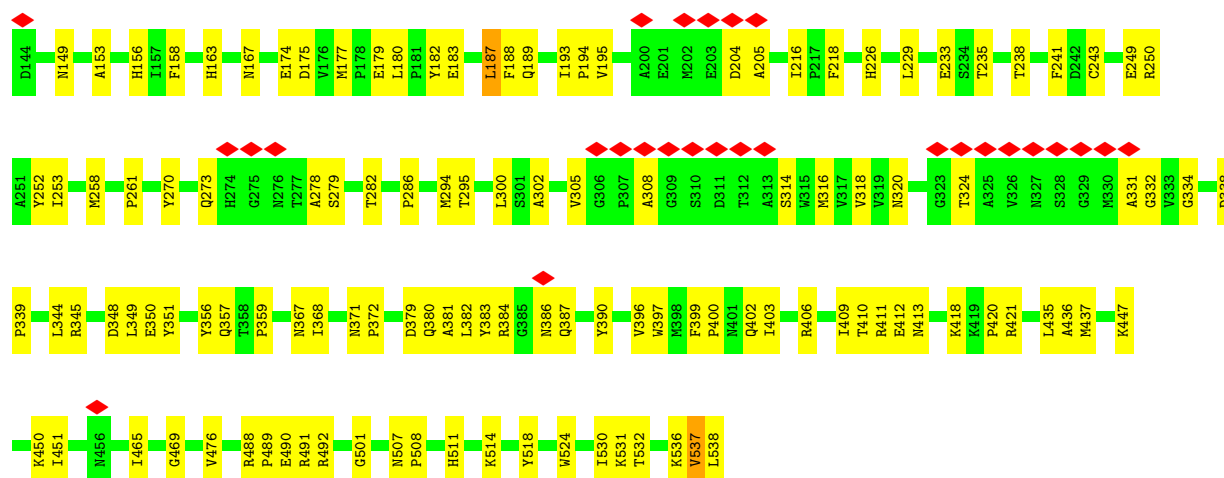


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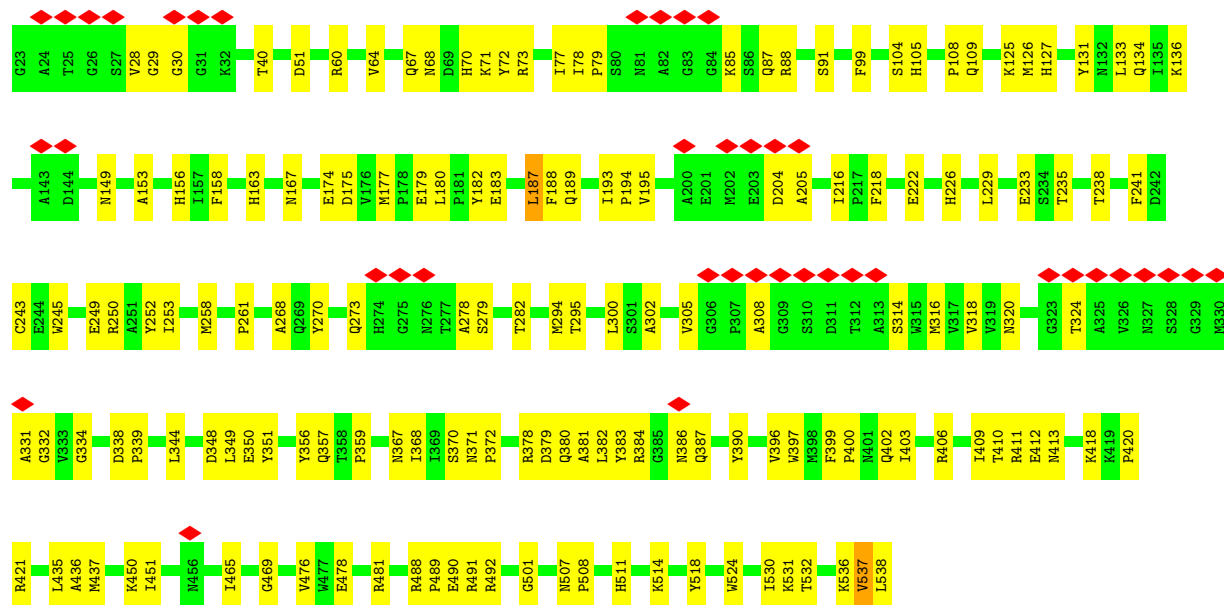


- Molecule 1: VP2

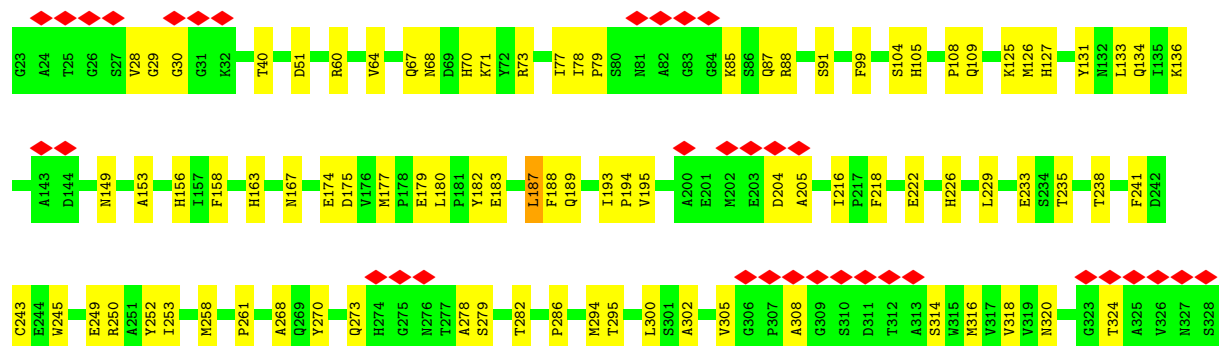


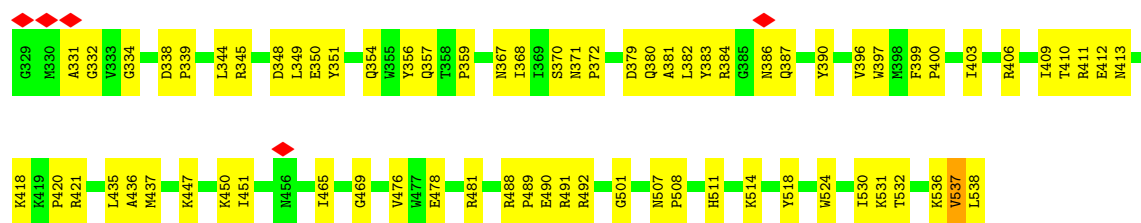


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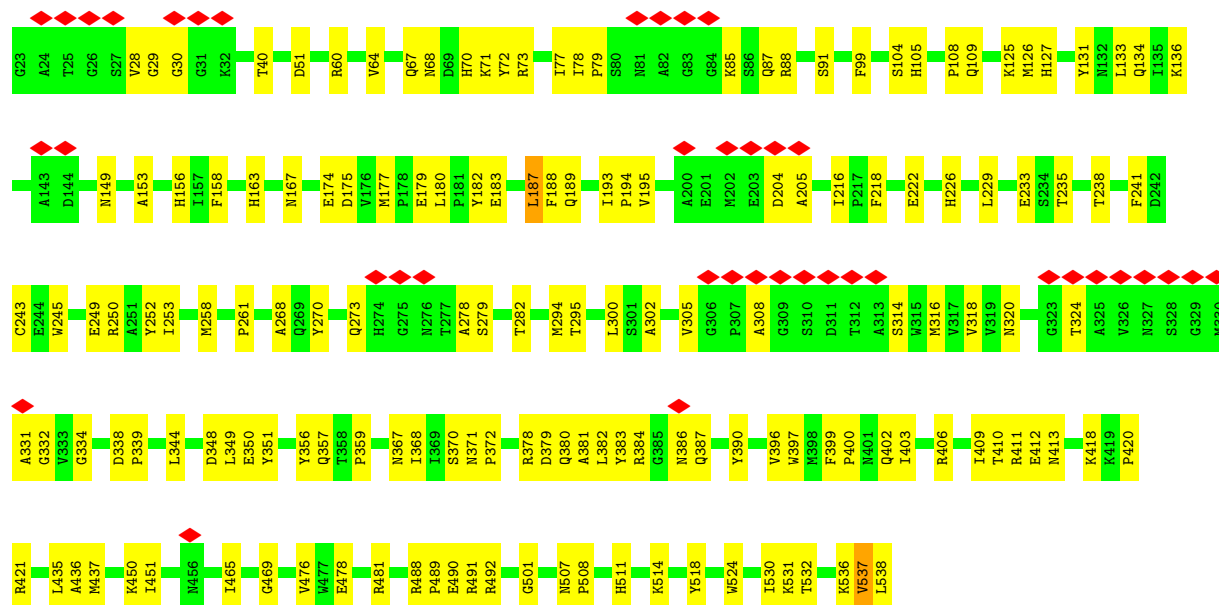


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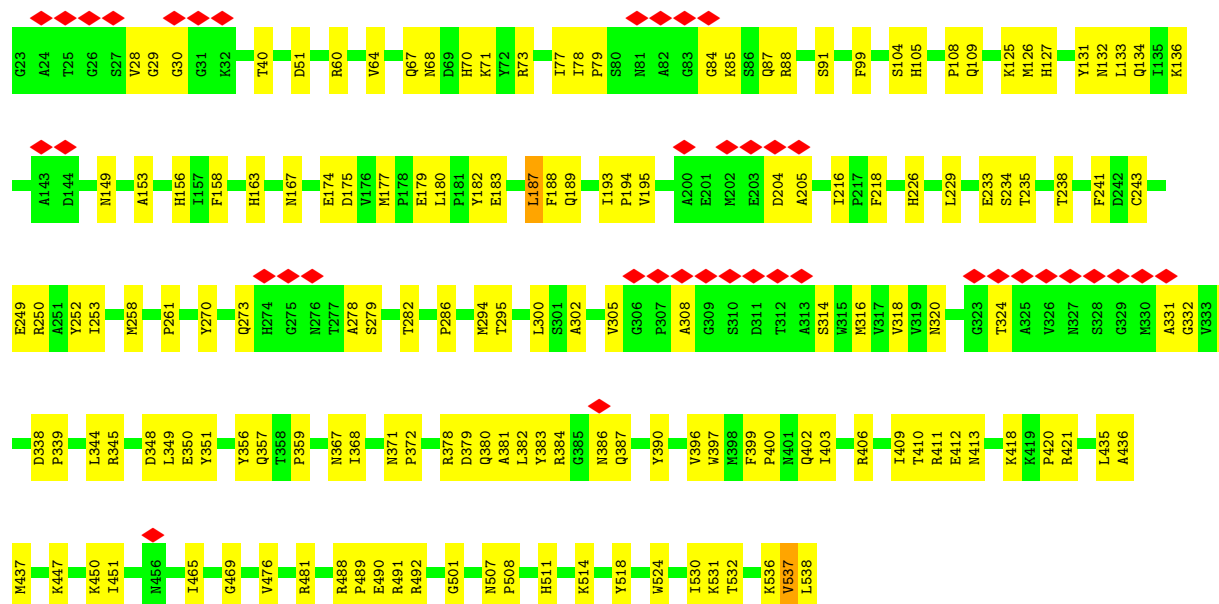




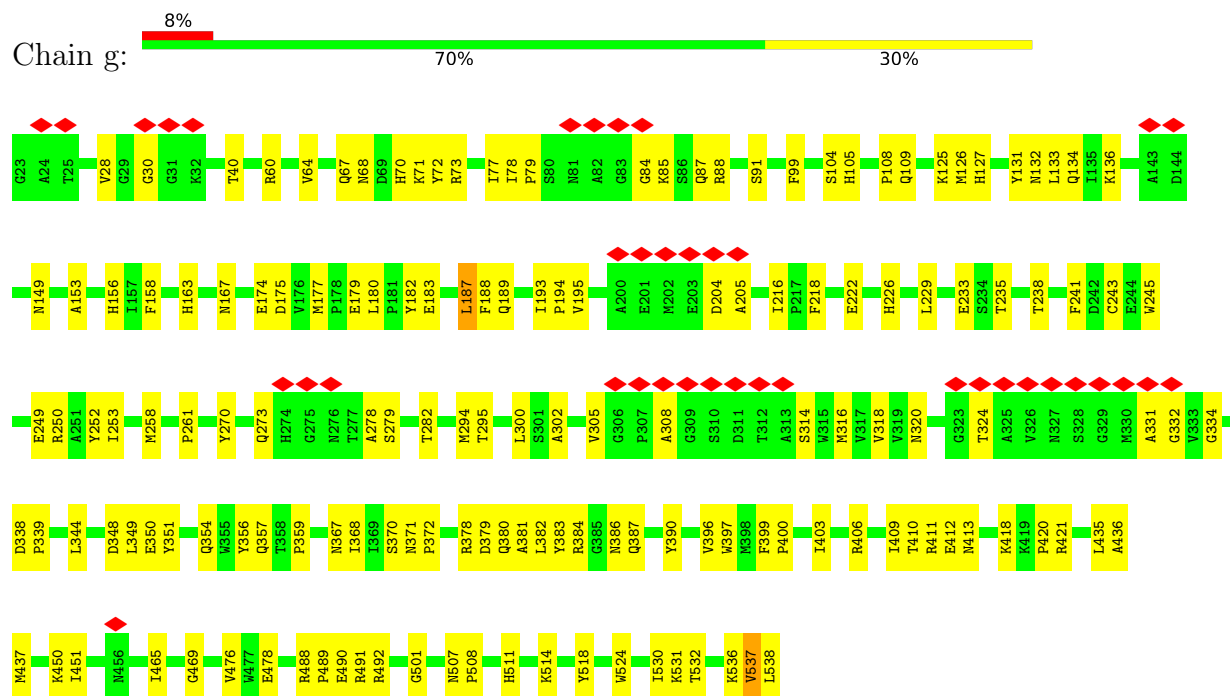
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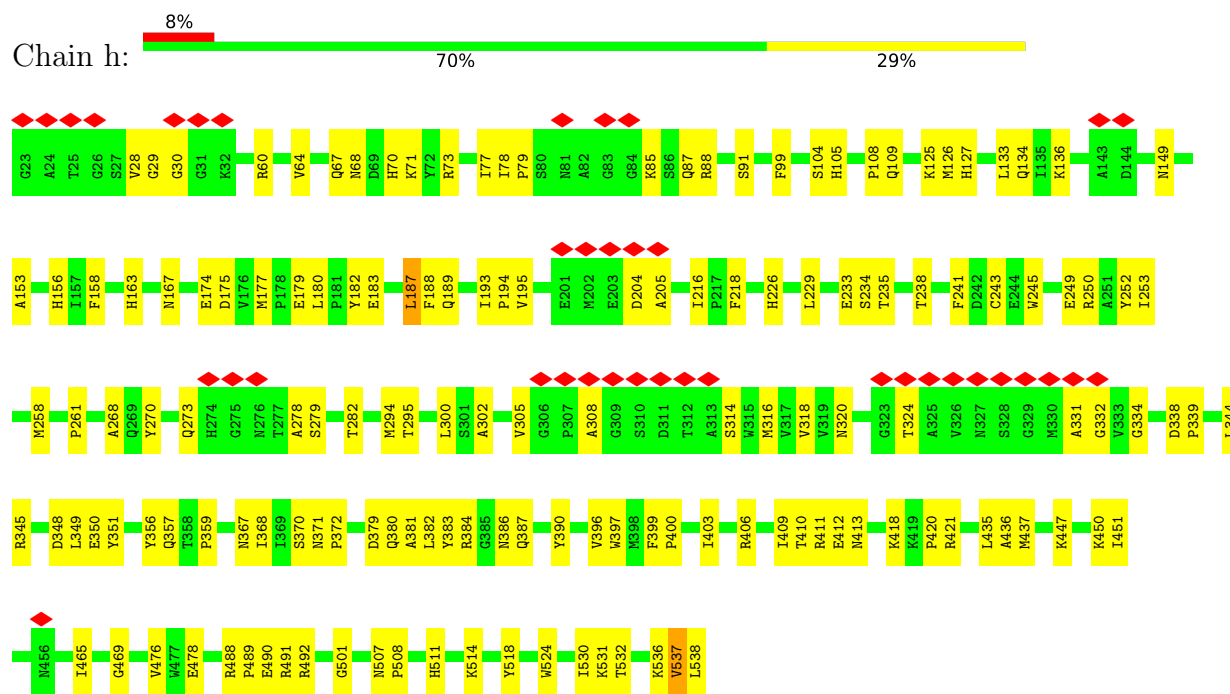
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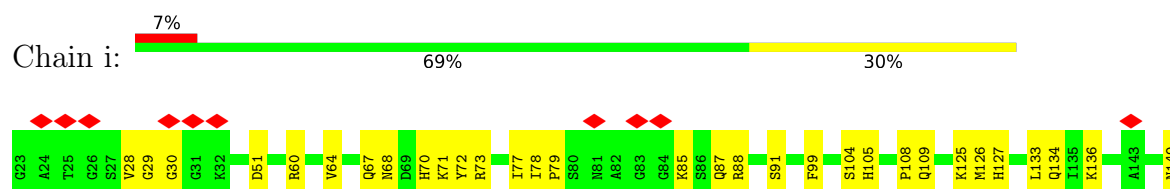
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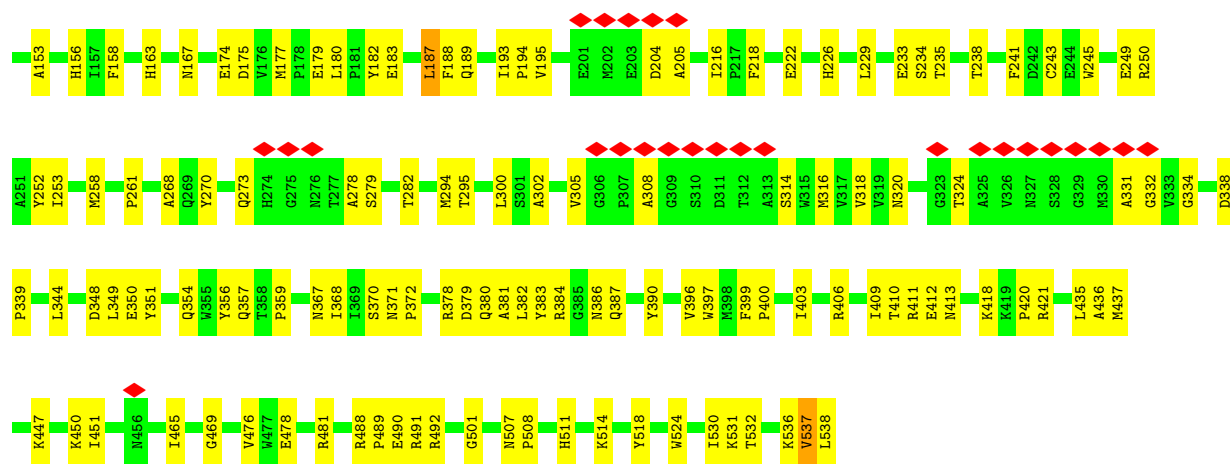


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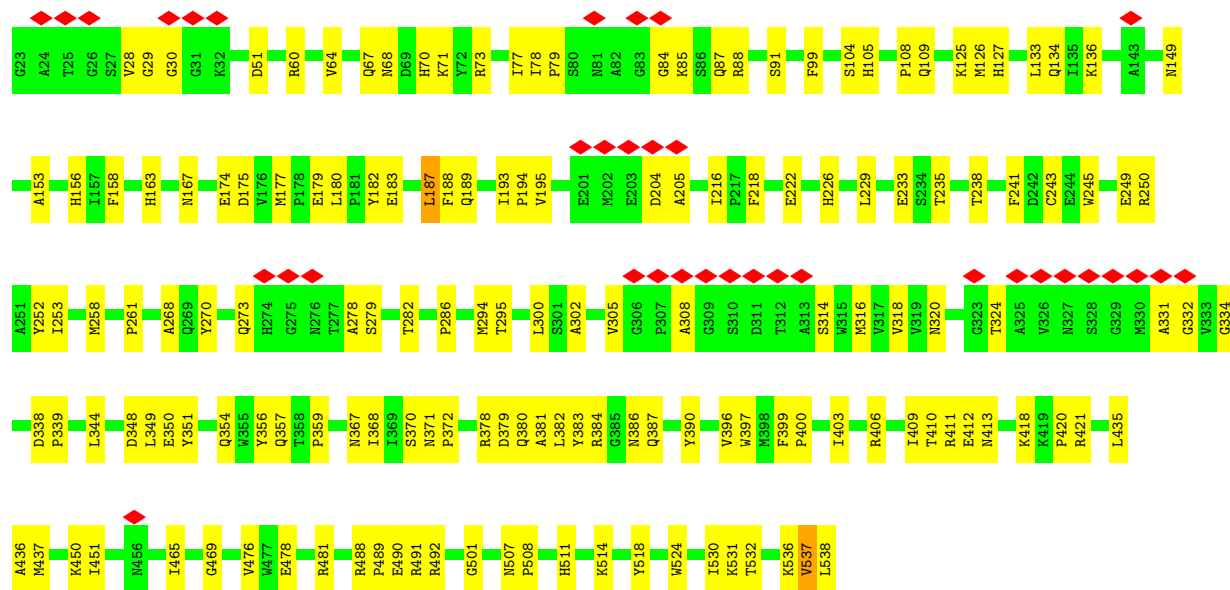


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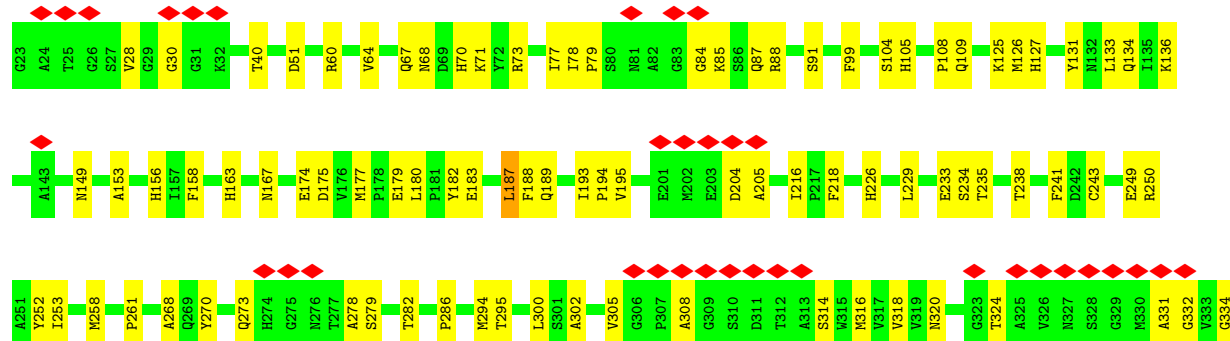


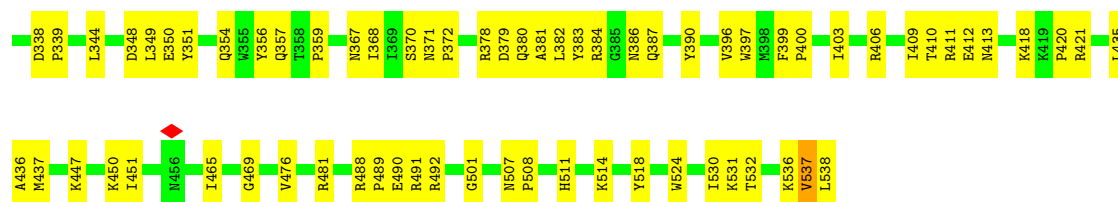


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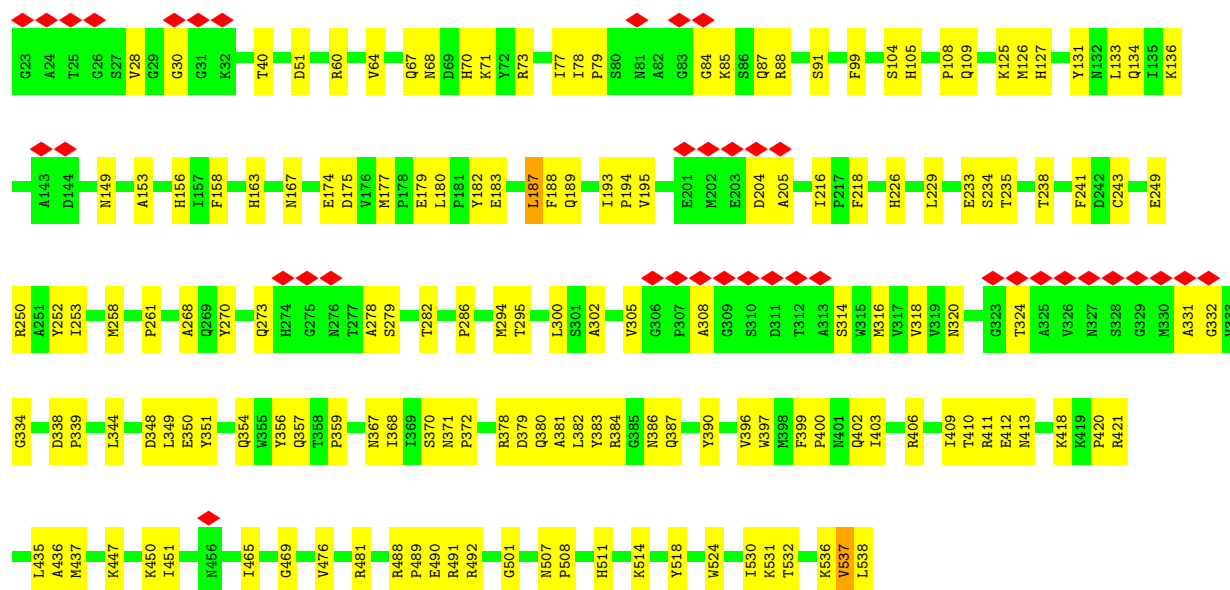


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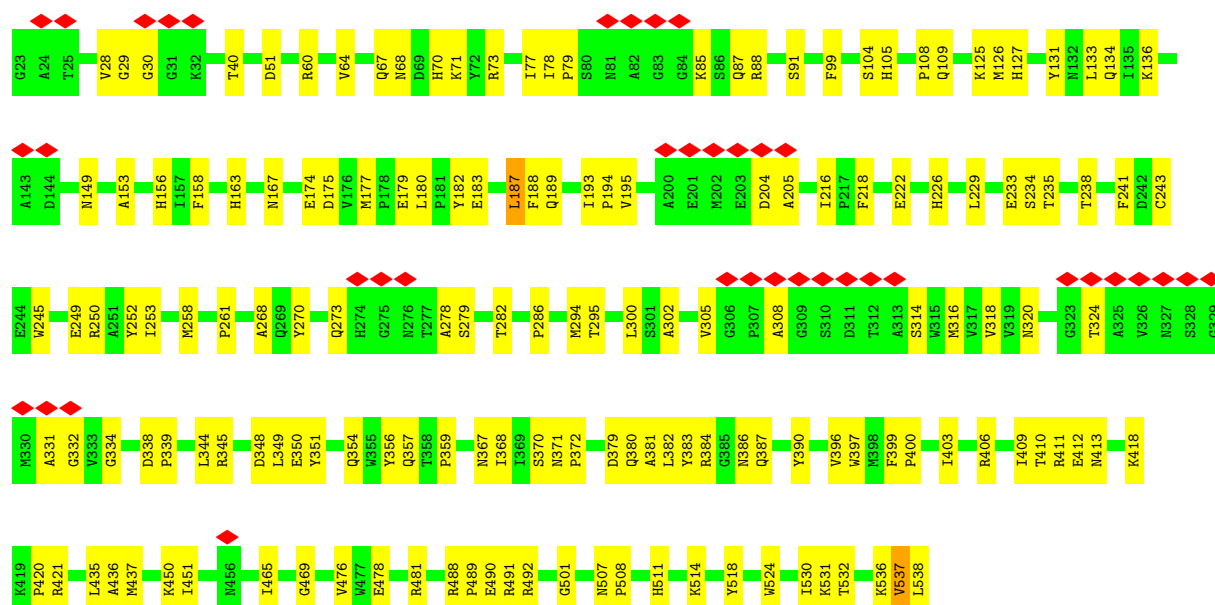




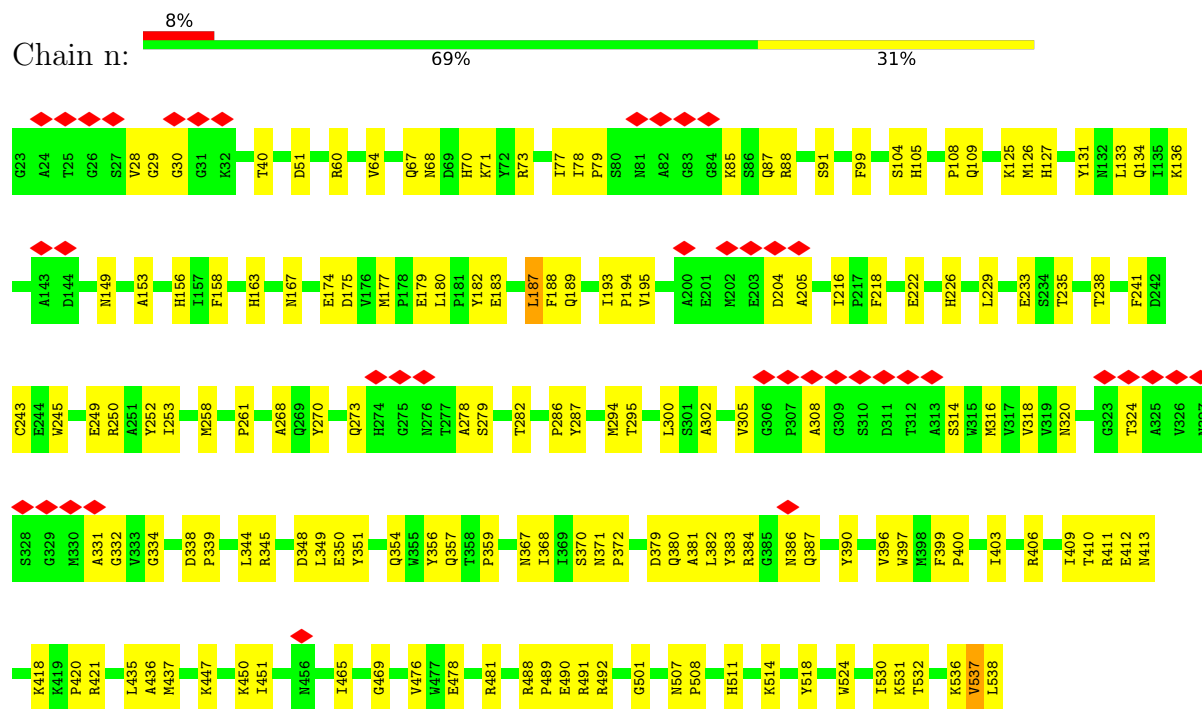
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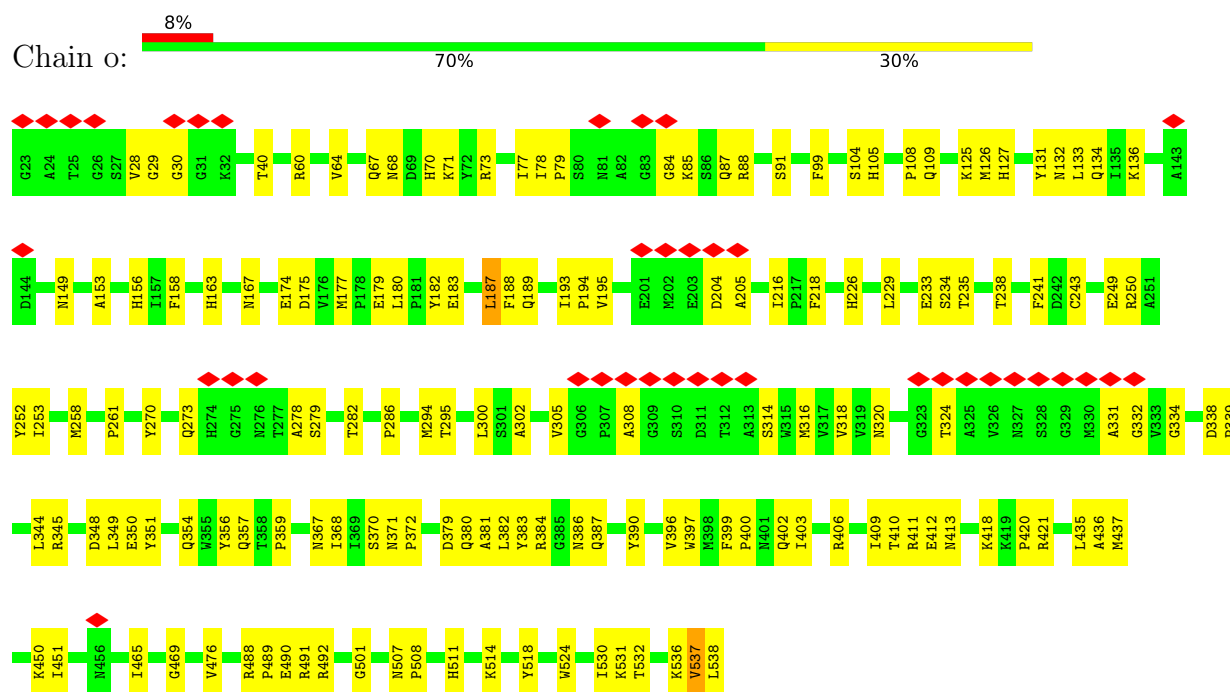
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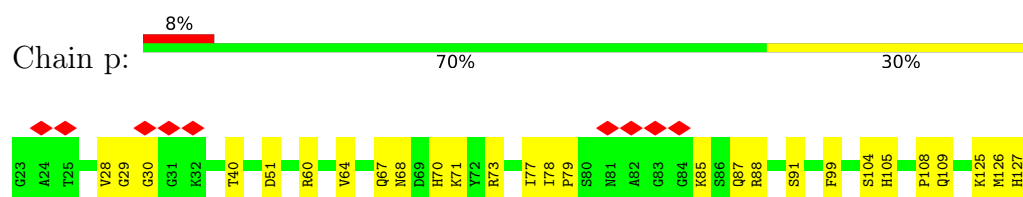
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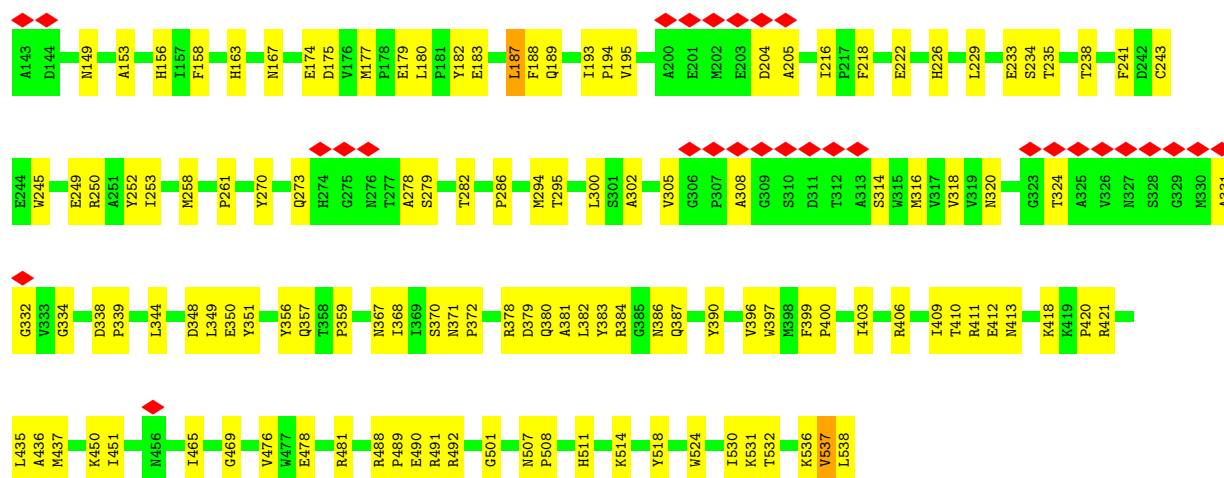


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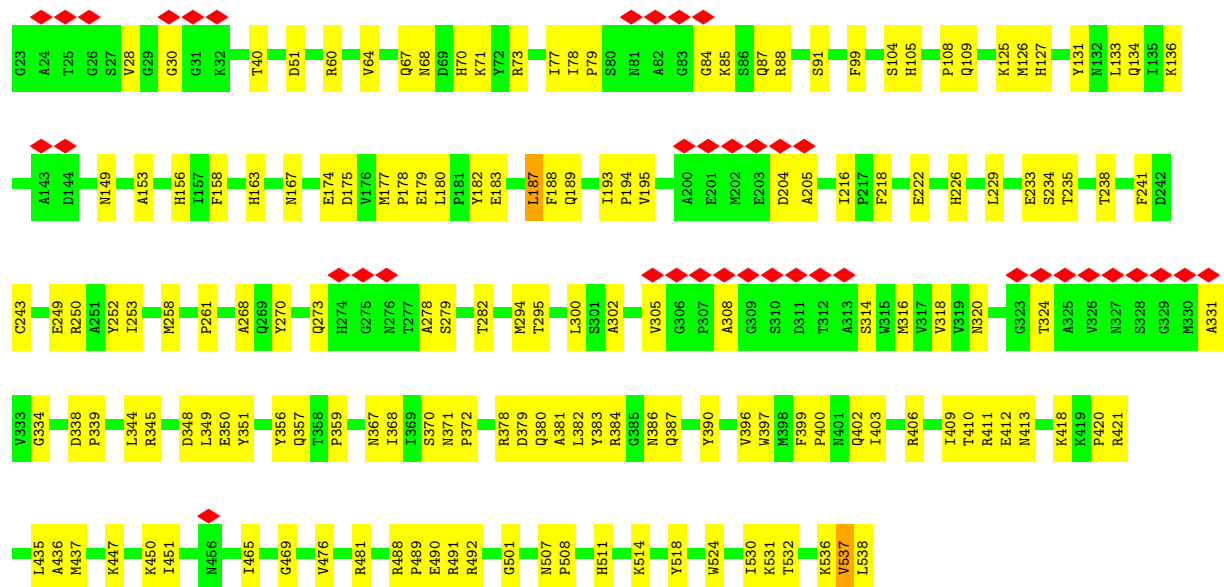


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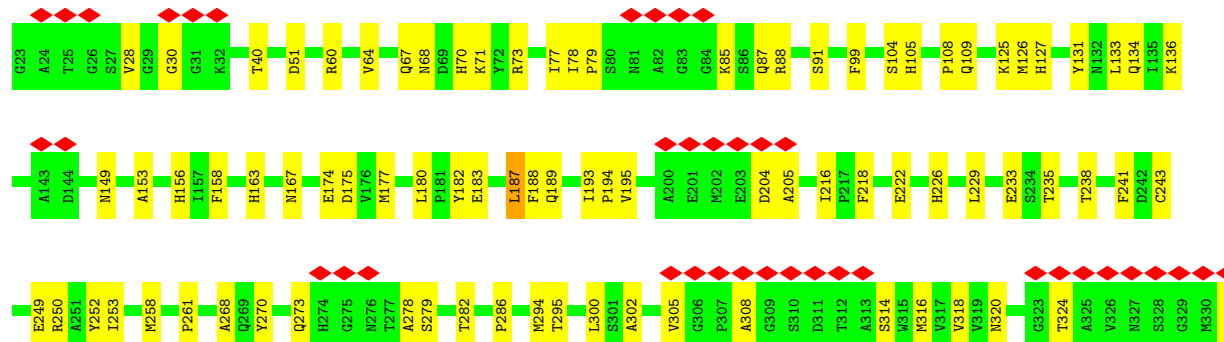


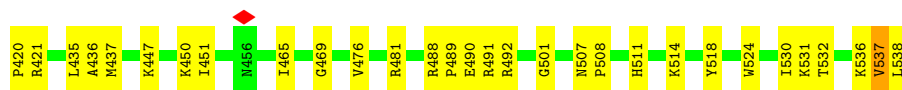
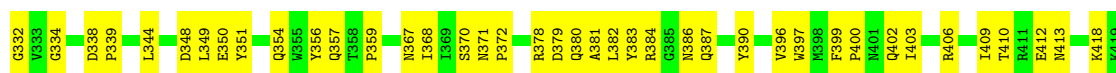


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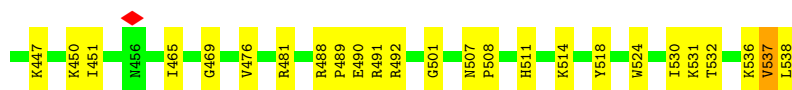
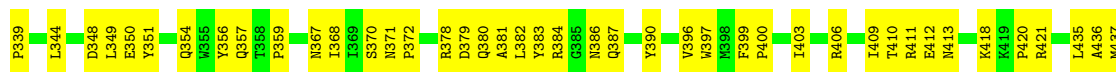
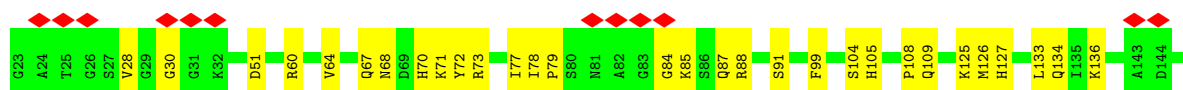


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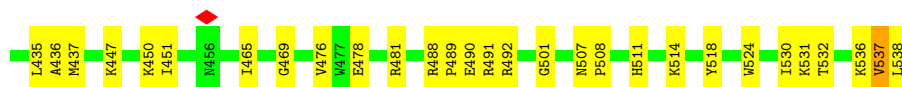
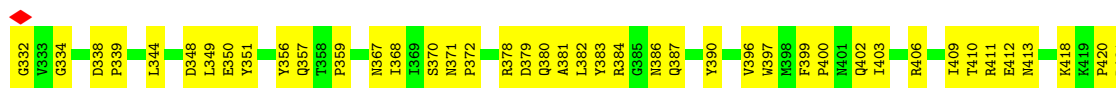
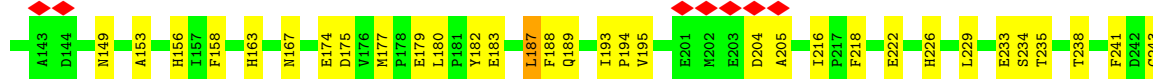
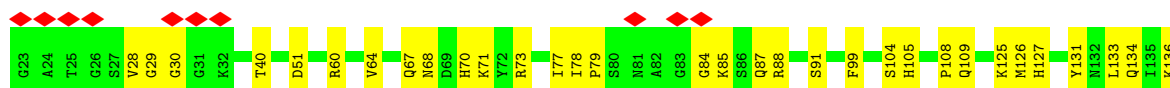




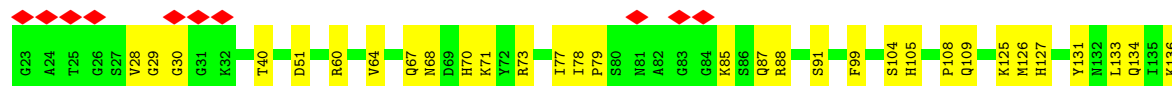
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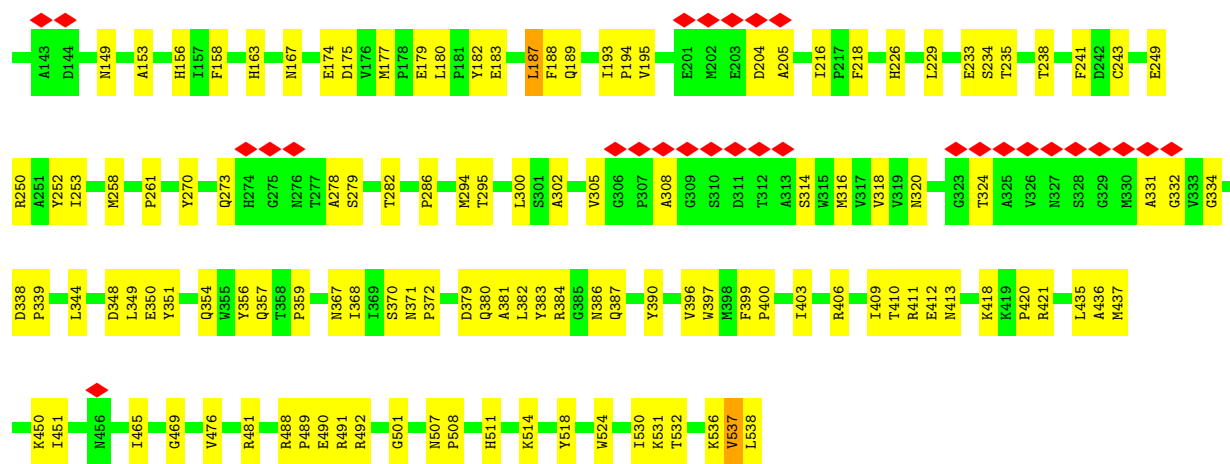


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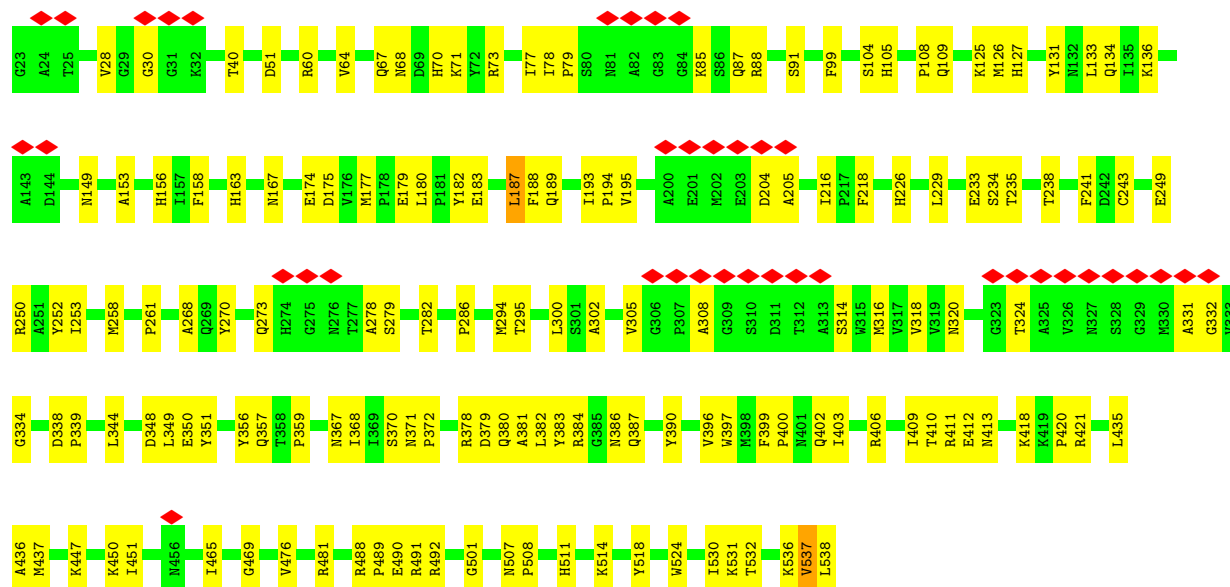


Chain u: 

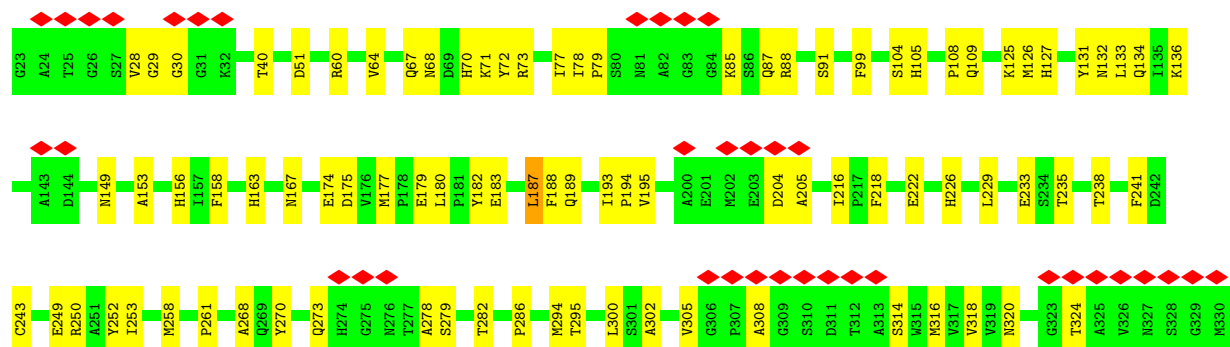


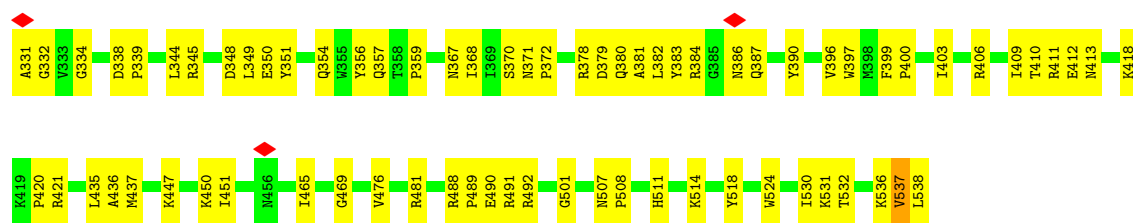


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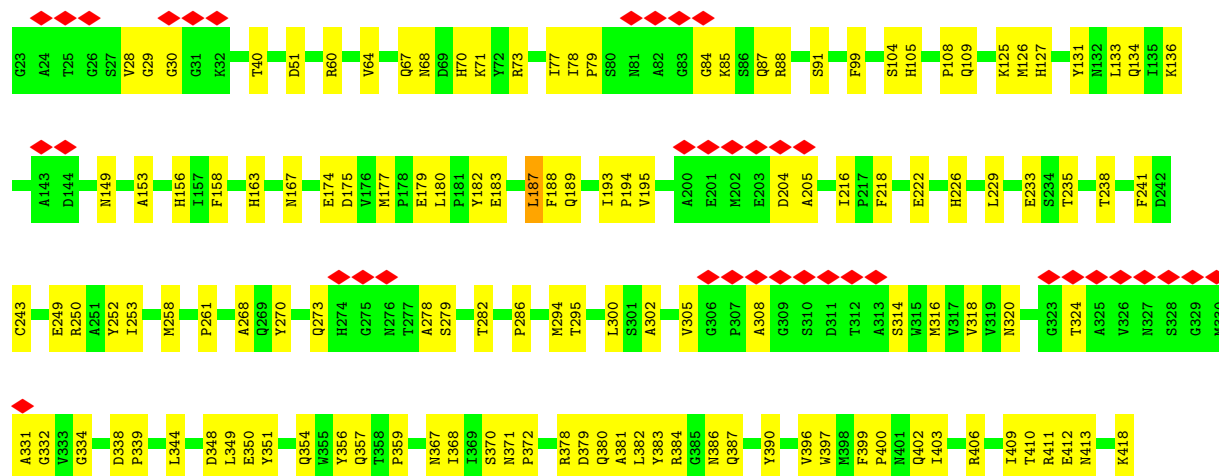


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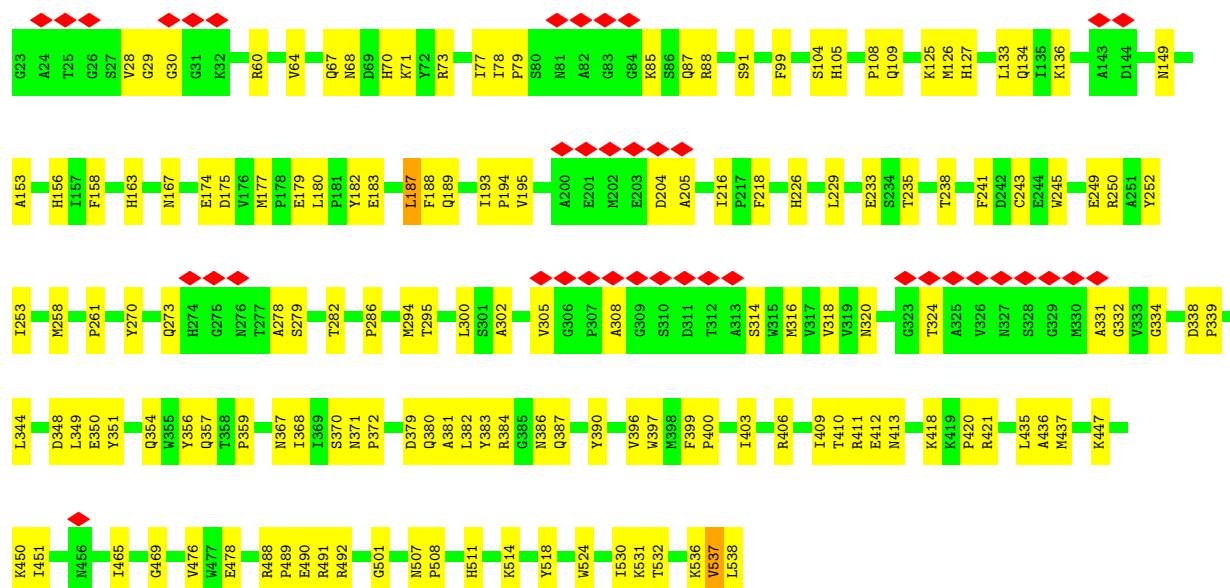




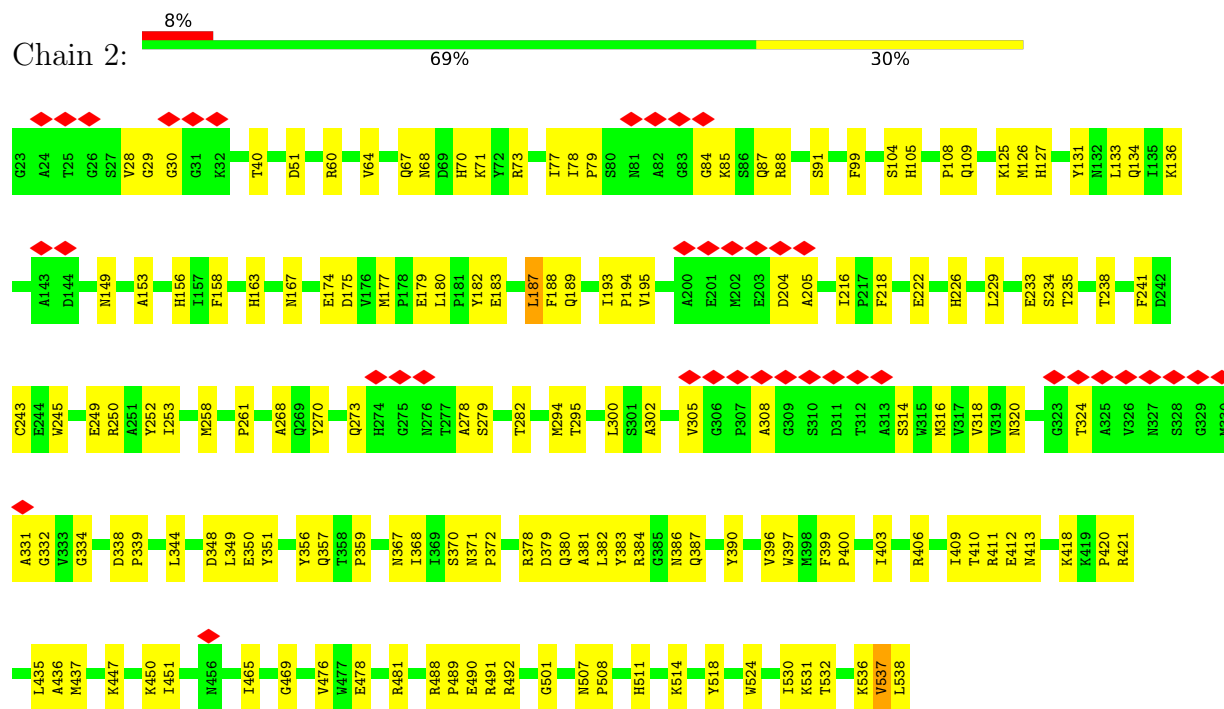
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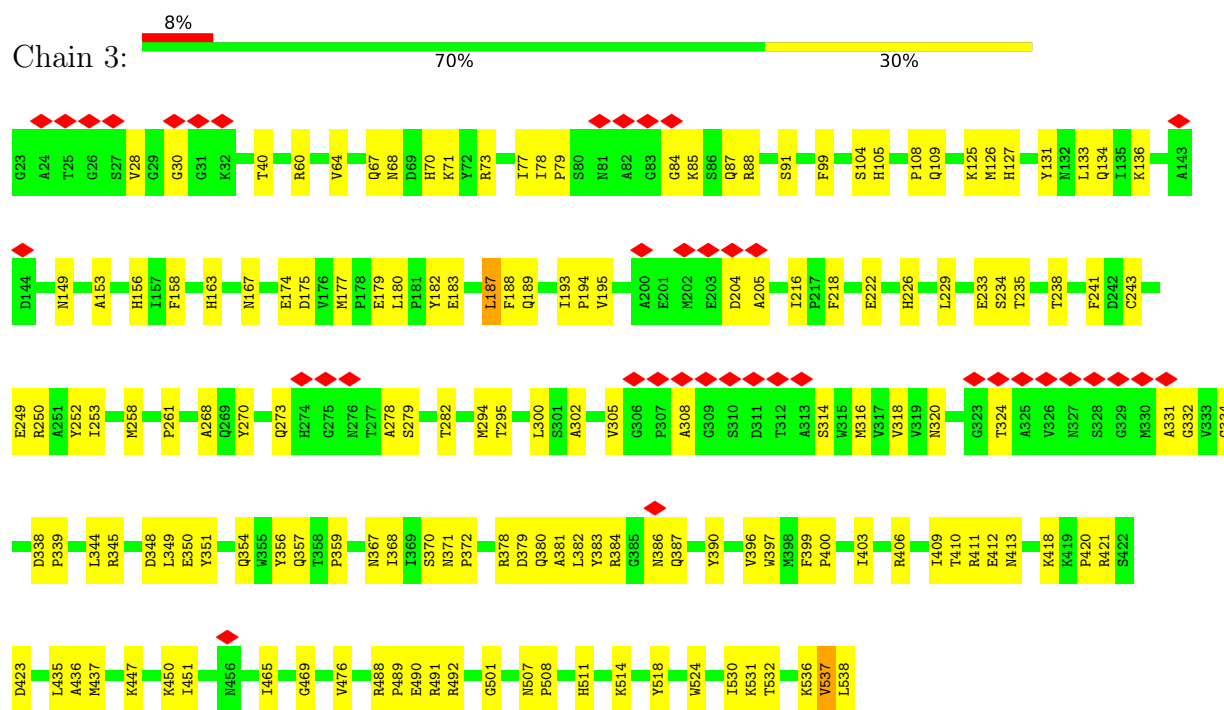
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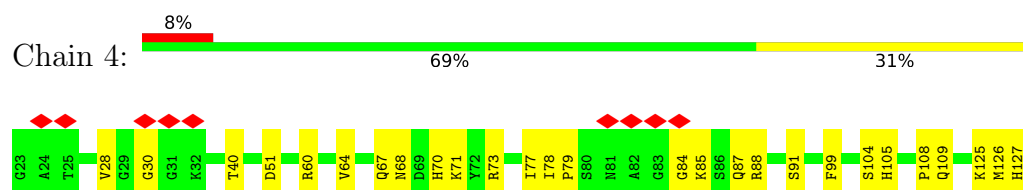
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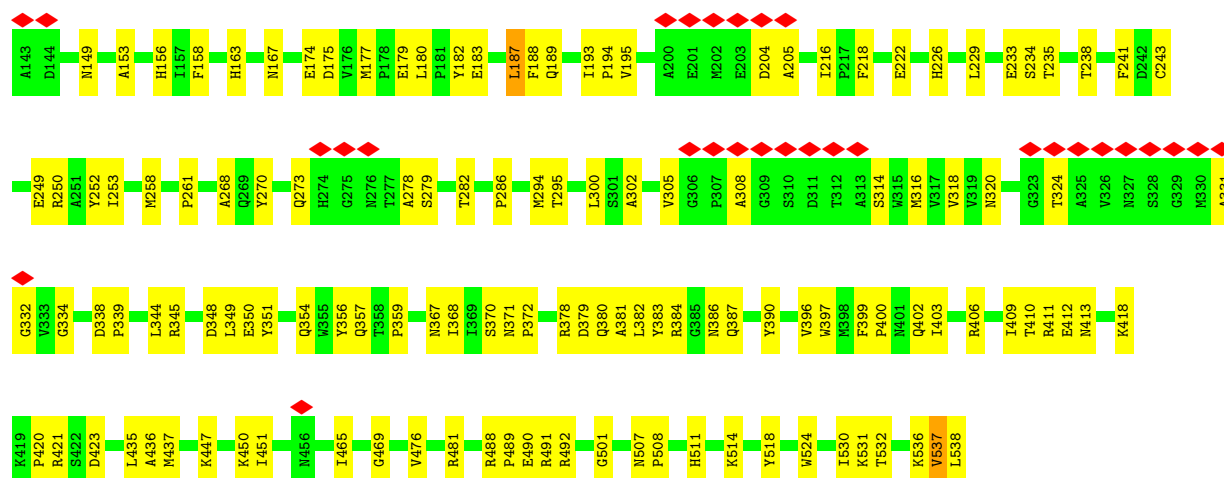


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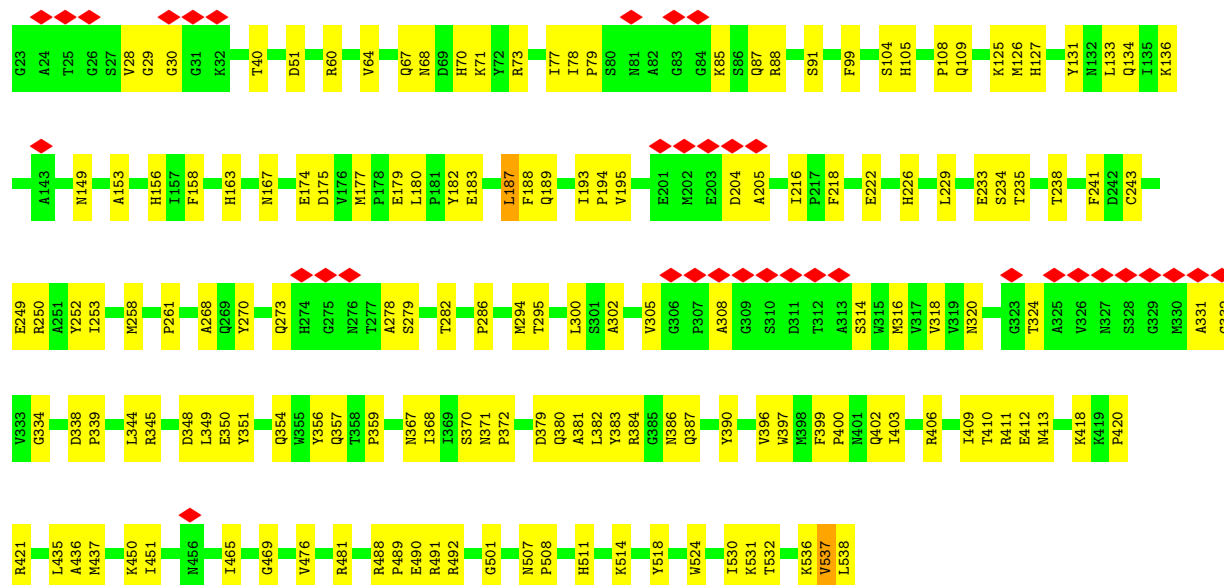


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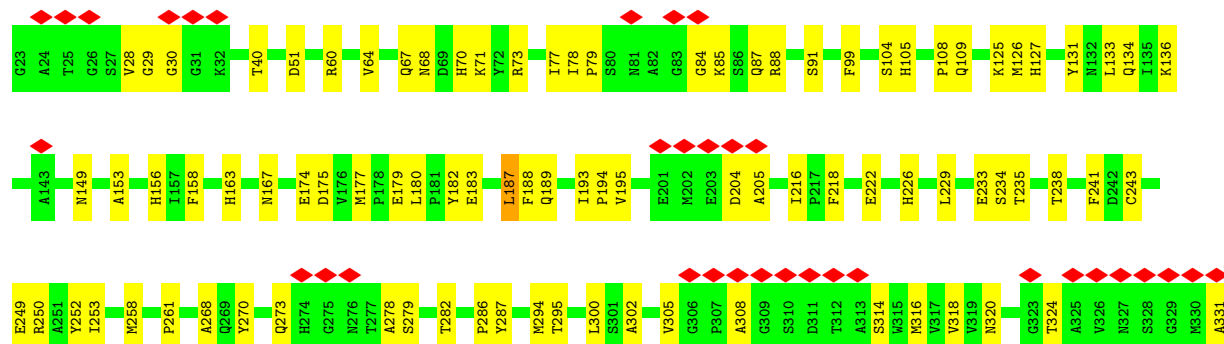


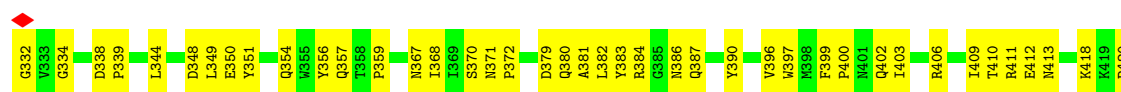


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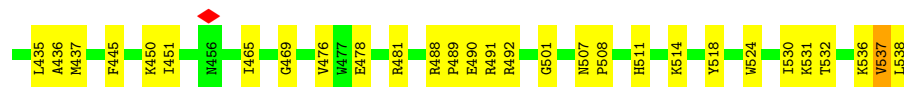
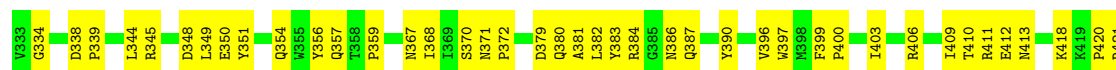
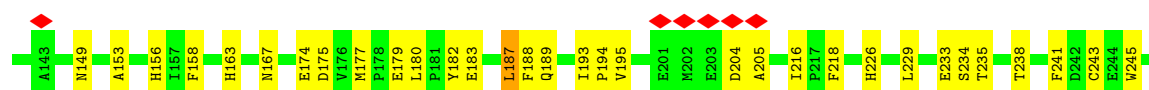
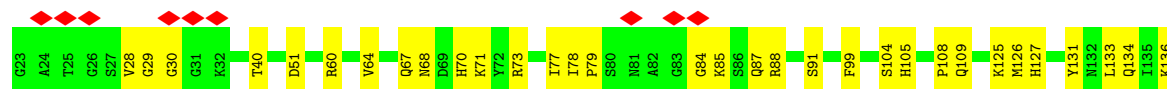


• Molecule 1: VP2

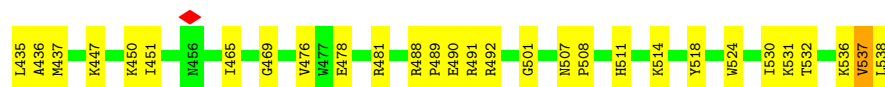
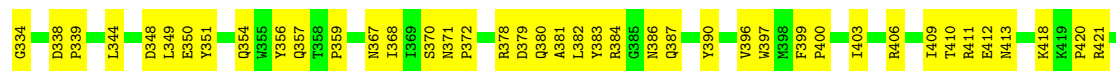
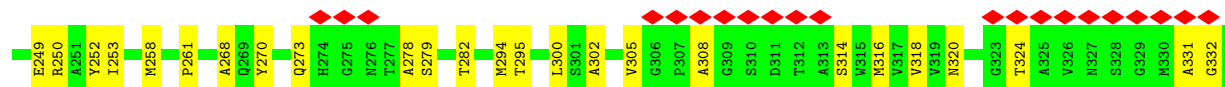
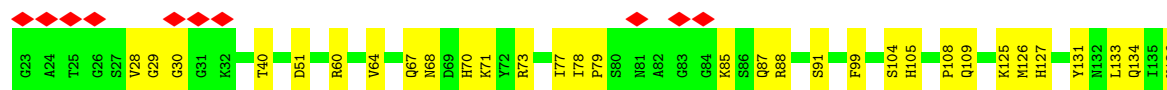




• Molecule 1: VP2



• Molecule 1: VP2



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 19648                                   | 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 ( $e^-/\text{\AA}^2$ ) | 64                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 18.698                                  | Depositor |
| Minimum map value                    | -10.397                                 | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 1.5                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 406.35, 406.35, 406.35                  | wwPDB     |
| Map dimensions                       | 450, 450, 450                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.903, 0.903, 0.903                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | 1     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | 2     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | 3     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | 4     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | 5     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | 6     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | 7     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | 8     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | A     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | B     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | C     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | D     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | E     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | F     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | G     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | H     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | I     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | J     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | K     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | L     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | M     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | N     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | O     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | P     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | Q     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | R     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | S     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | T     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | U     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | V     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | W     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | X     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | Y     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |
| 1   | Z     | 0.40         | 0/4232      | 0.59        | 2/5771 (0.0%) |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 1   | a     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | b     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | c     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | d     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | e     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | f     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | g     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | h     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | i     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | j     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | k     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | l     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | m     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | n     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | o     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | p     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | q     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | r     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | s     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | t     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | u     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | v     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | w     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | x     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | y     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| 1   | z     | 0.40         | 0/4232   | 0.59        | 2/5771 (0.0%)     |
| All | All   | 0.40         | 0/253920 | 0.59        | 120/346260 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 1     | 0                   | 1                   |
| 1   | 2     | 0                   | 1                   |
| 1   | 3     | 0                   | 1                   |
| 1   | 4     | 0                   | 1                   |
| 1   | 5     | 0                   | 1                   |
| 1   | 6     | 0                   | 1                   |
| 1   | 7     | 0                   | 1                   |
| 1   | 8     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| 1   | H     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 1   | J     | 0                   | 1                   |
| 1   | K     | 0                   | 1                   |
| 1   | L     | 0                   | 1                   |
| 1   | M     | 0                   | 1                   |
| 1   | N     | 0                   | 1                   |
| 1   | O     | 0                   | 1                   |
| 1   | P     | 0                   | 1                   |
| 1   | Q     | 0                   | 1                   |
| 1   | R     | 0                   | 1                   |
| 1   | S     | 0                   | 1                   |
| 1   | T     | 0                   | 1                   |
| 1   | U     | 0                   | 1                   |
| 1   | V     | 0                   | 1                   |
| 1   | W     | 0                   | 1                   |
| 1   | X     | 0                   | 1                   |
| 1   | Y     | 0                   | 1                   |
| 1   | Z     | 0                   | 1                   |
| 1   | a     | 0                   | 1                   |
| 1   | b     | 0                   | 1                   |
| 1   | c     | 0                   | 1                   |
| 1   | d     | 0                   | 1                   |
| 1   | e     | 0                   | 1                   |
| 1   | f     | 0                   | 1                   |
| 1   | g     | 0                   | 1                   |
| 1   | h     | 0                   | 1                   |
| 1   | i     | 0                   | 1                   |
| 1   | j     | 0                   | 1                   |
| 1   | k     | 0                   | 1                   |
| 1   | l     | 0                   | 1                   |
| 1   | m     | 0                   | 1                   |
| 1   | n     | 0                   | 1                   |
| 1   | o     | 0                   | 1                   |
| 1   | p     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | q     | 0                   | 1                   |
| 1   | r     | 0                   | 1                   |
| 1   | s     | 0                   | 1                   |
| 1   | t     | 0                   | 1                   |
| 1   | u     | 0                   | 1                   |
| 1   | v     | 0                   | 1                   |
| 1   | w     | 0                   | 1                   |
| 1   | x     | 0                   | 1                   |
| 1   | y     | 0                   | 1                   |
| 1   | z     | 0                   | 1                   |
| All | All   | 0                   | 60                  |

There are no bond length outliers.

All (120) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | V     | 537 | VAL  | O-C-N | -11.12 | 109.37      | 122.94   |
| 1   | g     | 537 | VAL  | O-C-N | -11.12 | 109.37      | 122.94   |
| 1   | p     | 537 | VAL  | O-C-N | -11.12 | 109.37      | 122.94   |
| 1   | L     | 537 | VAL  | O-C-N | -11.12 | 109.37      | 122.94   |
| 1   | B     | 537 | VAL  | O-C-N | -11.11 | 109.39      | 122.94   |
| 1   | O     | 537 | VAL  | O-C-N | -11.10 | 109.41      | 122.94   |
| 1   | Z     | 537 | VAL  | O-C-N | -11.10 | 109.41      | 122.94   |
| 1   | d     | 537 | VAL  | O-C-N | -11.10 | 109.40      | 122.94   |
| 1   | l     | 537 | VAL  | O-C-N | -11.10 | 109.41      | 122.94   |
| 1   | n     | 537 | VAL  | O-C-N | -11.10 | 109.40      | 122.94   |
| 1   | 3     | 537 | VAL  | O-C-N | -11.10 | 109.40      | 122.94   |
| 1   | 8     | 537 | VAL  | O-C-N | -11.10 | 109.41      | 122.94   |
| 1   | C     | 537 | VAL  | O-C-N | -11.09 | 109.41      | 122.94   |
| 1   | Q     | 537 | VAL  | O-C-N | -11.09 | 109.41      | 122.94   |
| 1   | c     | 537 | VAL  | O-C-N | -11.09 | 109.41      | 122.94   |
| 1   | e     | 537 | VAL  | O-C-N | -11.09 | 109.41      | 122.94   |
| 1   | f     | 537 | VAL  | O-C-N | -11.09 | 109.41      | 122.94   |
| 1   | u     | 537 | VAL  | O-C-N | -11.09 | 109.41      | 122.94   |
| 1   | x     | 537 | VAL  | O-C-N | -11.09 | 109.41      | 122.94   |
| 1   | E     | 537 | VAL  | O-C-N | -11.08 | 109.42      | 122.94   |
| 1   | G     | 537 | VAL  | O-C-N | -11.08 | 109.42      | 122.94   |
| 1   | H     | 537 | VAL  | O-C-N | -11.08 | 109.42      | 122.94   |
| 1   | I     | 537 | VAL  | O-C-N | -11.08 | 109.42      | 122.94   |
| 1   | P     | 537 | VAL  | O-C-N | -11.08 | 109.42      | 122.94   |
| 1   | j     | 537 | VAL  | O-C-N | -11.08 | 109.42      | 122.94   |
| 1   | 5     | 537 | VAL  | O-C-N | -11.08 | 109.42      | 122.94   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | t     | 537 | VAL  | O-C-N  | -11.08 | 109.42      | 122.94   |
| 1   | w     | 537 | VAL  | O-C-N  | -11.08 | 109.42      | 122.94   |
| 1   | A     | 537 | VAL  | O-C-N  | -11.08 | 109.42      | 122.94   |
| 1   | F     | 537 | VAL  | O-C-N  | -11.08 | 109.42      | 122.94   |
| 1   | a     | 537 | VAL  | O-C-N  | -11.08 | 109.42      | 122.94   |
| 1   | v     | 537 | VAL  | O-C-N  | -11.08 | 109.42      | 122.94   |
| 1   | y     | 537 | VAL  | O-C-N  | -11.08 | 109.42      | 122.94   |
| 1   | U     | 537 | VAL  | O-C-N  | -11.07 | 109.43      | 122.94   |
| 1   | z     | 537 | VAL  | O-C-N  | -11.07 | 109.44      | 122.94   |
| 1   | S     | 537 | VAL  | O-C-N  | -11.06 | 109.44      | 122.94   |
| 1   | r     | 537 | VAL  | O-C-N  | -11.06 | 109.44      | 122.94   |
| 1   | 2     | 537 | VAL  | O-C-N  | -11.06 | 109.44      | 122.94   |
| 1   | K     | 537 | VAL  | O-C-N  | -11.06 | 109.45      | 122.94   |
| 1   | T     | 537 | VAL  | O-C-N  | -11.06 | 109.45      | 122.94   |
| 1   | m     | 537 | VAL  | O-C-N  | -11.06 | 109.45      | 122.94   |
| 1   | 4     | 537 | VAL  | O-C-N  | -11.06 | 109.45      | 122.94   |
| 1   | N     | 537 | VAL  | O-C-N  | -11.05 | 109.46      | 122.94   |
| 1   | Y     | 537 | VAL  | O-C-N  | -11.05 | 109.46      | 122.94   |
| 1   | i     | 537 | VAL  | O-C-N  | -11.05 | 109.46      | 122.94   |
| 1   | 7     | 537 | VAL  | O-C-N  | -11.05 | 109.46      | 122.94   |
| 1   | J     | 537 | VAL  | O-C-N  | -11.05 | 109.46      | 122.94   |
| 1   | b     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | M     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | R     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | X     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | h     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | o     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | q     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | l     | 537 | VAL  | O-C-N  | -11.04 | 109.47      | 122.94   |
| 1   | s     | 537 | VAL  | O-C-N  | -11.03 | 109.48      | 122.94   |
| 1   | D     | 537 | VAL  | O-C-N  | -11.03 | 109.49      | 122.94   |
| 1   | W     | 537 | VAL  | O-C-N  | -11.03 | 109.49      | 122.94   |
| 1   | k     | 537 | VAL  | O-C-N  | -11.03 | 109.49      | 122.94   |
| 1   | 6     | 537 | VAL  | O-C-N  | -11.03 | 109.49      | 122.94   |
| 1   | B     | 187 | LEU  | N-CA-C | 5.57   | 118.14      | 110.35   |
| 1   | K     | 187 | LEU  | N-CA-C | 5.56   | 118.13      | 110.35   |
| 1   | C     | 187 | LEU  | N-CA-C | 5.56   | 118.13      | 110.35   |
| 1   | V     | 187 | LEU  | N-CA-C | 5.56   | 118.13      | 110.35   |
| 1   | a     | 187 | LEU  | N-CA-C | 5.56   | 118.13      | 110.35   |
| 1   | g     | 187 | LEU  | N-CA-C | 5.56   | 118.13      | 110.35   |
| 1   | p     | 187 | LEU  | N-CA-C | 5.56   | 118.13      | 110.35   |
| 1   | I     | 187 | LEU  | N-CA-C | 5.55   | 118.12      | 110.35   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | M     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | W     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | X     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | h     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | k     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | o     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | 6     | 187 | LEU  | N-CA-C | 5.55 | 118.12      | 110.35   |
| 1   | H     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | O     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | P     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | Z     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | j     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | l     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | 1     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | 5     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | 8     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | N     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | Y     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | i     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | 7     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | A     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | F     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | v     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | y     | 187 | LEU  | N-CA-C | 5.54 | 118.11      | 110.35   |
| 1   | Q     | 187 | LEU  | N-CA-C | 5.54 | 118.10      | 110.35   |
| 1   | u     | 187 | LEU  | N-CA-C | 5.54 | 118.10      | 110.35   |
| 1   | x     | 187 | LEU  | N-CA-C | 5.54 | 118.10      | 110.35   |
| 1   | U     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | s     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | z     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | 2     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | L     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | R     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | S     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | q     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | r     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | E     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | G     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | t     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | w     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | b     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | c     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | d     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | e     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | f     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | n     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | 3     | 187 | LEU  | N-CA-C | 5.52 | 118.08      | 110.35   |
| 1   | J     | 187 | LEU  | N-CA-C | 5.52 | 118.07      | 110.35   |
| 1   | T     | 187 | LEU  | N-CA-C | 5.52 | 118.07      | 110.35   |
| 1   | m     | 187 | LEU  | N-CA-C | 5.52 | 118.07      | 110.35   |
| 1   | 4     | 187 | LEU  | N-CA-C | 5.52 | 118.07      | 110.35   |

There are no chirality outliers.

All (60) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 1     | 537 | VAL  | Mainchain |
| 1   | 2     | 537 | VAL  | Mainchain |
| 1   | 3     | 537 | VAL  | Mainchain |
| 1   | 4     | 537 | VAL  | Mainchain |
| 1   | 5     | 537 | VAL  | Mainchain |
| 1   | 6     | 537 | VAL  | Mainchain |
| 1   | 7     | 537 | VAL  | Mainchain |
| 1   | 8     | 537 | VAL  | Mainchain |
| 1   | A     | 537 | VAL  | Mainchain |
| 1   | B     | 537 | VAL  | Mainchain |
| 1   | C     | 537 | VAL  | Mainchain |
| 1   | D     | 537 | VAL  | Mainchain |
| 1   | E     | 537 | VAL  | Mainchain |
| 1   | F     | 537 | VAL  | Mainchain |
| 1   | G     | 537 | VAL  | Mainchain |
| 1   | H     | 537 | VAL  | Mainchain |
| 1   | I     | 537 | VAL  | Mainchain |
| 1   | J     | 537 | VAL  | Mainchain |
| 1   | K     | 537 | VAL  | Mainchain |
| 1   | L     | 537 | VAL  | Mainchain |
| 1   | M     | 537 | VAL  | Mainchain |
| 1   | N     | 537 | VAL  | Mainchain |
| 1   | O     | 537 | VAL  | Mainchain |
| 1   | P     | 537 | VAL  | Mainchain |
| 1   | Q     | 537 | VAL  | Mainchain |
| 1   | R     | 537 | VAL  | Mainchain |
| 1   | S     | 537 | VAL  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | T     | 537 | VAL  | Mainchain |
| 1   | U     | 537 | VAL  | Mainchain |
| 1   | V     | 537 | VAL  | Mainchain |
| 1   | W     | 537 | VAL  | Mainchain |
| 1   | X     | 537 | VAL  | Mainchain |
| 1   | Y     | 537 | VAL  | Mainchain |
| 1   | Z     | 537 | VAL  | Mainchain |
| 1   | a     | 537 | VAL  | Mainchain |
| 1   | b     | 537 | VAL  | Mainchain |
| 1   | c     | 537 | VAL  | Mainchain |
| 1   | d     | 537 | VAL  | Mainchain |
| 1   | e     | 537 | VAL  | Mainchain |
| 1   | f     | 537 | VAL  | Mainchain |
| 1   | g     | 537 | VAL  | Mainchain |
| 1   | h     | 537 | VAL  | Mainchain |
| 1   | i     | 537 | VAL  | Mainchain |
| 1   | j     | 537 | VAL  | Mainchain |
| 1   | k     | 537 | VAL  | Mainchain |
| 1   | l     | 537 | VAL  | Mainchain |
| 1   | m     | 537 | VAL  | Mainchain |
| 1   | n     | 537 | VAL  | Mainchain |
| 1   | o     | 537 | VAL  | Mainchain |
| 1   | p     | 537 | VAL  | Mainchain |
| 1   | q     | 537 | VAL  | Mainchain |
| 1   | r     | 537 | VAL  | Mainchain |
| 1   | s     | 537 | VAL  | Mainchain |
| 1   | t     | 537 | VAL  | Mainchain |
| 1   | u     | 537 | VAL  | Mainchain |
| 1   | v     | 537 | VAL  | Mainchain |
| 1   | w     | 537 | VAL  | Mainchain |
| 1   | x     | 537 | VAL  | Mainchain |
| 1   | y     | 537 | VAL  | Mainchain |
| 1   | z     | 537 | VAL  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 4108  | 0        | 3916     | 141     | 0            |
| 1   | 2     | 4108  | 0        | 3916     | 148     | 0            |
| 1   | 3     | 4108  | 0        | 3916     | 149     | 0            |
| 1   | 4     | 4108  | 0        | 3916     | 151     | 0            |
| 1   | 5     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | 6     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | 7     | 4108  | 0        | 3916     | 149     | 0            |
| 1   | 8     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | A     | 4108  | 0        | 3916     | 145     | 0            |
| 1   | B     | 4108  | 0        | 3916     | 143     | 0            |
| 1   | C     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | D     | 4108  | 0        | 3916     | 148     | 0            |
| 1   | E     | 4108  | 0        | 3916     | 143     | 0            |
| 1   | F     | 4108  | 0        | 3916     | 144     | 0            |
| 1   | G     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | H     | 4108  | 0        | 3916     | 148     | 0            |
| 1   | I     | 4108  | 0        | 3916     | 149     | 0            |
| 1   | J     | 4108  | 0        | 3916     | 150     | 0            |
| 1   | K     | 4108  | 0        | 3916     | 149     | 0            |
| 1   | L     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | M     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | N     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | O     | 4108  | 0        | 3916     | 150     | 0            |
| 1   | P     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | Q     | 4108  | 0        | 3916     | 145     | 0            |
| 1   | R     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | S     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | T     | 4108  | 0        | 3916     | 149     | 0            |
| 1   | U     | 4108  | 0        | 3916     | 144     | 0            |
| 1   | V     | 4108  | 0        | 3916     | 142     | 0            |
| 1   | W     | 4108  | 0        | 3916     | 144     | 0            |
| 1   | X     | 4108  | 0        | 3916     | 145     | 0            |
| 1   | Y     | 4108  | 0        | 3916     | 148     | 0            |
| 1   | Z     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | a     | 4108  | 0        | 3916     | 148     | 0            |
| 1   | b     | 4108  | 0        | 3916     | 143     | 0            |
| 1   | c     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | d     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | e     | 4108  | 0        | 3916     | 146     | 0            |
| 1   | f     | 4108  | 0        | 3916     | 147     | 0            |
| 1   | g     | 4108  | 0        | 3916     | 145     | 0            |
| 1   | h     | 4108  | 0        | 3916     | 145     | 0            |
| 1   | i     | 4108  | 0        | 3916     | 148     | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | j     | 4108   | 0        | 3916     | 147     | 0            |
| 1   | k     | 4108   | 0        | 3916     | 147     | 0            |
| 1   | l     | 4108   | 0        | 3916     | 148     | 0            |
| 1   | m     | 4108   | 0        | 3916     | 149     | 0            |
| 1   | n     | 4108   | 0        | 3916     | 148     | 0            |
| 1   | o     | 4108   | 0        | 3916     | 146     | 0            |
| 1   | p     | 4108   | 0        | 3916     | 145     | 0            |
| 1   | q     | 4108   | 0        | 3916     | 147     | 0            |
| 1   | r     | 4108   | 0        | 3916     | 146     | 0            |
| 1   | s     | 4108   | 0        | 3916     | 146     | 0            |
| 1   | t     | 4108   | 0        | 3916     | 147     | 0            |
| 1   | u     | 4108   | 0        | 3916     | 149     | 0            |
| 1   | v     | 4108   | 0        | 3916     | 146     | 0            |
| 1   | w     | 4108   | 0        | 3916     | 143     | 0            |
| 1   | x     | 4108   | 0        | 3916     | 146     | 0            |
| 1   | y     | 4108   | 0        | 3916     | 146     | 0            |
| 1   | z     | 4108   | 0        | 3916     | 148     | 0            |
| All | All   | 246480 | 0        | 234960   | 7170    | 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 15.

All (7170) 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:O:175:ASP:HB2 | 1:O:188:PHE:CZ | 2.08                     | 0.89              |
| 1:S:175:ASP:HB2 | 1:S:188:PHE:CZ | 2.08                     | 0.89              |
| 1:l:175:ASP:HB2 | 1:l:188:PHE:CZ | 2.08                     | 0.89              |
| 1:r:175:ASP:HB2 | 1:r:188:PHE:CZ | 2.08                     | 0.89              |
| 1:H:175:ASP:HB2 | 1:H:188:PHE:CZ | 2.08                     | 0.89              |
| 1:V:175:ASP:HB2 | 1:V:188:PHE:CZ | 2.08                     | 0.89              |
| 1:a:175:ASP:HB2 | 1:a:188:PHE:CZ | 2.08                     | 0.89              |
| 1:b:175:ASP:HB2 | 1:b:188:PHE:CZ | 2.08                     | 0.89              |
| 1:p:175:ASP:HB2 | 1:p:188:PHE:CZ | 2.08                     | 0.89              |
| 1:3:175:ASP:HB2 | 1:3:188:PHE:CZ | 2.08                     | 0.89              |
| 1:5:175:ASP:HB2 | 1:5:188:PHE:CZ | 2.08                     | 0.89              |
| 1:f:175:ASP:HB2 | 1:f:188:PHE:CZ | 2.08                     | 0.89              |
| 1:B:175:ASP:HB2 | 1:B:188:PHE:CZ | 2.08                     | 0.89              |
| 1:F:175:ASP:HB2 | 1:F:188:PHE:CZ | 2.08                     | 0.89              |
| 1:I:175:ASP:HB2 | 1:I:188:PHE:CZ | 2.08                     | 0.89              |
| 1:1:175:ASP:HB2 | 1:1:188:PHE:CZ | 2.08                     | 0.89              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:D:175:ASP:HB2 | 1:D:188:PHE:CZ | 2.08                     | 0.89              |
| 1:X:175:ASP:HB2 | 1:X:188:PHE:CZ | 2.08                     | 0.89              |
| 1:u:175:ASP:HB2 | 1:u:188:PHE:CZ | 2.08                     | 0.89              |
| 1:y:175:ASP:HB2 | 1:y:188:PHE:CZ | 2.08                     | 0.89              |
| 1:c:175:ASP:HB2 | 1:c:188:PHE:CZ | 2.08                     | 0.89              |
| 1:k:175:ASP:HB2 | 1:k:188:PHE:CZ | 2.08                     | 0.89              |
| 1:o:175:ASP:HB2 | 1:o:188:PHE:CZ | 2.08                     | 0.89              |
| 1:U:175:ASP:HB2 | 1:U:188:PHE:CZ | 2.08                     | 0.89              |
| 1:e:175:ASP:HB2 | 1:e:188:PHE:CZ | 2.08                     | 0.89              |
| 1:J:175:ASP:HB2 | 1:J:188:PHE:CZ | 2.08                     | 0.89              |
| 1:g:175:ASP:HB2 | 1:g:188:PHE:CZ | 2.08                     | 0.89              |
| 1:s:175:ASP:HB2 | 1:s:188:PHE:CZ | 2.08                     | 0.89              |
| 1:v:175:ASP:HB2 | 1:v:188:PHE:CZ | 2.08                     | 0.89              |
| 1:2:175:ASP:HB2 | 1:2:188:PHE:CZ | 2.08                     | 0.89              |
| 1:A:175:ASP:HB2 | 1:A:188:PHE:CZ | 2.08                     | 0.89              |
| 1:C:175:ASP:HB2 | 1:C:188:PHE:CZ | 2.08                     | 0.89              |
| 1:Q:175:ASP:HB2 | 1:Q:188:PHE:CZ | 2.08                     | 0.89              |
| 1:x:175:ASP:HB2 | 1:x:188:PHE:CZ | 2.08                     | 0.89              |
| 1:N:175:ASP:HB2 | 1:N:188:PHE:CZ | 2.08                     | 0.89              |
| 1:R:175:ASP:HB2 | 1:R:188:PHE:CZ | 2.08                     | 0.89              |
| 1:h:175:ASP:HB2 | 1:h:188:PHE:CZ | 2.08                     | 0.89              |
| 1:i:175:ASP:HB2 | 1:i:188:PHE:CZ | 2.08                     | 0.89              |
| 1:z:175:ASP:HB2 | 1:z:188:PHE:CZ | 2.08                     | 0.89              |
| 1:L:175:ASP:HB2 | 1:L:188:PHE:CZ | 2.08                     | 0.88              |
| 1:q:175:ASP:HB2 | 1:q:188:PHE:CZ | 2.08                     | 0.88              |
| 1:K:175:ASP:HB2 | 1:K:188:PHE:CZ | 2.08                     | 0.88              |
| 1:M:175:ASP:HB2 | 1:M:188:PHE:CZ | 2.08                     | 0.88              |
| 1:W:175:ASP:HB2 | 1:W:188:PHE:CZ | 2.08                     | 0.88              |
| 1:Z:175:ASP:HB2 | 1:Z:188:PHE:CZ | 2.08                     | 0.88              |
| 1:4:175:ASP:HB2 | 1:4:188:PHE:CZ | 2.08                     | 0.88              |
| 1:n:175:ASP:HB2 | 1:n:188:PHE:CZ | 2.08                     | 0.88              |
| 1:6:175:ASP:HB2 | 1:6:188:PHE:CZ | 2.08                     | 0.88              |
| 1:T:175:ASP:HB2 | 1:T:188:PHE:CZ | 2.08                     | 0.88              |
| 1:d:175:ASP:HB2 | 1:d:188:PHE:CZ | 2.08                     | 0.88              |
| 1:j:175:ASP:HB2 | 1:j:188:PHE:CZ | 2.08                     | 0.88              |
| 1:8:175:ASP:HB2 | 1:8:188:PHE:CZ | 2.08                     | 0.88              |
| 1:P:175:ASP:HB2 | 1:P:188:PHE:CZ | 2.08                     | 0.88              |
| 1:G:175:ASP:HB2 | 1:G:188:PHE:CZ | 2.08                     | 0.88              |
| 1:7:175:ASP:HB2 | 1:7:188:PHE:CZ | 2.08                     | 0.88              |
| 1:m:175:ASP:HB2 | 1:m:188:PHE:CZ | 2.08                     | 0.88              |
| 1:t:175:ASP:HB2 | 1:t:188:PHE:CZ | 2.08                     | 0.88              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Y:175:ASP:HB2 | 1:Y:188:PHE:CZ  | 2.08                     | 0.88              |
| 1:w:175:ASP:HB2 | 1:w:188:PHE:CZ  | 2.08                     | 0.87              |
| 1:E:175:ASP:HB2 | 1:E:188:PHE:CZ  | 2.08                     | 0.87              |
| 1:a:67:GLN:HE21 | 1:a:189:GLN:HB2 | 1.49                     | 0.78              |
| 1:3:67:GLN:HE21 | 1:3:189:GLN:HB2 | 1.49                     | 0.78              |
| 1:j:67:GLN:HE21 | 1:j:189:GLN:HB2 | 1.49                     | 0.78              |
| 1:P:67:GLN:HE21 | 1:P:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:t:67:GLN:HE21 | 1:t:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:x:67:GLN:HE21 | 1:x:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:G:67:GLN:HE21 | 1:G:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:Q:67:GLN:HE21 | 1:Q:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:c:67:GLN:HE21 | 1:c:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:B:67:GLN:HE21 | 1:B:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:R:67:GLN:HE21 | 1:R:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:e:67:GLN:HE21 | 1:e:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:1:67:GLN:HE21 | 1:1:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:l:67:GLN:HE21 | 1:l:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:q:67:GLN:HE21 | 1:q:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:h:67:GLN:HE21 | 1:h:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:v:67:GLN:HE21 | 1:v:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:A:67:GLN:HE21 | 1:A:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:I:67:GLN:HE21 | 1:I:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:O:67:GLN:HE21 | 1:O:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:W:67:GLN:HE21 | 1:W:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:8:67:GLN:HE21 | 1:8:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:M:67:GLN:HE21 | 1:M:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:u:67:GLN:HE21 | 1:u:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:Z:67:GLN:HE21 | 1:Z:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:6:67:GLN:HE21 | 1:6:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:C:67:GLN:HE21 | 1:C:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:d:67:GLN:HE21 | 1:d:189:GLN:HB2 | 1.49                     | 0.77              |
| 1:g:67:GLN:HE21 | 1:g:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:E:67:GLN:HE21 | 1:E:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:U:67:GLN:HE21 | 1:U:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:s:67:GLN:HE21 | 1:s:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:w:67:GLN:HE21 | 1:w:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:n:67:GLN:HE21 | 1:n:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:i:67:GLN:HE21 | 1:i:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:D:67:GLN:HE21 | 1:D:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:K:67:GLN:HE21 | 1:K:189:GLN:HB2 | 1.49                     | 0.76              |
| 1:N:67:GLN:HE21 | 1:N:189:GLN:HB2 | 1.49                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:67:GLN:HE21  | 1:b:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:o:67:GLN:HE21  | 1:o:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:f:67:GLN:HE21  | 1:f:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:T:67:GLN:HE21  | 1:T:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:k:67:GLN:HE21  | 1:k:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:m:67:GLN:HE21  | 1:m:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:z:67:GLN:HE21  | 1:z:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:4:67:GLN:HE21  | 1:4:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:X:67:GLN:HE21  | 1:X:189:GLN:HB2  | 1.49                     | 0.76              |
| 1:H:67:GLN:HE21  | 1:H:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:L:67:GLN:HE21  | 1:L:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:p:67:GLN:HE21  | 1:p:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:Y:67:GLN:HE21  | 1:Y:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:5:67:GLN:HE21  | 1:5:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:V:67:GLN:HE21  | 1:V:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:S:67:GLN:HE21  | 1:S:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:7:67:GLN:HE21  | 1:7:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:F:67:GLN:HE21  | 1:F:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:r:67:GLN:HE21  | 1:r:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:2:67:GLN:HE21  | 1:2:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:y:67:GLN:HE21  | 1:y:189:GLN:HB2  | 1.49                     | 0.75              |
| 1:J:67:GLN:HE21  | 1:J:189:GLN:HB2  | 1.49                     | 0.74              |
| 1:J:258:MET:HE3  | 1:L:167:ASN:HD21 | 1.53                     | 0.74              |
| 1:B:258:MET:HE3  | 1:J:167:ASN:HD21 | 1.53                     | 0.73              |
| 1:S:258:MET:HE3  | 1:U:167:ASN:HD21 | 1.55                     | 0.72              |
| 1:r:258:MET:HE3  | 1:s:167:ASN:HD21 | 1.55                     | 0.72              |
| 1:z:167:ASN:HD21 | 1:2:258:MET:HE3  | 1.55                     | 0.72              |
| 1:V:167:ASN:HD21 | 1:X:258:MET:HE3  | 1.55                     | 0.72              |
| 1:o:258:MET:HE3  | 1:p:167:ASN:HD21 | 1.55                     | 0.72              |
| 1:C:167:ASN:HD21 | 1:M:258:MET:HE3  | 1.55                     | 0.72              |
| 1:1:258:MET:HE3  | 1:2:167:ASN:HD21 | 1.55                     | 0.72              |
| 1:6:302:ALA:O    | 1:6:351:TYR:OH   | 2.08                     | 0.72              |
| 1:V:258:MET:HE3  | 1:e:167:ASN:HD21 | 1.55                     | 0.72              |
| 1:g:167:ASN:HD21 | 1:h:258:MET:HE3  | 1.55                     | 0.72              |
| 1:j:258:MET:HE3  | 1:k:167:ASN:HD21 | 1.55                     | 0.72              |
| 1:D:167:ASN:HD21 | 1:P:258:MET:HE3  | 1.55                     | 0.72              |
| 1:c:167:ASN:HD21 | 1:p:258:MET:HE3  | 1.55                     | 0.72              |
| 1:A:302:ALA:O    | 1:A:351:TYR:OH   | 2.08                     | 0.71              |
| 1:J:258:MET:HE3  | 1:L:167:ASN:ND2  | 2.05                     | 0.71              |
| 1:M:167:ASN:HD21 | 1:b:258:MET:HE3  | 1.55                     | 0.71              |
| 1:P:302:ALA:O    | 1:P:351:TYR:OH   | 2.08                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:302:ALA:O    | 1:v:351:TYR:OH   | 2.08                     | 0.71              |
| 1:f:258:MET:HE3  | 1:h:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:i:258:MET:HE3  | 1:j:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:n:302:ALA:O    | 1:n:351:TYR:OH   | 2.08                     | 0.71              |
| 1:N:258:MET:HE3  | 1:P:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:d:302:ALA:O    | 1:d:351:TYR:OH   | 2.08                     | 0.71              |
| 1:E:167:ASN:HD21 | 1:F:258:MET:HE3  | 1.55                     | 0.71              |
| 1:H:258:MET:HE3  | 1:W:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:p:302:ALA:O    | 1:p:351:TYR:OH   | 2.08                     | 0.71              |
| 1:w:167:ASN:HD21 | 1:y:258:MET:HE3  | 1.55                     | 0.71              |
| 1:O:258:MET:HE3  | 1:m:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:T:167:ASN:HD21 | 1:l:258:MET:HE3  | 1.55                     | 0.71              |
| 1:V:302:ALA:O    | 1:V:351:TYR:OH   | 2.08                     | 0.71              |
| 1:u:258:MET:HE3  | 1:v:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:5:258:MET:HE3  | 1:6:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:z:258:MET:HE3  | 1:1:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:A:167:ASN:HD21 | 1:I:258:MET:HE3  | 1.56                     | 0.71              |
| 1:A:258:MET:HE3  | 1:G:167:ASN:HD21 | 1.56                     | 0.71              |
| 1:C:258:MET:HE3  | 1:b:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:G:258:MET:HE3  | 1:I:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:W:258:MET:HE3  | 1:Y:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:b:302:ALA:O    | 1:b:351:TYR:OH   | 2.08                     | 0.71              |
| 1:f:167:ASN:HD21 | 1:g:258:MET:HE3  | 1.55                     | 0.71              |
| 1:t:258:MET:HE3  | 1:u:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:6:258:MET:HE3  | 1:7:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:t:167:ASN:HD21 | 1:v:258:MET:HE3  | 1.55                     | 0.71              |
| 1:E:258:MET:HE3  | 1:Q:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:m:258:MET:HE3  | 1:n:167:ASN:HD21 | 1.56                     | 0.71              |
| 1:w:258:MET:HE3  | 1:x:167:ASN:HD21 | 1.55                     | 0.71              |
| 1:M:302:ALA:O    | 1:M:351:TYR:OH   | 2.08                     | 0.70              |
| 1:R:167:ASN:HD21 | 1:U:258:MET:HE3  | 1.55                     | 0.70              |
| 1:T:258:MET:HE3  | 1:d:167:ASN:HD21 | 1.56                     | 0.70              |
| 1:q:167:ASN:HD21 | 1:s:258:MET:HE3  | 1.55                     | 0.70              |
| 1:H:167:ASN:HD21 | 1:Y:258:MET:HE3  | 1.55                     | 0.70              |
| 1:h:302:ALA:O    | 1:h:351:TYR:OH   | 2.08                     | 0.70              |
| 1:B:167:ASN:HD21 | 1:L:258:MET:HE3  | 1.55                     | 0.70              |
| 1:F:167:ASN:HD21 | 1:Q:258:MET:HE3  | 1.55                     | 0.70              |
| 1:5:167:ASN:HD21 | 1:7:258:MET:HE3  | 1.55                     | 0.70              |
| 1:P:175:ASP:CB   | 1:P:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:a:175:ASP:CB   | 1:a:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:j:175:ASP:CB   | 1:j:188:PHE:CE2  | 2.75                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:175:ASP:CB   | 1:l:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:3:175:ASP:CB   | 1:3:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:O:175:ASP:CB   | 1:O:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:d:258:MET:HE3  | 1:l:167:ASN:HD21 | 1.55                     | 0.70              |
| 1:x:258:MET:HE3  | 1:y:167:ASN:HD21 | 1.55                     | 0.70              |
| 1:D:175:ASP:CB   | 1:D:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:K:175:ASP:CB   | 1:K:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:R:175:ASP:CB   | 1:R:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:k:175:ASP:CB   | 1:k:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:q:175:ASP:CB   | 1:q:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:4:175:ASP:CB   | 1:4:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:A:175:ASP:CB   | 1:A:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:B:258:MET:HE3  | 1:J:167:ASN:ND2  | 2.06                     | 0.70              |
| 1:Z:175:ASP:CB   | 1:Z:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:b:175:ASP:CB   | 1:b:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:c:175:ASP:CB   | 1:c:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:e:175:ASP:CB   | 1:e:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:f:175:ASP:CB   | 1:f:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:m:175:ASP:CB   | 1:m:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:q:167:ASN:ND2  | 1:s:258:MET:HE3  | 2.07                     | 0.70              |
| 1:v:175:ASP:CB   | 1:v:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:1:302:ALA:O    | 1:1:351:TYR:OH   | 2.08                     | 0.70              |
| 1:8:175:ASP:CB   | 1:8:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:O:167:ASN:HD21 | 1:n:258:MET:HE3  | 1.55                     | 0.70              |
| 1:R:167:ASN:ND2  | 1:U:258:MET:HE3  | 2.07                     | 0.70              |
| 1:T:175:ASP:CB   | 1:T:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:V:175:ASP:CB   | 1:V:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:X:167:ASN:HD21 | 1:e:258:MET:HE3  | 1.55                     | 0.70              |
| 1:c:258:MET:HE3  | 1:o:167:ASN:HD21 | 1.55                     | 0.70              |
| 1:i:167:ASN:HD21 | 1:k:258:MET:HE3  | 1.55                     | 0.70              |
| 1:p:175:ASP:CB   | 1:p:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:7:175:ASP:CB   | 1:7:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:B:302:ALA:O    | 1:B:351:TYR:OH   | 2.08                     | 0.70              |
| 1:C:175:ASP:CB   | 1:C:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:E:175:ASP:CB   | 1:E:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:I:175:ASP:CB   | 1:I:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:I:302:ALA:O    | 1:I:351:TYR:OH   | 2.08                     | 0.70              |
| 1:Y:175:ASP:CB   | 1:Y:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:o:175:ASP:CB   | 1:o:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:u:175:ASP:CB   | 1:u:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:w:175:ASP:CB   | 1:w:188:PHE:CE2  | 2.75                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:y:302:ALA:O    | 1:y:351:TYR:OH   | 2.08                     | 0.70              |
| 1:8:302:ALA:O    | 1:8:351:TYR:OH   | 2.08                     | 0.70              |
| 1:F:302:ALA:O    | 1:F:351:TYR:OH   | 2.08                     | 0.70              |
| 1:H:175:ASP:CB   | 1:H:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:X:175:ASP:CB   | 1:X:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:a:258:MET:HE3  | 1:8:167:ASN:HD21 | 1.55                     | 0.70              |
| 1:g:175:ASP:CB   | 1:g:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:u:302:ALA:O    | 1:u:351:TYR:OH   | 2.08                     | 0.70              |
| 1:z:167:ASN:ND2  | 1:2:258:MET:HE3  | 2.07                     | 0.70              |
| 1:5:175:ASP:CB   | 1:5:188:PHE:CE2  | 2.75                     | 0.70              |
| 1:D:258:MET:HE3  | 1:N:167:ASN:HD21 | 1.55                     | 0.69              |
| 1:K:167:ASN:HD21 | 1:8:258:MET:HE3  | 1.55                     | 0.69              |
| 1:K:258:MET:HE3  | 1:a:167:ASN:HD21 | 1.55                     | 0.69              |
| 1:U:175:ASP:CB   | 1:U:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:Z:302:ALA:O    | 1:Z:351:TYR:OH   | 2.08                     | 0.69              |
| 1:r:258:MET:HE3  | 1:s:167:ASN:ND2  | 2.07                     | 0.69              |
| 1:t:175:ASP:CB   | 1:t:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:G:175:ASP:CB   | 1:G:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:S:175:ASP:CB   | 1:S:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:S:258:MET:HE3  | 1:U:167:ASN:ND2  | 2.07                     | 0.69              |
| 1:i:175:ASP:CB   | 1:i:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:r:175:ASP:CB   | 1:r:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:s:175:ASP:CB   | 1:s:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:z:258:MET:HE3  | 1:1:167:ASN:ND2  | 2.07                     | 0.69              |
| 1:N:175:ASP:CB   | 1:N:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:Z:167:ASN:HD21 | 1:3:258:MET:HE3  | 1.55                     | 0.69              |
| 1:Z:258:MET:HE3  | 1:4:167:ASN:HD21 | 1.55                     | 0.69              |
| 1:f:302:ALA:O    | 1:f:351:TYR:OH   | 2.08                     | 0.69              |
| 1:2:175:ASP:CB   | 1:2:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:6:175:ASP:CB   | 1:6:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:D:258:MET:HE3  | 1:N:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:L:175:ASP:CB   | 1:L:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:M:175:ASP:CB   | 1:M:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:O:167:ASN:ND2  | 1:n:258:MET:HE3  | 2.08                     | 0.69              |
| 1:R:258:MET:HE3  | 1:S:167:ASN:HD21 | 1.55                     | 0.69              |
| 1:W:175:ASP:CB   | 1:W:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:d:258:MET:HE3  | 1:l:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:i:167:ASN:ND2  | 1:k:258:MET:HE3  | 2.08                     | 0.69              |
| 1:z:175:ASP:CB   | 1:z:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:J:175:ASP:CB   | 1:J:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:N:258:MET:HE3  | 1:P:167:ASN:ND2  | 2.08                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:258:MET:HE3  | 1:m:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:R:258:MET:HE3  | 1:S:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:T:167:ASN:ND2  | 1:l:258:MET:HE3  | 2.08                     | 0.69              |
| 1:h:175:ASP:CB   | 1:h:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:q:258:MET:HE3  | 1:r:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:u:258:MET:HE3  | 1:v:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:x:175:ASP:CB   | 1:x:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:3:167:ASN:HD21 | 1:4:258:MET:HE3  | 1.56                     | 0.69              |
| 1:B:175:ASP:CB   | 1:B:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:c:258:MET:HE3  | 1:o:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:i:258:MET:HE3  | 1:j:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:q:258:MET:HE3  | 1:r:167:ASN:HD21 | 1.55                     | 0.69              |
| 1:l:175:ASP:CB   | 1:l:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:A:167:ASN:ND2  | 1:I:258:MET:HE3  | 2.08                     | 0.69              |
| 1:H:258:MET:HE3  | 1:W:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:Q:175:ASP:CB   | 1:Q:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:X:167:ASN:ND2  | 1:e:258:MET:HE3  | 2.08                     | 0.69              |
| 1:C:258:MET:HE3  | 1:b:167:ASN:ND2  | 2.07                     | 0.69              |
| 1:E:167:ASN:ND2  | 1:F:258:MET:HE3  | 2.08                     | 0.69              |
| 1:K:302:ALA:O    | 1:K:351:TYR:OH   | 2.08                     | 0.69              |
| 1:M:167:ASN:ND2  | 1:b:258:MET:HE3  | 2.08                     | 0.69              |
| 1:W:258:MET:HE3  | 1:Y:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:d:175:ASP:CB   | 1:d:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:f:167:ASN:ND2  | 1:g:258:MET:HE3  | 2.07                     | 0.69              |
| 1:f:258:MET:HE3  | 1:h:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:n:175:ASP:CB   | 1:n:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:w:167:ASN:ND2  | 1:y:258:MET:HE3  | 2.08                     | 0.69              |
| 1:y:175:ASP:CB   | 1:y:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:4:302:ALA:O    | 1:4:351:TYR:OH   | 2.08                     | 0.69              |
| 1:5:258:MET:HE3  | 1:6:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:F:175:ASP:CB   | 1:F:188:PHE:CE2  | 2.75                     | 0.69              |
| 1:K:258:MET:HE3  | 1:a:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:U:302:ALA:O    | 1:U:351:TYR:OH   | 2.08                     | 0.69              |
| 1:s:302:ALA:O    | 1:s:351:TYR:OH   | 2.08                     | 0.69              |
| 1:6:258:MET:HE3  | 1:7:167:ASN:ND2  | 2.08                     | 0.69              |
| 1:B:167:ASN:ND2  | 1:L:258:MET:HE3  | 2.08                     | 0.69              |
| 1:G:302:ALA:O    | 1:G:351:TYR:OH   | 2.08                     | 0.69              |
| 1:T:158:PHE:HB2  | 1:T:226:HIS:HB3  | 1.76                     | 0.69              |
| 1:V:258:MET:HE3  | 1:e:167:ASN:ND2  | 2.07                     | 0.69              |
| 1:m:158:PHE:HB2  | 1:m:226:HIS:HB3  | 1.76                     | 0.69              |
| 1:y:158:PHE:HB2  | 1:y:226:HIS:HB3  | 1.75                     | 0.69              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:1:258:MET:HE3 | 1:2:167:ASN:ND2 | 2.08                     | 0.69              |
| 1:3:302:ALA:O   | 1:3:351:TYR:OH  | 2.08                     | 0.69              |
| 1:D:158:PHE:HB2 | 1:D:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:F:158:PHE:HB2 | 1:F:226:HIS:HB3 | 1.75                     | 0.68              |
| 1:J:384:ARG:HG3 | 1:L:302:ALA:HB2 | 1.74                     | 0.68              |
| 1:N:302:ALA:O   | 1:N:351:TYR:OH  | 2.08                     | 0.68              |
| 1:U:158:PHE:HB2 | 1:U:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:a:258:MET:HE3 | 1:8:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:c:167:ASN:ND2 | 1:p:258:MET:HE3 | 2.07                     | 0.68              |
| 1:c:450:LYS:NZ  | 1:s:182:TYR:O   | 2.26                     | 0.68              |
| 1:i:302:ALA:O   | 1:i:351:TYR:OH  | 2.08                     | 0.68              |
| 1:k:158:PHE:HB2 | 1:k:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:t:302:ALA:O   | 1:t:351:TYR:OH  | 2.08                     | 0.68              |
| 1:D:167:ASN:ND2 | 1:P:258:MET:HE3 | 2.08                     | 0.68              |
| 1:U:182:TYR:O   | 1:e:450:LYS:NZ  | 2.26                     | 0.68              |
| 1:Y:302:ALA:O   | 1:Y:351:TYR:OH  | 2.08                     | 0.68              |
| 1:q:302:ALA:O   | 1:q:351:TYR:OH  | 2.08                     | 0.68              |
| 1:s:158:PHE:HB2 | 1:s:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:G:258:MET:HE3 | 1:I:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:O:450:LYS:NZ  | 1:d:182:TYR:O   | 2.26                     | 0.68              |
| 1:Z:167:ASN:ND2 | 1:3:258:MET:HE3 | 2.08                     | 0.68              |
| 1:a:158:PHE:HB2 | 1:a:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:a:302:ALA:O   | 1:a:351:TYR:OH  | 2.08                     | 0.68              |
| 1:c:158:PHE:HB2 | 1:c:226:HIS:HB3 | 1.75                     | 0.68              |
| 1:e:158:PHE:HB2 | 1:e:226:HIS:HB3 | 1.75                     | 0.68              |
| 1:e:302:ALA:O   | 1:e:351:TYR:OH  | 2.08                     | 0.68              |
| 1:l:450:LYS:NZ  | 1:n:182:TYR:O   | 2.26                     | 0.68              |
| 1:o:258:MET:HE3 | 1:p:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:3:158:PHE:HB2 | 1:3:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:3:167:ASN:ND2 | 1:4:258:MET:HE3 | 2.08                     | 0.68              |
| 1:5:167:ASN:ND2 | 1:7:258:MET:HE3 | 2.08                     | 0.68              |
| 1:H:167:ASN:ND2 | 1:Y:258:MET:HE3 | 2.08                     | 0.68              |
| 1:K:167:ASN:ND2 | 1:8:258:MET:HE3 | 2.08                     | 0.68              |
| 1:O:182:TYR:O   | 1:P:450:LYS:NZ  | 2.26                     | 0.68              |
| 1:Z:258:MET:HE3 | 1:4:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:j:258:MET:HE3 | 1:k:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:r:158:PHE:HB2 | 1:r:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:t:258:MET:HE3 | 1:u:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:K:158:PHE:HB2 | 1:K:226:HIS:HB3 | 1.75                     | 0.68              |
| 1:O:158:PHE:HB2 | 1:O:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:R:302:ALA:O   | 1:R:351:TYR:OH  | 2.08                     | 0.68              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:450:LYS:NZ  | 1:V:182:TYR:O   | 2.26                     | 0.68              |
| 1:V:167:ASN:ND2 | 1:X:258:MET:HE3 | 2.08                     | 0.68              |
| 1:j:450:LYS:NZ  | 1:l:182:TYR:O   | 2.26                     | 0.68              |
| 1:p:158:PHE:HB2 | 1:p:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:p:182:TYR:O   | 1:q:450:LYS:NZ  | 2.26                     | 0.68              |
| 1:x:302:ALA:O   | 1:x:351:TYR:OH  | 2.08                     | 0.68              |
| 1:7:302:ALA:O   | 1:7:351:TYR:OH  | 2.08                     | 0.68              |
| 1:Q:158:PHE:HB2 | 1:Q:226:HIS:HB3 | 1.75                     | 0.68              |
| 1:S:302:ALA:O   | 1:S:351:TYR:OH  | 2.08                     | 0.68              |
| 1:V:158:PHE:HB2 | 1:V:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:c:302:ALA:O   | 1:c:351:TYR:OH  | 2.08                     | 0.68              |
| 1:g:167:ASN:ND2 | 1:h:258:MET:HE3 | 2.08                     | 0.68              |
| 1:C:167:ASN:ND2 | 1:M:258:MET:HE3 | 2.08                     | 0.68              |
| 1:E:258:MET:HE3 | 1:Q:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:S:158:PHE:HB2 | 1:S:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:l:158:PHE:HB2 | 1:l:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:o:302:ALA:O   | 1:o:351:TYR:OH  | 2.08                     | 0.68              |
| 1:r:302:ALA:O   | 1:r:351:TYR:OH  | 2.08                     | 0.68              |
| 1:x:158:PHE:HB2 | 1:x:226:HIS:HB3 | 1.75                     | 0.68              |
| 1:I:182:TYR:O   | 1:J:450:LYS:NZ  | 2.24                     | 0.68              |
| 1:O:302:ALA:O   | 1:O:351:TYR:OH  | 2.08                     | 0.68              |
| 1:w:258:MET:HE3 | 1:x:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:4:158:PHE:HB2 | 1:4:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:F:167:ASN:ND2 | 1:Q:258:MET:HE3 | 2.08                     | 0.68              |
| 1:Q:302:ALA:O   | 1:Q:351:TYR:OH  | 2.08                     | 0.68              |
| 1:x:258:MET:HE3 | 1:y:167:ASN:ND2 | 2.08                     | 0.68              |
| 1:W:158:PHE:HB2 | 1:W:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:j:158:PHE:HB2 | 1:j:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:m:302:ALA:O   | 1:m:351:TYR:OH  | 2.08                     | 0.68              |
| 1:n:158:PHE:HB2 | 1:n:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:o:158:PHE:HB2 | 1:o:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:v:158:PHE:HB2 | 1:v:226:HIS:HB3 | 1.75                     | 0.68              |
| 1:z:158:PHE:HB2 | 1:z:226:HIS:HB3 | 1.76                     | 0.68              |
| 1:A:158:PHE:HB2 | 1:A:226:HIS:HB3 | 1.75                     | 0.67              |
| 1:E:302:ALA:O   | 1:E:351:TYR:OH  | 2.08                     | 0.67              |
| 1:L:158:PHE:HB2 | 1:L:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:T:258:MET:HE3 | 1:d:167:ASN:ND2 | 2.08                     | 0.67              |
| 1:q:302:ALA:HB2 | 1:s:384:ARG:HG3 | 1.76                     | 0.67              |
| 1:6:158:PHE:HB2 | 1:6:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:A:258:MET:HE3 | 1:G:167:ASN:ND2 | 2.08                     | 0.67              |
| 1:P:158:PHE:HB2 | 1:P:226:HIS:HB3 | 1.76                     | 0.67              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:302:ALA:HB2 | 1:U:384:ARG:HG3 | 1.76                     | 0.67              |
| 1:X:158:PHE:HB2 | 1:X:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:X:450:LYS:NZ  | 1:f:182:TYR:O   | 2.26                     | 0.67              |
| 1:Z:158:PHE:HB2 | 1:Z:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:d:158:PHE:HB2 | 1:d:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:m:258:MET:HE3 | 1:n:167:ASN:ND2 | 2.08                     | 0.67              |
| 1:n:450:LYS:NZ  | 1:r:182:TYR:O   | 2.27                     | 0.67              |
| 1:t:167:ASN:ND2 | 1:v:258:MET:HE3 | 2.08                     | 0.67              |
| 1:t:182:TYR:O   | 1:6:450:LYS:NZ  | 2.26                     | 0.67              |
| 1:w:302:ALA:O   | 1:w:351:TYR:OH  | 2.08                     | 0.67              |
| 1:b:182:TYR:O   | 1:o:450:LYS:NZ  | 2.26                     | 0.67              |
| 1:8:158:PHE:HB2 | 1:8:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:G:182:TYR:O   | 1:W:450:LYS:NZ  | 2.26                     | 0.67              |
| 1:S:182:TYR:O   | 1:d:450:LYS:NZ  | 2.27                     | 0.67              |
| 1:T:302:ALA:O   | 1:T:351:TYR:OH  | 2.08                     | 0.67              |
| 1:T:450:LYS:NZ  | 1:i:182:TYR:O   | 2.26                     | 0.67              |
| 1:3:175:ASP:HB3 | 1:3:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:F:182:TYR:O   | 1:G:450:LYS:NZ  | 2.27                     | 0.67              |
| 1:I:175:ASP:HB3 | 1:I:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:N:182:TYR:O   | 1:m:450:LYS:NZ  | 2.26                     | 0.67              |
| 1:a:175:ASP:HB3 | 1:a:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:i:175:ASP:HB3 | 1:i:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:B:384:ARG:HG3 | 1:J:302:ALA:HB2 | 1.76                     | 0.67              |
| 1:N:175:ASP:HB3 | 1:N:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:T:175:ASP:HB3 | 1:T:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:U:175:ASP:HB3 | 1:U:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:Z:175:ASP:HB3 | 1:Z:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:g:249:GLU:HG3 | 1:g:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:k:175:ASP:HB3 | 1:k:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:m:175:ASP:HB3 | 1:m:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:o:384:ARG:HG3 | 1:p:302:ALA:HB2 | 1.77                     | 0.67              |
| 1:s:175:ASP:HB3 | 1:s:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:t:450:LYS:NZ  | 1:y:182:TYR:O   | 2.27                     | 0.67              |
| 1:u:158:PHE:HB2 | 1:u:226:HIS:HB3 | 1.75                     | 0.67              |
| 1:u:175:ASP:HB3 | 1:u:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:5:249:GLU:HG3 | 1:5:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:8:175:ASP:HB3 | 1:8:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:A:175:ASP:HB3 | 1:A:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:C:249:GLU:HG3 | 1:C:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:C:302:ALA:O   | 1:C:351:TYR:OH  | 2.08                     | 0.67              |
| 1:D:175:ASP:HB3 | 1:D:188:PHE:CE2 | 2.30                     | 0.67              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:158:PHE:HB2  | 1:G:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:H:249:GLU:HG3  | 1:H:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:I:158:PHE:HB2  | 1:I:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:m:249:GLU:HG3  | 1:m:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:t:158:PHE:HB2  | 1:t:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:v:175:ASP:HB3  | 1:v:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:B:175:ASP:HB3  | 1:B:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:G:249:GLU:HG3  | 1:G:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:N:158:PHE:HB2  | 1:N:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:Q:175:ASP:HB3  | 1:Q:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:T:182:TYR:O    | 1:U:450:LYS:NZ  | 2.26                     | 0.67              |
| 1:T:249:GLU:HG3  | 1:T:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:V:302:ALA:HB2  | 1:X:384:ARG:HG3 | 1.77                     | 0.67              |
| 1:W:175:ASP:HB3  | 1:W:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:Z:450:LYS:NZ   | 1:a:182:TYR:O   | 2.26                     | 0.67              |
| 1:e:175:ASP:HB3  | 1:e:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:g:109:GLN:HE22 | 1:z:490:GLU:HG3 | 1.60                     | 0.67              |
| 1:g:302:ALA:O    | 1:g:351:TYR:OH  | 2.08                     | 0.67              |
| 1:k:302:ALA:O    | 1:k:351:TYR:OH  | 2.08                     | 0.67              |
| 1:x:175:ASP:HB3  | 1:x:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:1:175:ASP:HB3  | 1:1:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:6:175:ASP:HB3  | 1:6:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:H:175:ASP:HB3  | 1:H:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:J:158:PHE:HB2  | 1:J:226:HIS:HB3 | 1.75                     | 0.67              |
| 1:M:450:LYS:NZ   | 1:c:182:TYR:O   | 2.26                     | 0.67              |
| 1:U:249:GLU:HG3  | 1:U:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:c:175:ASP:HB3  | 1:c:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:h:249:GLU:HG3  | 1:h:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:t:249:GLU:HG3  | 1:t:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:3:182:TYR:O    | 1:8:450:LYS:NZ  | 2.26                     | 0.67              |
| 1:3:249:GLU:HG3  | 1:3:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:5:158:PHE:HB2  | 1:5:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:G:175:ASP:HB3  | 1:G:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:M:249:GLU:HG3  | 1:M:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:R:158:PHE:HB2  | 1:R:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:S:384:ARG:HG3  | 1:U:302:ALA:HB2 | 1.77                     | 0.67              |
| 1:W:384:ARG:HG3  | 1:Y:302:ALA:HB2 | 1.77                     | 0.67              |
| 1:Z:302:ALA:HB2  | 1:3:384:ARG:HG3 | 1.78                     | 0.67              |
| 1:a:249:GLU:HG3  | 1:a:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:a:384:ARG:HG3  | 1:8:302:ALA:HB2 | 1.77                     | 0.67              |
| 1:i:158:PHE:HB2  | 1:i:226:HIS:HB3 | 1.76                     | 0.67              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:m:182:TYR:O    | 1:s:450:LYS:NZ  | 2.26                     | 0.67              |
| 1:s:249:GLU:HG3  | 1:s:536:LYS:HD3 | 1.77                     | 0.67              |
| 1:2:158:PHE:HB2  | 1:2:226:HIS:HB3 | 1.76                     | 0.67              |
| 1:5:175:ASP:HB3  | 1:5:188:PHE:CE2 | 2.30                     | 0.67              |
| 1:D:302:ALA:O    | 1:D:351:TYR:OH  | 2.08                     | 0.66              |
| 1:H:158:PHE:HB2  | 1:H:226:HIS:HB3 | 1.76                     | 0.66              |
| 1:H:302:ALA:HB2  | 1:Y:384:ARG:HG3 | 1.77                     | 0.66              |
| 1:P:182:TYR:O    | 1:Q:450:LYS:NZ  | 2.26                     | 0.66              |
| 1:c:249:GLU:HG3  | 1:c:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:e:182:TYR:O    | 1:h:450:LYS:NZ  | 2.26                     | 0.66              |
| 1:n:175:ASP:HB3  | 1:n:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:q:158:PHE:HB2  | 1:q:226:HIS:HB3 | 1.76                     | 0.66              |
| 1:r:384:ARG:HG3  | 1:s:302:ALA:HB2 | 1.77                     | 0.66              |
| 1:t:175:ASP:HB3  | 1:t:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:z:249:GLU:HG3  | 1:z:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:6:384:ARG:HG3  | 1:7:302:ALA:HB2 | 1.77                     | 0.66              |
| 1:D:302:ALA:HB2  | 1:P:384:ARG:HG3 | 1.77                     | 0.66              |
| 1:J:175:ASP:HB3  | 1:J:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:L:249:GLU:HG3  | 1:L:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:L:302:ALA:O    | 1:L:351:TYR:OH  | 2.08                     | 0.66              |
| 1:Q:249:GLU:HG3  | 1:Q:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:X:175:ASP:HB3  | 1:X:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:d:175:ASP:HB3  | 1:d:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:d:249:GLU:HG3  | 1:d:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:e:249:GLU:HG3  | 1:e:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:f:450:LYS:NZ   | 1:z:182:TYR:O   | 2.26                     | 0.66              |
| 1:g:158:PHE:HB2  | 1:g:226:HIS:HB3 | 1.76                     | 0.66              |
| 1:n:249:GLU:HG3  | 1:n:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:r:249:GLU:HG3  | 1:r:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:y:175:ASP:HB3  | 1:y:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:2:175:ASP:HB3  | 1:2:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:2:249:GLU:HG3  | 1:2:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:4:175:ASP:HB3  | 1:4:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:C:158:PHE:HB2  | 1:C:226:HIS:HB3 | 1.76                     | 0.66              |
| 1:K:175:ASP:HB3  | 1:K:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:L:182:TYR:O    | 1:b:450:LYS:NZ  | 2.27                     | 0.66              |
| 1:Q:182:TYR:O    | 1:S:450:LYS:NZ  | 2.26                     | 0.66              |
| 1:S:249:GLU:HG3  | 1:S:536:LYS:HD3 | 1.77                     | 0.66              |
| 1:Y:175:ASP:HB3  | 1:Y:188:PHE:CE2 | 2.30                     | 0.66              |
| 1:b:109:GLN:HE22 | 1:c:490:GLU:HG3 | 1.61                     | 0.66              |
| 1:b:175:ASP:HB3  | 1:b:188:PHE:CE2 | 2.30                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:158:PHE:HB2  | 1:f:226:HIS:HB3  | 1.75                     | 0.66              |
| 1:f:175:ASP:HB3  | 1:f:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:j:175:ASP:HB3  | 1:j:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:j:182:TYR:O    | 1:x:450:LYS:NZ   | 2.26                     | 0.66              |
| 1:j:384:ARG:HG3  | 1:k:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:o:175:ASP:HB3  | 1:o:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:w:158:PHE:HB2  | 1:w:226:HIS:HB3  | 1.76                     | 0.66              |
| 1:x:249:GLU:HG3  | 1:x:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:z:302:ALA:O    | 1:z:351:TYR:OH   | 2.08                     | 0.66              |
| 1:5:302:ALA:HB2  | 1:7:384:ARG:HG3  | 1.77                     | 0.66              |
| 1:7:175:ASP:HB3  | 1:7:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:B:403:ILE:HD13 | 1:J:420:PRO:HG2  | 1.78                     | 0.66              |
| 1:E:158:PHE:HB2  | 1:E:226:HIS:HB3  | 1.76                     | 0.66              |
| 1:F:175:ASP:HB3  | 1:F:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:J:249:GLU:HG3  | 1:J:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:J:490:GLU:HG3  | 1:K:109:GLN:HE22 | 1.60                     | 0.66              |
| 1:O:249:GLU:HG3  | 1:O:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:P:175:ASP:HB3  | 1:P:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:X:302:ALA:O    | 1:X:351:TYR:OH   | 2.08                     | 0.66              |
| 1:b:158:PHE:HB2  | 1:b:226:HIS:HB3  | 1.76                     | 0.66              |
| 1:e:490:GLU:HG3  | 1:f:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:g:302:ALA:HB2  | 1:h:384:ARG:HG3  | 1.77                     | 0.66              |
| 1:l:249:GLU:HG3  | 1:l:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:r:450:LYS:NZ   | 1:x:182:TYR:O    | 2.26                     | 0.66              |
| 1:u:182:TYR:O    | 1:2:450:LYS:NZ   | 2.26                     | 0.66              |
| 1:C:302:ALA:HB2  | 1:M:384:ARG:HG3  | 1.77                     | 0.66              |
| 1:K:384:ARG:HG3  | 1:a:302:ALA:HB2  | 1.78                     | 0.66              |
| 1:O:175:ASP:HB3  | 1:O:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:Y:158:PHE:HB2  | 1:Y:226:HIS:HB3  | 1.76                     | 0.66              |
| 1:Y:249:GLU:HG3  | 1:Y:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:m:384:ARG:HG3  | 1:n:302:ALA:HB2  | 1.78                     | 0.66              |
| 1:o:490:GLU:HG3  | 1:6:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:p:450:LYS:NZ   | 1:6:182:TYR:O    | 2.26                     | 0.66              |
| 1:w:175:ASP:HB3  | 1:w:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:z:175:ASP:HB3  | 1:z:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:3:302:ALA:HB2  | 1:4:384:ARG:HG3  | 1.78                     | 0.66              |
| 1:7:249:GLU:HG3  | 1:7:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:A:450:LYS:NZ   | 1:B:182:TYR:O    | 2.27                     | 0.66              |
| 1:K:249:GLU:HG3  | 1:K:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:T:384:ARG:HG3  | 1:d:302:ALA:HB2  | 1.78                     | 0.66              |
| 1:W:249:GLU:HG3  | 1:W:536:LYS:HD3  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:175:ASP:HB3  | 1:l:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:v:490:GLU:HG3  | 1:y:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:4:249:GLU:HG3  | 1:4:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:B:158:PHE:HB2  | 1:B:226:HIS:HB3  | 1.75                     | 0.66              |
| 1:E:175:ASP:HB3  | 1:E:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:H:384:ARG:HG3  | 1:W:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:L:175:ASP:HB3  | 1:L:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:R:175:ASP:HB3  | 1:R:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:R:384:ARG:HG3  | 1:S:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:V:450:LYS:NZ   | 1:W:182:TYR:O    | 2.26                     | 0.66              |
| 1:W:109:GLN:HE22 | 1:X:490:GLU:HG3  | 1.61                     | 0.66              |
| 1:g:182:TYR:O    | 1:1:450:LYS:NZ   | 2.26                     | 0.66              |
| 1:v:450:LYS:NZ   | 1:1:182:TYR:O    | 2.27                     | 0.66              |
| 1:6:249:GLU:HG3  | 1:6:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:B:450:LYS:NZ   | 1:C:182:TYR:O    | 2.26                     | 0.66              |
| 1:C:490:GLU:HG3  | 1:L:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:D:249:GLU:HG3  | 1:D:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:D:490:GLU:HG3  | 1:M:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:E:384:ARG:HG3  | 1:Q:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:M:302:ALA:HB2  | 1:b:384:ARG:HG3  | 1.78                     | 0.66              |
| 1:P:249:GLU:HG3  | 1:P:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:S:175:ASP:HB3  | 1:S:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:V:175:ASP:HB3  | 1:V:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:Y:490:GLU:HG3  | 1:Z:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:b:249:GLU:HG3  | 1:b:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:f:249:GLU:HG3  | 1:f:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:f:384:ARG:HG3  | 1:h:302:ALA:HB2  | 1.78                     | 0.66              |
| 1:h:109:GLN:HE22 | 1:k:490:GLU:HG3  | 1.61                     | 0.66              |
| 1:j:249:GLU:HG3  | 1:j:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:q:175:ASP:HB3  | 1:q:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:r:175:ASP:HB3  | 1:r:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:w:384:ARG:HG3  | 1:x:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:1:158:PHE:HB2  | 1:1:226:HIS:HB3  | 1.76                     | 0.66              |
| 1:7:158:PHE:HB2  | 1:7:226:HIS:HB3  | 1.76                     | 0.66              |
| 1:A:109:GLN:HE22 | 1:F:490:GLU:HG3  | 1.61                     | 0.66              |
| 1:A:490:GLU:HG3  | 1:F:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:G:384:ARG:HG3  | 1:I:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:h:158:PHE:HB2  | 1:h:226:HIS:HB3  | 1.76                     | 0.66              |
| 1:k:249:GLU:HG3  | 1:k:536:LYS:HD3  | 1.77                     | 0.66              |
| 1:p:175:ASP:HB3  | 1:p:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:q:384:ARG:HG3  | 1:r:302:ALA:HB2  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:384:ARG:HG3  | 1:u:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:5:384:ARG:HG3  | 1:6:302:ALA:HB2  | 1.77                     | 0.66              |
| 1:7:490:GLU:HG3  | 1:8:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:H:450:LYS:NZ   | 1:Z:182:TYR:O    | 2.26                     | 0.66              |
| 1:K:182:TYR:O    | 1:L:450:LYS:NZ   | 2.26                     | 0.66              |
| 1:N:490:GLU:HG3  | 1:O:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:O:302:ALA:HB2  | 1:n:384:ARG:HG3  | 1.77                     | 0.66              |
| 1:g:175:ASP:HB3  | 1:g:188:PHE:CE2  | 2.30                     | 0.66              |
| 1:g:450:LYS:NZ   | 1:k:182:TYR:O    | 2.26                     | 0.66              |
| 1:i:490:GLU:HG3  | 1:l:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:v:109:GLN:HE22 | 1:y:490:GLU:HG3  | 1.61                     | 0.66              |
| 1:z:384:ARG:HG3  | 1:1:302:ALA:HB2  | 1.76                     | 0.66              |
| 1:2:490:GLU:HG3  | 1:4:109:GLN:HE22 | 1.61                     | 0.66              |
| 1:A:384:ARG:HG3  | 1:G:302:ALA:HB2  | 1.78                     | 0.65              |
| 1:C:109:GLN:HE22 | 1:L:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:o:249:GLU:HG3  | 1:o:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:t:302:ALA:HB2  | 1:v:384:ARG:HG3  | 1.78                     | 0.65              |
| 1:5:450:LYS:NZ   | 1:8:182:TYR:O    | 2.26                     | 0.65              |
| 1:C:104:SER:HB2  | 1:C:177:MET:CE   | 2.27                     | 0.65              |
| 1:E:302:ALA:HB2  | 1:F:384:ARG:HG3  | 1.78                     | 0.65              |
| 1:M:158:PHE:HB2  | 1:M:226:HIS:HB3  | 1.76                     | 0.65              |
| 1:X:249:GLU:HG3  | 1:X:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:d:384:ARG:HG3  | 1:l:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:g:104:SER:HB2  | 1:g:177:MET:CE   | 2.27                     | 0.65              |
| 1:w:302:ALA:HB2  | 1:y:384:ARG:HG3  | 1.78                     | 0.65              |
| 1:C:175:ASP:HB3  | 1:C:188:PHE:CE2  | 2.30                     | 0.65              |
| 1:C:450:LYS:NZ   | 1:D:182:TYR:O    | 2.26                     | 0.65              |
| 1:E:104:SER:HB2  | 1:E:177:MET:CE   | 2.27                     | 0.65              |
| 1:J:109:GLN:HE22 | 1:K:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:M:175:ASP:HB3  | 1:M:188:PHE:CE2  | 2.30                     | 0.65              |
| 1:Q:109:GLN:HE22 | 1:R:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:W:490:GLU:HG3  | 1:X:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:Z:104:SER:HB2  | 1:Z:177:MET:CE   | 2.27                     | 0.65              |
| 1:c:104:SER:HB2  | 1:c:177:MET:CE   | 2.27                     | 0.65              |
| 1:e:104:SER:HB2  | 1:e:177:MET:CE   | 2.27                     | 0.65              |
| 1:e:109:GLN:HE22 | 1:f:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:q:104:SER:HB2  | 1:q:177:MET:CE   | 2.27                     | 0.65              |
| 1:q:490:GLU:HG3  | 1:x:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:u:104:SER:HB2  | 1:u:177:MET:CE   | 2.27                     | 0.65              |
| 1:w:104:SER:HB2  | 1:w:177:MET:CE   | 2.27                     | 0.65              |
| 1:z:450:LYS:NZ   | 1:4:182:TYR:O    | 2.26                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:8:104:SER:HB2  | 1:8:177:MET:CE   | 2.27                     | 0.65              |
| 1:B:249:GLU:HG3  | 1:B:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:G:104:SER:HB2  | 1:G:177:MET:CE   | 2.27                     | 0.65              |
| 1:H:104:SER:HB2  | 1:H:177:MET:CE   | 2.27                     | 0.65              |
| 1:I:104:SER:HB2  | 1:I:177:MET:CE   | 2.27                     | 0.65              |
| 1:L:104:SER:HB2  | 1:L:177:MET:CE   | 2.27                     | 0.65              |
| 1:R:104:SER:HB2  | 1:R:177:MET:CE   | 2.27                     | 0.65              |
| 1:l:302:ALA:O    | 1:l:351:TYR:OH   | 2.08                     | 0.65              |
| 1:u:450:LYS:NZ   | 1:5:182:TYR:O    | 2.26                     | 0.65              |
| 1:v:104:SER:HB2  | 1:v:177:MET:CE   | 2.27                     | 0.65              |
| 1:A:104:SER:HB2  | 1:A:177:MET:CE   | 2.27                     | 0.65              |
| 1:B:490:GLU:HG3  | 1:I:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:D:384:ARG:HG3  | 1:N:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:H:182:TYR:O    | 1:I:450:LYS:NZ   | 2.26                     | 0.65              |
| 1:K:104:SER:HB2  | 1:K:177:MET:CE   | 2.27                     | 0.65              |
| 1:K:450:LYS:NZ   | 1:7:182:TYR:O    | 2.26                     | 0.65              |
| 1:N:104:SER:HB2  | 1:N:177:MET:CE   | 2.27                     | 0.65              |
| 1:T:175:ASP:HB2  | 1:T:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:Z:384:ARG:HG3  | 1:4:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:g:490:GLU:HG3  | 1:z:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:m:175:ASP:HB2  | 1:m:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:o:109:GLN:HE22 | 1:6:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:t:104:SER:HB2  | 1:t:177:MET:CE   | 2.27                     | 0.65              |
| 1:y:104:SER:HB2  | 1:y:177:MET:CE   | 2.27                     | 0.65              |
| 1:z:104:SER:HB2  | 1:z:177:MET:CE   | 2.27                     | 0.65              |
| 1:2:302:ALA:O    | 1:2:351:TYR:OH   | 2.08                     | 0.65              |
| 1:5:104:SER:HB2  | 1:5:177:MET:CE   | 2.27                     | 0.65              |
| 1:B:109:GLN:HE22 | 1:I:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:E:249:GLU:HG3  | 1:E:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:F:104:SER:HB2  | 1:F:177:MET:CE   | 2.27                     | 0.65              |
| 1:K:302:ALA:HB2  | 1:8:384:ARG:HG3  | 1.77                     | 0.65              |
| 1:M:104:SER:HB2  | 1:M:177:MET:CE   | 2.27                     | 0.65              |
| 1:O:104:SER:HB2  | 1:O:177:MET:CE   | 2.27                     | 0.65              |
| 1:P:104:SER:HB2  | 1:P:177:MET:CE   | 2.27                     | 0.65              |
| 1:X:302:ALA:HB2  | 1:e:384:ARG:HG3  | 1.78                     | 0.65              |
| 1:b:104:SER:HB2  | 1:b:177:MET:CE   | 2.27                     | 0.65              |
| 1:b:490:GLU:HG3  | 1:c:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:c:384:ARG:HG3  | 1:o:302:ALA:HB2  | 1.78                     | 0.65              |
| 1:h:104:SER:HB2  | 1:h:177:MET:CE   | 2.27                     | 0.65              |
| 1:h:175:ASP:HB3  | 1:h:188:PHE:CE2  | 2.30                     | 0.65              |
| 1:i:104:SER:HB2  | 1:i:177:MET:CE   | 2.27                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:302:ALA:O    | 1:j:351:TYR:OH   | 2.08                     | 0.65              |
| 1:k:450:LYS:NZ   | 1:w:182:TYR:O    | 2.26                     | 0.65              |
| 1:p:249:GLU:HG3  | 1:p:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:t:490:GLU:HG3  | 1:5:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:u:384:ARG:HG3  | 1:v:302:ALA:HB2  | 1.78                     | 0.65              |
| 1:w:249:GLU:HG3  | 1:w:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:1:384:ARG:HG3  | 1:2:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:4:104:SER:HB2  | 1:4:177:MET:CE   | 2.27                     | 0.65              |
| 1:5:302:ALA:O    | 1:5:351:TYR:OH   | 2.08                     | 0.65              |
| 1:A:302:ALA:HB2  | 1:I:384:ARG:HG3  | 1.78                     | 0.65              |
| 1:B:104:SER:HB2  | 1:B:177:MET:CE   | 2.27                     | 0.65              |
| 1:D:109:GLN:HE22 | 1:M:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:G:490:GLU:HG3  | 1:H:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:K:175:ASP:HB2  | 1:K:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:N:109:GLN:HE22 | 1:O:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:N:249:GLU:HG3  | 1:N:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:R:175:ASP:HB2  | 1:R:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:U:104:SER:HB2  | 1:U:177:MET:CE   | 2.27                     | 0.65              |
| 1:V:175:ASP:HB2  | 1:V:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:V:249:GLU:HG3  | 1:V:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:X:104:SER:HB2  | 1:X:177:MET:CE   | 2.27                     | 0.65              |
| 1:i:249:GLU:HG3  | 1:i:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:i:302:ALA:HB2  | 1:k:384:ARG:HG3  | 1.77                     | 0.65              |
| 1:j:104:SER:HB2  | 1:j:177:MET:CE   | 2.27                     | 0.65              |
| 1:l:104:SER:HB2  | 1:l:177:MET:CE   | 2.27                     | 0.65              |
| 1:p:175:ASP:HB2  | 1:p:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:q:175:ASP:HB2  | 1:q:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:u:109:GLN:HE22 | 1:1:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:u:249:GLU:HG3  | 1:u:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:z:302:ALA:HB2  | 1:2:384:ARG:HG3  | 1.77                     | 0.65              |
| 1:1:104:SER:HB2  | 1:1:177:MET:CE   | 2.27                     | 0.65              |
| 1:2:109:GLN:HE22 | 1:4:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:F:249:GLU:HG3  | 1:F:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:N:175:ASP:HB2  | 1:N:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:S:104:SER:HB2  | 1:S:177:MET:CE   | 2.27                     | 0.65              |
| 1:S:175:ASP:HB2  | 1:S:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:i:109:GLN:HE22 | 1:l:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:i:175:ASP:HB2  | 1:i:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:o:104:SER:HB2  | 1:o:177:MET:CE   | 2.27                     | 0.65              |
| 1:r:104:SER:HB2  | 1:r:177:MET:CE   | 2.27                     | 0.65              |
| 1:s:104:SER:HB2  | 1:s:177:MET:CE   | 2.27                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:249:GLU:HG3  | 1:1:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:2:182:TYR:O    | 1:3:450:LYS:NZ   | 2.27                     | 0.65              |
| 1:4:175:ASP:HB2  | 1:4:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:8:249:GLU:HG3  | 1:8:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:D:450:LYS:NZ   | 1:E:182:TYR:O    | 2.26                     | 0.65              |
| 1:I:175:ASP:HB2  | 1:I:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:I:249:GLU:HG3  | 1:I:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:J:104:SER:HB2  | 1:J:177:MET:CE   | 2.27                     | 0.65              |
| 1:N:384:ARG:HG3  | 1:P:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:O:384:ARG:HG3  | 1:m:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:R:249:GLU:HG3  | 1:R:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:U:490:GLU:HG3  | 1:V:109:GLN:HE22 | 1.60                     | 0.65              |
| 1:V:104:SER:HB2  | 1:V:177:MET:CE   | 2.27                     | 0.65              |
| 1:V:384:ARG:HG3  | 1:e:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:Y:182:TYR:O    | 1:4:450:LYS:NZ   | 2.26                     | 0.65              |
| 1:Z:249:GLU:HG3  | 1:Z:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:c:302:ALA:HB2  | 1:p:384:ARG:HG3  | 1.77                     | 0.65              |
| 1:f:104:SER:HB2  | 1:f:177:MET:CE   | 2.27                     | 0.65              |
| 1:h:490:GLU:HG3  | 1:k:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:i:384:ARG:HG3  | 1:j:302:ALA:HB2  | 1.77                     | 0.65              |
| 1:m:109:GLN:HE22 | 1:r:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:q:109:GLN:HE22 | 1:x:490:GLU:HG3  | 1.61                     | 0.65              |
| 1:q:249:GLU:HG3  | 1:q:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:r:175:ASP:HB2  | 1:r:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:u:175:ASP:HB2  | 1:u:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:u:490:GLU:HG3  | 1:1:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:x:104:SER:HB2  | 1:x:177:MET:CE   | 2.27                     | 0.65              |
| 1:E:490:GLU:HG3  | 1:P:109:GLN:HE22 | 1.61                     | 0.65              |
| 1:F:175:ASP:HB2  | 1:F:188:PHE:CE2  | 2.32                     | 0.65              |
| 1:H:302:ALA:O    | 1:H:351:TYR:OH   | 2.08                     | 0.65              |
| 1:J:302:ALA:O    | 1:J:351:TYR:OH   | 2.08                     | 0.65              |
| 1:M:182:TYR:O    | 1:N:450:LYS:NZ   | 2.26                     | 0.65              |
| 1:W:104:SER:HB2  | 1:W:177:MET:CE   | 2.27                     | 0.65              |
| 1:p:104:SER:HB2  | 1:p:177:MET:CE   | 2.27                     | 0.65              |
| 1:v:249:GLU:HG3  | 1:v:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:y:249:GLU:HG3  | 1:y:536:LYS:HD3  | 1.77                     | 0.65              |
| 1:A:249:GLU:HG3  | 1:A:536:LYS:HD3  | 1.77                     | 0.64              |
| 1:B:302:ALA:HB2  | 1:L:384:ARG:HG3  | 1.77                     | 0.64              |
| 1:Q:104:SER:HB2  | 1:Q:177:MET:CE   | 2.27                     | 0.64              |
| 1:Q:490:GLU:HG3  | 1:R:109:GLN:HE22 | 1.61                     | 0.64              |
| 1:R:420:PRO:HG2  | 1:U:403:ILE:HD13 | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:302:ALA:HB2  | 1:l:384:ARG:HG3  | 1.77                     | 0.64              |
| 1:d:104:SER:HB2  | 1:d:177:MET:CE   | 2.27                     | 0.64              |
| 1:j:109:GLN:HE22 | 1:w:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:m:490:GLU:HG3  | 1:r:109:GLN:HE22 | 1.61                     | 0.64              |
| 1:p:109:GLN:HE22 | 1:s:490:GLU:HG3  | 1.60                     | 0.64              |
| 1:q:420:PRO:HG2  | 1:s:403:ILE:HD13 | 1.79                     | 0.64              |
| 1:y:175:ASP:HB2  | 1:y:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:2:104:SER:HB2  | 1:2:177:MET:CE   | 2.27                     | 0.64              |
| 1:2:175:ASP:HB2  | 1:2:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:6:104:SER:HB2  | 1:6:177:MET:CE   | 2.27                     | 0.64              |
| 1:8:175:ASP:HB2  | 1:8:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:F:450:LYS:NZ   | 1:R:182:TYR:O    | 2.27                     | 0.64              |
| 1:J:175:ASP:HB2  | 1:J:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:O:175:ASP:HB2  | 1:O:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:S:109:GLN:HE22 | 1:T:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:S:403:ILE:HD13 | 1:U:420:PRO:HG2  | 1.79                     | 0.64              |
| 1:S:490:GLU:HG3  | 1:T:109:GLN:HE22 | 1.61                     | 0.64              |
| 1:Z:175:ASP:HB2  | 1:Z:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:e:175:ASP:HB2  | 1:e:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:n:104:SER:HB2  | 1:n:177:MET:CE   | 2.27                     | 0.64              |
| 1:n:175:ASP:HB2  | 1:n:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:r:403:ILE:HD13 | 1:s:420:PRO:HG2  | 1.79                     | 0.64              |
| 1:H:175:ASP:HB2  | 1:H:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:Y:104:SER:HB2  | 1:Y:177:MET:CE   | 2.27                     | 0.64              |
| 1:a:490:GLU:HG3  | 1:3:109:GLN:HE22 | 1.61                     | 0.64              |
| 1:c:175:ASP:HB2  | 1:c:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:f:302:ALA:HB2  | 1:g:384:ARG:HG3  | 1.77                     | 0.64              |
| 1:h:182:TYR:O    | 1:i:450:LYS:NZ   | 2.26                     | 0.64              |
| 1:7:175:ASP:HB2  | 1:7:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:C:403:ILE:HD13 | 1:b:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:G:109:GLN:HE22 | 1:H:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:J:182:TYR:O    | 1:a:450:LYS:NZ   | 2.27                     | 0.64              |
| 1:J:403:ILE:HD13 | 1:L:420:PRO:HG2  | 1.78                     | 0.64              |
| 1:K:420:PRO:HG2  | 1:8:403:ILE:HD13 | 1.80                     | 0.64              |
| 1:N:403:ILE:HD13 | 1:P:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:X:420:PRO:HG2  | 1:e:403:ILE:HD13 | 1.80                     | 0.64              |
| 1:Y:175:ASP:HB2  | 1:Y:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:Z:403:ILE:HD13 | 1:4:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:c:403:ILE:HD13 | 1:o:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:d:175:ASP:HB2  | 1:d:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:f:420:PRO:HG2  | 1:g:403:ILE:HD13 | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:175:ASP:HB2  | 1:l:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:7:104:SER:HB2  | 1:7:177:MET:CE   | 2.27                     | 0.64              |
| 1:C:384:ARG:HG3  | 1:b:302:ALA:HB2  | 1.77                     | 0.64              |
| 1:D:175:ASP:HB2  | 1:D:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:F:302:ALA:HB2  | 1:Q:384:ARG:HG3  | 1.78                     | 0.64              |
| 1:I:435:LEU:HB3  | 1:I:437:MET:HE3  | 1.80                     | 0.64              |
| 1:W:302:ALA:O    | 1:W:351:TYR:OH   | 2.08                     | 0.64              |
| 1:c:435:LEU:HB3  | 1:c:437:MET:HE3  | 1.80                     | 0.64              |
| 1:i:403:ILE:HD13 | 1:j:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:k:104:SER:HB2  | 1:k:177:MET:CE   | 2.27                     | 0.64              |
| 1:s:175:ASP:HB2  | 1:s:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:t:109:GLN:HE22 | 1:5:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:t:435:LEU:HB3  | 1:t:437:MET:HE3  | 1.80                     | 0.64              |
| 1:u:435:LEU:HB3  | 1:u:437:MET:HE3  | 1.80                     | 0.64              |
| 1:1:403:ILE:HD13 | 1:2:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:2:435:LEU:HB3  | 1:2:437:MET:HE3  | 1.80                     | 0.64              |
| 1:5:175:ASP:HB2  | 1:5:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:6:403:ILE:HD13 | 1:7:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:A:435:LEU:HB3  | 1:A:437:MET:HE3  | 1.80                     | 0.64              |
| 1:G:435:LEU:HB3  | 1:G:437:MET:HE3  | 1.80                     | 0.64              |
| 1:J:435:LEU:HB3  | 1:J:437:MET:HE3  | 1.80                     | 0.64              |
| 1:N:435:LEU:HB3  | 1:N:437:MET:HE3  | 1.80                     | 0.64              |
| 1:S:435:LEU:HB3  | 1:S:437:MET:HE3  | 1.80                     | 0.64              |
| 1:U:175:ASP:HB2  | 1:U:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:V:403:ILE:HD13 | 1:e:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:W:403:ILE:HD13 | 1:Y:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:a:104:SER:HB2  | 1:a:177:MET:CE   | 2.27                     | 0.64              |
| 1:a:109:GLN:HE22 | 1:3:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:c:420:PRO:HG2  | 1:p:403:ILE:HD13 | 1.80                     | 0.64              |
| 1:e:435:LEU:HB3  | 1:e:437:MET:HE3  | 1.80                     | 0.64              |
| 1:f:175:ASP:HB2  | 1:f:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:j:490:GLU:HG3  | 1:w:109:GLN:HE22 | 1.61                     | 0.64              |
| 1:m:104:SER:HB2  | 1:m:177:MET:CE   | 2.27                     | 0.64              |
| 1:q:182:TYR:O    | 1:y:450:LYS:NZ   | 2.27                     | 0.64              |
| 1:v:435:LEU:HB3  | 1:v:437:MET:HE3  | 1.80                     | 0.64              |
| 1:x:384:ARG:HG3  | 1:y:302:ALA:HB2  | 1.78                     | 0.64              |
| 1:3:175:ASP:HB2  | 1:3:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:6:175:ASP:HB2  | 1:6:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:A:175:ASP:HB2  | 1:A:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:D:104:SER:HB2  | 1:D:177:MET:CE   | 2.27                     | 0.64              |
| 1:E:109:GLN:HE22 | 1:P:490:GLU:HG3  | 1.61                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:403:ILE:HD13 | 1:W:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:L:435:LEU:HB3  | 1:L:437:MET:HE3  | 1.80                     | 0.64              |
| 1:W:175:ASP:HB2  | 1:W:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:X:175:ASP:HB2  | 1:X:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:Y:109:GLN:HE22 | 1:Z:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:d:490:GLU:HG3  | 1:n:109:GLN:HE22 | 1.61                     | 0.64              |
| 1:g:420:PRO:HG2  | 1:h:403:ILE:HD13 | 1.80                     | 0.64              |
| 1:i:435:LEU:HB3  | 1:i:437:MET:HE3  | 1.80                     | 0.64              |
| 1:k:175:ASP:HB2  | 1:k:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:r:435:LEU:HB3  | 1:r:437:MET:HE3  | 1.80                     | 0.64              |
| 1:x:175:ASP:HB2  | 1:x:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:z:435:LEU:HB3  | 1:z:437:MET:HE3  | 1.80                     | 0.64              |
| 1:C:420:PRO:HG2  | 1:M:403:ILE:HD13 | 1.80                     | 0.64              |
| 1:Q:175:ASP:HB2  | 1:Q:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:T:104:SER:HB2  | 1:T:177:MET:CE   | 2.27                     | 0.64              |
| 1:Z:435:LEU:HB3  | 1:Z:437:MET:HE3  | 1.80                     | 0.64              |
| 1:a:175:ASP:HB2  | 1:a:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:b:175:ASP:HB2  | 1:b:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:d:109:GLN:HE22 | 1:n:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:j:435:LEU:HB3  | 1:j:437:MET:HE3  | 1.80                     | 0.64              |
| 1:v:175:ASP:HB2  | 1:v:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:w:175:ASP:HB2  | 1:w:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:3:104:SER:HB2  | 1:3:177:MET:CE   | 2.27                     | 0.64              |
| 1:5:403:ILE:HD13 | 1:6:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:7:109:GLN:HE22 | 1:8:490:GLU:HG3  | 1.61                     | 0.64              |
| 1:G:175:ASP:HB2  | 1:G:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:P:175:ASP:HB2  | 1:P:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:P:435:LEU:HB3  | 1:P:437:MET:HE3  | 1.80                     | 0.64              |
| 1:U:435:LEU:HB3  | 1:U:437:MET:HE3  | 1.80                     | 0.64              |
| 1:X:182:TYR:O    | 1:Y:450:LYS:NZ   | 2.26                     | 0.64              |
| 1:h:175:ASP:HB2  | 1:h:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:s:435:LEU:HB3  | 1:s:437:MET:HE3  | 1.80                     | 0.64              |
| 1:t:175:ASP:HB2  | 1:t:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:8:435:LEU:HB3  | 1:8:437:MET:HE3  | 1.80                     | 0.64              |
| 1:E:175:ASP:HB2  | 1:E:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:F:420:PRO:HG2  | 1:Q:403:ILE:HD13 | 1.80                     | 0.64              |
| 1:d:435:LEU:HB3  | 1:d:437:MET:HE3  | 1.80                     | 0.64              |
| 1:g:175:ASP:HB2  | 1:g:188:PHE:CE2  | 2.32                     | 0.64              |
| 1:g:435:LEU:HB3  | 1:g:437:MET:HE3  | 1.80                     | 0.64              |
| 1:n:435:LEU:HB3  | 1:n:437:MET:HE3  | 1.80                     | 0.64              |
| 1:o:182:TYR:O    | 1:7:450:LYS:NZ   | 2.26                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:435:LEU:HB3  | 1:o:437:MET:HE3  | 1.80                     | 0.64              |
| 1:x:403:ILE:HD13 | 1:y:420:PRO:HG2  | 1.80                     | 0.64              |
| 1:4:435:LEU:HB3  | 1:4:437:MET:HE3  | 1.80                     | 0.64              |
| 1:C:435:LEU:HB3  | 1:C:437:MET:HE3  | 1.80                     | 0.63              |
| 1:E:420:PRO:HG2  | 1:F:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:K:435:LEU:HB3  | 1:K:437:MET:HE3  | 1.80                     | 0.63              |
| 1:M:175:ASP:HB2  | 1:M:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:M:420:PRO:HG2  | 1:b:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:R:435:LEU:HB3  | 1:R:437:MET:HE3  | 1.80                     | 0.63              |
| 1:U:109:GLN:HE22 | 1:V:490:GLU:HG3  | 1.61                     | 0.63              |
| 1:W:435:LEU:HB3  | 1:W:437:MET:HE3  | 1.80                     | 0.63              |
| 1:X:435:LEU:HB3  | 1:X:437:MET:HE3  | 1.80                     | 0.63              |
| 1:a:403:ILE:HD13 | 1:8:420:PRO:HG2  | 1.80                     | 0.63              |
| 1:j:175:ASP:HB2  | 1:j:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:p:490:GLU:HG3  | 1:s:109:GLN:HE22 | 1.61                     | 0.63              |
| 1:w:420:PRO:HG2  | 1:y:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:1:175:ASP:HB2  | 1:1:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:2:357:GLN:HE21 | 1:2:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:6:435:LEU:HB3  | 1:6:437:MET:HE3  | 1.80                     | 0.63              |
| 1:B:175:ASP:HB2  | 1:B:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:C:175:ASP:HB2  | 1:C:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:T:357:GLN:HE21 | 1:T:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:d:357:GLN:HE21 | 1:d:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:f:435:LEU:HB3  | 1:f:437:MET:HE3  | 1.80                     | 0.63              |
| 1:g:357:GLN:HE21 | 1:g:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:k:435:LEU:HB3  | 1:k:437:MET:HE3  | 1.80                     | 0.63              |
| 1:m:357:GLN:HE21 | 1:m:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:n:357:GLN:HE21 | 1:n:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:q:435:LEU:HB3  | 1:q:437:MET:HE3  | 1.80                     | 0.63              |
| 1:z:403:ILE:HD13 | 1:1:420:PRO:HG2  | 1.79                     | 0.63              |
| 1:D:435:LEU:HB3  | 1:D:437:MET:HE3  | 1.80                     | 0.63              |
| 1:H:420:PRO:HG2  | 1:Y:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:J:357:GLN:HE21 | 1:J:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:L:175:ASP:HB2  | 1:L:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:N:357:GLN:HE21 | 1:N:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:P:357:GLN:HE21 | 1:P:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:Y:357:GLN:HE21 | 1:Y:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:Z:420:PRO:HG2  | 1:3:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:b:435:LEU:HB3  | 1:b:437:MET:HE3  | 1.80                     | 0.63              |
| 1:f:403:ILE:HD13 | 1:h:420:PRO:HG2  | 1.80                     | 0.63              |
| 1:i:357:GLN:HE21 | 1:i:368:ILE:HD12 | 1.64                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:357:GLN:HE21 | 1:j:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:o:175:ASP:HB2  | 1:o:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:5:420:PRO:HG2  | 1:7:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:C:357:GLN:HE21 | 1:C:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:T:435:LEU:HB3  | 1:T:437:MET:HE3  | 1.80                     | 0.63              |
| 1:V:420:PRO:HG2  | 1:X:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:Y:435:LEU:HB3  | 1:Y:437:MET:HE3  | 1.80                     | 0.63              |
| 1:m:435:LEU:HB3  | 1:m:437:MET:HE3  | 1.80                     | 0.63              |
| 1:o:357:GLN:HE21 | 1:o:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:o:403:ILE:HD13 | 1:p:420:PRO:HG2  | 1.80                     | 0.63              |
| 1:7:357:GLN:HE21 | 1:7:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:7:435:LEU:HB3  | 1:7:437:MET:HE3  | 1.80                     | 0.63              |
| 1:B:357:GLN:HE21 | 1:B:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:F:435:LEU:HB3  | 1:F:437:MET:HE3  | 1.80                     | 0.63              |
| 1:L:357:GLN:HE21 | 1:L:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:Q:357:GLN:HE21 | 1:Q:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:X:357:GLN:HE21 | 1:X:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:v:357:GLN:HE21 | 1:v:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:y:435:LEU:HB3  | 1:y:437:MET:HE3  | 1.80                     | 0.63              |
| 1:z:175:ASP:HB2  | 1:z:188:PHE:CE2  | 2.32                     | 0.63              |
| 1:z:357:GLN:HE21 | 1:z:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:z:420:PRO:HG2  | 1:2:403:ILE:HD13 | 1.79                     | 0.63              |
| 1:Q:435:LEU:HB3  | 1:Q:437:MET:HE3  | 1.80                     | 0.63              |
| 1:x:357:GLN:HE21 | 1:x:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:x:435:LEU:HB3  | 1:x:437:MET:HE3  | 1.80                     | 0.63              |
| 1:1:357:GLN:HE21 | 1:1:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:A:357:GLN:HE21 | 1:A:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:B:420:PRO:HG2  | 1:L:403:ILE:HD13 | 1.80                     | 0.63              |
| 1:E:403:ILE:HD13 | 1:Q:420:PRO:HG2  | 1.80                     | 0.63              |
| 1:E:435:LEU:HB3  | 1:E:437:MET:HE3  | 1.80                     | 0.63              |
| 1:w:403:ILE:HD13 | 1:x:420:PRO:HG2  | 1.80                     | 0.63              |
| 1:8:357:GLN:HE21 | 1:8:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:I:357:GLN:HE21 | 1:I:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:R:403:ILE:HD13 | 1:S:420:PRO:HG2  | 1.80                     | 0.63              |
| 1:Z:357:GLN:HE21 | 1:Z:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:4:357:GLN:HE21 | 1:4:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:5:357:GLN:HE21 | 1:5:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:q:403:ILE:HD13 | 1:r:420:PRO:HG2  | 1.80                     | 0.63              |
| 1:u:357:GLN:HE21 | 1:u:368:ILE:HD12 | 1.64                     | 0.63              |
| 1:w:435:LEU:HB3  | 1:w:437:MET:HE3  | 1.80                     | 0.63              |
| 1:3:357:GLN:HE21 | 1:3:368:ILE:HD12 | 1.64                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:357:GLN:HE21 | 1:H:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:i:420:PRO:HG2  | 1:k:403:ILE:HD13 | 1.80                     | 0.62              |
| 1:D:403:ILE:HD13 | 1:N:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:K:357:GLN:HE21 | 1:K:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:k:357:GLN:HE21 | 1:k:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:s:357:GLN:HE21 | 1:s:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:3:420:PRO:HG2  | 1:4:403:ILE:HD13 | 1.80                     | 0.62              |
| 1:A:182:TYR:O    | 1:E:450:LYS:NZ   | 2.26                     | 0.62              |
| 1:A:420:PRO:HG2  | 1:I:403:ILE:HD13 | 1.80                     | 0.62              |
| 1:D:420:PRO:HG2  | 1:P:403:ILE:HD13 | 1.80                     | 0.62              |
| 1:O:435:LEU:HB3  | 1:O:437:MET:HE3  | 1.80                     | 0.62              |
| 1:U:357:GLN:HE21 | 1:U:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:a:357:GLN:HE21 | 1:a:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:l:435:LEU:HB3  | 1:l:437:MET:HE3  | 1.80                     | 0.62              |
| 1:m:403:ILE:HD13 | 1:n:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:u:403:ILE:HD13 | 1:v:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:1:435:LEU:HB3  | 1:1:437:MET:HE3  | 1.80                     | 0.62              |
| 1:B:435:LEU:HB3  | 1:B:437:MET:HE3  | 1.80                     | 0.62              |
| 1:D:357:GLN:HE21 | 1:D:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:O:403:ILE:HD13 | 1:m:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:S:357:GLN:HE21 | 1:S:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:T:403:ILE:HD13 | 1:d:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:T:420:PRO:HG2  | 1:l:403:ILE:HD13 | 1.80                     | 0.62              |
| 1:a:435:LEU:HB3  | 1:a:437:MET:HE3  | 1.80                     | 0.62              |
| 1:v:182:TYR:O    | 1:w:450:LYS:NZ   | 2.27                     | 0.62              |
| 1:3:435:LEU:HB3  | 1:3:437:MET:HE3  | 1.80                     | 0.62              |
| 1:H:435:LEU:HB3  | 1:H:437:MET:HE3  | 1.80                     | 0.62              |
| 1:O:420:PRO:HG2  | 1:n:403:ILE:HD13 | 1.80                     | 0.62              |
| 1:d:403:ILE:HD13 | 1:l:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:l:357:GLN:HE21 | 1:l:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:r:357:GLN:HE21 | 1:r:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:K:403:ILE:HD13 | 1:a:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:O:357:GLN:HE21 | 1:O:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:b:87:GLN:HE21  | 1:b:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:f:87:GLN:HE21  | 1:f:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:h:357:GLN:HE21 | 1:h:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:j:403:ILE:HD13 | 1:k:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:p:435:LEU:HB3  | 1:p:437:MET:HE3  | 1.80                     | 0.62              |
| 1:5:435:LEU:HB3  | 1:5:437:MET:HE3  | 1.80                     | 0.62              |
| 1:C:87:GLN:HE21  | 1:C:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:M:357:GLN:HE21 | 1:M:368:ILE:HD12 | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:435:LEU:HB3  | 1:V:437:MET:HE3  | 1.80                     | 0.62              |
| 1:d:194:PRO:HG2  | 1:d:195:VAL:HG23 | 1.82                     | 0.62              |
| 1:f:357:GLN:HE21 | 1:f:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:n:194:PRO:HG2  | 1:n:195:VAL:HG23 | 1.82                     | 0.62              |
| 1:p:194:PRO:HG2  | 1:p:195:VAL:HG23 | 1.82                     | 0.62              |
| 1:y:87:GLN:HE21  | 1:y:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:A:403:ILE:HD13 | 1:G:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:F:87:GLN:HE21  | 1:F:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:F:357:GLN:HE21 | 1:F:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:V:194:PRO:HG2  | 1:V:195:VAL:HG23 | 1.82                     | 0.62              |
| 1:Y:87:GLN:HE21  | 1:Y:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:b:357:GLN:HE21 | 1:b:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:g:87:GLN:HE21  | 1:g:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:t:357:GLN:HE21 | 1:t:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:7:87:GLN:HE21  | 1:7:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:A:87:GLN:HE21  | 1:A:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:M:435:LEU:HB3  | 1:M:437:MET:HE3  | 1.80                     | 0.62              |
| 1:U:87:GLN:HE21  | 1:U:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:c:357:GLN:HE21 | 1:c:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:i:87:GLN:HE21  | 1:i:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:s:87:GLN:HE21  | 1:s:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:t:403:ILE:HD13 | 1:u:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:t:420:PRO:HG2  | 1:v:403:ILE:HD13 | 1.80                     | 0.62              |
| 1:D:87:GLN:HE21  | 1:D:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:G:357:GLN:HE21 | 1:G:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:G:403:ILE:HD13 | 1:I:420:PRO:HG2  | 1.80                     | 0.62              |
| 1:K:87:GLN:HE21  | 1:K:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:N:87:GLN:HE21  | 1:N:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:T:87:GLN:HE21  | 1:T:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:V:357:GLN:HE21 | 1:V:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:b:194:PRO:HG2  | 1:b:195:VAL:HG23 | 1.82                     | 0.62              |
| 1:e:357:GLN:HE21 | 1:e:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:f:194:PRO:HG2  | 1:f:195:VAL:HG23 | 1.82                     | 0.62              |
| 1:h:435:LEU:HB3  | 1:h:437:MET:HE3  | 1.80                     | 0.62              |
| 1:v:87:GLN:HE21  | 1:v:193:ILE:HD13 | 1.65                     | 0.62              |
| 1:y:357:GLN:HE21 | 1:y:368:ILE:HD12 | 1.64                     | 0.62              |
| 1:G:87:GLN:HE21  | 1:G:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:e:175:ASP:CB   | 1:e:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:m:87:GLN:HE21  | 1:m:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:t:87:GLN:HE21  | 1:t:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:B:261:PRO:HB2  | 1:J:77:ILE:HG13  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:175:ASP:CB   | 1:R:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:g:194:PRO:HG2  | 1:g:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:k:87:GLN:HE21  | 1:k:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:w:308:ALA:HB1  | 1:y:282:THR:HG21 | 1.82                     | 0.61              |
| 1:4:87:GLN:HE21  | 1:4:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:C:194:PRO:HG2  | 1:C:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:E:308:ALA:HB1  | 1:F:282:THR:HG21 | 1.83                     | 0.61              |
| 1:H:87:GLN:HE21  | 1:H:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:O:87:GLN:HE21  | 1:O:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:Q:194:PRO:HG2  | 1:Q:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:V:87:GLN:HE21  | 1:V:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:W:357:GLN:HE21 | 1:W:368:ILE:HD12 | 1.64                     | 0.61              |
| 1:X:87:GLN:HE21  | 1:X:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:Z:87:GLN:HE21  | 1:Z:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:l:87:GLN:HE21  | 1:l:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:o:87:GLN:HE21  | 1:o:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:p:87:GLN:HE21  | 1:p:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:p:357:GLN:HE21 | 1:p:368:ILE:HD12 | 1.64                     | 0.61              |
| 1:q:175:ASP:CB   | 1:q:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:u:175:ASP:CB   | 1:u:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:x:194:PRO:HG2  | 1:x:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:5:87:GLN:HE21  | 1:5:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:I:175:ASP:CB   | 1:I:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:a:194:PRO:HG2  | 1:a:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:3:194:PRO:HG2  | 1:3:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:H:194:PRO:HG2  | 1:H:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:R:357:GLN:HE21 | 1:R:368:ILE:HD12 | 1.64                     | 0.61              |
| 1:q:194:PRO:HG2  | 1:q:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:u:282:THR:HG21 | 1:v:308:ALA:HB1  | 1.83                     | 0.61              |
| 1:6:357:GLN:HE21 | 1:6:368:ILE:HD12 | 1.64                     | 0.61              |
| 1:8:87:GLN:HE21  | 1:8:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:A:308:ALA:HB1  | 1:I:282:THR:HG21 | 1.83                     | 0.61              |
| 1:R:194:PRO:HG2  | 1:R:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:c:87:GLN:HE21  | 1:c:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:e:87:GLN:HE21  | 1:e:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:q:357:GLN:HE21 | 1:q:368:ILE:HD12 | 1.64                     | 0.61              |
| 1:t:308:ALA:HB1  | 1:v:282:THR:HG21 | 1.82                     | 0.61              |
| 1:5:194:PRO:HG2  | 1:5:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:A:282:THR:HG21 | 1:G:308:ALA:HB1  | 1.82                     | 0.61              |
| 1:J:87:GLN:HE21  | 1:J:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:P:87:GLN:HE21  | 1:P:193:ILE:HD13 | 1.65                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:175:ASP:CB   | 1:a:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:t:175:ASP:CB   | 1:t:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:w:357:GLN:HE21 | 1:w:368:ILE:HD12 | 1.64                     | 0.61              |
| 1:F:308:ALA:HB1  | 1:Q:282:THR:HG21 | 1.83                     | 0.61              |
| 1:G:175:ASP:CB   | 1:G:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:I:87:GLN:HE21  | 1:I:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:P:194:PRO:HG2  | 1:P:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:S:282:THR:HG21 | 1:U:308:ALA:HB1  | 1.83                     | 0.61              |
| 1:j:87:GLN:HE21  | 1:j:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:u:87:GLN:HE21  | 1:u:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:x:282:THR:HG21 | 1:y:308:ALA:HB1  | 1.83                     | 0.61              |
| 1:z:87:GLN:HE21  | 1:z:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:3:175:ASP:CB   | 1:3:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:8:194:PRO:HG2  | 1:8:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:B:87:GLN:HE21  | 1:B:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:E:357:GLN:HE21 | 1:E:368:ILE:HD12 | 1.64                     | 0.61              |
| 1:M:194:PRO:HG2  | 1:M:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:Z:194:PRO:HG2  | 1:Z:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:f:282:THR:HG21 | 1:h:308:ALA:HB1  | 1.83                     | 0.61              |
| 1:h:194:PRO:HG2  | 1:h:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:j:194:PRO:HG2  | 1:j:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:q:87:GLN:HE21  | 1:q:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:r:282:THR:HG21 | 1:s:308:ALA:HB1  | 1.83                     | 0.61              |
| 1:z:308:ALA:HB1  | 1:2:282:THR:HG21 | 1.83                     | 0.61              |
| 1:2:87:GLN:HE21  | 1:2:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:E:87:GLN:HE21  | 1:E:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:N:282:THR:HG21 | 1:P:308:ALA:HB1  | 1.83                     | 0.61              |
| 1:W:87:GLN:HE21  | 1:W:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:W:175:ASP:CB   | 1:W:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:X:175:ASP:CB   | 1:X:188:PHE:CZ   | 2.83                     | 0.61              |
| 1:a:87:GLN:HE21  | 1:a:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:i:282:THR:HG21 | 1:j:308:ALA:HB1  | 1.83                     | 0.61              |
| 1:s:194:PRO:HG2  | 1:s:195:VAL:HG23 | 1.82                     | 0.61              |
| 1:3:87:GLN:HE21  | 1:3:193:ILE:HD13 | 1.65                     | 0.61              |
| 1:A:194:PRO:HG2  | 1:A:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:D:175:ASP:CB   | 1:D:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:L:87:GLN:HE21  | 1:L:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:M:308:ALA:HB1  | 1:b:282:THR:HG21 | 1.83                     | 0.60              |
| 1:Q:87:GLN:HE21  | 1:Q:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:R:87:GLN:HE21  | 1:R:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:U:194:PRO:HG2  | 1:U:195:VAL:HG23 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:175:ASP:CB   | 1:V:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:X:77:ILE:HG13  | 1:e:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:X:194:PRO:HG2  | 1:X:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:k:175:ASP:CB   | 1:k:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:o:175:ASP:CB   | 1:o:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:p:175:ASP:CB   | 1:p:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:v:194:PRO:HG2  | 1:v:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:w:87:GLN:HE21  | 1:w:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:1:282:THR:HG21 | 1:2:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:6:175:ASP:CB   | 1:6:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:A:261:PRO:HB2  | 1:G:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:F:175:ASP:CB   | 1:F:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:O:194:PRO:HG2  | 1:O:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:S:194:PRO:HG2  | 1:S:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:c:261:PRO:HB2  | 1:o:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:i:77:ILE:HG13  | 1:k:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:i:175:ASP:CB   | 1:i:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:q:261:PRO:HB2  | 1:r:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:x:87:GLN:HE21  | 1:x:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:y:175:ASP:CB   | 1:y:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:1:87:GLN:HE21  | 1:1:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:1:261:PRO:HB2  | 1:2:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:5:308:ALA:HB1  | 1:7:282:THR:HG21 | 1.83                     | 0.60              |
| 1:6:87:GLN:HE21  | 1:6:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:B:77:ILE:HG13  | 1:L:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:B:194:PRO:HG2  | 1:B:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:D:261:PRO:HB2  | 1:N:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:H:308:ALA:HB1  | 1:Y:282:THR:HG21 | 1.83                     | 0.60              |
| 1:O:282:THR:HG21 | 1:m:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:R:261:PRO:HB2  | 1:S:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:T:308:ALA:HB1  | 1:l:282:THR:HG21 | 1.83                     | 0.60              |
| 1:l:194:PRO:HG2  | 1:l:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:o:194:PRO:HG2  | 1:o:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:t:77:ILE:HG13  | 1:v:261:PRO:HB2  | 1.84                     | 0.60              |
| 1:D:77:ILE:HG13  | 1:P:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:J:261:PRO:HB2  | 1:L:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:N:175:ASP:CB   | 1:N:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:P:175:ASP:CB   | 1:P:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:S:261:PRO:HB2  | 1:U:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:W:194:PRO:HG2  | 1:W:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:W:282:THR:HG21 | 1:Y:308:ALA:HB1  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:175:ASP:CB   | 1:j:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:r:194:PRO:HG2  | 1:r:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:1:194:PRO:HG2  | 1:1:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:6:194:PRO:HG2  | 1:6:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:6:282:THR:HG21 | 1:7:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:7:194:PRO:HG2  | 1:7:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:B:308:ALA:HB1  | 1:L:282:THR:HG21 | 1.83                     | 0.60              |
| 1:D:194:PRO:HG2  | 1:D:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:E:194:PRO:HG2  | 1:E:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:G:261:PRO:HB2  | 1:I:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:K:194:PRO:HG2  | 1:K:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:j:261:PRO:HB2  | 1:k:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:k:194:PRO:HG2  | 1:k:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:r:261:PRO:HB2  | 1:s:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:z:77:ILE:HG13  | 1:2:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:z:282:THR:HG21 | 1:1:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:3:77:ILE:HG13  | 1:4:261:PRO:HB2  | 1.84                     | 0.60              |
| 1:E:282:THR:HG21 | 1:Q:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:J:194:PRO:HG2  | 1:J:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:K:261:PRO:HB2  | 1:a:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:N:261:PRO:HB2  | 1:P:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:Y:194:PRO:HG2  | 1:Y:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:Z:282:THR:HG21 | 1:4:308:ALA:HB1  | 1.84                     | 0.60              |
| 1:i:261:PRO:HB2  | 1:j:77:ILE:HG13  | 1.83                     | 0.60              |
| 1:t:261:PRO:HB2  | 1:u:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:4:194:PRO:HG2  | 1:4:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:5:77:ILE:HG13  | 1:7:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:F:194:PRO:HG2  | 1:F:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:H:77:ILE:HG13  | 1:Y:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:K:308:ALA:HB1  | 1:8:282:THR:HG21 | 1.84                     | 0.60              |
| 1:L:194:PRO:HG2  | 1:L:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:M:87:GLN:HE21  | 1:M:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:S:87:GLN:HE21  | 1:S:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:T:194:PRO:HG2  | 1:T:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:X:308:ALA:HB1  | 1:e:282:THR:HG21 | 1.83                     | 0.60              |
| 1:Z:261:PRO:HB2  | 1:4:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:a:282:THR:HG21 | 1:8:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:c:282:THR:HG21 | 1:o:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:m:194:PRO:HG2  | 1:m:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:v:175:ASP:CB   | 1:v:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:w:194:PRO:HG2  | 1:w:195:VAL:HG23 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:282:THR:HG21 | 1:x:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:5:175:ASP:CB   | 1:5:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:B:282:THR:HG21 | 1:J:308:ALA:HB1  | 1.84                     | 0.60              |
| 1:K:77:ILE:HG13  | 1:8:261:PRO:HB2  | 1.84                     | 0.60              |
| 1:Z:308:ALA:HB1  | 1:3:282:THR:HG21 | 1.83                     | 0.60              |
| 1:h:87:GLN:HE21  | 1:h:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:n:87:GLN:HE21  | 1:n:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:p:70:HIS:HB3   | 1:p:450:LYS:HE3  | 1.84                     | 0.60              |
| 1:r:87:GLN:HE21  | 1:r:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:t:194:PRO:HG2  | 1:t:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:w:261:PRO:HB2  | 1:x:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:y:194:PRO:HG2  | 1:y:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:z:194:PRO:HG2  | 1:z:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:z:261:PRO:HB2  | 1:1:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:A:175:ASP:CB   | 1:A:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:E:261:PRO:HB2  | 1:Q:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:H:175:ASP:CB   | 1:H:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:H:406:ARG:HB2  | 1:H:531:LYS:HZ1  | 1.67                     | 0.60              |
| 1:O:70:HIS:HB3   | 1:O:450:LYS:HE3  | 1.84                     | 0.60              |
| 1:V:70:HIS:HB3   | 1:V:450:LYS:HE3  | 1.84                     | 0.60              |
| 1:V:282:THR:HG21 | 1:e:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:f:308:ALA:HB1  | 1:g:282:THR:HG21 | 1.83                     | 0.60              |
| 1:i:194:PRO:HG2  | 1:i:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:2:194:PRO:HG2  | 1:2:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:5:406:ARG:HB2  | 1:5:531:LYS:HZ1  | 1.67                     | 0.60              |
| 1:C:282:THR:HG21 | 1:b:308:ALA:HB1  | 1.83                     | 0.60              |
| 1:M:77:ILE:HG13  | 1:b:261:PRO:HB2  | 1.83                     | 0.60              |
| 1:O:175:ASP:CB   | 1:O:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:W:70:HIS:HB3   | 1:W:450:LYS:HE3  | 1.84                     | 0.60              |
| 1:c:308:ALA:HB1  | 1:p:282:THR:HG21 | 1.83                     | 0.60              |
| 1:d:87:GLN:HE21  | 1:d:193:ILE:HD13 | 1.65                     | 0.60              |
| 1:e:194:PRO:HG2  | 1:e:195:VAL:HG23 | 1.82                     | 0.60              |
| 1:l:70:HIS:HB3   | 1:l:450:LYS:HE3  | 1.84                     | 0.60              |
| 1:l:175:ASP:CB   | 1:l:188:PHE:CZ   | 2.83                     | 0.60              |
| 1:o:261:PRO:HB2  | 1:p:77:ILE:HG13  | 1.84                     | 0.60              |
| 1:6:70:HIS:HB3   | 1:6:450:LYS:HE3  | 1.84                     | 0.60              |
| 1:C:308:ALA:HB1  | 1:M:282:THR:HG21 | 1.84                     | 0.59              |
| 1:G:194:PRO:HG2  | 1:G:195:VAL:HG23 | 1.82                     | 0.59              |
| 1:J:70:HIS:HB3   | 1:J:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:T:511:HIS:CD2  | 1:U:218:PHE:HB2  | 2.37                     | 0.59              |
| 1:V:77:ILE:HG13  | 1:X:261:PRO:HB2  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:70:HIS:HB3   | 1:X:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:c:194:PRO:HG2  | 1:c:195:VAL:HG23 | 1.82                     | 0.59              |
| 1:f:261:PRO:HB2  | 1:h:77:ILE:HG13  | 1.83                     | 0.59              |
| 1:m:511:HIS:CD2  | 1:s:218:PHE:HB2  | 2.37                     | 0.59              |
| 1:o:70:HIS:HB3   | 1:o:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:x:261:PRO:HB2  | 1:y:77:ILE:HG13  | 1.84                     | 0.59              |
| 1:z:218:PHE:HB2  | 1:4:511:HIS:CD2  | 2.37                     | 0.59              |
| 1:2:70:HIS:HB3   | 1:2:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:4:316:MET:HE3  | 1:4:331:ALA:HA   | 1.85                     | 0.59              |
| 1:5:70:HIS:HB3   | 1:5:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:B:70:HIS:HB3   | 1:B:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:K:175:ASP:CB   | 1:K:188:PHE:CZ   | 2.84                     | 0.59              |
| 1:K:316:MET:HE3  | 1:K:331:ALA:HA   | 1.85                     | 0.59              |
| 1:N:194:PRO:HG2  | 1:N:195:VAL:HG23 | 1.82                     | 0.59              |
| 1:Z:316:MET:HE3  | 1:Z:331:ALA:HA   | 1.84                     | 0.59              |
| 1:a:70:HIS:HB3   | 1:a:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:d:175:ASP:CB   | 1:d:188:PHE:CZ   | 2.83                     | 0.59              |
| 1:g:308:ALA:HB1  | 1:h:282:THR:HG21 | 1.84                     | 0.59              |
| 1:v:511:HIS:CD2  | 1:w:218:PHE:HB2  | 2.37                     | 0.59              |
| 1:x:70:HIS:HB3   | 1:x:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:3:70:HIS:HB3   | 1:3:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:4:175:ASP:CB   | 1:4:188:PHE:CZ   | 2.83                     | 0.59              |
| 1:8:316:MET:HE3  | 1:8:331:ALA:HA   | 1.84                     | 0.59              |
| 1:A:511:HIS:CD2  | 1:E:218:PHE:HB2  | 2.37                     | 0.59              |
| 1:C:316:MET:HE3  | 1:C:331:ALA:HA   | 1.84                     | 0.59              |
| 1:E:77:ILE:HG13  | 1:F:261:PRO:HB2  | 1.84                     | 0.59              |
| 1:F:77:ILE:HG13  | 1:Q:261:PRO:HB2  | 1.84                     | 0.59              |
| 1:H:70:HIS:HB3   | 1:H:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:O:308:ALA:HB1  | 1:n:282:THR:HG21 | 1.83                     | 0.59              |
| 1:P:70:HIS:HB3   | 1:P:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:Q:70:HIS:HB3   | 1:Q:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:R:282:THR:HG21 | 1:S:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:S:70:HIS:HB3   | 1:S:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:g:70:HIS:HB3   | 1:g:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:g:316:MET:HE3  | 1:g:331:ALA:HA   | 1.85                     | 0.59              |
| 1:j:70:HIS:HB3   | 1:j:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:n:175:ASP:CB   | 1:n:188:PHE:CZ   | 2.83                     | 0.59              |
| 1:u:70:HIS:HB3   | 1:u:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:1:70:HIS:HB3   | 1:1:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:5:282:THR:HG21 | 1:6:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:C:70:HIS:HB3   | 1:C:450:LYS:HE3  | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:316:MET:HE3  | 1:F:331:ALA:HA   | 1.84                     | 0.59              |
| 1:H:282:THR:HG21 | 1:W:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:Q:316:MET:HE3  | 1:Q:331:ALA:HA   | 1.84                     | 0.59              |
| 1:R:70:HIS:HB3   | 1:R:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:R:316:MET:HE3  | 1:R:331:ALA:HA   | 1.84                     | 0.59              |
| 1:T:282:THR:HG21 | 1:d:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:b:511:HIS:CD2  | 1:o:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:c:316:MET:HE3  | 1:c:331:ALA:HA   | 1.84                     | 0.59              |
| 1:e:316:MET:HE3  | 1:e:331:ALA:HA   | 1.84                     | 0.59              |
| 1:m:261:PRO:HB2  | 1:n:77:ILE:HG13  | 1.84                     | 0.59              |
| 1:m:282:THR:HG21 | 1:n:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:n:70:HIS:HB3   | 1:n:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:q:70:HIS:HB3   | 1:q:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:q:282:THR:HG21 | 1:r:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:q:316:MET:HE3  | 1:q:331:ALA:HA   | 1.84                     | 0.59              |
| 1:r:70:HIS:HB3   | 1:r:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:u:194:PRO:HG2  | 1:u:195:VAL:HG23 | 1.82                     | 0.59              |
| 1:x:316:MET:HE3  | 1:x:331:ALA:HA   | 1.84                     | 0.59              |
| 1:5:316:MET:HE3  | 1:5:331:ALA:HA   | 1.85                     | 0.59              |
| 1:H:316:MET:HE3  | 1:H:331:ALA:HA   | 1.85                     | 0.59              |
| 1:S:511:HIS:CD2  | 1:d:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:T:261:PRO:HB2  | 1:d:77:ILE:HG13  | 1.84                     | 0.59              |
| 1:X:218:PHE:HB2  | 1:f:511:HIS:CD2  | 2.38                     | 0.59              |
| 1:d:70:HIS:HB3   | 1:d:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:d:282:THR:HG21 | 1:l:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:d:316:MET:HE3  | 1:d:331:ALA:HA   | 1.84                     | 0.59              |
| 1:f:218:PHE:HB2  | 1:z:511:HIS:CD2  | 2.37                     | 0.59              |
| 1:g:77:ILE:HG13  | 1:h:261:PRO:HB2  | 1.83                     | 0.59              |
| 1:n:218:PHE:HB2  | 1:r:511:HIS:CD2  | 2.38                     | 0.59              |
| 1:n:316:MET:HE3  | 1:n:331:ALA:HA   | 1.84                     | 0.59              |
| 1:w:77:ILE:HG13  | 1:y:261:PRO:HB2  | 1.84                     | 0.59              |
| 1:y:316:MET:HE3  | 1:y:331:ALA:HA   | 1.84                     | 0.59              |
| 1:E:70:HIS:HB3   | 1:E:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:F:218:PHE:HB2  | 1:R:511:HIS:CD2  | 2.37                     | 0.59              |
| 1:G:70:HIS:HB3   | 1:G:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:I:70:HIS:HB3   | 1:I:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:I:194:PRO:HG2  | 1:I:195:VAL:HG23 | 1.82                     | 0.59              |
| 1:L:70:HIS:HB3   | 1:L:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:O:316:MET:HE3  | 1:O:331:ALA:HA   | 1.84                     | 0.59              |
| 1:R:308:ALA:HB1  | 1:U:282:THR:HG21 | 1.83                     | 0.59              |
| 1:V:316:MET:HE3  | 1:V:331:ALA:HA   | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:316:MET:HE3  | 1:j:331:ALA:HA   | 1.85                     | 0.59              |
| 1:l:316:MET:HE3  | 1:l:331:ALA:HA   | 1.84                     | 0.59              |
| 1:p:316:MET:HE3  | 1:p:331:ALA:HA   | 1.85                     | 0.59              |
| 1:q:511:HIS:CD2  | 1:y:218:PHE:HB2  | 2.37                     | 0.59              |
| 1:z:316:MET:HE3  | 1:z:331:ALA:HA   | 1.84                     | 0.59              |
| 1:1:316:MET:HE3  | 1:1:331:ALA:HA   | 1.84                     | 0.59              |
| 1:B:316:MET:HE3  | 1:B:331:ALA:HA   | 1.85                     | 0.59              |
| 1:C:77:ILE:HG13  | 1:M:261:PRO:HB2  | 1.84                     | 0.59              |
| 1:E:316:MET:HE3  | 1:E:331:ALA:HA   | 1.85                     | 0.59              |
| 1:F:511:HIS:CD2  | 1:G:218:PHE:HB2  | 2.37                     | 0.59              |
| 1:K:218:PHE:HB2  | 1:7:511:HIS:CD2  | 2.38                     | 0.59              |
| 1:L:316:MET:HE3  | 1:L:331:ALA:HA   | 1.85                     | 0.59              |
| 1:P:316:MET:HE3  | 1:P:331:ALA:HA   | 1.85                     | 0.59              |
| 1:Y:511:HIS:CD2  | 1:4:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:f:175:ASP:CB   | 1:f:188:PHE:CZ   | 2.83                     | 0.59              |
| 1:q:308:ALA:HB1  | 1:s:282:THR:HG21 | 1.83                     | 0.59              |
| 1:t:70:HIS:HB3   | 1:t:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:t:218:PHE:HB2  | 1:y:511:HIS:CD2  | 2.37                     | 0.59              |
| 1:u:261:PRO:HB2  | 1:v:77:ILE:HG13  | 1.84                     | 0.59              |
| 1:w:70:HIS:HB3   | 1:w:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:w:316:MET:HE3  | 1:w:331:ALA:HA   | 1.85                     | 0.59              |
| 1:D:282:THR:HG21 | 1:N:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:D:308:ALA:HB1  | 1:P:282:THR:HG21 | 1.83                     | 0.59              |
| 1:G:511:HIS:CD2  | 1:W:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:H:261:PRO:HB2  | 1:W:77:ILE:HG13  | 1.83                     | 0.59              |
| 1:W:261:PRO:HB2  | 1:Y:77:ILE:HG13  | 1.83                     | 0.59              |
| 1:b:175:ASP:CB   | 1:b:188:PHE:CZ   | 2.83                     | 0.59              |
| 1:e:511:HIS:CD2  | 1:h:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:h:316:MET:HE3  | 1:h:331:ALA:HA   | 1.84                     | 0.59              |
| 1:i:308:ALA:HB1  | 1:k:282:THR:HG21 | 1.83                     | 0.59              |
| 1:z:70:HIS:HB3   | 1:z:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:6:261:PRO:HB2  | 1:7:77:ILE:HG13  | 1.83                     | 0.59              |
| 1:A:77:ILE:HG13  | 1:I:261:PRO:HB2  | 1.84                     | 0.59              |
| 1:A:218:PHE:HB2  | 1:B:511:HIS:CD2  | 2.37                     | 0.59              |
| 1:C:261:PRO:HB2  | 1:b:77:ILE:HG13  | 1.84                     | 0.59              |
| 1:K:282:THR:HG21 | 1:a:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:L:511:HIS:CD2  | 1:b:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:M:218:PHE:HB2  | 1:c:511:HIS:CD2  | 2.38                     | 0.59              |
| 1:T:70:HIS:HB3   | 1:T:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:j:282:THR:HG21 | 1:k:308:ALA:HB1  | 1.83                     | 0.59              |
| 1:m:70:HIS:HB3   | 1:m:450:LYS:HE3  | 1.84                     | 0.59              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:t:511:HIS:CD2 | 1:6:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:5:261:PRO:HB2 | 1:6:77:ILE:HG13  | 1.83                     | 0.59              |
| 1:H:511:HIS:CD2 | 1:I:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:X:511:HIS:CD2 | 1:Y:218:PHE:HB2  | 2.38                     | 0.59              |
| 1:f:77:ILE:HG13 | 1:g:261:PRO:HB2  | 1.84                     | 0.59              |
| 1:o:316:MET:HE3 | 1:o:331:ALA:HA   | 1.84                     | 0.59              |
| 1:v:218:PHE:HB2 | 1:1:511:HIS:CD2  | 2.37                     | 0.59              |
| 1:7:70:HIS:HB3  | 1:7:450:LYS:HE3  | 1.84                     | 0.59              |
| 1:M:70:HIS:HB3  | 1:M:450:LYS:HE3  | 1.84                     | 0.58              |
| 1:M:316:MET:HE3 | 1:M:331:ALA:HA   | 1.84                     | 0.58              |
| 1:O:218:PHE:HB2 | 1:d:511:HIS:CD2  | 2.38                     | 0.58              |
| 1:P:511:HIS:CD2 | 1:Q:218:PHE:HB2  | 2.38                     | 0.58              |
| 1:T:316:MET:HE3 | 1:T:331:ALA:HA   | 1.85                     | 0.58              |
| 1:Y:70:HIS:HB3  | 1:Y:450:LYS:HE3  | 1.84                     | 0.58              |
| 1:a:261:PRO:HB2 | 1:8:77:ILE:HG13  | 1.83                     | 0.58              |
| 1:d:261:PRO:HB2 | 1:l:77:ILE:HG13  | 1.83                     | 0.58              |
| 1:l:218:PHE:HB2 | 1:n:511:HIS:CD2  | 2.38                     | 0.58              |
| 1:m:316:MET:HE3 | 1:m:331:ALA:HA   | 1.85                     | 0.58              |
| 1:o:511:HIS:CD2 | 1:7:218:PHE:HB2  | 2.38                     | 0.58              |
| 1:u:218:PHE:HB2 | 1:5:511:HIS:CD2  | 2.38                     | 0.58              |
| 1:2:511:HIS:CD2 | 1:3:218:PHE:HB2  | 2.38                     | 0.58              |
| 1:3:308:ALA:HB1 | 1:4:282:THR:HG21 | 1.83                     | 0.58              |
| 1:C:175:ASP:CB  | 1:C:188:PHE:CZ   | 2.83                     | 0.58              |
| 1:C:218:PHE:HB2 | 1:D:511:HIS:CD2  | 2.38                     | 0.58              |
| 1:D:70:HIS:HB3  | 1:D:450:LYS:HE3  | 1.84                     | 0.58              |
| 1:M:511:HIS:CD2 | 1:N:218:PHE:HB2  | 2.38                     | 0.58              |
| 1:V:261:PRO:HB2 | 1:e:77:ILE:HG13  | 1.84                     | 0.58              |
| 1:V:308:ALA:HB1 | 1:X:282:THR:HG21 | 1.84                     | 0.58              |
| 1:c:70:HIS:HB3  | 1:c:450:LYS:HE3  | 1.84                     | 0.58              |
| 1:c:218:PHE:HB2 | 1:s:511:HIS:CD2  | 2.37                     | 0.58              |
| 1:g:218:PHE:HB2 | 1:k:511:HIS:CD2  | 2.38                     | 0.58              |
| 1:j:511:HIS:CD2 | 1:x:218:PHE:HB2  | 2.38                     | 0.58              |
| 1:k:70:HIS:HB3  | 1:k:450:LYS:HE3  | 1.84                     | 0.58              |
| 1:F:70:HIS:HB3  | 1:F:450:LYS:HE3  | 1.84                     | 0.58              |
| 1:O:77:ILE:HG13 | 1:n:261:PRO:HB2  | 1.83                     | 0.58              |
| 1:R:77:ILE:HG13 | 1:U:261:PRO:HB2  | 1.84                     | 0.58              |
| 1:U:511:HIS:CD2 | 1:e:218:PHE:HB2  | 2.37                     | 0.58              |
| 1:X:316:MET:HE3 | 1:X:331:ALA:HA   | 1.84                     | 0.58              |
| 1:Z:77:ILE:HG13 | 1:3:261:PRO:HB2  | 1.83                     | 0.58              |
| 1:Z:175:ASP:CB  | 1:Z:188:PHE:CZ   | 2.83                     | 0.58              |
| 1:h:70:HIS:HB3  | 1:h:450:LYS:HE3  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:h:511:HIS:CD2  | 1:i:218:PHE:HB2 | 2.38                     | 0.58              |
| 1:q:77:ILE:HG13  | 1:s:261:PRO:HB2 | 1.84                     | 0.58              |
| 1:7:175:ASP:CB   | 1:7:188:PHE:CZ  | 2.83                     | 0.58              |
| 1:U:70:HIS:HB3   | 1:U:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:b:70:HIS:HB3   | 1:b:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:c:77:ILE:HG13  | 1:p:261:PRO:HB2 | 1.84                     | 0.58              |
| 1:e:70:HIS:HB3   | 1:e:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:g:175:ASP:CB   | 1:g:188:PHE:CZ  | 2.83                     | 0.58              |
| 1:o:282:THR:HG21 | 1:p:308:ALA:HB1 | 1.84                     | 0.58              |
| 1:s:70:HIS:HB3   | 1:s:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:u:511:HIS:CD2  | 1:2:218:PHE:HB2 | 2.38                     | 0.58              |
| 1:y:70:HIS:HB3   | 1:y:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:6:316:MET:HE3  | 1:6:331:ALA:HA  | 1.84                     | 0.58              |
| 1:G:282:THR:HG21 | 1:I:308:ALA:HB1 | 1.83                     | 0.58              |
| 1:K:511:HIS:CD2  | 1:L:218:PHE:HB2 | 2.39                     | 0.58              |
| 1:N:511:HIS:CD2  | 1:m:218:PHE:HB2 | 2.38                     | 0.58              |
| 1:T:218:PHE:HB2  | 1:i:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:W:316:MET:HE3  | 1:W:331:ALA:HA  | 1.84                     | 0.58              |
| 1:f:70:HIS:HB3   | 1:f:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:p:218:PHE:HB2  | 1:6:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:p:511:HIS:CD2  | 1:q:218:PHE:HB2 | 2.39                     | 0.58              |
| 1:A:316:MET:HE3  | 1:A:331:ALA:HA  | 1.84                     | 0.58              |
| 1:K:70:HIS:HB3   | 1:K:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:R:218:PHE:HB2  | 1:V:511:HIS:CD2 | 2.39                     | 0.58              |
| 1:V:218:PHE:HB2  | 1:W:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:Y:175:ASP:CB   | 1:Y:188:PHE:CZ  | 2.83                     | 0.58              |
| 1:4:70:HIS:HB3   | 1:4:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:5:218:PHE:HB2  | 1:8:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:8:175:ASP:CB   | 1:8:188:PHE:CZ  | 2.83                     | 0.58              |
| 1:H:218:PHE:HB2  | 1:Z:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:J:316:MET:HE3  | 1:J:331:ALA:HA  | 1.84                     | 0.58              |
| 1:J:511:HIS:CD2  | 1:a:218:PHE:HB2 | 2.39                     | 0.58              |
| 1:O:261:PRO:HB2  | 1:m:77:ILE:HG13 | 1.84                     | 0.58              |
| 1:O:511:HIS:CD2  | 1:P:218:PHE:HB2 | 2.38                     | 0.58              |
| 1:T:77:ILE:HG13  | 1:l:261:PRO:HB2 | 1.84                     | 0.58              |
| 1:r:218:PHE:HB2  | 1:x:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:t:282:THR:HG21 | 1:u:308:ALA:HB1 | 1.83                     | 0.58              |
| 1:v:70:HIS:HB3   | 1:v:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:7:316:MET:HE3  | 1:7:331:ALA:HA  | 1.85                     | 0.58              |
| 1:J:282:THR:HG21 | 1:L:308:ALA:HB1 | 1.86                     | 0.58              |
| 1:Q:511:HIS:CD2  | 1:S:218:PHE:HB2 | 2.38                     | 0.58              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:f:316:MET:HE3 | 1:f:331:ALA:HA  | 1.84                     | 0.58              |
| 1:i:70:HIS:HB3  | 1:i:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:j:218:PHE:HB2 | 1:l:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:s:316:MET:HE3 | 1:s:331:ALA:HA  | 1.84                     | 0.58              |
| 1:v:316:MET:HE3 | 1:v:331:ALA:HA  | 1.84                     | 0.58              |
| 1:w:175:ASP:CB  | 1:w:188:PHE:CZ  | 2.83                     | 0.58              |
| 1:2:316:MET:HE3 | 1:2:331:ALA:HA  | 1.85                     | 0.58              |
| 1:3:511:HIS:CD2 | 1:8:218:PHE:HB2 | 2.38                     | 0.58              |
| 1:A:70:HIS:HB3  | 1:A:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:B:218:PHE:HB2 | 1:C:511:HIS:CD2 | 2.39                     | 0.58              |
| 1:N:70:HIS:HB3  | 1:N:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:S:406:ARG:HB2 | 1:S:531:LYS:HZ1 | 1.69                     | 0.58              |
| 1:U:316:MET:HE3 | 1:U:331:ALA:HA  | 1.84                     | 0.58              |
| 1:Y:316:MET:HE3 | 1:Y:331:ALA:HA  | 1.85                     | 0.58              |
| 1:Z:218:PHE:HB2 | 1:a:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:g:511:HIS:CD2 | 1:l:218:PHE:HB2 | 2.39                     | 0.58              |
| 1:k:218:PHE:HB2 | 1:w:511:HIS:CD2 | 2.38                     | 0.58              |
| 1:B:175:ASP:CB  | 1:B:188:PHE:CZ  | 2.83                     | 0.58              |
| 1:Z:70:HIS:HB3  | 1:Z:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:b:316:MET:HE3 | 1:b:331:ALA:HA  | 1.84                     | 0.58              |
| 1:8:70:HIS:HB3  | 1:8:450:LYS:HE3 | 1.84                     | 0.58              |
| 1:D:218:PHE:HB2 | 1:E:511:HIS:CD2 | 2.38                     | 0.57              |
| 1:E:175:ASP:CB  | 1:E:188:PHE:CZ  | 2.83                     | 0.57              |
| 1:I:316:MET:HE3 | 1:I:331:ALA:HA  | 1.84                     | 0.57              |
| 1:u:316:MET:HE3 | 1:u:331:ALA:HA  | 1.84                     | 0.57              |
| 1:S:316:MET:HE3 | 1:S:331:ALA:HA  | 1.85                     | 0.57              |
| 1:t:406:ARG:HB2 | 1:t:531:LYS:HZ1 | 1.69                     | 0.57              |
| 1:3:316:MET:HE3 | 1:3:331:ALA:HA  | 1.84                     | 0.57              |
| 1:D:316:MET:HE3 | 1:D:331:ALA:HA  | 1.84                     | 0.57              |
| 1:I:511:HIS:CD2 | 1:J:218:PHE:HB2 | 2.40                     | 0.57              |
| 1:a:316:MET:HE3 | 1:a:331:ALA:HA  | 1.85                     | 0.57              |
| 1:k:316:MET:HE3 | 1:k:331:ALA:HA  | 1.84                     | 0.57              |
| 1:r:316:MET:HE3 | 1:r:331:ALA:HA  | 1.85                     | 0.57              |
| 1:t:316:MET:HE3 | 1:t:331:ALA:HA  | 1.85                     | 0.57              |
| 1:1:175:ASP:CB  | 1:1:188:PHE:CZ  | 2.83                     | 0.57              |
| 1:G:316:MET:HE3 | 1:G:331:ALA:HA  | 1.85                     | 0.57              |
| 1:A:406:ARG:HB2 | 1:A:531:LYS:HZ1 | 1.70                     | 0.57              |
| 1:N:273:GLN:HG3 | 1:N:278:ALA:HA  | 1.87                     | 0.57              |
| 1:Z:273:GLN:HG3 | 1:Z:278:ALA:HA  | 1.87                     | 0.57              |
| 1:i:273:GLN:HG3 | 1:i:278:ALA:HA  | 1.87                     | 0.57              |
| 1:8:273:GLN:HG3 | 1:8:278:ALA:HA  | 1.87                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:348:ASP:OD1 | 1:H:349:LEU:N   | 2.38                     | 0.57              |
| 1:N:316:MET:HE3 | 1:N:331:ALA:HA  | 1.85                     | 0.57              |
| 1:Q:273:GLN:HG3 | 1:Q:278:ALA:HA  | 1.87                     | 0.57              |
| 1:c:273:GLN:HG3 | 1:c:278:ALA:HA  | 1.87                     | 0.57              |
| 1:e:273:GLN:HG3 | 1:e:278:ALA:HA  | 1.87                     | 0.57              |
| 1:i:316:MET:HE3 | 1:i:331:ALA:HA  | 1.85                     | 0.57              |
| 1:x:273:GLN:HG3 | 1:x:278:ALA:HA  | 1.87                     | 0.57              |
| 1:A:348:ASP:OD1 | 1:A:349:LEU:N   | 2.38                     | 0.57              |
| 1:E:348:ASP:OD1 | 1:E:349:LEU:N   | 2.38                     | 0.57              |
| 1:E:406:ARG:HB2 | 1:E:531:LYS:HZ1 | 1.69                     | 0.57              |
| 1:r:273:GLN:HG3 | 1:r:278:ALA:HA  | 1.87                     | 0.57              |
| 1:v:348:ASP:OD1 | 1:v:349:LEU:N   | 2.38                     | 0.57              |
| 1:v:406:ARG:HB2 | 1:v:531:LYS:HZ2 | 1.70                     | 0.57              |
| 1:w:348:ASP:OD1 | 1:w:349:LEU:N   | 2.38                     | 0.57              |
| 1:5:348:ASP:OD1 | 1:5:349:LEU:N   | 2.38                     | 0.57              |
| 1:B:273:GLN:HG3 | 1:B:278:ALA:HA  | 1.87                     | 0.57              |
| 1:G:406:ARG:HB2 | 1:G:531:LYS:HZ1 | 1.70                     | 0.57              |
| 1:O:348:ASP:OD1 | 1:O:349:LEU:N   | 2.38                     | 0.57              |
| 1:P:406:ARG:HB2 | 1:P:531:LYS:HZ1 | 1.69                     | 0.57              |
| 1:Q:406:ARG:HB2 | 1:Q:531:LYS:HZ1 | 1.69                     | 0.57              |
| 1:S:273:GLN:HG3 | 1:S:278:ALA:HA  | 1.87                     | 0.57              |
| 1:U:30:GLY:HA3  | 1:e:233:GLU:HG2 | 1.87                     | 0.57              |
| 1:a:348:ASP:OD1 | 1:a:349:LEU:N   | 2.38                     | 0.57              |
| 1:c:233:GLU:HG2 | 1:s:30:GLY:HA3  | 1.87                     | 0.57              |
| 1:l:348:ASP:OD1 | 1:l:349:LEU:N   | 2.38                     | 0.57              |
| 1:p:348:ASP:OD1 | 1:p:349:LEU:N   | 2.38                     | 0.57              |
| 1:r:175:ASP:CB  | 1:r:188:PHE:CZ  | 2.83                     | 0.57              |
| 1:s:273:GLN:HG3 | 1:s:278:ALA:HA  | 1.87                     | 0.57              |
| 1:x:406:ARG:HB2 | 1:x:531:LYS:HZ1 | 1.69                     | 0.57              |
| 1:3:348:ASP:OD1 | 1:3:349:LEU:N   | 2.38                     | 0.57              |
| 1:6:273:GLN:HG3 | 1:6:278:ALA:HA  | 1.87                     | 0.57              |
| 1:8:348:ASP:OD1 | 1:8:349:LEU:N   | 2.38                     | 0.57              |
| 1:C:273:GLN:HG3 | 1:C:278:ALA:HA  | 1.87                     | 0.57              |
| 1:U:273:GLN:HG3 | 1:U:278:ALA:HA  | 1.87                     | 0.57              |
| 1:U:406:ARG:HB2 | 1:U:531:LYS:HZ1 | 1.69                     | 0.57              |
| 1:V:348:ASP:OD1 | 1:V:349:LEU:N   | 2.38                     | 0.57              |
| 1:W:273:GLN:HG3 | 1:W:278:ALA:HA  | 1.87                     | 0.57              |
| 1:Y:348:ASP:OD1 | 1:Y:349:LEU:N   | 2.38                     | 0.57              |
| 1:Z:348:ASP:OD1 | 1:Z:349:LEU:N   | 2.38                     | 0.57              |
| 1:b:273:GLN:HG3 | 1:b:278:ALA:HA  | 1.87                     | 0.57              |
| 1:j:406:ARG:HB2 | 1:j:531:LYS:HZ1 | 1.69                     | 0.57              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:s:406:ARG:HB2 | 1:s:531:LYS:HZ1 | 1.69                     | 0.57              |
| 1:1:273:GLN:HG3 | 1:1:278:ALA:HA  | 1.87                     | 0.57              |
| 1:H:273:GLN:HG3 | 1:H:278:ALA:HA  | 1.87                     | 0.56              |
| 1:M:348:ASP:OD1 | 1:M:349:LEU:N   | 2.38                     | 0.56              |
| 1:f:273:GLN:HG3 | 1:f:278:ALA:HA  | 1.87                     | 0.56              |
| 1:g:273:GLN:HG3 | 1:g:278:ALA:HA  | 1.87                     | 0.56              |
| 1:h:348:ASP:OD1 | 1:h:349:LEU:N   | 2.38                     | 0.56              |
| 1:r:348:ASP:OD1 | 1:r:349:LEU:N   | 2.38                     | 0.56              |
| 1:7:348:ASP:OD1 | 1:7:349:LEU:N   | 2.38                     | 0.56              |
| 1:C:28:VAL:HG12 | 1:C:30:GLY:H    | 1.71                     | 0.56              |
| 1:J:538:LEU:O   | 1:L:418:LYS:NZ  | 2.38                     | 0.56              |
| 1:K:383:TYR:HB3 | 1:K:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:S:175:ASP:CB  | 1:S:188:PHE:CZ  | 2.83                     | 0.56              |
| 1:S:348:ASP:OD1 | 1:S:349:LEU:N   | 2.38                     | 0.56              |
| 1:g:28:VAL:HG12 | 1:g:30:GLY:H    | 1.71                     | 0.56              |
| 1:h:273:GLN:HG3 | 1:h:278:ALA:HA  | 1.87                     | 0.56              |
| 1:5:273:GLN:HG3 | 1:5:278:ALA:HA  | 1.87                     | 0.56              |
| 1:A:383:TYR:HB3 | 1:A:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:D:28:VAL:HG12 | 1:D:30:GLY:H    | 1.71                     | 0.56              |
| 1:E:383:TYR:HB3 | 1:E:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:F:418:LYS:NZ  | 1:Q:538:LEU:O   | 2.39                     | 0.56              |
| 1:G:383:TYR:HB3 | 1:G:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:I:28:VAL:HG12 | 1:I:30:GLY:H    | 1.71                     | 0.56              |
| 1:L:28:VAL:HG12 | 1:L:30:GLY:H    | 1.71                     | 0.56              |
| 1:M:28:VAL:HG12 | 1:M:30:GLY:H    | 1.71                     | 0.56              |
| 1:M:30:GLY:HA3  | 1:N:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:M:273:GLN:HG3 | 1:M:278:ALA:HA  | 1.87                     | 0.56              |
| 1:Q:28:VAL:HG12 | 1:Q:30:GLY:H    | 1.71                     | 0.56              |
| 1:R:233:GLU:HG2 | 1:V:30:GLY:HA3  | 1.87                     | 0.56              |
| 1:T:383:TYR:HB3 | 1:T:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:V:233:GLU:HG2 | 1:W:30:GLY:HA3  | 1.88                     | 0.56              |
| 1:V:273:GLN:HG3 | 1:V:278:ALA:HA  | 1.87                     | 0.56              |
| 1:V:406:ARG:HB2 | 1:V:531:LYS:HZ1 | 1.70                     | 0.56              |
| 1:X:348:ASP:OD1 | 1:X:349:LEU:N   | 2.38                     | 0.56              |
| 1:Y:273:GLN:HG3 | 1:Y:278:ALA:HA  | 1.87                     | 0.56              |
| 1:h:28:VAL:HG12 | 1:h:30:GLY:H    | 1.71                     | 0.56              |
| 1:k:28:VAL:HG12 | 1:k:30:GLY:H    | 1.71                     | 0.56              |
| 1:m:383:TYR:HB3 | 1:m:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:o:348:ASP:OD1 | 1:o:349:LEU:N   | 2.38                     | 0.56              |
| 1:p:30:GLY:HA3  | 1:q:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:p:233:GLU:HG2 | 1:6:30:GLY:HA3  | 1.88                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:p:273:GLN:HG3 | 1:p:278:ALA:HA  | 1.87                     | 0.56              |
| 1:s:348:ASP:OD1 | 1:s:349:LEU:N   | 2.38                     | 0.56              |
| 1:t:383:TYR:HB3 | 1:t:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:u:28:VAL:HG12 | 1:u:30:GLY:H    | 1.71                     | 0.56              |
| 1:v:383:TYR:HB3 | 1:v:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:w:383:TYR:HB3 | 1:w:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:x:538:LEU:O   | 1:y:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:z:28:VAL:HG12 | 1:z:30:GLY:H    | 1.71                     | 0.56              |
| 1:2:28:VAL:HG12 | 1:2:30:GLY:H    | 1.71                     | 0.56              |
| 1:4:383:TYR:HB3 | 1:4:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:7:273:GLN:HG3 | 1:7:278:ALA:HA  | 1.87                     | 0.56              |
| 1:A:30:GLY:HA3  | 1:E:233:GLU:HG2 | 1.88                     | 0.56              |
| 1:A:418:LYS:NZ  | 1:I:538:LEU:O   | 2.38                     | 0.56              |
| 1:B:386:ASN:O   | 1:B:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:F:273:GLN:HG3 | 1:F:278:ALA:HA  | 1.87                     | 0.56              |
| 1:G:538:LEU:O   | 1:I:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:H:383:TYR:HB3 | 1:H:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:I:30:GLY:HA3  | 1:J:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:K:104:SER:HB2 | 1:K:177:MET:HE2 | 1.88                     | 0.56              |
| 1:L:273:GLN:HG3 | 1:L:278:ALA:HA  | 1.87                     | 0.56              |
| 1:M:386:ASN:O   | 1:M:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:U:348:ASP:OD1 | 1:U:349:LEU:N   | 2.38                     | 0.56              |
| 1:U:383:TYR:HB3 | 1:U:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:Z:383:TYR:HB3 | 1:Z:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:c:28:VAL:HG12 | 1:c:30:GLY:H    | 1.71                     | 0.56              |
| 1:c:406:ARG:HB2 | 1:c:531:LYS:HZ1 | 1.69                     | 0.56              |
| 1:e:28:VAL:HG12 | 1:e:30:GLY:H    | 1.71                     | 0.56              |
| 1:e:406:ARG:HB2 | 1:e:531:LYS:HZ1 | 1.70                     | 0.56              |
| 1:h:30:GLY:HA3  | 1:i:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:h:175:ASP:CB  | 1:h:188:PHE:CZ  | 2.83                     | 0.56              |
| 1:h:386:ASN:O   | 1:h:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:n:348:ASP:OD1 | 1:n:349:LEU:N   | 2.38                     | 0.56              |
| 1:p:383:TYR:HB3 | 1:p:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:s:383:TYR:HB3 | 1:s:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:u:30:GLY:HA3  | 1:2:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:x:28:VAL:HG12 | 1:x:30:GLY:H    | 1.71                     | 0.56              |
| 1:z:175:ASP:CB  | 1:z:188:PHE:CZ  | 2.83                     | 0.56              |
| 1:z:273:GLN:HG3 | 1:z:278:ALA:HA  | 1.87                     | 0.56              |
| 1:1:386:ASN:O   | 1:1:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:4:28:VAL:HG12 | 1:4:30:GLY:H    | 1.71                     | 0.56              |
| 1:4:104:SER:HB2 | 1:4:177:MET:HE2 | 1.88                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:5:383:TYR:HB3 | 1:5:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:6:28:VAL:HG12 | 1:6:30:GLY:H    | 1.71                     | 0.56              |
| 1:8:383:TYR:HB3 | 1:8:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:E:538:LEU:O   | 1:Q:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:G:104:SER:HB2 | 1:G:177:MET:HE2 | 1.88                     | 0.56              |
| 1:G:386:ASN:O   | 1:G:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:K:28:VAL:HG12 | 1:K:30:GLY:H    | 1.71                     | 0.56              |
| 1:K:30:GLY:HA3  | 1:L:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:O:233:GLU:HG2 | 1:d:30:GLY:HA3  | 1.88                     | 0.56              |
| 1:P:30:GLY:HA3  | 1:Q:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:R:273:GLN:HG3 | 1:R:278:ALA:HA  | 1.87                     | 0.56              |
| 1:S:104:SER:HB2 | 1:S:177:MET:HE2 | 1.88                     | 0.56              |
| 1:T:386:ASN:O   | 1:T:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:V:383:TYR:HB3 | 1:V:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:V:386:ASN:O   | 1:V:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:W:28:VAL:HG12 | 1:W:30:GLY:H    | 1.71                     | 0.56              |
| 1:X:28:VAL:HG12 | 1:X:30:GLY:H    | 1.71                     | 0.56              |
| 1:b:104:SER:HB2 | 1:b:177:MET:HE2 | 1.88                     | 0.56              |
| 1:c:383:TYR:HB3 | 1:c:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:d:348:ASP:OD1 | 1:d:349:LEU:N   | 2.38                     | 0.56              |
| 1:f:233:GLU:HG2 | 1:z:30:GLY:HA3  | 1.87                     | 0.56              |
| 1:j:30:GLY:HA3  | 1:x:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:l:233:GLU:HG2 | 1:n:30:GLY:HA3  | 1.88                     | 0.56              |
| 1:l:386:ASN:O   | 1:l:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:m:386:ASN:O   | 1:m:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:p:28:VAL:HG12 | 1:p:30:GLY:H    | 1.71                     | 0.56              |
| 1:p:386:ASN:O   | 1:p:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:t:104:SER:HB2 | 1:t:177:MET:HE2 | 1.88                     | 0.56              |
| 1:t:386:ASN:O   | 1:t:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:t:538:LEU:O   | 1:u:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:w:538:LEU:O   | 1:x:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:y:273:GLN:HG3 | 1:y:278:ALA:HA  | 1.87                     | 0.56              |
| 1:3:30:GLY:HA3  | 1:8:233:GLU:HG2 | 1.88                     | 0.56              |
| 1:3:386:ASN:O   | 1:3:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:B:68:ASN:ND2  | 1:B:71:LYS:O    | 2.39                     | 0.56              |
| 1:H:104:SER:HB2 | 1:H:177:MET:HE2 | 1.88                     | 0.56              |
| 1:I:104:SER:HB2 | 1:I:177:MET:HE2 | 1.88                     | 0.56              |
| 1:I:348:ASP:OD1 | 1:I:349:LEU:N   | 2.38                     | 0.56              |
| 1:J:28:VAL:HG12 | 1:J:30:GLY:H    | 1.71                     | 0.56              |
| 1:M:175:ASP:CB  | 1:M:188:PHE:CZ  | 2.83                     | 0.56              |
| 1:N:30:GLY:HA3  | 1:m:233:GLU:HG2 | 1.88                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:N:538:LEU:O   | 1:P:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:O:30:GLY:HA3  | 1:P:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:O:386:ASN:O   | 1:O:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:Q:386:ASN:O   | 1:Q:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:S:386:ASN:O   | 1:S:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:V:538:LEU:O   | 1:e:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:Y:68:ASN:ND2  | 1:Y:71:LYS:O    | 2.39                     | 0.56              |
| 1:Z:233:GLU:HG2 | 1:a:30:GLY:HA3  | 1.88                     | 0.56              |
| 1:a:386:ASN:O   | 1:a:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:c:418:LYS:NZ  | 1:p:538:LEU:O   | 2.39                     | 0.56              |
| 1:e:383:TYR:HB3 | 1:e:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:g:348:ASP:OD1 | 1:g:349:LEU:N   | 2.38                     | 0.56              |
| 1:i:538:LEU:O   | 1:j:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:k:273:GLN:HG3 | 1:k:278:ALA:HA  | 1.87                     | 0.56              |
| 1:k:383:TYR:HB3 | 1:k:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:o:28:VAL:HG12 | 1:o:30:GLY:H    | 1.71                     | 0.56              |
| 1:o:406:ARG:HB2 | 1:o:531:LYS:HZ1 | 1.71                     | 0.56              |
| 1:q:273:GLN:HG3 | 1:q:278:ALA:HA  | 1.87                     | 0.56              |
| 1:r:386:ASN:O   | 1:r:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:u:104:SER:HB2 | 1:u:177:MET:HE2 | 1.88                     | 0.56              |
| 1:u:538:LEU:O   | 1:v:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:x:386:ASN:O   | 1:x:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:6:386:ASN:O   | 1:6:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:7:68:ASN:ND2  | 1:7:71:LYS:O    | 2.39                     | 0.56              |
| 1:B:348:ASP:OD1 | 1:B:349:LEU:N   | 2.38                     | 0.56              |
| 1:D:273:GLN:HG3 | 1:D:278:ALA:HA  | 1.87                     | 0.56              |
| 1:D:383:TYR:HB3 | 1:D:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:D:418:LYS:NZ  | 1:P:538:LEU:O   | 2.39                     | 0.56              |
| 1:F:68:ASN:ND2  | 1:F:71:LYS:O    | 2.39                     | 0.56              |
| 1:F:386:ASN:O   | 1:F:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:K:273:GLN:HG3 | 1:K:278:ALA:HA  | 1.87                     | 0.56              |
| 1:L:383:TYR:HB3 | 1:L:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:N:104:SER:HB2 | 1:N:177:MET:HE2 | 1.88                     | 0.56              |
| 1:N:386:ASN:O   | 1:N:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:O:28:VAL:HG12 | 1:O:30:GLY:H    | 1.71                     | 0.56              |
| 1:O:383:TYR:HB3 | 1:O:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:O:538:LEU:O   | 1:m:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:P:104:SER:HB2 | 1:P:177:MET:HE2 | 1.88                     | 0.56              |
| 1:P:386:ASN:O   | 1:P:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:Q:30:GLY:HA3  | 1:S:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:T:233:GLU:HG2 | 1:i:30:GLY:HA3  | 1.88                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:T:418:LYS:NZ  | 1:l:538:LEU:O   | 2.39                     | 0.56              |
| 1:V:28:VAL:HG12 | 1:V:30:GLY:H    | 1.71                     | 0.56              |
| 1:W:386:ASN:O   | 1:W:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:W:538:LEU:O   | 1:Y:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:X:30:GLY:HA3  | 1:Y:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:X:386:ASN:O   | 1:X:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:X:406:ARG:HB2 | 1:X:531:LYS:HZ1 | 1.71                     | 0.56              |
| 1:Y:386:ASN:O   | 1:Y:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:f:104:SER:HB2 | 1:f:177:MET:HE2 | 1.88                     | 0.56              |
| 1:f:348:ASP:OD1 | 1:f:349:LEU:N   | 2.38                     | 0.56              |
| 1:i:104:SER:HB2 | 1:i:177:MET:HE2 | 1.88                     | 0.56              |
| 1:i:386:ASN:O   | 1:i:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:j:104:SER:HB2 | 1:j:177:MET:HE2 | 1.88                     | 0.56              |
| 1:j:538:LEU:O   | 1:k:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:l:28:VAL:HG12 | 1:l:30:GLY:H    | 1.71                     | 0.56              |
| 1:l:383:TYR:HB3 | 1:l:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:o:386:ASN:O   | 1:o:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:o:538:LEU:O   | 1:p:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:q:386:ASN:O   | 1:q:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:r:233:GLU:HG2 | 1:x:30:GLY:HA3  | 1.87                     | 0.56              |
| 1:v:30:GLY:HA3  | 1:w:233:GLU:HG2 | 1.88                     | 0.56              |
| 1:w:406:ARG:HB2 | 1:w:531:LYS:HZ1 | 1.71                     | 0.56              |
| 1:y:68:ASN:ND2  | 1:y:71:LYS:O    | 2.39                     | 0.56              |
| 1:y:386:ASN:O   | 1:y:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:1:68:ASN:ND2  | 1:1:71:LYS:O    | 2.39                     | 0.56              |
| 1:4:273:GLN:HG3 | 1:4:278:ALA:HA  | 1.87                     | 0.56              |
| 1:5:104:SER:HB2 | 1:5:177:MET:HE2 | 1.88                     | 0.56              |
| 1:6:538:LEU:O   | 1:7:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:7:386:ASN:O   | 1:7:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:D:538:LEU:O   | 1:N:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:E:28:VAL:HG12 | 1:E:30:GLY:H    | 1.71                     | 0.56              |
| 1:I:383:TYR:HB3 | 1:I:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:I:386:ASN:O   | 1:I:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:J:68:ASN:ND2  | 1:J:71:LYS:O    | 2.39                     | 0.56              |
| 1:L:104:SER:HB2 | 1:L:177:MET:HE2 | 1.88                     | 0.56              |
| 1:L:175:ASP:CB  | 1:L:188:PHE:CZ  | 2.83                     | 0.56              |
| 1:Q:68:ASN:ND2  | 1:Q:71:LYS:O    | 2.39                     | 0.56              |
| 1:R:68:ASN:ND2  | 1:R:71:LYS:O    | 2.39                     | 0.56              |
| 1:R:386:ASN:O   | 1:R:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:V:418:LYS:NZ  | 1:X:538:LEU:O   | 2.39                     | 0.56              |
| 1:W:68:ASN:ND2  | 1:W:71:LYS:O    | 2.39                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:a:273:GLN:HG3 | 1:a:278:ALA:HA  | 1.87                     | 0.56              |
| 1:b:348:ASP:OD1 | 1:b:349:LEU:N   | 2.38                     | 0.56              |
| 1:g:233:GLU:HG2 | 1:k:30:GLY:HA3  | 1.88                     | 0.56              |
| 1:g:406:ARG:HB2 | 1:g:531:LYS:HZ1 | 1.71                     | 0.56              |
| 1:i:418:LYS:NZ  | 1:k:538:LEU:O   | 2.39                     | 0.56              |
| 1:j:233:GLU:HG2 | 1:l:30:GLY:HA3  | 1.87                     | 0.56              |
| 1:j:386:ASN:O   | 1:j:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:o:30:GLY:HA3  | 1:7:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:q:418:LYS:NZ  | 1:s:538:LEU:O   | 2.39                     | 0.56              |
| 1:u:383:TYR:HB3 | 1:u:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:w:28:VAL:HG12 | 1:w:30:GLY:H    | 1.71                     | 0.56              |
| 1:x:104:SER:HB2 | 1:x:177:MET:HE2 | 1.88                     | 0.56              |
| 1:z:348:ASP:OD1 | 1:z:349:LEU:N   | 2.38                     | 0.56              |
| 1:z:383:TYR:HB3 | 1:z:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:2:68:ASN:ND2  | 1:2:71:LYS:O    | 2.39                     | 0.56              |
| 1:3:273:GLN:HG3 | 1:3:278:ALA:HA  | 1.87                     | 0.56              |
| 1:6:68:ASN:ND2  | 1:6:71:LYS:O    | 2.39                     | 0.56              |
| 1:7:28:VAL:HG12 | 1:7:30:GLY:H    | 1.71                     | 0.56              |
| 1:A:99:PHE:O    | 1:A:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:A:104:SER:HB2 | 1:A:177:MET:HE2 | 1.88                     | 0.56              |
| 1:C:233:GLU:HG2 | 1:D:30:GLY:HA3  | 1.88                     | 0.56              |
| 1:C:383:TYR:HB3 | 1:C:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:C:406:ARG:HB2 | 1:C:531:LYS:HZ1 | 1.71                     | 0.56              |
| 1:K:418:LYS:NZ  | 1:8:538:LEU:O   | 2.39                     | 0.56              |
| 1:L:348:ASP:OD1 | 1:L:349:LEU:N   | 2.38                     | 0.56              |
| 1:P:28:VAL:HG12 | 1:P:30:GLY:H    | 1.71                     | 0.56              |
| 1:Q:99:PHE:O    | 1:Q:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:Q:104:SER:HB2 | 1:Q:177:MET:HE2 | 1.88                     | 0.56              |
| 1:R:418:LYS:NZ  | 1:U:538:LEU:O   | 2.39                     | 0.56              |
| 1:T:104:SER:HB2 | 1:T:177:MET:HE2 | 1.88                     | 0.56              |
| 1:U:28:VAL:HG12 | 1:U:30:GLY:H    | 1.71                     | 0.56              |
| 1:U:104:SER:HB2 | 1:U:177:MET:HE2 | 1.88                     | 0.56              |
| 1:Y:28:VAL:HG12 | 1:Y:30:GLY:H    | 1.71                     | 0.56              |
| 1:Y:99:PHE:O    | 1:Y:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:Y:104:SER:HB2 | 1:Y:177:MET:HE2 | 1.88                     | 0.56              |
| 1:Z:538:LEU:O   | 1:4:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:d:99:PHE:O    | 1:d:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:g:383:TYR:HB3 | 1:g:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:q:68:ASN:ND2  | 1:q:71:LYS:O    | 2.39                     | 0.56              |
| 1:s:28:VAL:HG12 | 1:s:30:GLY:H    | 1.71                     | 0.56              |
| 1:u:386:ASN:O   | 1:u:387:GLN:HG2 | 2.06                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:v:28:VAL:HG12 | 1:v:30:GLY:H    | 1.71                     | 0.56              |
| 1:v:99:PHE:O    | 1:v:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:x:68:ASN:ND2  | 1:x:71:LYS:O    | 2.39                     | 0.56              |
| 1:z:104:SER:HB2 | 1:z:177:MET:HE2 | 1.88                     | 0.56              |
| 1:z:418:LYS:NZ  | 1:2:538:LEU:O   | 2.39                     | 0.56              |
| 1:1:348:ASP:OD1 | 1:1:349:LEU:N   | 2.38                     | 0.56              |
| 1:2:99:PHE:O    | 1:2:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:5:538:LEU:O   | 1:6:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:7:99:PHE:O    | 1:7:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:7:104:SER:HB2 | 1:7:177:MET:HE2 | 1.88                     | 0.56              |
| 1:A:28:VAL:HG12 | 1:A:30:GLY:H    | 1.71                     | 0.56              |
| 1:A:386:ASN:O   | 1:A:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:F:30:GLY:HA3  | 1:G:233:GLU:HG2 | 1.88                     | 0.56              |
| 1:F:383:TYR:HB3 | 1:F:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:H:30:GLY:HA3  | 1:I:233:GLU:HG2 | 1.87                     | 0.56              |
| 1:H:538:LEU:O   | 1:W:418:LYS:NZ  | 2.39                     | 0.56              |
| 1:J:99:PHE:O    | 1:J:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:J:104:SER:HB2 | 1:J:177:MET:HE2 | 1.88                     | 0.56              |
| 1:M:383:TYR:HB3 | 1:M:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:N:68:ASN:ND2  | 1:N:71:LYS:O    | 2.39                     | 0.56              |
| 1:O:99:PHE:O    | 1:O:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:O:273:GLN:HG3 | 1:O:278:ALA:HA  | 1.87                     | 0.56              |
| 1:P:383:TYR:HB3 | 1:P:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:T:28:VAL:HG12 | 1:T:30:GLY:H    | 1.71                     | 0.56              |
| 1:U:175:ASP:CB  | 1:U:188:PHE:CZ  | 2.83                     | 0.56              |
| 1:U:386:ASN:O   | 1:U:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:Z:104:SER:HB2 | 1:Z:177:MET:HE2 | 1.88                     | 0.56              |
| 1:a:28:VAL:HG12 | 1:a:30:GLY:H    | 1.71                     | 0.56              |
| 1:a:99:PHE:O    | 1:a:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:f:28:VAL:HG12 | 1:f:30:GLY:H    | 1.71                     | 0.56              |
| 1:f:386:ASN:O   | 1:f:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:j:28:VAL:HG12 | 1:j:30:GLY:H    | 1.71                     | 0.56              |
| 1:j:383:TYR:HB3 | 1:j:390:TYR:HB3 | 1.88                     | 0.56              |
| 1:l:99:PHE:O    | 1:l:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:l:273:GLN:HG3 | 1:l:278:ALA:HA  | 1.87                     | 0.56              |
| 1:m:104:SER:HB2 | 1:m:177:MET:HE2 | 1.88                     | 0.56              |
| 1:n:99:PHE:O    | 1:n:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:s:99:PHE:O    | 1:s:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:s:104:SER:HB2 | 1:s:177:MET:HE2 | 1.88                     | 0.56              |
| 1:s:386:ASN:O   | 1:s:387:GLN:HG2 | 2.06                     | 0.56              |
| 1:t:233:GLU:HG2 | 1:y:30:GLY:HA3  | 1.88                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:t:418:LYS:NZ  | 1:v:538:LEU:O   | 2.39                     | 0.56              |
| 1:u:233:GLU:HG2 | 1:5:30:GLY:HA3  | 1.87                     | 0.56              |
| 1:u:273:GLN:HG3 | 1:u:278:ALA:HA  | 1.87                     | 0.56              |
| 1:v:104:SER:HB2 | 1:v:177:MET:HE2 | 1.88                     | 0.56              |
| 1:v:233:GLU:HG2 | 1:1:30:GLY:HA3  | 1.88                     | 0.56              |
| 1:w:418:LYS:NZ  | 1:y:538:LEU:O   | 2.39                     | 0.56              |
| 1:x:99:PHE:O    | 1:x:105:HIS:HE1 | 1.89                     | 0.56              |
| 1:y:348:ASP:OD1 | 1:y:349:LEU:N   | 2.38                     | 0.56              |
| 1:2:406:ARG:HB2 | 1:2:531:LYS:HZ1 | 1.71                     | 0.56              |
| 1:A:538:LEU:O   | 1:G:418:LYS:NZ  | 2.39                     | 0.55              |
| 1:C:99:PHE:O    | 1:C:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:E:418:LYS:NZ  | 1:F:538:LEU:O   | 2.39                     | 0.55              |
| 1:F:348:ASP:OD1 | 1:F:349:LEU:N   | 2.38                     | 0.55              |
| 1:J:406:ARG:HB2 | 1:J:531:LYS:HZ1 | 1.72                     | 0.55              |
| 1:M:410:THR:H   | 1:M:413:ASN:ND2 | 2.05                     | 0.55              |
| 1:T:348:ASP:OD1 | 1:T:349:LEU:N   | 2.38                     | 0.55              |
| 1:T:538:LEU:O   | 1:d:418:LYS:NZ  | 2.39                     | 0.55              |
| 1:U:99:PHE:O    | 1:U:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:X:68:ASN:ND2  | 1:X:71:LYS:O    | 2.39                     | 0.55              |
| 1:b:28:VAL:HG12 | 1:b:30:GLY:H    | 1.71                     | 0.55              |
| 1:b:386:ASN:O   | 1:b:387:GLN:HG2 | 2.06                     | 0.55              |
| 1:g:99:PHE:O    | 1:g:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:h:383:TYR:HB3 | 1:h:390:TYR:HB3 | 1.88                     | 0.55              |
| 1:i:68:ASN:ND2  | 1:i:71:LYS:O    | 2.39                     | 0.55              |
| 1:m:538:LEU:O   | 1:n:418:LYS:NZ  | 2.39                     | 0.55              |
| 1:n:28:VAL:HG12 | 1:n:30:GLY:H    | 1.71                     | 0.55              |
| 1:o:68:ASN:ND2  | 1:o:71:LYS:O    | 2.39                     | 0.55              |
| 1:s:175:ASP:CB  | 1:s:188:PHE:CZ  | 2.83                     | 0.55              |
| 1:v:386:ASN:O   | 1:v:387:GLN:HG2 | 2.06                     | 0.55              |
| 1:y:383:TYR:HB3 | 1:y:390:TYR:HB3 | 1.88                     | 0.55              |
| 1:2:104:SER:HB2 | 1:2:177:MET:HE2 | 1.88                     | 0.55              |
| 1:2:383:TYR:HB3 | 1:2:390:TYR:HB3 | 1.88                     | 0.55              |
| 1:3:28:VAL:HG12 | 1:3:30:GLY:H    | 1.71                     | 0.55              |
| 1:3:99:PHE:O    | 1:3:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:A:233:GLU:HG2 | 1:B:30:GLY:HA3  | 1.89                     | 0.55              |
| 1:C:386:ASN:O   | 1:C:387:GLN:HG2 | 2.06                     | 0.55              |
| 1:D:348:ASP:OD1 | 1:D:349:LEU:N   | 2.38                     | 0.55              |
| 1:E:273:GLN:HG3 | 1:E:278:ALA:HA  | 1.87                     | 0.55              |
| 1:G:30:GLY:HA3  | 1:W:233:GLU:HG2 | 1.88                     | 0.55              |
| 1:H:68:ASN:ND2  | 1:H:71:LYS:O    | 2.39                     | 0.55              |
| 1:J:383:TYR:HB3 | 1:J:390:TYR:HB3 | 1.88                     | 0.55              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:233:GLU:HG2 | 1:7:30:GLY:HA3  | 1.87                     | 0.55              |
| 1:K:538:LEU:O   | 1:a:418:LYS:NZ  | 2.39                     | 0.55              |
| 1:O:418:LYS:NZ  | 1:n:538:LEU:O   | 2.39                     | 0.55              |
| 1:P:99:PHE:O    | 1:P:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:Q:348:ASP:OD1 | 1:Q:349:LEU:N   | 2.38                     | 0.55              |
| 1:R:99:PHE:O    | 1:R:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:V:99:PHE:O    | 1:V:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:W:348:ASP:OD1 | 1:W:349:LEU:N   | 2.38                     | 0.55              |
| 1:Z:410:THR:H   | 1:Z:413:ASN:ND2 | 2.05                     | 0.55              |
| 1:b:68:ASN:ND2  | 1:b:71:LYS:O    | 2.39                     | 0.55              |
| 1:c:175:ASP:CB  | 1:c:188:PHE:CZ  | 2.83                     | 0.55              |
| 1:c:348:ASP:OD1 | 1:c:349:LEU:N   | 2.38                     | 0.55              |
| 1:d:28:VAL:HG12 | 1:d:30:GLY:H    | 1.71                     | 0.55              |
| 1:d:68:ASN:ND2  | 1:d:71:LYS:O    | 2.39                     | 0.55              |
| 1:d:538:LEU:O   | 1:l:418:LYS:NZ  | 2.39                     | 0.55              |
| 1:e:348:ASP:OD1 | 1:e:349:LEU:N   | 2.38                     | 0.55              |
| 1:h:99:PHE:O    | 1:h:105:HIS:HE1 | 1.89                     | 0.55              |
| 1:h:410:THR:H   | 1:h:413:ASN:ND2 | 2.05                     | 0.55              |
| 1:m:28:VAL:HG12 | 1:m:30:GLY:H    | 1.71                     | 0.55              |
| 1:m:68:ASN:ND2  | 1:m:71:LYS:O    | 2.39                     | 0.55              |
| 1:m:348:ASP:OD1 | 1:m:349:LEU:N   | 2.38                     | 0.55              |
| 1:o:273:GLN:HG3 | 1:o:278:ALA:HA  | 1.87                     | 0.55              |
| 1:w:104:SER:HB2 | 1:w:177:MET:HE2 | 1.88                     | 0.55              |
| 1:w:273:GLN:HG3 | 1:w:278:ALA:HA  | 1.87                     | 0.55              |
| 1:x:348:ASP:OD1 | 1:x:349:LEU:N   | 2.38                     | 0.55              |
| 1:z:538:LEU:O   | 1:1:418:LYS:NZ  | 2.39                     | 0.55              |
| 1:3:418:LYS:NZ  | 1:4:538:LEU:O   | 2.39                     | 0.55              |
| 1:4:348:ASP:OD1 | 1:4:349:LEU:N   | 2.38                     | 0.55              |
| 1:5:68:ASN:ND2  | 1:5:71:LYS:O    | 2.39                     | 0.55              |
| 1:8:104:SER:HB2 | 1:8:177:MET:HE2 | 1.88                     | 0.55              |
| 1:B:104:SER:HB2 | 1:B:177:MET:HE3 | 1.89                     | 0.55              |
| 1:B:233:GLU:HG2 | 1:C:30:GLY:HA3  | 1.87                     | 0.55              |
| 1:C:68:ASN:ND2  | 1:C:71:LYS:O    | 2.39                     | 0.55              |
| 1:C:418:LYS:NZ  | 1:M:538:LEU:O   | 2.39                     | 0.55              |
| 1:C:538:LEU:O   | 1:b:418:LYS:NZ  | 2.39                     | 0.55              |
| 1:E:104:SER:HB2 | 1:E:177:MET:HE2 | 1.88                     | 0.55              |
| 1:H:28:VAL:HG12 | 1:H:30:GLY:H    | 1.71                     | 0.55              |
| 1:I:273:GLN:HG3 | 1:I:278:ALA:HA  | 1.87                     | 0.55              |
| 1:J:348:ASP:OD1 | 1:J:349:LEU:N   | 2.38                     | 0.55              |
| 1:L:68:ASN:ND2  | 1:L:71:LYS:O    | 2.39                     | 0.55              |
| 1:M:99:PHE:O    | 1:M:105:HIS:HE1 | 1.89                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:410:THR:H   | 1:O:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:P:348:ASP:OD1 | 1:P:349:LEU:N    | 2.38                     | 0.55              |
| 1:T:68:ASN:ND2  | 1:T:71:LYS:O     | 2.39                     | 0.55              |
| 1:X:273:GLN:HG3 | 1:X:278:ALA:HA   | 1.87                     | 0.55              |
| 1:X:410:THR:H   | 1:X:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:Y:30:GLY:HA3  | 1:4:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:c:386:ASN:O   | 1:c:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:e:386:ASN:O   | 1:e:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:f:68:ASN:ND2  | 1:f:71:LYS:O     | 2.39                     | 0.55              |
| 1:f:538:LEU:O   | 1:h:418:LYS:NZ   | 2.39                     | 0.55              |
| 1:g:30:GLY:HA3  | 1:1:233:GLU:HG2  | 1.87                     | 0.55              |
| 1:g:418:LYS:NZ  | 1:h:538:LEU:O    | 2.39                     | 0.55              |
| 1:h:104:SER:HB2 | 1:h:177:MET:HE2  | 1.88                     | 0.55              |
| 1:j:99:PHE:O    | 1:j:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:k:348:ASP:OD1 | 1:k:349:LEU:N    | 2.38                     | 0.55              |
| 1:n:68:ASN:ND2  | 1:n:71:LYS:O     | 2.39                     | 0.55              |
| 1:o:104:SER:HB2 | 1:o:177:MET:HE3  | 1.89                     | 0.55              |
| 1:o:410:THR:H   | 1:o:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:p:99:PHE:O    | 1:p:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:q:99:PHE:O    | 1:q:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:t:30:GLY:HA3  | 1:6:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:z:68:ASN:ND2  | 1:z:71:LYS:O     | 2.39                     | 0.55              |
| 1:2:348:ASP:OD1 | 1:2:349:LEU:N    | 2.38                     | 0.55              |
| 1:5:386:ASN:O   | 1:5:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:6:348:ASP:OD1 | 1:6:349:LEU:N    | 2.38                     | 0.55              |
| 1:A:410:THR:H   | 1:A:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:C:410:THR:H   | 1:C:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:E:99:PHE:O    | 1:E:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:F:28:VAL:HG12 | 1:F:30:GLY:H     | 1.71                     | 0.55              |
| 1:H:104:SER:HB2 | 1:H:177:MET:HE3  | 1.89                     | 0.55              |
| 1:H:233:GLU:HG2 | 1:Z:30:GLY:HA3   | 1.87                     | 0.55              |
| 1:H:386:ASN:O   | 1:H:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:K:99:PHE:O    | 1:K:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:K:348:ASP:OD1 | 1:K:349:LEU:N    | 2.38                     | 0.55              |
| 1:K:386:ASN:O   | 1:K:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:L:104:SER:HB2 | 1:L:177:MET:HE3  | 1.89                     | 0.55              |
| 1:L:386:ASN:O   | 1:L:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:M:104:SER:HB2 | 1:M:177:MET:HE2  | 1.88                     | 0.55              |
| 1:M:418:LYS:NZ  | 1:b:538:LEU:O    | 2.39                     | 0.55              |
| 1:R:348:ASP:OD1 | 1:R:349:LEU:N    | 2.38                     | 0.55              |
| 1:S:383:TYR:HB3 | 1:S:390:TYR:HB3  | 1.88                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:V:410:THR:H   | 1:V:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:W:383:TYR:HB3 | 1:W:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:X:99:PHE:O    | 1:X:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:X:104:SER:HB2 | 1:X:177:MET:HE3  | 1.89                     | 0.55              |
| 1:Z:386:ASN:O   | 1:Z:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:Z:418:LYS:NZ  | 1:3:538:LEU:O    | 2.39                     | 0.55              |
| 1:a:383:TYR:HB3 | 1:a:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:a:410:THR:H   | 1:a:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:e:68:ASN:ND2  | 1:e:71:LYS:O     | 2.39                     | 0.55              |
| 1:f:418:LYS:NZ  | 1:g:538:LEU:O    | 2.39                     | 0.55              |
| 1:g:386:ASN:O   | 1:g:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:g:410:THR:H   | 1:g:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:i:348:ASP:OD1 | 1:i:349:LEU:N    | 2.38                     | 0.55              |
| 1:j:348:ASP:OD1 | 1:j:349:LEU:N    | 2.38                     | 0.55              |
| 1:o:99:PHE:O    | 1:o:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:p:410:THR:H   | 1:p:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:r:383:TYR:HB3 | 1:r:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:v:410:THR:H   | 1:v:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:w:99:PHE:O    | 1:w:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:y:28:VAL:HG12 | 1:y:30:GLY:H     | 1.71                     | 0.55              |
| 1:1:28:VAL:HG12 | 1:1:30:GLY:H     | 1.71                     | 0.55              |
| 1:1:99:PHE:O    | 1:1:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:3:383:TYR:HB3 | 1:3:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:3:410:THR:H   | 1:3:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:5:104:SER:HB2 | 1:5:177:MET:HE3  | 1.89                     | 0.55              |
| 1:7:410:THR:H   | 1:7:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:8:410:THR:H   | 1:8:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:B:28:VAL:HG12 | 1:B:30:GLY:H     | 1.71                     | 0.55              |
| 1:C:410:THR:H   | 1:C:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:F:104:SER:HB2 | 1:F:177:MET:HE3  | 1.89                     | 0.55              |
| 1:G:348:ASP:OD1 | 1:G:349:LEU:N    | 2.38                     | 0.55              |
| 1:H:410:THR:H   | 1:H:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:J:273:GLN:HG3 | 1:J:278:ALA:HA   | 1.87                     | 0.55              |
| 1:L:30:GLY:HA3  | 1:b:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:O:410:THR:H   | 1:O:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:R:28:VAL:HG12 | 1:R:30:GLY:H     | 1.71                     | 0.55              |
| 1:Y:410:THR:H   | 1:Y:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:c:68:ASN:ND2  | 1:c:71:LYS:O     | 2.39                     | 0.55              |
| 1:f:383:TYR:HB3 | 1:f:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:g:68:ASN:ND2  | 1:g:71:LYS:O     | 2.39                     | 0.55              |
| 1:l:410:THR:H   | 1:l:413:ASN:HD22 | 1.55                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:q:28:VAL:HG12 | 1:q:30:GLY:H     | 1.71                     | 0.55              |
| 1:q:348:ASP:OD1 | 1:q:349:LEU:N    | 2.38                     | 0.55              |
| 1:y:104:SER:HB2 | 1:y:177:MET:HE3  | 1.89                     | 0.55              |
| 1:z:233:GLU:HG2 | 1:4:30:GLY:HA3   | 1.88                     | 0.55              |
| 1:z:386:ASN:O   | 1:z:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:1:104:SER:HB2 | 1:1:177:MET:HE3  | 1.89                     | 0.55              |
| 1:4:99:PHE:O    | 1:4:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:4:386:ASN:O   | 1:4:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:5:28:VAL:HG12 | 1:5:30:GLY:H     | 1.71                     | 0.55              |
| 1:5:410:THR:H   | 1:5:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:6:383:TYR:HB3 | 1:6:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:B:99:PHE:O    | 1:B:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:B:383:TYR:HB3 | 1:B:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:I:410:THR:H   | 1:I:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:N:348:ASP:OD1 | 1:N:349:LEU:N    | 2.38                     | 0.55              |
| 1:P:273:GLN:HG3 | 1:P:278:ALA:HA   | 1.87                     | 0.55              |
| 1:S:30:GLY:HA3  | 1:d:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:S:538:LEU:O   | 1:U:418:LYS:NZ   | 2.39                     | 0.55              |
| 1:T:410:THR:H   | 1:T:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:V:68:ASN:OD1  | 1:V:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:W:294:MET:HE1 | 1:W:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:W:491:ARG:O   | 1:W:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:a:538:LEU:O   | 1:8:418:LYS:NZ   | 2.39                     | 0.55              |
| 1:c:538:LEU:O   | 1:o:418:LYS:NZ   | 2.39                     | 0.55              |
| 1:g:410:THR:H   | 1:g:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:l:410:THR:H   | 1:l:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:n:386:ASN:O   | 1:n:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:o:491:ARG:O   | 1:o:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:p:68:ASN:OD1  | 1:p:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:q:383:TYR:HB3 | 1:q:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:r:104:SER:HB2 | 1:r:177:MET:HE2  | 1.88                     | 0.55              |
| 1:y:406:ARG:HB2 | 1:y:531:LYS:HZ1  | 1.72                     | 0.55              |
| 1:z:104:SER:HB2 | 1:z:177:MET:HE3  | 1.89                     | 0.55              |
| 1:1:383:TYR:HB3 | 1:1:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:2:273:GLN:HG3 | 1:2:278:ALA:HA   | 1.87                     | 0.55              |
| 1:5:233:GLU:HG2 | 1:8:30:GLY:HA3   | 1.87                     | 0.55              |
| 1:8:386:ASN:O   | 1:8:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:B:68:ASN:OD1  | 1:B:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:B:418:LYS:NZ  | 1:L:538:LEU:O    | 2.39                     | 0.55              |
| 1:C:104:SER:HB2 | 1:C:177:MET:HE3  | 1.89                     | 0.55              |
| 1:D:249:GLU:CG  | 1:D:536:LYS:HD3  | 2.37                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:386:ASN:O   | 1:E:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:F:249:GLU:CG  | 1:F:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:K:294:MET:HE1 | 1:K:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:N:28:VAL:HG12 | 1:N:30:GLY:H     | 1.71                     | 0.55              |
| 1:N:383:TYR:HB3 | 1:N:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:Q:410:THR:H   | 1:Q:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:R:383:TYR:HB3 | 1:R:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:S:68:ASN:OD1  | 1:S:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:T:30:GLY:HA3  | 1:U:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:T:104:SER:HB2 | 1:T:177:MET:HE3  | 1.89                     | 0.55              |
| 1:V:249:GLU:CG  | 1:V:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:X:418:LYS:NZ  | 1:e:538:LEU:O    | 2.39                     | 0.55              |
| 1:X:491:ARG:O   | 1:X:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:b:383:TYR:HB3 | 1:b:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:c:491:ARG:O   | 1:c:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:d:273:GLN:HG3 | 1:d:278:ALA:HA   | 1.87                     | 0.55              |
| 1:e:30:GLY:HA3  | 1:h:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:g:104:SER:HB2 | 1:g:177:MET:HE3  | 1.89                     | 0.55              |
| 1:i:28:VAL:HG12 | 1:i:30:GLY:H     | 1.71                     | 0.55              |
| 1:i:383:TYR:HB3 | 1:i:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:k:249:GLU:CG  | 1:k:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:k:386:ASN:O   | 1:k:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:m:30:GLY:HA3  | 1:s:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:m:410:THR:H   | 1:m:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:n:104:SER:HB2 | 1:n:177:MET:HE2  | 1.88                     | 0.55              |
| 1:n:233:GLU:HG2 | 1:r:30:GLY:HA3   | 1.88                     | 0.55              |
| 1:p:249:GLU:CG  | 1:p:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:r:68:ASN:OD1  | 1:r:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:r:538:LEU:O   | 1:s:418:LYS:NZ   | 2.39                     | 0.55              |
| 1:t:273:GLN:HG3 | 1:t:278:ALA:HA   | 1.87                     | 0.55              |
| 1:t:348:ASP:OD1 | 1:t:349:LEU:N    | 2.38                     | 0.55              |
| 1:x:410:THR:H   | 1:x:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:y:249:GLU:CG  | 1:y:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:y:294:MET:HE1 | 1:y:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:z:249:GLU:CG  | 1:z:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:1:68:ASN:OD1  | 1:1:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:6:294:MET:HE1 | 1:6:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:6:410:THR:H   | 1:6:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:6:491:ARG:O   | 1:6:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:F:233:GLU:HG2 | 1:R:30:GLY:HA3   | 1.88                     | 0.55              |
| 1:F:294:MET:HE1 | 1:F:382:LEU:HD11 | 1.89                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:273:GLN:HG3 | 1:G:278:ALA:HA   | 1.87                     | 0.55              |
| 1:H:410:THR:H   | 1:H:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:H:418:LYS:NZ  | 1:Y:538:LEU:O    | 2.39                     | 0.55              |
| 1:J:30:GLY:HA3  | 1:a:233:GLU:HG2  | 1.87                     | 0.55              |
| 1:J:68:ASN:OD1  | 1:J:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:K:68:ASN:OD1  | 1:K:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:K:104:SER:HB2 | 1:K:177:MET:HE3  | 1.89                     | 0.55              |
| 1:L:249:GLU:CG  | 1:L:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:R:410:THR:H   | 1:R:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:T:273:GLN:HG3 | 1:T:278:ALA:HA   | 1.87                     | 0.55              |
| 1:U:294:MET:HE1 | 1:U:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:V:104:SER:HB2 | 1:V:177:MET:HE2  | 1.88                     | 0.55              |
| 1:V:410:THR:H   | 1:V:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:W:68:ASN:OD1  | 1:W:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:W:410:THR:H   | 1:W:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:X:249:GLU:CG  | 1:X:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:Y:68:ASN:OD1  | 1:Y:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:b:410:THR:H   | 1:b:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:d:386:ASN:O   | 1:d:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:f:410:THR:H   | 1:f:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:i:99:PHE:O    | 1:i:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:j:68:ASN:ND2  | 1:j:71:LYS:O     | 2.39                     | 0.55              |
| 1:j:273:GLN:HG3 | 1:j:278:ALA:HA   | 1.87                     | 0.55              |
| 1:m:104:SER:HB2 | 1:m:177:MET:HE3  | 1.89                     | 0.55              |
| 1:m:273:GLN:HG3 | 1:m:278:ALA:HA   | 1.87                     | 0.55              |
| 1:n:273:GLN:HG3 | 1:n:278:ALA:HA   | 1.87                     | 0.55              |
| 1:o:249:GLU:CG  | 1:o:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:q:30:GLY:HA3  | 1:y:233:GLU:HG2  | 1.88                     | 0.55              |
| 1:q:410:THR:H   | 1:q:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:q:491:ARG:O   | 1:q:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:q:538:LEU:O   | 1:r:418:LYS:NZ   | 2.39                     | 0.55              |
| 1:r:28:VAL:HG12 | 1:r:30:GLY:H     | 1.71                     | 0.55              |
| 1:s:294:MET:HE1 | 1:s:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:w:386:ASN:O   | 1:w:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:z:406:ARG:HB2 | 1:z:531:LYS:HZ1  | 1.70                     | 0.55              |
| 1:2:68:ASN:OD1  | 1:2:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:2:104:SER:HB2 | 1:2:177:MET:HE3  | 1.89                     | 0.55              |
| 1:4:68:ASN:OD1  | 1:4:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:4:104:SER:HB2 | 1:4:177:MET:HE3  | 1.89                     | 0.55              |
| 1:5:410:THR:H   | 1:5:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:5:418:LYS:NZ  | 1:7:538:LEU:O    | 2.39                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:6:68:ASN:OD1  | 1:6:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:6:104:SER:HB2 | 1:6:177:MET:HE2  | 1.88                     | 0.55              |
| 1:7:68:ASN:OD1  | 1:7:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:D:386:ASN:O   | 1:D:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:G:68:ASN:OD1  | 1:G:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:H:68:ASN:OD1  | 1:H:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:J:104:SER:HB2 | 1:J:177:MET:HE3  | 1.89                     | 0.55              |
| 1:J:386:ASN:O   | 1:J:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:J:410:THR:H   | 1:J:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:P:68:ASN:ND2  | 1:P:71:LYS:O     | 2.39                     | 0.55              |
| 1:Q:491:ARG:O   | 1:Q:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:R:538:LEU:O   | 1:S:418:LYS:NZ   | 2.39                     | 0.55              |
| 1:S:28:VAL:HG12 | 1:S:30:GLY:H     | 1.71                     | 0.55              |
| 1:S:294:MET:HE1 | 1:S:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:W:104:SER:HB2 | 1:W:177:MET:HE2  | 1.88                     | 0.55              |
| 1:X:104:SER:HB2 | 1:X:177:MET:HE2  | 1.88                     | 0.55              |
| 1:Y:249:GLU:CG  | 1:Y:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:Z:68:ASN:OD1  | 1:Z:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:Z:410:THR:H   | 1:Z:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:a:68:ASN:ND2  | 1:a:71:LYS:O     | 2.39                     | 0.55              |
| 1:b:99:PHE:O    | 1:b:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:b:104:SER:HB2 | 1:b:177:MET:HE3  | 1.89                     | 0.55              |
| 1:d:104:SER:HB2 | 1:d:177:MET:HE2  | 1.88                     | 0.55              |
| 1:f:99:PHE:O    | 1:f:105:HIS:HE1  | 1.90                     | 0.55              |
| 1:i:294:MET:HE1 | 1:i:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:p:410:THR:H   | 1:p:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:r:410:THR:H   | 1:r:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:s:410:THR:H   | 1:s:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:t:68:ASN:OD1  | 1:t:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:u:410:THR:H   | 1:u:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:x:491:ARG:O   | 1:x:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:2:410:THR:H   | 1:2:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:4:294:MET:HE1 | 1:4:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:5:68:ASN:OD1  | 1:5:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:6:249:GLU:CG  | 1:6:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:7:249:GLU:CG  | 1:7:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:8:28:VAL:HG12 | 1:8:30:GLY:H     | 1.71                     | 0.55              |
| 1:E:68:ASN:OD1  | 1:E:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:F:68:ASN:OD1  | 1:F:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:F:99:PHE:O    | 1:F:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:G:28:VAL:HG12 | 1:G:30:GLY:H     | 1.71                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:68:ASN:OD1  | 1:L:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:M:233:GLU:HG2 | 1:c:30:GLY:HA3   | 1.88                     | 0.55              |
| 1:N:99:PHE:O    | 1:N:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:N:294:MET:HE1 | 1:N:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:N:410:THR:H   | 1:N:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:P:410:THR:H   | 1:P:413:ASN:HD22 | 1.55                     | 0.55              |
| 1:R:68:ASN:OD1  | 1:R:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:R:491:ARG:O   | 1:R:492:ARG:NH1  | 2.40                     | 0.55              |
| 1:T:249:GLU:CG  | 1:T:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:W:249:GLU:CG  | 1:W:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:Z:28:VAL:HG12 | 1:Z:30:GLY:H     | 1.71                     | 0.55              |
| 1:a:68:ASN:OD1  | 1:a:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:b:294:MET:HE1 | 1:b:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:c:68:ASN:OD1  | 1:c:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:e:68:ASN:OD1  | 1:e:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:f:294:MET:HE1 | 1:f:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:i:410:THR:H   | 1:i:413:ASN:ND2  | 2.05                     | 0.55              |
| 1:k:233:GLU:HG2 | 1:w:30:GLY:HA3   | 1.88                     | 0.55              |
| 1:o:104:SER:HB2 | 1:o:177:MET:HE2  | 1.88                     | 0.55              |
| 1:p:104:SER:HB2 | 1:p:177:MET:HE2  | 1.88                     | 0.55              |
| 1:r:294:MET:HE1 | 1:r:382:LEU:HD11 | 1.89                     | 0.55              |
| 1:y:68:ASN:OD1  | 1:y:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:z:68:ASN:OD1  | 1:z:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:2:249:GLU:CG  | 1:2:536:LYS:HD3  | 2.37                     | 0.55              |
| 1:2:386:ASN:O   | 1:2:387:GLN:HG2  | 2.06                     | 0.55              |
| 1:6:99:PHE:O    | 1:6:105:HIS:HE1  | 1.89                     | 0.55              |
| 1:8:68:ASN:OD1  | 1:8:73:ARG:NH2   | 2.40                     | 0.55              |
| 1:A:68:ASN:OD1  | 1:A:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:A:410:THR:H   | 1:A:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:B:294:MET:HE1 | 1:B:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:D:68:ASN:OD1  | 1:D:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:E:410:THR:H   | 1:E:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:F:406:ARG:HB2 | 1:F:531:LYS:HZ1  | 1.73                     | 0.54              |
| 1:I:294:MET:HE1 | 1:I:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:I:410:THR:H   | 1:I:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:K:410:THR:H   | 1:K:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:N:104:SER:HB2 | 1:N:177:MET:HE3  | 1.89                     | 0.54              |
| 1:O:104:SER:HB2 | 1:O:177:MET:HE3  | 1.89                     | 0.54              |
| 1:S:410:THR:H   | 1:S:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:U:68:ASN:OD1  | 1:U:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:U:410:THR:H   | 1:U:413:ASN:ND2  | 2.05                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:W:99:PHE:O    | 1:W:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:W:406:ARG:HB2 | 1:W:531:LYS:HZ1  | 1.71                     | 0.54              |
| 1:X:68:ASN:OD1  | 1:X:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:a:249:GLU:CG  | 1:a:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:b:249:GLU:CG  | 1:b:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:c:104:SER:HB2 | 1:c:177:MET:HE2  | 1.88                     | 0.54              |
| 1:d:491:ARG:O   | 1:d:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:f:249:GLU:CG  | 1:f:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:i:410:THR:H   | 1:i:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:j:410:THR:H   | 1:j:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:l:68:ASN:OD1  | 1:l:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:l:104:SER:HB2 | 1:l:177:MET:HE3  | 1.89                     | 0.54              |
| 1:m:99:PHE:O    | 1:m:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:m:249:GLU:CG  | 1:m:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:m:410:THR:H   | 1:m:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:o:68:ASN:OD1  | 1:o:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:t:28:VAL:HG12 | 1:t:30:GLY:H     | 1.71                     | 0.54              |
| 1:v:68:ASN:OD1  | 1:v:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:w:68:ASN:OD1  | 1:w:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:y:99:PHE:O    | 1:y:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:1:294:MET:HE1 | 1:1:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:3:68:ASN:ND2  | 1:3:71:LYS:O     | 2.39                     | 0.54              |
| 1:3:68:ASN:OD1  | 1:3:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:3:249:GLU:CG  | 1:3:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:5:99:PHE:O    | 1:5:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:7:410:THR:H   | 1:7:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:A:273:GLN:HG3 | 1:A:278:ALA:HA   | 1.87                     | 0.54              |
| 1:C:348:ASP:OD1 | 1:C:349:LEU:N    | 2.38                     | 0.54              |
| 1:D:233:GLU:HG2 | 1:E:30:GLY:HA3   | 1.88                     | 0.54              |
| 1:D:410:THR:H   | 1:D:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:G:104:SER:HB2 | 1:G:177:MET:HE3  | 1.89                     | 0.54              |
| 1:I:68:ASN:ND2  | 1:I:71:LYS:O     | 2.39                     | 0.54              |
| 1:K:249:GLU:CG  | 1:K:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:M:104:SER:HB2 | 1:M:177:MET:HE3  | 1.89                     | 0.54              |
| 1:N:410:THR:H   | 1:N:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:O:68:ASN:OD1  | 1:O:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:S:68:ASN:ND2  | 1:S:71:LYS:O     | 2.39                     | 0.54              |
| 1:T:99:PHE:O    | 1:T:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:T:410:THR:H   | 1:T:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:W:64:VAL:HG22 | 1:W:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:W:410:THR:H   | 1:W:413:ASN:HD22 | 1.55                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:Y:410:THR:H   | 1:Y:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:a:104:SER:HB2 | 1:a:177:MET:HE2  | 1.88                     | 0.54              |
| 1:c:410:THR:H   | 1:c:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:e:410:THR:H   | 1:e:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:g:68:ASN:OD1  | 1:g:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:g:294:MET:HE1 | 1:g:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:h:104:SER:HB2 | 1:h:177:MET:HE3  | 1.89                     | 0.54              |
| 1:i:104:SER:HB2 | 1:i:177:MET:HE3  | 1.89                     | 0.54              |
| 1:j:410:THR:H   | 1:j:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:k:68:ASN:OD1  | 1:k:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:k:410:THR:H   | 1:k:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:r:68:ASN:ND2  | 1:r:71:LYS:O     | 2.39                     | 0.54              |
| 1:r:99:PHE:O    | 1:r:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:s:68:ASN:OD1  | 1:s:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:t:99:PHE:O    | 1:t:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:u:294:MET:HE1 | 1:u:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:v:410:THR:H   | 1:v:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:w:410:THR:H   | 1:w:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:x:249:GLU:CG  | 1:x:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:z:99:PHE:O    | 1:z:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:1:538:LEU:O   | 1:2:418:LYS:NZ   | 2.39                     | 0.54              |
| 1:2:410:THR:H   | 1:2:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:4:64:VAL:HG22 | 1:4:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:4:249:GLU:CG  | 1:4:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:4:410:THR:H   | 1:4:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:5:249:GLU:CG  | 1:5:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:6:64:VAL:HG22 | 1:6:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:6:410:THR:H   | 1:6:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:8:410:THR:H   | 1:8:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:A:64:VAL:HG22 | 1:A:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:A:104:SER:HB2 | 1:A:177:MET:HE3  | 1.89                     | 0.54              |
| 1:C:68:ASN:OD1  | 1:C:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:C:294:MET:HE1 | 1:C:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:D:99:PHE:O    | 1:D:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:F:410:THR:H   | 1:F:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:G:99:PHE:O    | 1:G:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:H:99:PHE:O    | 1:H:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:H:249:GLU:CG  | 1:H:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:I:249:GLU:CG  | 1:I:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:J:249:GLU:CG  | 1:J:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:J:410:THR:H   | 1:J:413:ASN:HD22 | 1.55                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:104:SER:HB2 | 1:O:177:MET:HE2  | 1.88                     | 0.54              |
| 1:P:68:ASN:OD1  | 1:P:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:Q:249:GLU:CG  | 1:Q:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:R:104:SER:HB2 | 1:R:177:MET:HE2  | 1.88                     | 0.54              |
| 1:S:99:PHE:O    | 1:S:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:S:249:GLU:CG  | 1:S:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:Z:99:PHE:O    | 1:Z:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:Z:249:GLU:CG  | 1:Z:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:c:99:PHE:O    | 1:c:105:HIS:HE1  | 1.90                     | 0.54              |
| 1:f:104:SER:HB2 | 1:f:177:MET:HE3  | 1.89                     | 0.54              |
| 1:j:68:ASN:OD1  | 1:j:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:k:99:PHE:O    | 1:k:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:l:64:VAL:HG22 | 1:l:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:l:104:SER:HB2 | 1:l:177:MET:HE2  | 1.88                     | 0.54              |
| 1:n:406:ARG:HB2 | 1:n:531:LYS:HZ1  | 1.72                     | 0.54              |
| 1:n:491:ARG:O   | 1:n:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:q:68:ASN:OD1  | 1:q:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:r:249:GLU:CG  | 1:r:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:u:68:ASN:ND2  | 1:u:71:LYS:O     | 2.39                     | 0.54              |
| 1:v:64:VAL:HG22 | 1:v:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:v:273:GLN:HG3 | 1:v:278:ALA:HA   | 1.87                     | 0.54              |
| 1:z:64:VAL:HG22 | 1:z:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:4:68:ASN:ND2  | 1:4:71:LYS:O     | 2.39                     | 0.54              |
| 1:A:491:ARG:O   | 1:A:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:D:64:VAL:HG22 | 1:D:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:I:68:ASN:OD1  | 1:I:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:K:64:VAL:HG22 | 1:K:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:L:64:VAL:HG22 | 1:L:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:L:99:PHE:O    | 1:L:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:O:64:VAL:HG22 | 1:O:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:P:104:SER:HB2 | 1:P:177:MET:HE3  | 1.89                     | 0.54              |
| 1:P:410:THR:H   | 1:P:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:Q:410:THR:H   | 1:Q:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:R:410:THR:H   | 1:R:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:Y:104:SER:HB2 | 1:Y:177:MET:HE3  | 1.89                     | 0.54              |
| 1:a:410:THR:H   | 1:a:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:d:406:ARG:HB2 | 1:d:531:LYS:HZ1  | 1.71                     | 0.54              |
| 1:e:104:SER:HB2 | 1:e:177:MET:HE2  | 1.88                     | 0.54              |
| 1:j:104:SER:HB2 | 1:j:177:MET:HE3  | 1.89                     | 0.54              |
| 1:q:104:SER:HB2 | 1:q:177:MET:HE2  | 1.88                     | 0.54              |
| 1:t:104:SER:HB2 | 1:t:177:MET:HE3  | 1.89                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:u:99:PHE:O    | 1:u:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:u:249:GLU:CG  | 1:u:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:u:348:ASP:OD1 | 1:u:349:LEU:N    | 2.38                     | 0.54              |
| 1:u:410:THR:H   | 1:u:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:v:491:ARG:O   | 1:v:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:y:410:THR:H   | 1:y:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:y:410:THR:H   | 1:y:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:1:410:THR:H   | 1:1:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:3:104:SER:HB2 | 1:3:177:MET:HE2  | 1.88                     | 0.54              |
| 1:7:64:VAL:HG22 | 1:7:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:8:99:PHE:O    | 1:8:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:8:249:GLU:CG  | 1:8:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:B:410:THR:H   | 1:B:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:F:104:SER:HB2 | 1:F:177:MET:HE2  | 1.88                     | 0.54              |
| 1:I:99:PHE:O    | 1:I:105:HIS:HE1  | 1.89                     | 0.54              |
| 1:J:64:VAL:HG22 | 1:J:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:K:68:ASN:ND2  | 1:K:71:LYS:O     | 2.39                     | 0.54              |
| 1:M:294:MET:HE1 | 1:M:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:T:175:ASP:CB  | 1:T:188:PHE:CZ   | 2.83                     | 0.54              |
| 1:V:64:VAL:HG22 | 1:V:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:Y:64:VAL:HG22 | 1:Y:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:Y:383:TYR:HB3 | 1:Y:390:TYR:HB3  | 1.88                     | 0.54              |
| 1:b:64:VAL:HG22 | 1:b:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:e:99:PHE:O    | 1:e:105:HIS:HE1  | 1.90                     | 0.54              |
| 1:f:64:VAL:HG22 | 1:f:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:h:294:MET:HE1 | 1:h:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:k:64:VAL:HG22 | 1:k:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:m:68:ASN:OD1  | 1:m:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:n:104:SER:HB2 | 1:n:177:MET:HE3  | 1.89                     | 0.54              |
| 1:o:383:TYR:HB3 | 1:o:390:TYR:HB3  | 1.88                     | 0.54              |
| 1:p:64:VAL:HG22 | 1:p:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:p:406:ARG:HB2 | 1:p:531:LYS:HZ1  | 1.73                     | 0.54              |
| 1:s:104:SER:HB2 | 1:s:177:MET:HE3  | 1.89                     | 0.54              |
| 1:u:68:ASN:OD1  | 1:u:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:v:104:SER:HB2 | 1:v:177:MET:HE3  | 1.89                     | 0.54              |
| 1:x:410:THR:H   | 1:x:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:z:410:THR:H   | 1:z:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:7:104:SER:HB2 | 1:7:177:MET:HE3  | 1.89                     | 0.54              |
| 1:7:383:TYR:HB3 | 1:7:390:TYR:HB3  | 1.88                     | 0.54              |
| 1:E:104:SER:HB2 | 1:E:177:MET:HE3  | 1.89                     | 0.54              |
| 1:F:410:THR:H   | 1:F:413:ASN:ND2  | 2.05                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:64:VAL:HG22 | 1:H:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:J:294:MET:HE1 | 1:J:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:L:406:ARG:HB2 | 1:L:531:LYS:HZ1  | 1.71                     | 0.54              |
| 1:N:406:ARG:HB2 | 1:N:531:LYS:HZ1  | 1.73                     | 0.54              |
| 1:O:294:MET:HE1 | 1:O:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:T:68:ASN:OD1  | 1:T:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:Z:294:MET:HE1 | 1:Z:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:d:68:ASN:OD1  | 1:d:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:d:383:TYR:HB3 | 1:d:390:TYR:HB3  | 1.88                     | 0.54              |
| 1:i:406:ARG:HB2 | 1:i:531:LYS:HZ1  | 1.73                     | 0.54              |
| 1:l:294:MET:HE1 | 1:l:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:n:249:GLU:CG  | 1:n:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:q:249:GLU:CG  | 1:q:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:q:410:THR:H   | 1:q:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:t:249:GLU:CG  | 1:t:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:w:104:SER:HB2 | 1:w:177:MET:HE3  | 1.89                     | 0.54              |
| 1:w:249:GLU:CG  | 1:w:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:2:64:VAL:HG22 | 1:2:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:7:491:ARG:O   | 1:7:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:8:68:ASN:ND2  | 1:8:71:LYS:O     | 2.39                     | 0.54              |
| 1:B:249:GLU:CG  | 1:B:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:C:249:GLU:CG  | 1:C:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:E:249:GLU:CG  | 1:E:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:G:249:GLU:CG  | 1:G:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:L:410:THR:H   | 1:L:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:O:406:ARG:HB2 | 1:O:531:LYS:HZ1  | 1.73                     | 0.54              |
| 1:R:249:GLU:CG  | 1:R:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:U:104:SER:HB2 | 1:U:177:MET:HE3  | 1.89                     | 0.54              |
| 1:X:294:MET:HE1 | 1:X:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:X:410:THR:H   | 1:X:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:d:104:SER:HB2 | 1:d:177:MET:HE3  | 1.89                     | 0.54              |
| 1:d:249:GLU:CG  | 1:d:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:e:64:VAL:HG22 | 1:e:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:e:249:GLU:CG  | 1:e:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:f:410:THR:H   | 1:f:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:g:249:GLU:CG  | 1:g:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:i:68:ASN:OD1  | 1:i:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:m:175:ASP:CB  | 1:m:188:PHE:CZ   | 2.83                     | 0.54              |
| 1:n:383:TYR:HB3 | 1:n:390:TYR:HB3  | 1.88                     | 0.54              |
| 1:n:410:THR:H   | 1:n:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:o:294:MET:HE1 | 1:o:382:LEU:HD11 | 1.89                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:q:294:MET:HE1 | 1:q:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:w:68:ASN:ND2  | 1:w:71:LYS:O     | 2.39                     | 0.54              |
| 1:y:104:SER:HB2 | 1:y:177:MET:HE2  | 1.88                     | 0.54              |
| 1:2:30:GLY:HA3  | 1:3:233:GLU:HG2  | 1.88                     | 0.54              |
| 1:2:294:MET:HE1 | 1:2:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:3:410:THR:H   | 1:3:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:4:491:ARG:O   | 1:4:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:5:64:VAL:HG22 | 1:5:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:5:294:MET:HE1 | 1:5:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:8:294:MET:HE1 | 1:8:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:B:410:THR:H   | 1:B:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:D:68:ASN:ND2  | 1:D:71:LYS:O     | 2.39                     | 0.54              |
| 1:E:68:ASN:ND2  | 1:E:71:LYS:O     | 2.39                     | 0.54              |
| 1:H:294:MET:HE1 | 1:H:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:K:491:ARG:O   | 1:K:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:N:68:ASN:OD1  | 1:N:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:P:64:VAL:HG22 | 1:P:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:Q:383:TYR:HB3 | 1:Q:390:TYR:HB3  | 1.88                     | 0.54              |
| 1:R:294:MET:HE1 | 1:R:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:X:233:GLU:HG2 | 1:f:30:GLY:HA3   | 1.88                     | 0.54              |
| 1:X:383:TYR:HB3 | 1:X:390:TYR:HB3  | 1.88                     | 0.54              |
| 1:Z:68:ASN:ND2  | 1:Z:71:LYS:O     | 2.39                     | 0.54              |
| 1:b:30:GLY:HA3  | 1:o:233:GLU:HG2  | 1.88                     | 0.54              |
| 1:b:68:ASN:OD1  | 1:b:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:b:410:THR:H   | 1:b:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:c:64:VAL:HG22 | 1:c:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:f:68:ASN:OD1  | 1:f:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:g:104:SER:HB2 | 1:g:177:MET:HE2  | 1.88                     | 0.54              |
| 1:k:68:ASN:ND2  | 1:k:71:LYS:O     | 2.39                     | 0.54              |
| 1:l:68:ASN:ND2  | 1:l:71:LYS:O     | 2.39                     | 0.54              |
| 1:n:68:ASN:OD1  | 1:n:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:r:104:SER:HB2 | 1:r:177:MET:HE3  | 1.89                     | 0.54              |
| 1:s:249:GLU:CG  | 1:s:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:w:64:VAL:HG22 | 1:w:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:1:104:SER:HB2 | 1:1:177:MET:HE2  | 1.88                     | 0.54              |
| 1:6:406:ARG:HB2 | 1:6:531:LYS:HZ1  | 1.72                     | 0.54              |
| 1:B:104:SER:HB2 | 1:B:177:MET:HE2  | 1.88                     | 0.54              |
| 1:B:538:LEU:O   | 1:J:418:LYS:NZ   | 2.40                     | 0.54              |
| 1:C:104:SER:HB2 | 1:C:177:MET:HE2  | 1.88                     | 0.54              |
| 1:D:104:SER:HB2 | 1:D:177:MET:HE2  | 1.88                     | 0.54              |
| 1:E:64:VAL:HG22 | 1:E:187:LEU:HD12 | 1.90                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:64:VAL:HG22 | 1:F:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:G:410:THR:H   | 1:G:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:R:64:VAL:HG22 | 1:R:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:S:104:SER:HB2 | 1:S:177:MET:HE3  | 1.89                     | 0.54              |
| 1:T:64:VAL:HG22 | 1:T:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:U:249:GLU:CG  | 1:U:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:V:294:MET:HE1 | 1:V:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:Z:104:SER:HB2 | 1:Z:177:MET:HE3  | 1.89                     | 0.54              |
| 1:c:249:GLU:CG  | 1:c:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:d:410:THR:H   | 1:d:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:h:68:ASN:OD1  | 1:h:73:ARG:NH2   | 2.40                     | 0.54              |
| 1:h:249:GLU:CG  | 1:h:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:j:64:VAL:HG22 | 1:j:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:l:249:GLU:CG  | 1:l:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:o:410:THR:H   | 1:o:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:q:64:VAL:HG22 | 1:q:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:u:104:SER:HB2 | 1:u:177:MET:HE3  | 1.89                     | 0.54              |
| 1:x:294:MET:HE1 | 1:x:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:1:249:GLU:CG  | 1:1:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:1:410:THR:H   | 1:1:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:8:64:VAL:HG22 | 1:8:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:C:64:VAL:HG22 | 1:C:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:G:410:THR:H   | 1:G:413:ASN:HD22 | 1.55                     | 0.54              |
| 1:G:491:ARG:O   | 1:G:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:I:104:SER:HB2 | 1:I:177:MET:HE3  | 1.89                     | 0.54              |
| 1:J:491:ARG:O   | 1:J:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:L:294:MET:HE1 | 1:L:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:O:68:ASN:ND2  | 1:O:71:LYS:O     | 2.39                     | 0.54              |
| 1:O:249:GLU:CG  | 1:O:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:P:249:GLU:CG  | 1:P:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:T:294:MET:HE1 | 1:T:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:Z:64:VAL:HG22 | 1:Z:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:g:64:VAL:HG22 | 1:g:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:j:249:GLU:CG  | 1:j:536:LYS:HD3  | 2.37                     | 0.54              |
| 1:m:64:VAL:HG22 | 1:m:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:p:294:MET:HE1 | 1:p:382:LEU:HD11 | 1.89                     | 0.54              |
| 1:t:68:ASN:ND2  | 1:t:71:LYS:O     | 2.39                     | 0.54              |
| 1:t:410:THR:H   | 1:t:413:ASN:ND2  | 2.05                     | 0.54              |
| 1:y:64:VAL:HG22 | 1:y:187:LEU:HD12 | 1.90                     | 0.54              |
| 1:2:491:ARG:O   | 1:2:492:ARG:NH1  | 2.40                     | 0.54              |
| 1:8:104:SER:HB2 | 1:8:177:MET:HE3  | 1.89                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:175:ASP:HB3 | 1:A:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:B:491:ARG:O   | 1:B:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:D:294:MET:HE1 | 1:D:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:G:68:ASN:ND2  | 1:G:71:LYS:O     | 2.39                     | 0.53              |
| 1:M:68:ASN:OD1  | 1:M:73:ARG:NH2   | 2.40                     | 0.53              |
| 1:M:249:GLU:CG  | 1:M:536:LYS:HD3  | 2.37                     | 0.53              |
| 1:P:294:MET:HE1 | 1:P:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:Q:68:ASN:OD1  | 1:Q:73:ARG:NH2   | 2.40                     | 0.53              |
| 1:Q:294:MET:HE1 | 1:Q:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:W:104:SER:HB2 | 1:W:177:MET:HE3  | 1.89                     | 0.53              |
| 1:a:104:SER:HB2 | 1:a:177:MET:HE3  | 1.89                     | 0.53              |
| 1:k:104:SER:HB2 | 1:k:177:MET:HE2  | 1.88                     | 0.53              |
| 1:l:406:ARG:HB2 | 1:l:531:LYS:HZ1  | 1.73                     | 0.53              |
| 1:m:294:MET:HE1 | 1:m:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:q:406:ARG:HB2 | 1:q:531:LYS:HZ1  | 1.73                     | 0.53              |
| 1:v:175:ASP:HB3 | 1:v:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:x:68:ASN:OD1  | 1:x:73:ARG:NH2   | 2.40                     | 0.53              |
| 1:x:383:TYR:HB3 | 1:x:390:TYR:HB3  | 1.88                     | 0.53              |
| 1:z:410:THR:H   | 1:z:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:1:491:ARG:O   | 1:1:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:E:294:MET:HE1 | 1:E:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:L:410:THR:H   | 1:L:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:U:410:THR:H   | 1:U:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:U:491:ARG:O   | 1:U:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:d:294:MET:HE1 | 1:d:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:e:104:SER:HB2 | 1:e:177:MET:HE3  | 1.89                     | 0.53              |
| 1:j:294:MET:HE1 | 1:j:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:k:294:MET:HE1 | 1:k:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:t:410:THR:H   | 1:t:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:t:491:ARG:O   | 1:t:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:v:68:ASN:ND2  | 1:v:71:LYS:O     | 2.39                     | 0.53              |
| 1:v:249:GLU:CG  | 1:v:536:LYS:HD3  | 2.37                     | 0.53              |
| 1:z:294:MET:HE1 | 1:z:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:3:104:SER:HB2 | 1:3:177:MET:HE3  | 1.89                     | 0.53              |
| 1:L:175:ASP:HB3 | 1:L:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:M:406:ARG:HB2 | 1:M:531:LYS:HZ1  | 1.73                     | 0.53              |
| 1:N:175:ASP:HB3 | 1:N:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:T:175:ASP:HB3 | 1:T:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:V:104:SER:HB2 | 1:V:177:MET:HE3  | 1.89                     | 0.53              |
| 1:W:175:ASP:HB3 | 1:W:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:c:104:SER:HB2 | 1:c:177:MET:HE3  | 1.89                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:h:406:ARG:HB2 | 1:h:531:LYS:HZ1  | 1.73                     | 0.53              |
| 1:i:175:ASP:HB3 | 1:i:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:m:175:ASP:HB3 | 1:m:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:n:294:MET:HE1 | 1:n:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:s:410:THR:H   | 1:s:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:s:491:ARG:O   | 1:s:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:w:294:MET:HE1 | 1:w:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:x:175:ASP:HB3 | 1:x:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:1:64:VAL:HG22 | 1:1:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:6:104:SER:HB2 | 1:6:177:MET:HE3  | 1.89                     | 0.53              |
| 1:A:68:ASN:ND2  | 1:A:71:LYS:O     | 2.39                     | 0.53              |
| 1:A:249:GLU:CG  | 1:A:536:LYS:HD3  | 2.37                     | 0.53              |
| 1:B:64:VAL:HG22 | 1:B:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:D:104:SER:HB2 | 1:D:177:MET:HE3  | 1.89                     | 0.53              |
| 1:F:175:ASP:HB3 | 1:F:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:I:64:VAL:HG22 | 1:I:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:M:175:ASP:HB3 | 1:M:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:Q:104:SER:HB2 | 1:Q:177:MET:HE3  | 1.89                     | 0.53              |
| 1:Q:175:ASP:HB3 | 1:Q:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:a:294:MET:HE1 | 1:a:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:b:406:ARG:HB2 | 1:b:531:LYS:HZ1  | 1.73                     | 0.53              |
| 1:c:410:THR:H   | 1:c:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:f:406:ARG:HB2 | 1:f:531:LYS:HZ1  | 1.73                     | 0.53              |
| 1:r:410:THR:H   | 1:r:413:ASN:ND2  | 2.05                     | 0.53              |
| 1:u:64:VAL:HG22 | 1:u:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:v:294:MET:HE1 | 1:v:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:x:104:SER:HB2 | 1:x:177:MET:HE3  | 1.89                     | 0.53              |
| 1:y:175:ASP:HB3 | 1:y:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:z:175:ASP:HB3 | 1:z:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:3:64:VAL:HG22 | 1:3:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:6:175:ASP:HB3 | 1:6:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:A:294:MET:HE1 | 1:A:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:C:175:ASP:HB3 | 1:C:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:D:491:ARG:O   | 1:D:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:H:175:ASP:HB3 | 1:H:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:T:406:ARG:HB2 | 1:T:531:LYS:HZ1  | 1.74                     | 0.53              |
| 1:X:64:VAL:HG22 | 1:X:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:Y:294:MET:HE1 | 1:Y:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:Z:175:ASP:HB3 | 1:Z:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:a:64:VAL:HG22 | 1:a:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:c:294:MET:HE1 | 1:c:382:LEU:HD11 | 1.89                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:g:175:ASP:HB3 | 1:g:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:k:104:SER:HB2 | 1:k:177:MET:HE3  | 1.89                     | 0.53              |
| 1:m:406:ARG:HB2 | 1:m:531:LYS:HZ1  | 1.74                     | 0.53              |
| 1:n:64:VAL:HG22 | 1:n:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:o:64:VAL:HG22 | 1:o:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:p:104:SER:HB2 | 1:p:177:MET:HE3  | 1.89                     | 0.53              |
| 1:8:175:ASP:HB3 | 1:8:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:B:175:ASP:HB3 | 1:B:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:R:406:ARG:HB2 | 1:R:531:LYS:HZ1  | 1.73                     | 0.53              |
| 1:S:410:THR:H   | 1:S:413:ASN:ND2  | 2.05                     | 0.53              |
| 1:U:64:VAL:HG22 | 1:U:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:d:64:VAL:HG22 | 1:d:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:e:294:MET:HE1 | 1:e:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:h:175:ASP:HB3 | 1:h:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:k:491:ARG:O   | 1:k:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:s:64:VAL:HG22 | 1:s:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:3:294:MET:HE1 | 1:3:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:5:175:ASP:HB3 | 1:5:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:7:294:MET:HE1 | 1:7:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:N:249:GLU:CG  | 1:N:536:LYS:HD3  | 2.37                     | 0.53              |
| 1:e:410:THR:H   | 1:e:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:i:249:GLU:CG  | 1:i:536:LYS:HD3  | 2.37                     | 0.53              |
| 1:l:491:ARG:O   | 1:l:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:1:175:ASP:HB3 | 1:1:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:E:410:THR:H   | 1:E:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:G:294:MET:HE1 | 1:G:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:S:64:VAL:HG22 | 1:S:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:U:68:ASN:ND2  | 1:U:71:LYS:O     | 2.39                     | 0.53              |
| 1:r:64:VAL:HG22 | 1:r:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:E:175:ASP:HB3 | 1:E:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:O:491:ARG:O   | 1:O:492:ARG:NH1  | 2.40                     | 0.53              |
| 1:d:175:ASP:HB3 | 1:d:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:M:64:VAL:HG22 | 1:M:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:M:410:THR:H   | 1:M:413:ASN:HD22 | 1.55                     | 0.53              |
| 1:Q:64:VAL:HG22 | 1:Q:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:t:294:MET:HE1 | 1:t:382:LEU:HD11 | 1.89                     | 0.53              |
| 1:w:175:ASP:HB3 | 1:w:188:PHE:CD2  | 2.44                     | 0.53              |
| 1:x:64:VAL:HG22 | 1:x:187:LEU:HD12 | 1.90                     | 0.53              |
| 1:S:491:ARG:O   | 1:S:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:d:410:THR:H   | 1:d:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:h:64:VAL:HG22 | 1:h:187:LEU:HD12 | 1.90                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:n:175:ASP:HB3 | 1:n:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:s:68:ASN:ND2  | 1:s:71:LYS:O     | 2.39                     | 0.52              |
| 1:w:410:THR:H   | 1:w:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:4:175:ASP:HB3 | 1:4:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:K:175:ASP:HB3 | 1:K:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:a:175:ASP:HB3 | 1:a:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:q:104:SER:HB2 | 1:q:177:MET:HE3  | 1.89                     | 0.52              |
| 1:r:175:ASP:HB3 | 1:r:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:u:175:ASP:HB3 | 1:u:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:I:175:ASP:HB3 | 1:I:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:P:491:ARG:O   | 1:P:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:S:175:ASP:HB3 | 1:S:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:Y:175:ASP:HB3 | 1:Y:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:h:410:THR:H   | 1:h:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:j:491:ARG:O   | 1:j:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:n:410:THR:H   | 1:n:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:t:64:VAL:HG22 | 1:t:187:LEU:HD12 | 1.90                     | 0.52              |
| 1:2:175:ASP:CB  | 1:2:188:PHE:CZ   | 2.83                     | 0.52              |
| 1:3:175:ASP:HB3 | 1:3:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:G:64:VAL:HG22 | 1:G:187:LEU:HD12 | 1.90                     | 0.52              |
| 1:P:175:ASP:HB3 | 1:P:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:V:175:ASP:HB3 | 1:V:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:V:491:ARG:O   | 1:V:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:b:491:ARG:O   | 1:b:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:p:175:ASP:HB3 | 1:p:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:r:491:ARG:O   | 1:r:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:2:175:ASP:HB3 | 1:2:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:3:136:LYS:NZ  | 1:3:149:ASN:OD1  | 2.37                     | 0.52              |
| 1:7:175:ASP:HB3 | 1:7:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:I:491:ARG:O   | 1:I:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:J:175:ASP:HB3 | 1:J:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:N:64:VAL:HG22 | 1:N:187:LEU:HD12 | 1.90                     | 0.52              |
| 1:R:104:SER:HB2 | 1:R:177:MET:HE3  | 1.89                     | 0.52              |
| 1:b:175:ASP:HB3 | 1:b:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:e:175:ASP:HB3 | 1:e:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:f:175:ASP:HB3 | 1:f:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:f:491:ARG:O   | 1:f:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:j:175:ASP:HB3 | 1:j:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:o:175:ASP:HB3 | 1:o:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:s:175:ASP:HB3 | 1:s:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:O:175:ASP:HB3 | 1:O:188:PHE:CD2  | 2.44                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:64:VAL:HG22  | 1:i:187:LEU:HD12 | 1.90                     | 0.52              |
| 1:k:410:THR:H    | 1:k:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:l:175:ASP:HB3  | 1:l:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:p:68:ASN:ND2   | 1:p:71:LYS:O     | 2.39                     | 0.52              |
| 1:p:491:ARG:O    | 1:p:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:x:175:ASP:CB   | 1:x:188:PHE:CZ   | 2.83                     | 0.52              |
| 1:G:357:GLN:HE22 | 1:G:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:J:175:ASP:CB   | 1:J:188:PHE:CZ   | 2.83                     | 0.52              |
| 1:K:410:THR:H    | 1:K:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:M:68:ASN:ND2   | 1:M:71:LYS:O     | 2.39                     | 0.52              |
| 1:R:175:ASP:HB3  | 1:R:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:U:175:ASP:HB3  | 1:U:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:X:175:ASP:HB3  | 1:X:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:Z:156:HIS:HD2  | 1:Z:226:HIS:CD2  | 2.28                     | 0.52              |
| 1:c:175:ASP:HB3  | 1:c:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:g:491:ARG:O    | 1:g:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:o:357:GLN:HE22 | 1:o:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:t:357:GLN:HE22 | 1:t:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:u:491:ARG:O    | 1:u:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:4:410:THR:H    | 1:4:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:8:156:HIS:HD2  | 1:8:226:HIS:CD2  | 2.28                     | 0.52              |
| 1:M:357:GLN:HE22 | 1:M:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:Q:175:ASP:CB   | 1:Q:188:PHE:CZ   | 2.83                     | 0.52              |
| 1:X:357:GLN:HE22 | 1:X:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:h:68:ASN:ND2   | 1:h:71:LYS:O     | 2.39                     | 0.52              |
| 1:h:357:GLN:HE22 | 1:h:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:m:156:HIS:HD2  | 1:m:226:HIS:CD2  | 2.28                     | 0.52              |
| 1:q:175:ASP:HB3  | 1:q:188:PHE:CD2  | 2.44                     | 0.52              |
| 1:B:156:HIS:HD2  | 1:B:226:HIS:CD2  | 2.28                     | 0.52              |
| 1:D:410:THR:H    | 1:D:413:ASN:HD22 | 1.55                     | 0.52              |
| 1:T:156:HIS:HD2  | 1:T:226:HIS:CD2  | 2.28                     | 0.52              |
| 1:V:68:ASN:ND2   | 1:V:71:LYS:O     | 2.39                     | 0.52              |
| 1:6:357:GLN:HE22 | 1:6:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:7:406:ARG:HB2  | 1:7:531:LYS:HZ1  | 1.75                     | 0.52              |
| 1:B:406:ARG:HB2  | 1:B:531:LYS:HZ1  | 1.74                     | 0.52              |
| 1:C:491:ARG:O    | 1:C:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:E:357:GLN:HE22 | 1:E:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:N:491:ARG:O    | 1:N:492:ARG:NH1  | 2.40                     | 0.52              |
| 1:S:156:HIS:HD2  | 1:S:226:HIS:CD2  | 2.28                     | 0.52              |
| 1:W:357:GLN:HE22 | 1:W:412:GLU:HG2  | 1.75                     | 0.52              |
| 1:m:491:ARG:O    | 1:m:492:ARG:NH1  | 2.40                     | 0.52              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:r:156:HIS:HD2  | 1:r:226:HIS:CD2 | 2.28                     | 0.52              |
| 1:v:156:HIS:HD2  | 1:v:226:HIS:CD2 | 2.28                     | 0.52              |
| 1:A:156:HIS:HD2  | 1:A:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:B:390:TYR:HE2  | 1:J:331:ALA:HB2 | 1.75                     | 0.51              |
| 1:E:156:HIS:HD2  | 1:E:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:F:302:ALA:C    | 1:F:314:SER:HB2 | 2.35                     | 0.51              |
| 1:L:302:ALA:C    | 1:L:314:SER:HB2 | 2.36                     | 0.51              |
| 1:N:156:HIS:HD2  | 1:N:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:T:491:ARG:O    | 1:T:492:ARG:NH1 | 2.40                     | 0.51              |
| 1:f:357:GLN:HE22 | 1:f:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:i:156:HIS:HD2  | 1:i:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:q:156:HIS:HD2  | 1:q:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:s:302:ALA:C    | 1:s:314:SER:HB2 | 2.36                     | 0.51              |
| 1:u:156:HIS:HD2  | 1:u:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:w:156:HIS:HD2  | 1:w:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:w:357:GLN:HE22 | 1:w:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:y:302:ALA:C    | 1:y:314:SER:HB2 | 2.36                     | 0.51              |
| 1:1:156:HIS:HD2  | 1:1:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:1:406:ARG:HB2  | 1:1:531:LYS:HZ1 | 1.74                     | 0.51              |
| 1:4:302:ALA:C    | 1:4:314:SER:HB2 | 2.35                     | 0.51              |
| 1:D:175:ASP:HB3  | 1:D:188:PHE:CD2 | 2.44                     | 0.51              |
| 1:D:357:GLN:HE22 | 1:D:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:H:302:ALA:C    | 1:H:314:SER:HB2 | 2.36                     | 0.51              |
| 1:I:156:HIS:HD2  | 1:I:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:K:156:HIS:HD2  | 1:K:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:O:357:GLN:HE22 | 1:O:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:R:156:HIS:HD2  | 1:R:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:U:302:ALA:C    | 1:U:314:SER:HB2 | 2.36                     | 0.51              |
| 1:X:302:ALA:C    | 1:X:314:SER:HB2 | 2.36                     | 0.51              |
| 1:Z:302:ALA:C    | 1:Z:314:SER:HB2 | 2.36                     | 0.51              |
| 1:b:156:HIS:HD2  | 1:b:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:b:357:GLN:HE22 | 1:b:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:c:302:ALA:C    | 1:c:314:SER:HB2 | 2.36                     | 0.51              |
| 1:e:302:ALA:C    | 1:e:314:SER:HB2 | 2.36                     | 0.51              |
| 1:i:491:ARG:O    | 1:i:492:ARG:NH1 | 2.40                     | 0.51              |
| 1:k:175:ASP:HB3  | 1:k:188:PHE:CD2 | 2.44                     | 0.51              |
| 1:k:357:GLN:HE22 | 1:k:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:o:302:ALA:C    | 1:o:314:SER:HB2 | 2.36                     | 0.51              |
| 1:s:357:GLN:HE22 | 1:s:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:y:156:HIS:HD2  | 1:y:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:z:302:ALA:C    | 1:z:314:SER:HB2 | 2.36                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:4:156:HIS:HD2  | 1:4:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:5:491:ARG:O    | 1:5:492:ARG:NH1 | 2.40                     | 0.51              |
| 1:8:302:ALA:C    | 1:8:314:SER:HB2 | 2.36                     | 0.51              |
| 1:E:302:ALA:C    | 1:E:314:SER:HB2 | 2.36                     | 0.51              |
| 1:F:156:HIS:HD2  | 1:F:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:H:357:GLN:HE22 | 1:H:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:H:491:ARG:O    | 1:H:492:ARG:NH1 | 2.40                     | 0.51              |
| 1:K:302:ALA:C    | 1:K:314:SER:HB2 | 2.36                     | 0.51              |
| 1:Q:156:HIS:HD2  | 1:Q:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:c:156:HIS:HD2  | 1:c:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:d:156:HIS:HD2  | 1:d:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:h:491:ARG:O    | 1:h:492:ARG:NH1 | 2.40                     | 0.51              |
| 1:l:357:GLN:HE22 | 1:l:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:t:175:ASP:HB3  | 1:t:188:PHE:CD2 | 2.44                     | 0.51              |
| 1:w:302:ALA:C    | 1:w:314:SER:HB2 | 2.36                     | 0.51              |
| 1:x:156:HIS:HD2  | 1:x:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:5:302:ALA:C    | 1:5:314:SER:HB2 | 2.36                     | 0.51              |
| 1:G:175:ASP:HB3  | 1:G:188:PHE:CD2 | 2.44                     | 0.51              |
| 1:I:302:ALA:C    | 1:I:314:SER:HB2 | 2.36                     | 0.51              |
| 1:J:302:ALA:C    | 1:J:314:SER:HB2 | 2.36                     | 0.51              |
| 1:K:273:GLN:HB2  | 1:K:279:SER:HB2 | 1.93                     | 0.51              |
| 1:K:357:GLN:HE22 | 1:K:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:M:491:ARG:O    | 1:M:492:ARG:NH1 | 2.40                     | 0.51              |
| 1:N:273:GLN:HB2  | 1:N:279:SER:HB2 | 1.93                     | 0.51              |
| 1:P:357:GLN:HE22 | 1:P:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:U:357:GLN:HE22 | 1:U:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:V:156:HIS:HD2  | 1:V:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:c:357:GLN:HE22 | 1:c:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:f:156:HIS:HD2  | 1:f:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:f:273:GLN:HB2  | 1:f:279:SER:HB2 | 1.93                     | 0.51              |
| 1:j:357:GLN:HE22 | 1:j:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:n:156:HIS:HD2  | 1:n:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:2:302:ALA:C    | 1:2:314:SER:HB2 | 2.36                     | 0.51              |
| 1:5:357:GLN:HE22 | 1:5:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:7:357:GLN:HE22 | 1:7:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:E:273:GLN:HB2  | 1:E:279:SER:HB2 | 1.93                     | 0.51              |
| 1:H:273:GLN:HB2  | 1:H:279:SER:HB2 | 1.93                     | 0.51              |
| 1:M:156:HIS:HD2  | 1:M:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:P:302:ALA:C    | 1:P:314:SER:HB2 | 2.36                     | 0.51              |
| 1:T:302:ALA:C    | 1:T:314:SER:HB2 | 2.35                     | 0.51              |
| 1:Y:156:HIS:HD2  | 1:Y:226:HIS:CD2 | 2.28                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:Y:357:GLN:HE22 | 1:Y:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:a:302:ALA:C    | 1:a:314:SER:HB2 | 2.36                     | 0.51              |
| 1:b:273:GLN:HB2  | 1:b:279:SER:HB2 | 1.93                     | 0.51              |
| 1:d:273:GLN:HB2  | 1:d:279:SER:HB2 | 1.93                     | 0.51              |
| 1:e:156:HIS:HD2  | 1:e:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:e:357:GLN:HE22 | 1:e:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:i:273:GLN:HB2  | 1:i:279:SER:HB2 | 1.93                     | 0.51              |
| 1:l:156:HIS:HD2  | 1:l:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:m:302:ALA:C    | 1:m:314:SER:HB2 | 2.36                     | 0.51              |
| 1:t:302:ALA:C    | 1:t:314:SER:HB2 | 2.36                     | 0.51              |
| 1:u:302:ALA:C    | 1:u:314:SER:HB2 | 2.36                     | 0.51              |
| 1:w:273:GLN:HB2  | 1:w:279:SER:HB2 | 1.93                     | 0.51              |
| 1:4:273:GLN:HB2  | 1:4:279:SER:HB2 | 1.93                     | 0.51              |
| 1:5:156:HIS:HD2  | 1:5:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:5:273:GLN:HB2  | 1:5:279:SER:HB2 | 1.93                     | 0.51              |
| 1:7:156:HIS:HD2  | 1:7:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:A:302:ALA:C    | 1:A:314:SER:HB2 | 2.36                     | 0.51              |
| 1:G:302:ALA:C    | 1:G:314:SER:HB2 | 2.36                     | 0.51              |
| 1:H:156:HIS:HD2  | 1:H:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:N:357:GLN:HE22 | 1:N:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:O:156:HIS:HD2  | 1:O:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:U:273:GLN:HB2  | 1:U:279:SER:HB2 | 1.93                     | 0.51              |
| 1:W:302:ALA:C    | 1:W:314:SER:HB2 | 2.36                     | 0.51              |
| 1:b:302:ALA:C    | 1:b:314:SER:HB2 | 2.36                     | 0.51              |
| 1:h:156:HIS:HD2  | 1:h:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:i:357:GLN:HE22 | 1:i:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:n:273:GLN:HB2  | 1:n:279:SER:HB2 | 1.93                     | 0.51              |
| 1:p:156:HIS:HD2  | 1:p:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:u:406:ARG:HB2  | 1:u:531:LYS:HZ1 | 1.75                     | 0.51              |
| 1:v:302:ALA:C    | 1:v:314:SER:HB2 | 2.36                     | 0.51              |
| 1:3:302:ALA:C    | 1:3:314:SER:HB2 | 2.36                     | 0.51              |
| 1:6:302:ALA:C    | 1:6:314:SER:HB2 | 2.36                     | 0.51              |
| 1:I:357:GLN:HE22 | 1:I:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:J:390:TYR:HE2  | 1:L:331:ALA:HB2 | 1.75                     | 0.51              |
| 1:P:273:GLN:HB2  | 1:P:279:SER:HB2 | 1.93                     | 0.51              |
| 1:U:156:HIS:HD2  | 1:U:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:V:273:GLN:HB2  | 1:V:279:SER:HB2 | 1.93                     | 0.51              |
| 1:Y:406:ARG:HB2  | 1:Y:531:LYS:HZ1 | 1.75                     | 0.51              |
| 1:j:302:ALA:C    | 1:j:314:SER:HB2 | 2.36                     | 0.51              |
| 1:o:156:HIS:HD2  | 1:o:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:p:273:GLN:HB2  | 1:p:279:SER:HB2 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:p:357:GLN:HE22 | 1:p:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:q:273:GLN:HB2  | 1:q:279:SER:HB2 | 1.93                     | 0.51              |
| 1:q:357:GLN:HE22 | 1:q:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:s:273:GLN:HB2  | 1:s:279:SER:HB2 | 1.93                     | 0.51              |
| 1:1:357:GLN:HE22 | 1:1:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:3:406:ARG:HB2  | 1:3:531:LYS:HZ1 | 1.75                     | 0.51              |
| 1:4:357:GLN:HE22 | 1:4:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:B:357:GLN:HE22 | 1:B:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:C:156:HIS:HD2  | 1:C:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:D:302:ALA:C    | 1:D:314:SER:HB2 | 2.36                     | 0.51              |
| 1:L:156:HIS:HD2  | 1:L:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:Q:357:GLN:HE22 | 1:Q:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:R:273:GLN:HB2  | 1:R:279:SER:HB2 | 1.93                     | 0.51              |
| 1:T:273:GLN:HB2  | 1:T:279:SER:HB2 | 1.93                     | 0.51              |
| 1:T:357:GLN:HE22 | 1:T:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:X:156:HIS:HD2  | 1:X:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:f:302:ALA:C    | 1:f:314:SER:HB2 | 2.36                     | 0.51              |
| 1:g:156:HIS:HD2  | 1:g:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:j:273:GLN:HB2  | 1:j:279:SER:HB2 | 1.93                     | 0.51              |
| 1:s:156:HIS:HD2  | 1:s:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:x:357:GLN:HE22 | 1:x:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:6:156:HIS:HD2  | 1:6:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:8:357:GLN:HE22 | 1:8:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:D:273:GLN:HB2  | 1:D:279:SER:HB2 | 1.93                     | 0.51              |
| 1:L:136:LYS:NZ   | 1:L:149:ASN:OD1 | 2.37                     | 0.51              |
| 1:L:273:GLN:HB2  | 1:L:279:SER:HB2 | 1.93                     | 0.51              |
| 1:L:357:GLN:HE22 | 1:L:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:R:357:GLN:HE22 | 1:R:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:V:357:GLN:HE22 | 1:V:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:W:156:HIS:HD2  | 1:W:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:k:273:GLN:HB2  | 1:k:279:SER:HB2 | 1.93                     | 0.51              |
| 1:k:302:ALA:C    | 1:k:314:SER:HB2 | 2.36                     | 0.51              |
| 1:m:273:GLN:HB2  | 1:m:279:SER:HB2 | 1.93                     | 0.51              |
| 1:m:357:GLN:HE22 | 1:m:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:z:136:LYS:NZ   | 1:z:149:ASN:OD1 | 2.37                     | 0.51              |
| 1:z:156:HIS:HD2  | 1:z:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:z:273:GLN:HB2  | 1:z:279:SER:HB2 | 1.93                     | 0.51              |
| 1:z:357:GLN:HE22 | 1:z:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:3:273:GLN:HB2  | 1:3:279:SER:HB2 | 1.93                     | 0.51              |
| 1:H:204:ASP:OD1  | 1:H:205:ALA:N   | 2.44                     | 0.51              |
| 1:R:174:GLU:OE1  | 1:R:359:PRO:HG3 | 2.11                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:V:302:ALA:C    | 1:V:314:SER:HB2 | 2.36                     | 0.51              |
| 1:X:273:GLN:HB2  | 1:X:279:SER:HB2 | 1.93                     | 0.51              |
| 1:Z:357:GLN:HE22 | 1:Z:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:d:302:ALA:C    | 1:d:314:SER:HB2 | 2.36                     | 0.51              |
| 1:g:302:ALA:C    | 1:g:314:SER:HB2 | 2.36                     | 0.51              |
| 1:i:302:ALA:C    | 1:i:314:SER:HB2 | 2.36                     | 0.51              |
| 1:o:273:GLN:HB2  | 1:o:279:SER:HB2 | 1.93                     | 0.51              |
| 1:p:302:ALA:C    | 1:p:314:SER:HB2 | 2.36                     | 0.51              |
| 1:q:174:GLU:OE1  | 1:q:359:PRO:HG3 | 2.11                     | 0.51              |
| 1:u:357:GLN:HE22 | 1:u:412:GLU:HG2 | 1.75                     | 0.51              |
| 1:3:156:HIS:HD2  | 1:3:226:HIS:CD2 | 2.28                     | 0.51              |
| 1:5:204:ASP:OD1  | 1:5:205:ALA:N   | 2.44                     | 0.51              |
| 1:A:273:GLN:HB2  | 1:A:279:SER:HB2 | 1.93                     | 0.50              |
| 1:C:357:GLN:HE22 | 1:C:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:D:156:HIS:HD2  | 1:D:226:HIS:CD2 | 2.28                     | 0.50              |
| 1:E:174:GLU:OE1  | 1:E:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:E:204:ASP:OD1  | 1:E:205:ALA:N   | 2.45                     | 0.50              |
| 1:F:491:ARG:O    | 1:F:492:ARG:NH1 | 2.40                     | 0.50              |
| 1:G:204:ASP:OD1  | 1:G:205:ALA:N   | 2.45                     | 0.50              |
| 1:M:174:GLU:OE1  | 1:M:359:PRO:HG3 | 2.11                     | 0.50              |
| 1:N:302:ALA:C    | 1:N:314:SER:HB2 | 2.36                     | 0.50              |
| 1:Y:174:GLU:OE1  | 1:Y:359:PRO:HG3 | 2.11                     | 0.50              |
| 1:a:156:HIS:HD2  | 1:a:226:HIS:CD2 | 2.28                     | 0.50              |
| 1:b:204:ASP:OD1  | 1:b:205:ALA:N   | 2.45                     | 0.50              |
| 1:d:357:GLN:HE22 | 1:d:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:e:204:ASP:OD1  | 1:e:205:ALA:N   | 2.45                     | 0.50              |
| 1:f:204:ASP:OD1  | 1:f:205:ALA:N   | 2.45                     | 0.50              |
| 1:h:174:GLU:OE1  | 1:h:359:PRO:HG3 | 2.11                     | 0.50              |
| 1:h:302:ALA:C    | 1:h:314:SER:HB2 | 2.36                     | 0.50              |
| 1:k:156:HIS:HD2  | 1:k:226:HIS:CD2 | 2.28                     | 0.50              |
| 1:n:357:GLN:HE22 | 1:n:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:v:273:GLN:HB2  | 1:v:279:SER:HB2 | 1.93                     | 0.50              |
| 1:w:174:GLU:OE1  | 1:w:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:y:491:ARG:O    | 1:y:492:ARG:NH1 | 2.40                     | 0.50              |
| 1:2:156:HIS:HD2  | 1:2:226:HIS:CD2 | 2.28                     | 0.50              |
| 1:8:491:ARG:O    | 1:8:492:ARG:NH1 | 2.40                     | 0.50              |
| 1:A:357:GLN:HE22 | 1:A:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:C:204:ASP:OD1  | 1:C:205:ALA:N   | 2.45                     | 0.50              |
| 1:C:302:ALA:C    | 1:C:314:SER:HB2 | 2.36                     | 0.50              |
| 1:G:136:LYS:NZ   | 1:G:149:ASN:OD1 | 2.37                     | 0.50              |
| 1:G:273:GLN:HB2  | 1:G:279:SER:HB2 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:H:174:GLU:OE1  | 1:H:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:I:174:GLU:OE1  | 1:I:359:PRO:HG3 | 2.11                     | 0.50              |
| 1:M:273:GLN:HB2  | 1:M:279:SER:HB2 | 1.93                     | 0.50              |
| 1:M:302:ALA:C    | 1:M:314:SER:HB2 | 2.36                     | 0.50              |
| 1:P:136:LYS:NZ   | 1:P:149:ASN:OD1 | 2.37                     | 0.50              |
| 1:P:156:HIS:HD2  | 1:P:226:HIS:CD2 | 2.28                     | 0.50              |
| 1:S:357:GLN:HE22 | 1:S:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:T:174:GLU:OE1  | 1:T:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:a:273:GLN:HB2  | 1:a:279:SER:HB2 | 1.93                     | 0.50              |
| 1:c:204:ASP:OD1  | 1:c:205:ALA:N   | 2.45                     | 0.50              |
| 1:g:357:GLN:HE22 | 1:g:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:j:136:LYS:NZ   | 1:j:149:ASN:OD1 | 2.37                     | 0.50              |
| 1:l:302:ALA:C    | 1:l:314:SER:HB2 | 2.36                     | 0.50              |
| 1:m:174:GLU:OE1  | 1:m:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:n:302:ALA:C    | 1:n:314:SER:HB2 | 2.36                     | 0.50              |
| 1:t:204:ASP:OD1  | 1:t:205:ALA:N   | 2.45                     | 0.50              |
| 1:t:273:GLN:HB2  | 1:t:279:SER:HB2 | 1.93                     | 0.50              |
| 1:u:273:GLN:HB2  | 1:u:279:SER:HB2 | 1.93                     | 0.50              |
| 1:v:357:GLN:HE22 | 1:v:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:w:204:ASP:OD1  | 1:w:205:ALA:N   | 2.45                     | 0.50              |
| 1:5:174:GLU:OE1  | 1:5:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:7:174:GLU:OE1  | 1:7:359:PRO:HG3 | 2.11                     | 0.50              |
| 1:J:156:HIS:HD2  | 1:J:226:HIS:CD2 | 2.28                     | 0.50              |
| 1:K:174:GLU:OE1  | 1:K:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:N:204:ASP:OD1  | 1:N:205:ALA:N   | 2.45                     | 0.50              |
| 1:O:174:GLU:OE1  | 1:O:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:O:302:ALA:C    | 1:O:314:SER:HB2 | 2.36                     | 0.50              |
| 1:Q:302:ALA:C    | 1:Q:314:SER:HB2 | 2.36                     | 0.50              |
| 1:U:204:ASP:OD1  | 1:U:205:ALA:N   | 2.45                     | 0.50              |
| 1:V:204:ASP:OD1  | 1:V:205:ALA:N   | 2.45                     | 0.50              |
| 1:a:357:GLN:HE22 | 1:a:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:a:406:ARG:HB2  | 1:a:531:LYS:HZ1 | 1.76                     | 0.50              |
| 1:g:204:ASP:OD1  | 1:g:205:ALA:N   | 2.45                     | 0.50              |
| 1:h:273:GLN:HB2  | 1:h:279:SER:HB2 | 1.93                     | 0.50              |
| 1:j:156:HIS:HD2  | 1:j:226:HIS:CD2 | 2.28                     | 0.50              |
| 1:l:174:GLU:OE1  | 1:l:359:PRO:HG3 | 2.12                     | 0.50              |
| 1:r:357:GLN:HE22 | 1:r:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:1:204:ASP:OD1  | 1:1:205:ALA:N   | 2.44                     | 0.50              |
| 1:3:357:GLN:HE22 | 1:3:412:GLU:HG2 | 1.75                     | 0.50              |
| 1:6:204:ASP:OD1  | 1:6:205:ALA:N   | 2.44                     | 0.50              |
| 1:B:204:ASP:OD1  | 1:B:205:ALA:N   | 2.45                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:302:ALA:C    | 1:B:314:SER:HB2  | 2.36                     | 0.50              |
| 1:G:156:HIS:HD2  | 1:G:226:HIS:CD2  | 2.28                     | 0.50              |
| 1:I:273:GLN:HB2  | 1:I:279:SER:HB2  | 1.93                     | 0.50              |
| 1:O:273:GLN:HB2  | 1:O:279:SER:HB2  | 1.93                     | 0.50              |
| 1:Q:174:GLU:OE1  | 1:Q:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:S:204:ASP:OD1  | 1:S:205:ALA:N    | 2.45                     | 0.50              |
| 1:U:174:GLU:OE1  | 1:U:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:W:204:ASP:OD1  | 1:W:205:ALA:N    | 2.44                     | 0.50              |
| 1:Z:273:GLN:HB2  | 1:Z:279:SER:HB2  | 1.93                     | 0.50              |
| 1:Z:491:ARG:O    | 1:Z:492:ARG:NH1  | 2.40                     | 0.50              |
| 1:i:204:ASP:OD1  | 1:i:205:ALA:N    | 2.45                     | 0.50              |
| 1:k:174:GLU:OE1  | 1:k:359:PRO:HG3  | 2.11                     | 0.50              |
| 1:l:273:GLN:HB2  | 1:l:279:SER:HB2  | 1.93                     | 0.50              |
| 1:p:204:ASP:OD1  | 1:p:205:ALA:N    | 2.45                     | 0.50              |
| 1:r:302:ALA:C    | 1:r:314:SER:HB2  | 2.36                     | 0.50              |
| 1:s:204:ASP:OD1  | 1:s:205:ALA:N    | 2.45                     | 0.50              |
| 1:t:156:HIS:HD2  | 1:t:226:HIS:CD2  | 2.28                     | 0.50              |
| 1:u:174:GLU:OE1  | 1:u:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:x:174:GLU:OE1  | 1:x:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:y:204:ASP:OD1  | 1:y:205:ALA:N    | 2.45                     | 0.50              |
| 1:1:302:ALA:C    | 1:1:314:SER:HB2  | 2.36                     | 0.50              |
| 1:4:174:GLU:OE1  | 1:4:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:8:273:GLN:HB2  | 1:8:279:SER:HB2  | 1.93                     | 0.50              |
| 1:F:204:ASP:OD1  | 1:F:205:ALA:N    | 2.45                     | 0.50              |
| 1:F:357:GLN:HE22 | 1:F:412:GLU:HG2  | 1.75                     | 0.50              |
| 1:S:273:GLN:HB2  | 1:S:279:SER:HB2  | 1.93                     | 0.50              |
| 1:S:302:ALA:C    | 1:S:314:SER:HB2  | 2.36                     | 0.50              |
| 1:Y:491:ARG:O    | 1:Y:492:ARG:NH1  | 2.40                     | 0.50              |
| 1:a:204:ASP:OD1  | 1:a:205:ALA:N    | 2.45                     | 0.50              |
| 1:a:387:GLN:HA   | 1:8:305:VAL:HG22 | 1.94                     | 0.50              |
| 1:j:204:ASP:OD1  | 1:j:205:ALA:N    | 2.44                     | 0.50              |
| 1:m:241:PHE:HB3  | 1:m:243:CYS:SG   | 2.52                     | 0.50              |
| 1:n:204:ASP:OD1  | 1:n:205:ALA:N    | 2.45                     | 0.50              |
| 1:r:204:ASP:OD1  | 1:r:205:ALA:N    | 2.45                     | 0.50              |
| 1:r:273:GLN:HB2  | 1:r:279:SER:HB2  | 1.93                     | 0.50              |
| 1:s:174:GLU:OE1  | 1:s:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:s:241:PHE:HB3  | 1:s:243:CYS:SG   | 2.52                     | 0.50              |
| 1:v:204:ASP:OD1  | 1:v:205:ALA:N    | 2.45                     | 0.50              |
| 1:x:204:ASP:OD1  | 1:x:205:ALA:N    | 2.45                     | 0.50              |
| 1:x:302:ALA:C    | 1:x:314:SER:HB2  | 2.36                     | 0.50              |
| 1:y:357:GLN:HE22 | 1:y:412:GLU:HG2  | 1.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:163:HIS:HB2  | 1:A:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:A:204:ASP:OD1  | 1:A:205:ALA:N    | 2.45                     | 0.50              |
| 1:D:174:GLU:OE1  | 1:D:359:PRO:HG3  | 2.11                     | 0.50              |
| 1:D:241:PHE:HB3  | 1:D:243:CYS:SG   | 2.52                     | 0.50              |
| 1:D:406:ARG:HB2  | 1:D:531:LYS:HZ1  | 1.75                     | 0.50              |
| 1:G:241:PHE:HB3  | 1:G:243:CYS:SG   | 2.52                     | 0.50              |
| 1:P:204:ASP:OD1  | 1:P:205:ALA:N    | 2.44                     | 0.50              |
| 1:Q:204:ASP:OD1  | 1:Q:205:ALA:N    | 2.45                     | 0.50              |
| 1:T:241:PHE:HB3  | 1:T:243:CYS:SG   | 2.52                     | 0.50              |
| 1:U:241:PHE:HB3  | 1:U:243:CYS:SG   | 2.52                     | 0.50              |
| 1:X:204:ASP:OD1  | 1:X:205:ALA:N    | 2.45                     | 0.50              |
| 1:Z:305:VAL:HG22 | 1:3:387:GLN:HA   | 1.94                     | 0.50              |
| 1:a:174:GLU:OE1  | 1:a:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:a:241:PHE:HB3  | 1:a:243:CYS:SG   | 2.52                     | 0.50              |
| 1:c:163:HIS:HB2  | 1:c:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:c:241:PHE:HB3  | 1:c:243:CYS:SG   | 2.52                     | 0.50              |
| 1:c:273:GLN:HB2  | 1:c:279:SER:HB2  | 1.93                     | 0.50              |
| 1:d:204:ASP:OD1  | 1:d:205:ALA:N    | 2.45                     | 0.50              |
| 1:e:163:HIS:HB2  | 1:e:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:e:241:PHE:HB3  | 1:e:243:CYS:SG   | 2.52                     | 0.50              |
| 1:e:273:GLN:HB2  | 1:e:279:SER:HB2  | 1.93                     | 0.50              |
| 1:f:163:HIS:HB2  | 1:f:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:j:241:PHE:HB3  | 1:j:243:CYS:SG   | 2.52                     | 0.50              |
| 1:k:241:PHE:HB3  | 1:k:243:CYS:SG   | 2.52                     | 0.50              |
| 1:k:406:ARG:HB2  | 1:k:531:LYS:HZ1  | 1.75                     | 0.50              |
| 1:m:204:ASP:OD1  | 1:m:205:ALA:N    | 2.45                     | 0.50              |
| 1:t:136:LYS:NZ   | 1:t:149:ASN:OD1  | 2.37                     | 0.50              |
| 1:t:174:GLU:OE1  | 1:t:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:t:241:PHE:HB3  | 1:t:243:CYS:SG   | 2.52                     | 0.50              |
| 1:z:204:ASP:OD1  | 1:z:205:ALA:N    | 2.45                     | 0.50              |
| 1:2:174:GLU:OE1  | 1:2:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:3:241:PHE:HB3  | 1:3:243:CYS:SG   | 2.52                     | 0.50              |
| 1:4:204:ASP:OD1  | 1:4:205:ALA:N    | 2.45                     | 0.50              |
| 1:G:174:GLU:OE1  | 1:G:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:K:204:ASP:OD1  | 1:K:205:ALA:N    | 2.44                     | 0.50              |
| 1:L:204:ASP:OD1  | 1:L:205:ALA:N    | 2.45                     | 0.50              |
| 1:O:204:ASP:OD1  | 1:O:205:ALA:N    | 2.45                     | 0.50              |
| 1:P:241:PHE:HB3  | 1:P:243:CYS:SG   | 2.52                     | 0.50              |
| 1:R:331:ALA:HB2  | 1:U:390:TYR:HE2  | 1.76                     | 0.50              |
| 1:T:204:ASP:OD1  | 1:T:205:ALA:N    | 2.45                     | 0.50              |
| 1:W:241:PHE:HB3  | 1:W:243:CYS:SG   | 2.52                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:241:PHE:HB3  | 1:Y:243:CYS:SG   | 2.52                     | 0.50              |
| 1:Y:273:GLN:HB2  | 1:Y:279:SER:HB2  | 1.93                     | 0.50              |
| 1:Z:174:GLU:OE1  | 1:Z:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:Z:204:ASP:OD1  | 1:Z:205:ALA:N    | 2.45                     | 0.50              |
| 1:b:163:HIS:HB2  | 1:b:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:o:174:GLU:OE1  | 1:o:359:PRO:HG3  | 2.11                     | 0.50              |
| 1:o:204:ASP:OD1  | 1:o:205:ALA:N    | 2.45                     | 0.50              |
| 1:q:331:ALA:HB2  | 1:s:390:TYR:HE2  | 1.76                     | 0.50              |
| 1:v:163:HIS:HB2  | 1:v:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:2:241:PHE:HB3  | 1:2:243:CYS:SG   | 2.52                     | 0.50              |
| 1:2:357:GLN:HE22 | 1:2:412:GLU:HG2  | 1.75                     | 0.50              |
| 1:3:204:ASP:OD1  | 1:3:205:ALA:N    | 2.45                     | 0.50              |
| 1:A:241:PHE:HB3  | 1:A:243:CYS:SG   | 2.52                     | 0.50              |
| 1:D:204:ASP:OD1  | 1:D:205:ALA:N    | 2.44                     | 0.50              |
| 1:I:241:PHE:HB3  | 1:I:243:CYS:SG   | 2.52                     | 0.50              |
| 1:I:406:ARG:HB2  | 1:I:531:LYS:HZ1  | 1.76                     | 0.50              |
| 1:J:163:HIS:HB2  | 1:J:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:J:174:GLU:OE1  | 1:J:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:J:241:PHE:HB3  | 1:J:243:CYS:SG   | 2.52                     | 0.50              |
| 1:K:163:HIS:HB2  | 1:K:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:X:174:GLU:OE1  | 1:X:359:PRO:HG3  | 2.11                     | 0.50              |
| 1:b:174:GLU:OE1  | 1:b:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:f:174:GLU:OE1  | 1:f:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:k:204:ASP:OD1  | 1:k:205:ALA:N    | 2.44                     | 0.50              |
| 1:l:204:ASP:OD1  | 1:l:205:ALA:N    | 2.45                     | 0.50              |
| 1:o:241:PHE:HB3  | 1:o:243:CYS:SG   | 2.52                     | 0.50              |
| 1:t:305:VAL:HG22 | 1:v:387:GLN:HA   | 1.93                     | 0.50              |
| 1:u:241:PHE:HB3  | 1:u:243:CYS:SG   | 2.52                     | 0.50              |
| 1:v:241:PHE:HB3  | 1:v:243:CYS:SG   | 2.52                     | 0.50              |
| 1:z:305:VAL:HG22 | 1:2:387:GLN:HA   | 1.94                     | 0.50              |
| 1:3:174:GLU:OE1  | 1:3:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:6:241:PHE:HB3  | 1:6:243:CYS:SG   | 2.52                     | 0.50              |
| 1:7:273:GLN:HB2  | 1:7:279:SER:HB2  | 1.93                     | 0.50              |
| 1:8:204:ASP:OD1  | 1:8:205:ALA:N    | 2.45                     | 0.50              |
| 1:A:387:GLN:HA   | 1:G:305:VAL:HG22 | 1.93                     | 0.50              |
| 1:F:241:PHE:HB3  | 1:F:243:CYS:SG   | 2.52                     | 0.50              |
| 1:F:273:GLN:HB2  | 1:F:279:SER:HB2  | 1.93                     | 0.50              |
| 1:H:163:HIS:HB2  | 1:H:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:H:331:ALA:HB2  | 1:Y:390:TYR:HE2  | 1.77                     | 0.50              |
| 1:J:204:ASP:OD1  | 1:J:205:ALA:N    | 2.45                     | 0.50              |
| 1:J:357:GLN:HE22 | 1:J:412:GLU:HG2  | 1.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:88:ARG:O     | 1:P:194:PRO:HD2  | 2.12                     | 0.50              |
| 1:Q:136:LYS:NZ   | 1:Q:149:ASN:OD1  | 2.37                     | 0.50              |
| 1:S:241:PHE:HB3  | 1:S:243:CYS:SG   | 2.52                     | 0.50              |
| 1:X:241:PHE:HB3  | 1:X:243:CYS:SG   | 2.52                     | 0.50              |
| 1:Y:204:ASP:OD1  | 1:Y:205:ALA:N    | 2.45                     | 0.50              |
| 1:Y:302:ALA:C    | 1:Y:314:SER:HB2  | 2.36                     | 0.50              |
| 1:Z:88:ARG:O     | 1:Z:194:PRO:HD2  | 2.12                     | 0.50              |
| 1:Z:163:HIS:HB2  | 1:Z:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:b:88:ARG:O     | 1:b:194:PRO:HD2  | 2.12                     | 0.50              |
| 1:i:88:ARG:O     | 1:i:194:PRO:HD2  | 2.12                     | 0.50              |
| 1:i:390:TYR:HE2  | 1:j:331:ALA:HB2  | 1.77                     | 0.50              |
| 1:j:88:ARG:O     | 1:j:194:PRO:HD2  | 2.12                     | 0.50              |
| 1:q:302:ALA:C    | 1:q:314:SER:HB2  | 2.36                     | 0.50              |
| 1:r:163:HIS:HB2  | 1:r:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:x:136:LYS:NZ   | 1:x:149:ASN:OD1  | 2.37                     | 0.50              |
| 1:y:241:PHE:HB3  | 1:y:243:CYS:SG   | 2.52                     | 0.50              |
| 1:4:163:HIS:HB2  | 1:4:421:ARG:HH22 | 1.77                     | 0.50              |
| 1:4:241:PHE:HB3  | 1:4:243:CYS:SG   | 2.52                     | 0.50              |
| 1:5:331:ALA:HB2  | 1:7:390:TYR:HE2  | 1.77                     | 0.50              |
| 1:7:204:ASP:OD1  | 1:7:205:ALA:N    | 2.45                     | 0.50              |
| 1:7:241:PHE:HB3  | 1:7:243:CYS:SG   | 2.52                     | 0.50              |
| 1:7:302:ALA:C    | 1:7:314:SER:HB2  | 2.36                     | 0.50              |
| 1:8:88:ARG:O     | 1:8:194:PRO:HD2  | 2.12                     | 0.50              |
| 1:8:174:GLU:OE1  | 1:8:359:PRO:HG3  | 2.12                     | 0.50              |
| 1:8:241:PHE:HB3  | 1:8:243:CYS:SG   | 2.52                     | 0.50              |
| 1:B:163:HIS:HB2  | 1:B:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:E:88:ARG:O     | 1:E:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:E:163:HIS:HB2  | 1:E:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:F:163:HIS:HB2  | 1:F:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:G:163:HIS:HB2  | 1:G:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:I:88:ARG:O     | 1:I:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:K:241:PHE:HB3  | 1:K:243:CYS:SG   | 2.52                     | 0.49              |
| 1:N:88:ARG:O     | 1:N:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:N:390:TYR:HE2  | 1:P:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:S:163:HIS:HB2  | 1:S:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:S:382:LEU:HD12 | 1:S:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:U:229:LEU:HA   | 1:U:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:V:241:PHE:HB3  | 1:V:243:CYS:SG   | 2.52                     | 0.49              |
| 1:Z:241:PHE:HB3  | 1:Z:243:CYS:SG   | 2.52                     | 0.49              |
| 1:e:229:LEU:HA   | 1:e:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:f:88:ARG:O     | 1:f:194:PRO:HD2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:331:ALA:HB2  | 1:h:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:i:241:PHE:HB3  | 1:i:243:CYS:SG   | 2.52                     | 0.49              |
| 1:i:382:LEU:HD12 | 1:i:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:q:204:ASP:OD1  | 1:q:205:ALA:N    | 2.44                     | 0.49              |
| 1:s:229:LEU:HA   | 1:s:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:t:163:HIS:HB2  | 1:t:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:u:88:ARG:O     | 1:u:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:w:88:ARG:O     | 1:w:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:x:229:LEU:HA   | 1:x:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:1:163:HIS:HB2  | 1:1:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:2:163:HIS:HB2  | 1:2:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:2:204:ASP:OD1  | 1:2:205:ALA:N    | 2.45                     | 0.49              |
| 1:5:163:HIS:HB2  | 1:5:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:8:163:HIS:HB2  | 1:8:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:A:88:ARG:O     | 1:A:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:C:163:HIS:HB2  | 1:C:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:C:331:ALA:HB2  | 1:M:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:D:60:ARG:HG3   | 1:D:177:MET:HG3  | 1.95                     | 0.49              |
| 1:D:229:LEU:HA   | 1:D:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:K:305:VAL:HG22 | 1:8:387:GLN:HA   | 1.94                     | 0.49              |
| 1:K:387:GLN:HA   | 1:a:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:L:88:ARG:O     | 1:L:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:N:382:LEU:HD12 | 1:N:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:O:88:ARG:O     | 1:O:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:Q:163:HIS:HB2  | 1:Q:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:Q:229:LEU:HA   | 1:Q:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:R:163:HIS:HB2  | 1:R:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:R:204:ASP:OD1  | 1:R:205:ALA:N    | 2.44                     | 0.49              |
| 1:R:302:ALA:C    | 1:R:314:SER:HB2  | 2.36                     | 0.49              |
| 1:S:390:TYR:HE2  | 1:U:331:ALA:HB2  | 1.76                     | 0.49              |
| 1:T:305:VAL:HG22 | 1:l:387:GLN:HA   | 1.94                     | 0.49              |
| 1:T:372:PRO:HB3  | 1:T:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:V:88:ARG:O     | 1:V:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:W:60:ARG:HG3   | 1:W:177:MET:HG3  | 1.95                     | 0.49              |
| 1:Z:387:GLN:HA   | 1:4:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:c:229:LEU:HA   | 1:c:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:c:331:ALA:HB2  | 1:p:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:g:163:HIS:HB2  | 1:g:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:h:88:ARG:O     | 1:h:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:k:60:ARG:HG3   | 1:k:177:MET:HG3  | 1.95                     | 0.49              |
| 1:k:229:LEU:HA   | 1:k:233:GLU:OE1  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:372:PRO:HB3  | 1:m:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:n:163:HIS:HB2  | 1:n:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:p:241:PHE:HB3  | 1:p:243:CYS:SG   | 2.52                     | 0.49              |
| 1:q:387:GLN:HA   | 1:r:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:r:241:PHE:HB3  | 1:r:243:CYS:SG   | 2.52                     | 0.49              |
| 1:r:382:LEU:HD12 | 1:r:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:t:88:ARG:O     | 1:t:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:u:204:ASP:OD1  | 1:u:205:ALA:N    | 2.45                     | 0.49              |
| 1:u:382:LEU:HD12 | 1:u:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:v:88:ARG:O     | 1:v:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:v:382:LEU:HD12 | 1:v:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:w:163:HIS:HB2  | 1:w:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:w:331:ALA:HB2  | 1:y:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:w:372:PRO:HB3  | 1:w:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:x:163:HIS:HB2  | 1:x:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:y:163:HIS:HB2  | 1:y:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:y:273:GLN:HB2  | 1:y:279:SER:HB2  | 1.93                     | 0.49              |
| 1:z:372:PRO:HB3  | 1:z:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:1:273:GLN:HB2  | 1:1:279:SER:HB2  | 1.93                     | 0.49              |
| 1:3:305:VAL:HG22 | 1:4:387:GLN:HA   | 1.94                     | 0.49              |
| 1:6:60:ARG:HG3   | 1:6:177:MET:HG3  | 1.95                     | 0.49              |
| 1:A:382:LEU:HD12 | 1:A:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:B:273:GLN:HB2  | 1:B:279:SER:HB2  | 1.93                     | 0.49              |
| 1:C:88:ARG:O     | 1:C:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:C:174:GLU:OE1  | 1:C:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:C:273:GLN:HB2  | 1:C:279:SER:HB2  | 1.93                     | 0.49              |
| 1:E:331:ALA:HB2  | 1:F:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:E:372:PRO:HB3  | 1:E:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:F:136:LYS:NZ   | 1:F:149:ASN:OD1  | 2.37                     | 0.49              |
| 1:G:88:ARG:O     | 1:G:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:G:387:GLN:HA   | 1:I:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:I:204:ASP:OD1  | 1:I:205:ALA:N    | 2.45                     | 0.49              |
| 1:I:372:PRO:HB3  | 1:I:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:I:382:LEU:HD12 | 1:I:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:L:60:ARG:HG3   | 1:L:177:MET:HG3  | 1.95                     | 0.49              |
| 1:L:372:PRO:HB3  | 1:L:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:L:382:LEU:HD12 | 1:L:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:M:88:ARG:O     | 1:M:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:M:382:LEU:HD12 | 1:M:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:N:174:GLU:OE1  | 1:N:359:PRO:HG3  | 2.11                     | 0.49              |
| 1:N:241:PHE:HB3  | 1:N:243:CYS:SG   | 2.52                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:387:GLN:HA   | 1:m:305:VAL:HG22 | 1.95                     | 0.49              |
| 1:P:174:GLU:OE1  | 1:P:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:P:229:LEU:HA   | 1:P:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:Q:382:LEU:HD12 | 1:Q:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:R:387:GLN:HA   | 1:S:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:T:88:ARG:O     | 1:T:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:V:174:GLU:OE1  | 1:V:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:V:387:GLN:HA   | 1:e:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:V:390:TYR:HE2  | 1:e:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:W:174:GLU:OE1  | 1:W:359:PRO:HG3  | 2.11                     | 0.49              |
| 1:Y:60:ARG:HG3   | 1:Y:177:MET:HG3  | 1.95                     | 0.49              |
| 1:Z:331:ALA:HB2  | 1:3:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:a:390:TYR:HE2  | 1:8:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:b:60:ARG:HG3   | 1:b:177:MET:HG3  | 1.95                     | 0.49              |
| 1:c:174:GLU:OE1  | 1:c:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:c:305:VAL:HG22 | 1:p:387:GLN:HA   | 1.94                     | 0.49              |
| 1:d:229:LEU:HA   | 1:d:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:e:174:GLU:OE1  | 1:e:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:g:88:ARG:O     | 1:g:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:g:174:GLU:OE1  | 1:g:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:g:273:GLN:HB2  | 1:g:279:SER:HB2  | 1.93                     | 0.49              |
| 1:h:382:LEU:HD12 | 1:h:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:j:229:LEU:HA   | 1:j:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:l:88:ARG:O     | 1:l:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:m:88:ARG:O     | 1:m:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:m:163:HIS:HB2  | 1:m:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:n:60:ARG:HG3   | 1:n:177:MET:HG3  | 1.95                     | 0.49              |
| 1:n:229:LEU:HA   | 1:n:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:o:387:GLN:HA   | 1:p:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:p:88:ARG:O     | 1:p:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:q:163:HIS:HB2  | 1:q:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:t:387:GLN:HA   | 1:u:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:z:60:ARG:HG3   | 1:z:177:MET:HG3  | 1.95                     | 0.49              |
| 1:z:88:ARG:O     | 1:z:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:z:331:ALA:HB2  | 1:2:390:TYR:HE2  | 1.76                     | 0.49              |
| 1:z:382:LEU:HD12 | 1:z:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:6:229:LEU:HA   | 1:6:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:6:273:GLN:HB2  | 1:6:279:SER:HB2  | 1.93                     | 0.49              |
| 1:7:60:ARG:HG3   | 1:7:177:MET:HG3  | 1.95                     | 0.49              |
| 1:8:406:ARG:HB2  | 1:8:531:LYS:HZ1  | 1.76                     | 0.49              |
| 1:A:305:VAL:HG22 | 1:I:387:GLN:HA   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:174:GLU:OE1  | 1:F:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:G:382:LEU:HD12 | 1:G:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:G:390:TYR:HE2  | 1:I:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:H:229:LEU:HA   | 1:H:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:M:229:LEU:HA   | 1:M:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:O:390:TYR:HE2  | 1:m:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:R:305:VAL:HG22 | 1:U:387:GLN:HA   | 1.94                     | 0.49              |
| 1:T:163:HIS:HB2  | 1:T:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:W:229:LEU:HA   | 1:W:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:W:273:GLN:HB2  | 1:W:279:SER:HB2  | 1.93                     | 0.49              |
| 1:Z:382:LEU:HD12 | 1:Z:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:d:60:ARG:HG3   | 1:d:177:MET:HG3  | 1.95                     | 0.49              |
| 1:d:163:HIS:HB2  | 1:d:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:f:60:ARG:HG3   | 1:f:177:MET:HG3  | 1.95                     | 0.49              |
| 1:h:229:LEU:HA   | 1:h:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:i:174:GLU:OE1  | 1:i:359:PRO:HG3  | 2.11                     | 0.49              |
| 1:n:174:GLU:OE1  | 1:n:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:p:174:GLU:OE1  | 1:p:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:q:241:PHE:HB3  | 1:q:243:CYS:SG   | 2.52                     | 0.49              |
| 1:r:60:ARG:HG3   | 1:r:177:MET:HG3  | 1.95                     | 0.49              |
| 1:r:390:TYR:HE2  | 1:s:331:ALA:HB2  | 1.76                     | 0.49              |
| 1:u:372:PRO:HB3  | 1:u:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:x:382:LEU:HD12 | 1:x:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:5:229:LEU:HA   | 1:5:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:6:174:GLU:OE1  | 1:6:359:PRO:HG3  | 2.11                     | 0.49              |
| 1:B:174:GLU:OE1  | 1:B:359:PRO:HG3  | 2.11                     | 0.49              |
| 1:B:229:LEU:HA   | 1:B:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:C:60:ARG:HG3   | 1:C:177:MET:HG3  | 1.95                     | 0.49              |
| 1:C:241:PHE:HB3  | 1:C:243:CYS:SG   | 2.52                     | 0.49              |
| 1:E:241:PHE:HB3  | 1:E:243:CYS:SG   | 2.52                     | 0.49              |
| 1:H:241:PHE:HB3  | 1:H:243:CYS:SG   | 2.52                     | 0.49              |
| 1:I:163:HIS:HB2  | 1:I:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:I:229:LEU:HA   | 1:I:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:K:60:ARG:HG3   | 1:K:177:MET:HG3  | 1.95                     | 0.49              |
| 1:L:163:HIS:HB2  | 1:L:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:L:174:GLU:OE1  | 1:L:359:PRO:HG3  | 2.11                     | 0.49              |
| 1:L:241:PHE:HB3  | 1:L:243:CYS:SG   | 2.52                     | 0.49              |
| 1:M:331:ALA:HB2  | 1:b:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:N:372:PRO:HB3  | 1:N:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:O:60:ARG:HG3   | 1:O:177:MET:HG3  | 1.95                     | 0.49              |
| 1:Q:372:PRO:HB3  | 1:Q:379:ASP:OD2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:241:PHE:HB3  | 1:R:243:CYS:SG   | 2.52                     | 0.49              |
| 1:R:372:PRO:HB3  | 1:R:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:T:331:ALA:HB2  | 1:I:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:a:491:ARG:O    | 1:a:492:ARG:NH1  | 2.40                     | 0.49              |
| 1:d:174:GLU:OE1  | 1:d:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:f:331:ALA:HB2  | 1:g:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:g:60:ARG:HG3   | 1:g:177:MET:HG3  | 1.95                     | 0.49              |
| 1:j:174:GLU:OE1  | 1:j:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:l:60:ARG:HG3   | 1:l:177:MET:HG3  | 1.95                     | 0.49              |
| 1:n:372:PRO:HB3  | 1:n:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:p:372:PRO:HB3  | 1:p:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:q:305:VAL:HG22 | 1:s:387:GLN:HA   | 1.94                     | 0.49              |
| 1:r:88:ARG:O     | 1:r:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:t:382:LEU:HD12 | 1:t:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:t:390:TYR:HE2  | 1:u:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:u:163:HIS:HB2  | 1:u:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:u:387:GLN:HA   | 1:v:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:u:390:TYR:HE2  | 1:v:331:ALA:HB2  | 1.78                     | 0.49              |
| 1:w:241:PHE:HB3  | 1:w:243:CYS:SG   | 2.52                     | 0.49              |
| 1:w:390:TYR:HE2  | 1:x:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:x:241:PHE:HB3  | 1:x:243:CYS:SG   | 2.52                     | 0.49              |
| 1:x:372:PRO:HB3  | 1:x:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:y:174:GLU:OE1  | 1:y:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:z:163:HIS:HB2  | 1:z:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:z:390:TYR:HE2  | 1:1:331:ALA:HB2  | 1.76                     | 0.49              |
| 1:2:273:GLN:HB2  | 1:2:279:SER:HB2  | 1.93                     | 0.49              |
| 1:3:88:ARG:O     | 1:3:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:4:60:ARG:HG3   | 1:4:177:MET:HG3  | 1.95                     | 0.49              |
| 1:5:241:PHE:HB3  | 1:5:243:CYS:SG   | 2.52                     | 0.49              |
| 1:A:331:ALA:HB2  | 1:I:390:TYR:HE2  | 1.78                     | 0.49              |
| 1:C:382:LEU:HD12 | 1:C:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:D:163:HIS:HB2  | 1:D:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:E:390:TYR:HE2  | 1:Q:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:J:88:ARG:O     | 1:J:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:J:338:ASP:HA   | 1:J:339:PRO:C    | 2.38                     | 0.49              |
| 1:J:372:PRO:HB3  | 1:J:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:M:241:PHE:HB3  | 1:M:243:CYS:SG   | 2.52                     | 0.49              |
| 1:O:241:PHE:HB3  | 1:O:243:CYS:SG   | 2.52                     | 0.49              |
| 1:O:338:ASP:HA   | 1:O:339:PRO:C    | 2.38                     | 0.49              |
| 1:P:382:LEU:HD12 | 1:P:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:Q:241:PHE:HB3  | 1:Q:243:CYS:SG   | 2.52                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:273:GLN:HB2  | 1:Q:279:SER:HB2  | 1.93                     | 0.49              |
| 1:R:88:ARG:O     | 1:R:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:S:60:ARG:HG3   | 1:S:177:MET:HG3  | 1.95                     | 0.49              |
| 1:S:88:ARG:O     | 1:S:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:S:372:PRO:HB3  | 1:S:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:V:372:PRO:HB3  | 1:V:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:Y:88:ARG:O     | 1:Y:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:a:88:ARG:O     | 1:a:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:b:372:PRO:HB3  | 1:b:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:c:60:ARG:HG3   | 1:c:177:MET:HG3  | 1.95                     | 0.49              |
| 1:c:372:PRO:HB3  | 1:c:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:d:372:PRO:HB3  | 1:d:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:e:372:PRO:HB3  | 1:e:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:f:372:PRO:HB3  | 1:f:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:g:241:PHE:HB3  | 1:g:243:CYS:SG   | 2.52                     | 0.49              |
| 1:h:241:PHE:HB3  | 1:h:243:CYS:SG   | 2.52                     | 0.49              |
| 1:i:372:PRO:HB3  | 1:i:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:k:163:HIS:HB2  | 1:k:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:l:229:LEU:HA   | 1:l:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:l:241:PHE:HB3  | 1:l:243:CYS:SG   | 2.52                     | 0.49              |
| 1:n:241:PHE:HB3  | 1:n:243:CYS:SG   | 2.52                     | 0.49              |
| 1:o:60:ARG:HG3   | 1:o:177:MET:HG3  | 1.95                     | 0.49              |
| 1:o:88:ARG:O     | 1:o:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:p:163:HIS:HB2  | 1:p:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:p:382:LEU:HD12 | 1:p:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:q:372:PRO:HB3  | 1:q:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:r:372:PRO:HB3  | 1:r:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:x:88:ARG:O     | 1:x:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:z:241:PHE:HB3  | 1:z:243:CYS:SG   | 2.52                     | 0.49              |
| 1:z:387:GLN:HA   | 1:1:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:1:174:GLU:OE1  | 1:1:359:PRO:HG3  | 2.11                     | 0.49              |
| 1:1:229:LEU:HA   | 1:1:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:4:88:ARG:O     | 1:4:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:7:88:ARG:O     | 1:7:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:7:229:LEU:HD22 | 1:7:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:8:382:LEU:HD12 | 1:8:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:B:60:ARG:HG3   | 1:B:177:MET:HG3  | 1.95                     | 0.49              |
| 1:B:241:PHE:HB3  | 1:B:243:CYS:SG   | 2.52                     | 0.49              |
| 1:C:390:TYR:HE2  | 1:b:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:D:331:ALA:HB2  | 1:P:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:F:372:PRO:HB3  | 1:F:379:ASP:OD2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:382:LEU:HD12 | 1:F:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:G:229:LEU:HA   | 1:G:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:G:372:PRO:HB3  | 1:G:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:J:273:GLN:HB2  | 1:J:279:SER:HB2  | 1.93                     | 0.49              |
| 1:M:204:ASP:OD1  | 1:M:205:ALA:N    | 2.45                     | 0.49              |
| 1:N:163:HIS:HB2  | 1:N:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:O:229:LEU:HA   | 1:O:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:Q:60:ARG:HG3   | 1:Q:177:MET:HG3  | 1.95                     | 0.49              |
| 1:Q:88:ARG:O     | 1:Q:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:V:163:HIS:HB2  | 1:V:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:V:305:VAL:HG22 | 1:X:387:GLN:HA   | 1.94                     | 0.49              |
| 1:V:382:LEU:HD12 | 1:V:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:X:88:ARG:O     | 1:X:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:Y:229:LEU:HD22 | 1:Y:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:b:241:PHE:HB3  | 1:b:243:CYS:SG   | 2.52                     | 0.49              |
| 1:c:387:GLN:HA   | 1:o:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:d:241:PHE:HB3  | 1:d:243:CYS:SG   | 2.52                     | 0.49              |
| 1:e:60:ARG:HG3   | 1:e:177:MET:HG3  | 1.95                     | 0.49              |
| 1:f:390:TYR:HE2  | 1:h:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:g:382:LEU:HD12 | 1:g:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:h:204:ASP:OD1  | 1:h:205:ALA:N    | 2.45                     | 0.49              |
| 1:j:390:TYR:HE2  | 1:k:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:n:88:ARG:O     | 1:n:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:q:88:ARG:O     | 1:q:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:r:174:GLU:OE1  | 1:r:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:t:229:LEU:HA   | 1:t:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:u:229:LEU:HA   | 1:u:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:x:60:ARG:HG3   | 1:x:177:MET:HG3  | 1.95                     | 0.49              |
| 1:y:136:LYS:NZ   | 1:y:149:ASN:OD1  | 2.37                     | 0.49              |
| 1:y:382:LEU:HD12 | 1:y:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:z:174:GLU:OE1  | 1:z:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:1:60:ARG:HG3   | 1:1:177:MET:HG3  | 1.95                     | 0.49              |
| 1:1:241:PHE:HB3  | 1:1:243:CYS:SG   | 2.52                     | 0.49              |
| 1:1:390:TYR:HE2  | 1:2:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:2:88:ARG:O     | 1:2:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:2:338:ASP:HA   | 1:2:339:PRO:C    | 2.38                     | 0.49              |
| 1:2:372:PRO:HB3  | 1:2:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:A:229:LEU:HD22 | 1:A:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:A:338:ASP:HA   | 1:A:339:PRO:C    | 2.38                     | 0.49              |
| 1:B:338:ASP:HA   | 1:B:339:PRO:C    | 2.38                     | 0.49              |
| 1:E:338:ASP:HA   | 1:E:339:PRO:C    | 2.38                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:60:ARG:HG3   | 1:F:177:MET:HG3  | 1.95                     | 0.49              |
| 1:F:229:LEU:HD22 | 1:F:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:F:229:LEU:HA   | 1:F:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:G:229:LEU:HD22 | 1:G:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:H:387:GLN:HA   | 1:W:305:VAL:HG22 | 1.95                     | 0.49              |
| 1:K:270:TYR:O    | 1:a:350:GLU:HG2  | 2.13                     | 0.49              |
| 1:O:305:VAL:HG22 | 1:n:387:GLN:HA   | 1.94                     | 0.49              |
| 1:O:331:ALA:HB2  | 1:n:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:R:78:ILE:HD12  | 1:R:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:S:229:LEU:HD22 | 1:S:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:X:60:ARG:HG3   | 1:X:177:MET:HG3  | 1.95                     | 0.49              |
| 1:X:305:VAL:HG22 | 1:e:387:GLN:HA   | 1.94                     | 0.49              |
| 1:Z:229:LEU:HA   | 1:Z:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:a:338:ASP:HA   | 1:a:339:PRO:C    | 2.38                     | 0.49              |
| 1:d:88:ARG:O     | 1:d:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:g:78:ILE:HD12  | 1:g:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:h:60:ARG:HG3   | 1:h:177:MET:HG3  | 1.95                     | 0.49              |
| 1:j:382:LEU:HD12 | 1:j:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:k:88:ARG:O     | 1:k:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:l:229:LEU:HD22 | 1:l:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:l:338:ASP:HA   | 1:l:339:PRO:C    | 2.38                     | 0.49              |
| 1:o:78:ILE:HD12  | 1:o:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:r:229:LEU:HD22 | 1:r:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:t:372:PRO:HB3  | 1:t:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:v:229:LEU:HD22 | 1:v:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:v:338:ASP:HA   | 1:v:339:PRO:C    | 2.38                     | 0.49              |
| 1:w:305:VAL:HG22 | 1:y:387:GLN:HA   | 1.93                     | 0.49              |
| 1:w:338:ASP:HA   | 1:w:339:PRO:C    | 2.38                     | 0.49              |
| 1:x:273:GLN:HB2  | 1:x:279:SER:HB2  | 1.93                     | 0.49              |
| 1:x:338:ASP:HA   | 1:x:339:PRO:C    | 2.38                     | 0.49              |
| 1:y:60:ARG:HG3   | 1:y:177:MET:HG3  | 1.95                     | 0.49              |
| 1:y:229:LEU:HA   | 1:y:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:y:229:LEU:HD22 | 1:y:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:y:372:PRO:HB3  | 1:y:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:1:78:ILE:HD12  | 1:1:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:3:350:GLU:HG2  | 1:4:270:TYR:O    | 2.13                     | 0.49              |
| 1:5:60:ARG:HG3   | 1:5:177:MET:HG3  | 1.95                     | 0.49              |
| 1:5:372:PRO:HB3  | 1:5:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:5:387:GLN:HA   | 1:6:305:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:390:TYR:HE2  | 1:G:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:B:229:LEU:HD22 | 1:B:233:GLU:HB3  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:387:GLN:HA   | 1:b:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:D:88:ARG:O     | 1:D:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:E:491:ARG:O    | 1:E:492:ARG:NH1  | 2.40                     | 0.49              |
| 1:H:60:ARG:HG3   | 1:H:177:MET:HG3  | 1.95                     | 0.49              |
| 1:H:78:ILE:HD12  | 1:H:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:H:372:PRO:HB3  | 1:H:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:K:78:ILE:HD12  | 1:K:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:K:88:ARG:O     | 1:K:194:PRO:HD2  | 2.12                     | 0.49              |
| 1:M:60:ARG:HG3   | 1:M:177:MET:HG3  | 1.95                     | 0.49              |
| 1:M:163:HIS:HB2  | 1:M:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:O:229:LEU:HD22 | 1:O:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:P:78:ILE:HD12  | 1:P:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:P:163:HIS:HB2  | 1:P:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:Q:338:ASP:HA   | 1:Q:339:PRO:C    | 2.38                     | 0.49              |
| 1:R:338:ASP:HA   | 1:R:339:PRO:C    | 2.38                     | 0.49              |
| 1:S:174:GLU:OE1  | 1:S:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:T:60:ARG:HG3   | 1:T:177:MET:HG3  | 1.95                     | 0.49              |
| 1:T:229:LEU:HA   | 1:T:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:T:270:TYR:O    | 1:d:350:GLU:HG2  | 2.13                     | 0.49              |
| 1:U:179:GLU:OE2  | 1:U:411:ARG:NH1  | 2.38                     | 0.49              |
| 1:V:229:LEU:HA   | 1:V:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:V:331:ALA:HB2  | 1:X:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:X:78:ILE:HD12  | 1:X:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:X:338:ASP:HA   | 1:X:339:PRO:C    | 2.38                     | 0.49              |
| 1:a:372:PRO:HB3  | 1:a:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:c:229:LEU:HD22 | 1:c:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:d:387:GLN:HA   | 1:l:305:VAL:HG22 | 1.94                     | 0.49              |
| 1:e:229:LEU:HD22 | 1:e:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:f:305:VAL:HG22 | 1:g:387:GLN:HA   | 1.94                     | 0.49              |
| 1:h:136:LYS:NZ   | 1:h:149:ASN:OD1  | 2.37                     | 0.49              |
| 1:i:163:HIS:HB2  | 1:i:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:j:78:ILE:HD12  | 1:j:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:j:163:HIS:HB2  | 1:j:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:j:229:LEU:HD22 | 1:j:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:m:60:ARG:HG3   | 1:m:177:MET:HG3  | 1.95                     | 0.49              |
| 1:m:229:LEU:HD22 | 1:m:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:m:229:LEU:HA   | 1:m:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:m:270:TYR:O    | 1:n:350:GLU:HG2  | 2.13                     | 0.49              |
| 1:m:390:TYR:HE2  | 1:n:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:p:229:LEU:HA   | 1:p:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:q:78:ILE:HD12  | 1:q:79:PRO:HD2   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:229:LEU:HD22 | 1:t:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:v:174:GLU:OE1  | 1:v:359:PRO:HG3  | 2.12                     | 0.49              |
| 1:x:390:TYR:HE2  | 1:y:331:ALA:HB2  | 1.78                     | 0.49              |
| 1:z:229:LEU:HA   | 1:z:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:1:338:ASP:HA   | 1:1:339:PRO:C    | 2.38                     | 0.49              |
| 1:3:338:ASP:HA   | 1:3:339:PRO:C    | 2.38                     | 0.49              |
| 1:3:491:ARG:O    | 1:3:492:ARG:NH1  | 2.40                     | 0.49              |
| 1:5:78:ILE:HD12  | 1:5:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:6:338:ASP:HA   | 1:6:339:PRO:C    | 2.38                     | 0.49              |
| 1:7:163:HIS:HB2  | 1:7:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:7:229:LEU:HA   | 1:7:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:8:229:LEU:HA   | 1:8:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:A:78:ILE:HD12  | 1:A:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:B:78:ILE:HD12  | 1:B:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:B:133:LEU:HD23 | 1:B:469:GLY:HA3  | 1.95                     | 0.49              |
| 1:B:350:GLU:HG2  | 1:L:270:TYR:O    | 2.13                     | 0.49              |
| 1:D:270:TYR:O    | 1:N:350:GLU:HG2  | 2.13                     | 0.49              |
| 1:D:305:VAL:HG22 | 1:P:387:GLN:HA   | 1.95                     | 0.49              |
| 1:E:305:VAL:HG22 | 1:F:387:GLN:HA   | 1.93                     | 0.49              |
| 1:F:305:VAL:HG22 | 1:Q:387:GLN:HA   | 1.94                     | 0.49              |
| 1:F:331:ALA:HB2  | 1:Q:390:TYR:HE2  | 1.78                     | 0.49              |
| 1:J:229:LEU:HA   | 1:J:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:K:372:PRO:HB3  | 1:K:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:L:229:LEU:HA   | 1:L:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:M:78:ILE:HD12  | 1:M:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:M:133:LEU:HD23 | 1:M:469:GLY:HA3  | 1.95                     | 0.49              |
| 1:M:305:VAL:HG22 | 1:b:387:GLN:HA   | 1.94                     | 0.49              |
| 1:M:372:PRO:HB3  | 1:M:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:O:270:TYR:O    | 1:m:350:GLU:HG2  | 2.13                     | 0.49              |
| 1:P:60:ARG:HG3   | 1:P:177:MET:HG3  | 1.95                     | 0.49              |
| 1:P:229:LEU:HD22 | 1:P:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:T:229:LEU:HD22 | 1:T:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:T:350:GLU:HG2  | 1:l:270:TYR:O    | 2.13                     | 0.49              |
| 1:T:390:TYR:HE2  | 1:d:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:U:163:HIS:HB2  | 1:U:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:W:387:GLN:HA   | 1:Y:305:VAL:HG22 | 1.95                     | 0.49              |
| 1:Y:229:LEU:HA   | 1:Y:233:GLU:OE1  | 2.13                     | 0.49              |
| 1:b:78:ILE:HD12  | 1:b:79:PRO:HD2   | 1.95                     | 0.49              |
| 1:c:382:LEU:HD12 | 1:c:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:d:390:TYR:HE2  | 1:l:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:e:78:ILE:HD12  | 1:e:79:PRO:HD2   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:229:LEU:HA   | 1:f:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:f:241:PHE:HB3  | 1:f:243:CYS:SG   | 2.52                     | 0.49              |
| 1:g:229:LEU:HA   | 1:g:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:h:163:HIS:HB2  | 1:h:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:h:295:THR:HG23 | 1:h:380:GLN:HB3  | 1.95                     | 0.49              |
| 1:i:350:GLU:HG2  | 1:k:270:TYR:O    | 2.13                     | 0.49              |
| 1:j:60:ARG:HG3   | 1:j:177:MET:HG3  | 1.95                     | 0.49              |
| 1:j:387:GLN:HA   | 1:k:305:VAL:HG22 | 1.95                     | 0.49              |
| 1:o:338:ASP:HA   | 1:o:339:PRO:C    | 2.38                     | 0.49              |
| 1:o:382:LEU:HD12 | 1:o:396:VAL:HG22 | 1.94                     | 0.49              |
| 1:o:390:TYR:HE2  | 1:p:331:ALA:HB2  | 1.77                     | 0.49              |
| 1:s:163:HIS:HB2  | 1:s:421:ARG:HH22 | 1.77                     | 0.49              |
| 1:t:60:ARG:HG3   | 1:t:177:MET:HG3  | 1.95                     | 0.49              |
| 1:t:331:ALA:HB2  | 1:v:390:TYR:HE2  | 1.77                     | 0.49              |
| 1:u:133:LEU:HD23 | 1:u:469:GLY:HA3  | 1.95                     | 0.49              |
| 1:x:270:TYR:O    | 1:y:350:GLU:HG2  | 2.13                     | 0.49              |
| 1:y:133:LEU:HD23 | 1:y:469:GLY:HA3  | 1.95                     | 0.49              |
| 1:z:133:LEU:HD23 | 1:z:469:GLY:HA3  | 1.95                     | 0.49              |
| 1:1:133:LEU:HD23 | 1:1:469:GLY:HA3  | 1.95                     | 0.49              |
| 1:1:229:LEU:HD22 | 1:1:233:GLU:HB3  | 1.95                     | 0.49              |
| 1:2:229:LEU:HA   | 1:2:233:GLU:OE1  | 2.12                     | 0.49              |
| 1:4:372:PRO:HB3  | 1:4:379:ASP:OD2  | 2.12                     | 0.49              |
| 1:6:387:GLN:HA   | 1:7:305:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:174:GLU:OE1  | 1:A:359:PRO:HG3  | 2.12                     | 0.48              |
| 1:A:372:PRO:HB3  | 1:A:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:C:78:ILE:HD12  | 1:C:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:C:229:LEU:HA   | 1:C:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:E:270:TYR:O    | 1:Q:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:F:133:LEU:HD23 | 1:F:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:F:350:GLU:HG2  | 1:Q:270:TYR:O    | 2.13                     | 0.48              |
| 1:H:133:LEU:HD23 | 1:H:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:H:350:GLU:HG2  | 1:Y:270:TYR:O    | 2.13                     | 0.48              |
| 1:I:133:LEU:HD23 | 1:I:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:L:133:LEU:HD23 | 1:L:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:M:295:THR:HG23 | 1:M:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:O:372:PRO:HB3  | 1:O:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:P:372:PRO:HB3  | 1:P:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:Q:229:LEU:HD22 | 1:Q:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:S:229:LEU:HA   | 1:S:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:T:133:LEU:HD23 | 1:T:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:T:382:LEU:HD12 | 1:T:396:VAL:HG22 | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:372:PRO:HB3  | 1:U:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:W:295:THR:HG23 | 1:W:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:W:338:ASP:HA   | 1:W:339:PRO:C    | 2.38                     | 0.48              |
| 1:Y:163:HIS:HB2  | 1:Y:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:b:229:LEU:HA   | 1:b:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:c:78:ILE:HD12  | 1:c:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:e:382:LEU:HD12 | 1:e:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:f:78:ILE:HD12  | 1:f:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:f:387:GLN:HA   | 1:h:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:h:78:ILE:HD12  | 1:h:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:h:372:PRO:HB3  | 1:h:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:i:331:ALA:HB2  | 1:k:390:TYR:HE2  | 1.77                     | 0.48              |
| 1:l:372:PRO:HB3  | 1:l:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:m:382:LEU:HD12 | 1:m:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:q:338:ASP:HA   | 1:q:339:PRO:C    | 2.38                     | 0.48              |
| 1:r:229:LEU:HA   | 1:r:233:GLU:OE1  | 2.13                     | 0.48              |
| 1:v:372:PRO:HB3  | 1:v:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:w:270:TYR:O    | 1:x:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:x:229:LEU:HD22 | 1:x:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:3:331:ALA:HB2  | 1:4:390:TYR:HE2  | 1.77                     | 0.48              |
| 1:3:372:PRO:HB3  | 1:3:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:5:133:LEU:HD23 | 1:5:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:5:350:GLU:HG2  | 1:7:270:TYR:O    | 2.13                     | 0.48              |
| 1:6:295:THR:HG23 | 1:6:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:7:372:PRO:HB3  | 1:7:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:A:295:THR:HG23 | 1:A:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:B:382:LEU:HD12 | 1:B:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:D:390:TYR:HE2  | 1:N:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:G:60:ARG:HG3   | 1:G:177:MET:HG3  | 1.95                     | 0.48              |
| 1:H:229:LEU:HD22 | 1:H:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:K:390:TYR:HE2  | 1:a:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:N:133:LEU:HD23 | 1:N:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:N:338:ASP:HA   | 1:N:339:PRO:C    | 2.38                     | 0.48              |
| 1:R:295:THR:HG23 | 1:R:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:T:295:THR:HG23 | 1:T:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:T:387:GLN:HA   | 1:d:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:U:88:ARG:O     | 1:U:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:U:382:LEU:HD12 | 1:U:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:U:488:ARG:O    | 1:V:109:GLN:NE2  | 2.46                     | 0.48              |
| 1:V:78:ILE:HD12  | 1:V:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:X:295:THR:HG23 | 1:X:380:GLN:HB3  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:372:PRO:HB3  | 1:X:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:X:382:LEU:HD12 | 1:X:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:Y:133:LEU:HD23 | 1:Y:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:Y:372:PRO:HB3  | 1:Y:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:Z:133:LEU:HD23 | 1:Z:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:c:390:TYR:HE2  | 1:o:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:d:382:LEU:HD12 | 1:d:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:f:133:LEU:HD23 | 1:f:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:h:133:LEU:HD23 | 1:h:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:i:133:LEU:HD23 | 1:i:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:i:338:ASP:HA   | 1:i:339:PRO:C    | 2.38                     | 0.48              |
| 1:j:372:PRO:HB3  | 1:j:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:m:133:LEU:HD23 | 1:m:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:m:295:THR:HG23 | 1:m:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:n:382:LEU:HD12 | 1:n:396:VAL:HG22 | 1.95                     | 0.48              |
| 1:o:229:LEU:HA   | 1:o:233:GLU:OE1  | 2.13                     | 0.48              |
| 1:o:295:THR:HG23 | 1:o:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:o:372:PRO:HB3  | 1:o:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:p:109:GLN:NE2  | 1:s:488:ARG:O    | 2.46                     | 0.48              |
| 1:q:295:THR:HG23 | 1:q:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:v:78:ILE:HD12  | 1:v:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:v:295:THR:HG23 | 1:v:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:x:387:GLN:HA   | 1:y:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:1:382:LEU:HD12 | 1:1:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:3:163:HIS:HB2  | 1:3:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:4:229:LEU:HD22 | 1:4:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:6:390:TYR:HE2  | 1:7:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:7:133:LEU:HD23 | 1:7:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:8:78:ILE:HD12  | 1:8:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:8:133:LEU:HD23 | 1:8:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:8:338:ASP:HA   | 1:8:339:PRO:C    | 2.38                     | 0.48              |
| 1:B:372:PRO:HB3  | 1:B:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:C:436:ALA:C    | 1:C:437:MET:HG3  | 2.39                     | 0.48              |
| 1:D:372:PRO:HB3  | 1:D:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:D:382:LEU:HD12 | 1:D:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:H:382:LEU:HD12 | 1:H:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:K:229:LEU:HD22 | 1:K:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:M:136:LYS:NZ   | 1:M:149:ASN:OD1  | 2.37                     | 0.48              |
| 1:N:78:ILE:HD12  | 1:N:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:S:387:GLN:HA   | 1:U:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:Z:78:ILE:HD12  | 1:Z:79:PRO:HD2   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:338:ASP:HA   | 1:Z:339:PRO:C    | 2.38                     | 0.48              |
| 1:c:88:ARG:O     | 1:c:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:c:270:TYR:O    | 1:o:350:GLU:HG2  | 2.14                     | 0.48              |
| 1:d:78:ILE:HD12  | 1:d:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:e:88:ARG:O     | 1:e:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:g:436:ALA:C    | 1:g:437:MET:HG3  | 2.39                     | 0.48              |
| 1:i:78:ILE:HD12  | 1:i:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:i:229:LEU:HA   | 1:i:233:GLU:OE1  | 2.13                     | 0.48              |
| 1:l:295:THR:HG23 | 1:l:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:m:387:GLN:HA   | 1:n:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:n:78:ILE:HD12  | 1:n:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:p:78:ILE:HD12  | 1:p:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:q:270:TYR:O    | 1:r:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:s:372:PRO:HB3  | 1:s:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:s:382:LEU:HD12 | 1:s:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:w:491:ARG:O    | 1:w:492:ARG:NH1  | 2.40                     | 0.48              |
| 1:3:133:LEU:HD23 | 1:3:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:4:78:ILE:HD12  | 1:4:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:5:229:LEU:HD22 | 1:5:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:5:382:LEU:HD12 | 1:5:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:6:372:PRO:HB3  | 1:6:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:8:372:PRO:HB3  | 1:8:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:B:88:ARG:O     | 1:B:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:D:338:ASP:HA   | 1:D:339:PRO:C    | 2.38                     | 0.48              |
| 1:F:295:THR:HG23 | 1:F:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:J:109:GLN:NE2  | 1:K:488:ARG:O    | 2.47                     | 0.48              |
| 1:J:387:GLN:HA   | 1:L:305:VAL:HG22 | 1.95                     | 0.48              |
| 1:K:229:LEU:HA   | 1:K:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:K:436:ALA:C    | 1:K:437:MET:HG3  | 2.39                     | 0.48              |
| 1:O:295:THR:HG23 | 1:O:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:R:229:LEU:HD22 | 1:R:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:R:270:TYR:O    | 1:S:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:T:338:ASP:HA   | 1:T:339:PRO:C    | 2.38                     | 0.48              |
| 1:W:372:PRO:HB3  | 1:W:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:W:382:LEU:HD12 | 1:W:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:W:390:TYR:HE2  | 1:Y:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:X:229:LEU:HA   | 1:X:233:GLU:OE1  | 2.13                     | 0.48              |
| 1:X:331:ALA:HB2  | 1:e:390:TYR:HE2  | 1.77                     | 0.48              |
| 1:X:350:GLU:HG2  | 1:e:270:TYR:O    | 2.14                     | 0.48              |
| 1:a:163:HIS:HB2  | 1:a:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:b:133:LEU:HD23 | 1:b:469:GLY:HA3  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:179:GLU:OE2  | 1:c:411:ARG:NH1  | 2.38                     | 0.48              |
| 1:e:338:ASP:HA   | 1:e:339:PRO:C    | 2.38                     | 0.48              |
| 1:g:305:VAL:HG22 | 1:h:387:GLN:HA   | 1.94                     | 0.48              |
| 1:i:295:THR:HG23 | 1:i:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:k:372:PRO:HB3  | 1:k:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:k:382:LEU:HD12 | 1:k:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:o:229:LEU:HD22 | 1:o:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:r:387:GLN:HA   | 1:s:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:s:88:ARG:O     | 1:s:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:t:270:TYR:O    | 1:u:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:u:29:GLY:N     | 1:2:234:SER:O    | 2.32                     | 0.48              |
| 1:w:133:LEU:HD23 | 1:w:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:z:338:ASP:HA   | 1:z:339:PRO:C    | 2.38                     | 0.48              |
| 1:1:88:ARG:O     | 1:1:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:4:229:LEU:HA   | 1:4:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:5:305:VAL:HG22 | 1:7:387:GLN:HA   | 1.94                     | 0.48              |
| 1:5:338:ASP:HA   | 1:5:339:PRO:C    | 2.38                     | 0.48              |
| 1:6:382:LEU:HD12 | 1:6:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:E:350:GLU:HG2  | 1:F:270:TYR:O    | 2.14                     | 0.48              |
| 1:E:382:LEU:HD12 | 1:E:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:H:88:ARG:O     | 1:H:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:K:331:ALA:HB2  | 1:8:390:TYR:HE2  | 1.77                     | 0.48              |
| 1:L:436:ALA:C    | 1:L:437:MET:HG3  | 2.39                     | 0.48              |
| 1:N:229:LEU:HA   | 1:N:233:GLU:OE1  | 2.13                     | 0.48              |
| 1:N:295:THR:HG23 | 1:N:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:N:436:ALA:C    | 1:N:437:MET:HG3  | 2.39                     | 0.48              |
| 1:O:350:GLU:HG2  | 1:n:270:TYR:O    | 2.13                     | 0.48              |
| 1:O:382:LEU:HD12 | 1:O:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:O:436:ALA:C    | 1:O:437:MET:HG3  | 2.39                     | 0.48              |
| 1:R:390:TYR:HE2  | 1:S:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:X:229:LEU:HD22 | 1:X:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:Z:372:PRO:HB3  | 1:Z:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:a:133:LEU:HD23 | 1:a:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:c:295:THR:HG23 | 1:c:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:d:133:LEU:HD23 | 1:d:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:e:295:THR:HG23 | 1:e:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:f:338:ASP:HA   | 1:f:339:PRO:C    | 2.38                     | 0.48              |
| 1:f:436:ALA:C    | 1:f:437:MET:HG3  | 2.39                     | 0.48              |
| 1:g:372:PRO:HB3  | 1:g:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:i:305:VAL:HG22 | 1:k:387:GLN:HA   | 1.95                     | 0.48              |
| 1:i:436:ALA:C    | 1:i:437:MET:HG3  | 2.39                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:270:TYR:O    | 1:k:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:j:338:ASP:HA   | 1:j:339:PRO:C    | 2.38                     | 0.48              |
| 1:k:338:ASP:HA   | 1:k:339:PRO:C    | 2.38                     | 0.48              |
| 1:l:382:LEU:HD12 | 1:l:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:l:436:ALA:C    | 1:l:437:MET:HG3  | 2.39                     | 0.48              |
| 1:n:133:LEU:HD23 | 1:n:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:n:295:THR:HG23 | 1:n:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:o:163:HIS:HB2  | 1:o:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:o:270:TYR:O    | 1:p:350:GLU:HG2  | 2.14                     | 0.48              |
| 1:q:229:LEU:HD22 | 1:q:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:q:390:TYR:HE2  | 1:r:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:s:338:ASP:HA   | 1:s:339:PRO:C    | 2.38                     | 0.48              |
| 1:w:350:GLU:HG2  | 1:y:270:TYR:O    | 2.14                     | 0.48              |
| 1:y:295:THR:HG23 | 1:y:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:z:436:ALA:C    | 1:z:437:MET:HG3  | 2.39                     | 0.48              |
| 1:1:372:PRO:HB3  | 1:1:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:5:88:ARG:O     | 1:5:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:6:163:HIS:HB2  | 1:6:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:A:109:GLN:NE2  | 1:F:488:ARG:O    | 2.47                     | 0.48              |
| 1:A:350:GLU:HG2  | 1:I:270:TYR:O    | 2.13                     | 0.48              |
| 1:B:436:ALA:C    | 1:B:437:MET:HG3  | 2.39                     | 0.48              |
| 1:C:372:PRO:HB3  | 1:C:379:ASP:OD2  | 2.12                     | 0.48              |
| 1:D:350:GLU:HG2  | 1:P:270:TYR:O    | 2.13                     | 0.48              |
| 1:D:387:GLN:HA   | 1:N:305:VAL:HG22 | 1.95                     | 0.48              |
| 1:E:133:LEU:HD23 | 1:E:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:G:133:LEU:HD23 | 1:G:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:G:270:TYR:O    | 1:I:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:H:338:ASP:HA   | 1:H:339:PRO:C    | 2.38                     | 0.48              |
| 1:I:436:ALA:C    | 1:I:437:MET:HG3  | 2.39                     | 0.48              |
| 1:L:295:THR:HG23 | 1:L:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:L:338:ASP:HA   | 1:L:339:PRO:C    | 2.38                     | 0.48              |
| 1:O:409:ILE:H    | 1:O:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:P:295:THR:HG23 | 1:P:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:P:338:ASP:HA   | 1:P:339:PRO:C    | 2.38                     | 0.48              |
| 1:R:133:LEU:HD23 | 1:R:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:R:229:LEU:HA   | 1:R:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:S:270:TYR:O    | 1:U:350:GLU:HG2  | 2.14                     | 0.48              |
| 1:U:229:LEU:HD22 | 1:U:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:U:338:ASP:HA   | 1:U:339:PRO:C    | 2.38                     | 0.48              |
| 1:V:350:GLU:HG2  | 1:X:270:TYR:O    | 2.14                     | 0.48              |
| 1:W:133:LEU:HD23 | 1:W:469:GLY:HA3  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:163:HIS:HB2  | 1:X:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:Z:390:TYR:HE2  | 1:4:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:b:229:LEU:HD22 | 1:b:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:b:436:ALA:C    | 1:b:437:MET:HG3  | 2.39                     | 0.48              |
| 1:d:270:TYR:O    | 1:l:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:d:295:THR:HG23 | 1:d:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:f:382:LEU:HD12 | 1:f:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:g:109:GLN:NE2  | 1:z:488:ARG:O    | 2.46                     | 0.48              |
| 1:j:295:THR:HG23 | 1:j:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:p:133:LEU:HD23 | 1:p:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:q:229:LEU:HA   | 1:q:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:r:270:TYR:O    | 1:s:350:GLU:HG2  | 2.14                     | 0.48              |
| 1:t:133:LEU:HD23 | 1:t:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:w:382:LEU:HD12 | 1:w:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:w:436:ALA:C    | 1:w:437:MET:HG3  | 2.39                     | 0.48              |
| 1:1:436:ALA:C    | 1:1:437:MET:HG3  | 2.39                     | 0.48              |
| 1:4:357:GLN:NE2  | 1:4:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:4:436:ALA:C    | 1:4:437:MET:HG3  | 2.39                     | 0.48              |
| 1:A:133:LEU:HD23 | 1:A:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:A:229:LEU:HA   | 1:A:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:C:305:VAL:HG22 | 1:M:387:GLN:HA   | 1.95                     | 0.48              |
| 1:D:133:LEU:HD23 | 1:D:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:D:436:ALA:C    | 1:D:437:MET:HG3  | 2.39                     | 0.48              |
| 1:E:436:ALA:C    | 1:E:437:MET:HG3  | 2.39                     | 0.48              |
| 1:F:88:ARG:O     | 1:F:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:H:305:VAL:HG22 | 1:Y:387:GLN:HA   | 1.94                     | 0.48              |
| 1:J:78:ILE:HD12  | 1:J:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:J:133:LEU:HD23 | 1:J:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:K:133:LEU:HD23 | 1:K:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:K:338:ASP:HA   | 1:K:339:PRO:C    | 2.38                     | 0.48              |
| 1:K:357:GLN:NE2  | 1:K:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:R:60:ARG:HG3   | 1:R:177:MET:HG3  | 1.95                     | 0.48              |
| 1:U:295:THR:HG23 | 1:U:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:V:60:ARG:HG3   | 1:V:177:MET:HG3  | 1.95                     | 0.48              |
| 1:W:163:HIS:HB2  | 1:W:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:X:436:ALA:C    | 1:X:437:MET:HG3  | 2.39                     | 0.48              |
| 1:Y:109:GLN:NE2  | 1:Z:488:ARG:O    | 2.47                     | 0.48              |
| 1:Y:382:LEU:HD12 | 1:Y:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:b:382:LEU:HD12 | 1:b:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:c:338:ASP:HA   | 1:c:339:PRO:C    | 2.38                     | 0.48              |
| 1:f:229:LEU:HD22 | 1:f:233:GLU:HB3  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:133:LEU:HD23 | 1:k:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:l:409:ILE:H    | 1:l:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:m:338:ASP:HA   | 1:m:339:PRO:C    | 2.38                     | 0.48              |
| 1:o:133:LEU:HD23 | 1:o:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:p:51:ASP:OD1   | 1:p:481:ARG:NE   | 2.39                     | 0.48              |
| 1:p:60:ARG:HG3   | 1:p:177:MET:HG3  | 1.95                     | 0.48              |
| 1:q:60:ARG:HG3   | 1:q:177:MET:HG3  | 1.95                     | 0.48              |
| 1:q:133:LEU:HD23 | 1:q:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:r:295:THR:HG23 | 1:r:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:s:60:ARG:HG3   | 1:s:177:MET:HG3  | 1.95                     | 0.48              |
| 1:s:229:LEU:HD22 | 1:s:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:u:436:ALA:C    | 1:u:437:MET:HG3  | 2.39                     | 0.48              |
| 1:v:60:ARG:HG3   | 1:v:177:MET:HG3  | 1.95                     | 0.48              |
| 1:v:133:LEU:HD23 | 1:v:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:z:229:LEU:HD22 | 1:z:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:z:295:THR:HG23 | 1:z:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:1:409:ILE:H    | 1:1:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:3:409:ILE:H    | 1:3:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:4:133:LEU:HD23 | 1:4:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:4:136:LYS:NZ   | 1:4:149:ASN:OD1  | 2.37                     | 0.48              |
| 1:4:382:LEU:HD12 | 1:4:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:6:133:LEU:HD23 | 1:6:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:7:382:LEU:HD12 | 1:7:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:8:436:ALA:C    | 1:8:437:MET:HG3  | 2.39                     | 0.48              |
| 1:A:60:ARG:HG3   | 1:A:177:MET:HG3  | 1.95                     | 0.48              |
| 1:B:305:VAL:HG22 | 1:L:387:GLN:HA   | 1.95                     | 0.48              |
| 1:B:409:ILE:H    | 1:B:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:D:109:GLN:NE2  | 1:M:488:ARG:O    | 2.47                     | 0.48              |
| 1:E:60:ARG:HG3   | 1:E:177:MET:HG3  | 1.95                     | 0.48              |
| 1:G:338:ASP:HA   | 1:G:339:PRO:C    | 2.38                     | 0.48              |
| 1:I:29:GLY:N     | 1:J:234:SER:O    | 2.32                     | 0.48              |
| 1:J:382:LEU:HD12 | 1:J:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:J:436:ALA:C    | 1:J:437:MET:HG3  | 2.39                     | 0.48              |
| 1:L:229:LEU:HD22 | 1:L:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:O:163:HIS:HB2  | 1:O:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:U:78:ILE:HD12  | 1:U:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:X:133:LEU:HD23 | 1:X:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:a:409:ILE:H    | 1:a:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:b:409:ILE:H    | 1:b:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:d:436:ALA:C    | 1:d:437:MET:HG3  | 2.39                     | 0.48              |
| 1:e:179:GLU:OE2  | 1:e:411:ARG:NH1  | 2.38                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:409:ILE:H    | 1:f:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:g:133:LEU:HD23 | 1:g:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:h:229:LEU:HD22 | 1:h:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:h:488:ARG:O    | 1:k:109:GLN:NE2  | 2.47                     | 0.48              |
| 1:i:387:GLN:HA   | 1:j:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:k:436:ALA:C    | 1:k:437:MET:HG3  | 2.39                     | 0.48              |
| 1:n:436:ALA:C    | 1:n:437:MET:HG3  | 2.39                     | 0.48              |
| 1:o:436:ALA:C    | 1:o:437:MET:HG3  | 2.39                     | 0.48              |
| 1:r:338:ASP:HA   | 1:r:339:PRO:C    | 2.38                     | 0.48              |
| 1:s:295:THR:HG23 | 1:s:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:u:229:LEU:HD22 | 1:u:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:u:270:TYR:O    | 1:v:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:v:109:GLN:NE2  | 1:y:488:ARG:O    | 2.47                     | 0.48              |
| 1:w:60:ARG:HG3   | 1:w:177:MET:HG3  | 1.95                     | 0.48              |
| 1:w:78:ILE:HD12  | 1:w:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:1:387:GLN:HA   | 1:2:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:2:78:ILE:HD12  | 1:2:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:2:133:LEU:HD23 | 1:2:469:GLY:HA3  | 1.96                     | 0.48              |
| 1:2:382:LEU:HD12 | 1:2:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:2:436:ALA:C    | 1:2:437:MET:HG3  | 2.39                     | 0.48              |
| 1:3:60:ARG:HG3   | 1:3:177:MET:HG3  | 1.95                     | 0.48              |
| 1:4:338:ASP:HA   | 1:4:339:PRO:C    | 2.38                     | 0.48              |
| 1:7:109:GLN:NE2  | 1:8:488:ARG:O    | 2.47                     | 0.48              |
| 1:A:270:TYR:O    | 1:G:350:GLU:HG2  | 2.14                     | 0.48              |
| 1:E:78:ILE:HD12  | 1:E:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:E:229:LEU:HA   | 1:E:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:E:387:GLN:HA   | 1:Q:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:I:229:LEU:HD22 | 1:I:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:I:295:THR:HG23 | 1:I:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:I:409:ILE:H    | 1:I:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:K:382:LEU:HD12 | 1:K:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:M:229:LEU:HD22 | 1:M:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:M:338:ASP:HA   | 1:M:339:PRO:C    | 2.38                     | 0.48              |
| 1:N:387:GLN:HA   | 1:P:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:N:409:ILE:H    | 1:N:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:Q:295:THR:HG23 | 1:Q:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:S:338:ASP:HA   | 1:S:339:PRO:C    | 2.38                     | 0.48              |
| 1:S:436:ALA:C    | 1:S:437:MET:HG3  | 2.39                     | 0.48              |
| 1:T:179:GLU:OE2  | 1:T:411:ARG:NH1  | 2.38                     | 0.48              |
| 1:U:60:ARG:HG3   | 1:U:177:MET:HG3  | 1.95                     | 0.48              |
| 1:U:357:GLN:NE2  | 1:U:368:ILE:HD12 | 2.29                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:436:ALA:C    | 1:U:437:MET:HG3  | 2.39                     | 0.48              |
| 1:V:133:LEU:HD23 | 1:V:469:GLY:HA3  | 1.96                     | 0.48              |
| 1:W:78:ILE:HD12  | 1:W:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:W:409:ILE:H    | 1:W:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:Y:78:ILE:HD12  | 1:Y:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:Z:436:ALA:C    | 1:Z:437:MET:HG3  | 2.39                     | 0.48              |
| 1:a:60:ARG:HG3   | 1:a:177:MET:HG3  | 1.95                     | 0.48              |
| 1:a:78:ILE:HD12  | 1:a:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:b:338:ASP:HA   | 1:b:339:PRO:C    | 2.38                     | 0.48              |
| 1:e:491:ARG:O    | 1:e:492:ARG:NH1  | 2.40                     | 0.48              |
| 1:h:338:ASP:HA   | 1:h:339:PRO:C    | 2.38                     | 0.48              |
| 1:l:163:HIS:HB2  | 1:l:421:ARG:HH22 | 1.77                     | 0.48              |
| 1:n:338:ASP:HA   | 1:n:339:PRO:C    | 2.38                     | 0.48              |
| 1:r:436:ALA:C    | 1:r:437:MET:HG3  | 2.39                     | 0.48              |
| 1:s:78:ILE:HD12  | 1:s:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:s:357:GLN:NE2  | 1:s:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:s:436:ALA:C    | 1:s:437:MET:HG3  | 2.39                     | 0.48              |
| 1:t:338:ASP:HA   | 1:t:339:PRO:C    | 2.38                     | 0.48              |
| 1:t:350:GLU:HG2  | 1:v:270:TYR:O    | 2.14                     | 0.48              |
| 1:u:409:ILE:H    | 1:u:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:v:229:LEU:HA   | 1:v:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:w:229:LEU:HA   | 1:w:233:GLU:OE1  | 2.12                     | 0.48              |
| 1:y:88:ARG:O     | 1:y:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:y:338:ASP:HA   | 1:y:339:PRO:C    | 2.38                     | 0.48              |
| 1:2:109:GLN:NE2  | 1:4:488:ARG:O    | 2.47                     | 0.48              |
| 1:2:357:GLN:NE2  | 1:2:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:2:488:ARG:O    | 1:4:109:GLN:NE2  | 2.47                     | 0.48              |
| 1:3:78:ILE:HD12  | 1:3:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:F:436:ALA:C    | 1:F:437:MET:HG3  | 2.39                     | 0.48              |
| 1:G:357:GLN:NE2  | 1:G:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:J:229:LEU:HD22 | 1:J:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:J:295:THR:HG23 | 1:J:380:GLN:HB3  | 1.95                     | 0.48              |
| 1:J:357:GLN:NE2  | 1:J:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:K:350:GLU:HG2  | 1:8:270:TYR:O    | 2.13                     | 0.48              |
| 1:L:78:ILE:HD12  | 1:L:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:L:409:ILE:H    | 1:L:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:L:491:ARG:O    | 1:L:492:ARG:NH1  | 2.40                     | 0.48              |
| 1:M:409:ILE:H    | 1:M:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:Q:78:ILE:HD12  | 1:Q:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:R:382:LEU:HD12 | 1:R:396:VAL:HG22 | 1.94                     | 0.48              |
| 1:S:136:LYS:NZ   | 1:S:149:ASN:OD1  | 2.37                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:179:GLU:OE2  | 1:S:411:ARG:NH1  | 2.38                     | 0.48              |
| 1:S:295:THR:HG23 | 1:S:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:T:134:GLN:NE2  | 1:U:153:ALA:HA   | 2.29                     | 0.48              |
| 1:T:357:GLN:NE2  | 1:T:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:V:270:TYR:O    | 1:e:350:GLU:HG2  | 2.14                     | 0.48              |
| 1:V:338:ASP:HA   | 1:V:339:PRO:C    | 2.38                     | 0.48              |
| 1:W:88:ARG:O     | 1:W:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:W:109:GLN:NE2  | 1:X:488:ARG:O    | 2.47                     | 0.48              |
| 1:X:409:ILE:H    | 1:X:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:Y:488:ARG:O    | 1:Z:109:GLN:NE2  | 2.47                     | 0.48              |
| 1:Z:270:TYR:O    | 1:4:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:a:270:TYR:O    | 1:8:350:GLU:HG2  | 2.13                     | 0.48              |
| 1:d:109:GLN:NE2  | 1:n:488:ARG:O    | 2.47                     | 0.48              |
| 1:d:488:ARG:O    | 1:n:109:GLN:NE2  | 2.47                     | 0.48              |
| 1:i:409:ILE:H    | 1:i:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:j:378:ARG:HD2  | 1:j:378:ARG:HA   | 1.73                     | 0.48              |
| 1:m:134:GLN:NE2  | 1:s:153:ALA:HA   | 2.29                     | 0.48              |
| 1:o:109:GLN:NE2  | 1:6:488:ARG:O    | 2.47                     | 0.48              |
| 1:p:357:GLN:NE2  | 1:p:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:p:409:ILE:H    | 1:p:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:r:133:LEU:HD23 | 1:r:469:GLY:HA3  | 1.95                     | 0.48              |
| 1:t:357:GLN:NE2  | 1:t:368:ILE:HD12 | 2.29                     | 0.48              |
| 1:u:295:THR:HG23 | 1:u:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:v:409:ILE:H    | 1:v:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:w:387:GLN:HA   | 1:x:305:VAL:HG22 | 1.94                     | 0.48              |
| 1:x:78:ILE:HD12  | 1:x:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:x:295:THR:HG23 | 1:x:380:GLN:HB3  | 1.96                     | 0.48              |
| 1:z:78:ILE:HD12  | 1:z:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:z:409:ILE:H    | 1:z:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:z:491:ARG:O    | 1:z:492:ARG:NH1  | 2.40                     | 0.48              |
| 1:2:229:LEU:HD22 | 1:2:233:GLU:HB3  | 1.95                     | 0.48              |
| 1:5:390:TYR:HE2  | 1:6:331:ALA:HB2  | 1.77                     | 0.48              |
| 1:6:78:ILE:HD12  | 1:6:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:6:88:ARG:O     | 1:6:194:PRO:HD2  | 2.12                     | 0.48              |
| 1:6:409:ILE:H    | 1:6:530:ILE:HG12 | 1.79                     | 0.48              |
| 1:7:78:ILE:HD12  | 1:7:79:PRO:HD2   | 1.95                     | 0.48              |
| 1:7:488:ARG:O    | 1:8:109:GLN:NE2  | 2.47                     | 0.48              |
| 1:C:133:LEU:HD23 | 1:C:469:GLY:HA3  | 1.96                     | 0.47              |
| 1:D:136:LYS:NZ   | 1:D:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:E:229:LEU:HD22 | 1:E:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:E:295:THR:HG23 | 1:E:380:GLN:HB3  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:78:ILE:HD12  | 1:F:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:F:338:ASP:HA   | 1:F:339:PRO:C    | 2.38                     | 0.47              |
| 1:G:295:THR:HG23 | 1:G:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:K:136:LYS:NZ   | 1:K:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:L:357:GLN:NE2  | 1:L:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:S:133:LEU:HD23 | 1:S:469:GLY:HA3  | 1.96                     | 0.47              |
| 1:V:357:GLN:NE2  | 1:V:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:V:409:ILE:H    | 1:V:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:W:270:TYR:O    | 1:Y:350:GLU:HG2  | 2.13                     | 0.47              |
| 1:W:488:ARG:O    | 1:X:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:Z:350:GLU:HG2  | 1:3:270:TYR:O    | 2.13                     | 0.47              |
| 1:a:229:LEU:HD22 | 1:a:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:b:109:GLN:NE2  | 1:c:488:ARG:O    | 2.47                     | 0.47              |
| 1:c:350:GLU:HG2  | 1:p:270:TYR:O    | 2.14                     | 0.47              |
| 1:e:488:ARG:O    | 1:f:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:h:409:ILE:H    | 1:h:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:k:409:ILE:H    | 1:k:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:m:357:GLN:NE2  | 1:m:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:o:409:ILE:H    | 1:o:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:o:488:ARG:O    | 1:6:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:p:338:ASP:HA   | 1:p:339:PRO:C    | 2.38                     | 0.47              |
| 1:p:436:ALA:C    | 1:p:437:MET:HG3  | 2.39                     | 0.47              |
| 1:q:382:LEU:HD12 | 1:q:396:VAL:HG22 | 1.94                     | 0.47              |
| 1:t:295:THR:HG23 | 1:t:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:v:488:ARG:O    | 1:y:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:w:229:LEU:HD22 | 1:w:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:y:436:ALA:C    | 1:y:437:MET:HG3  | 2.39                     | 0.47              |
| 1:z:383:TYR:HE2  | 1:1:318:VAL:HG21 | 1.79                     | 0.47              |
| 1:5:357:GLN:NE2  | 1:5:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:7:295:THR:HG23 | 1:7:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:8:229:LEU:HD22 | 1:8:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:A:409:ILE:H    | 1:A:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:A:488:ARG:O    | 1:F:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:B:331:ALA:HB2  | 1:L:390:TYR:HE2  | 1.78                     | 0.47              |
| 1:B:390:TYR:CE2  | 1:J:331:ALA:HB2  | 2.48                     | 0.47              |
| 1:C:488:ARG:O    | 1:L:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:D:409:ILE:H    | 1:D:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:E:371:ASN:HB2  | 1:E:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:F:153:ALA:HA   | 1:R:134:GLN:NE2  | 2.29                     | 0.47              |
| 1:H:179:GLU:OE2  | 1:H:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:H:357:GLN:NE2  | 1:H:368:ILE:HD12 | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:390:TYR:HE2  | 1:W:331:ALA:HB2  | 1.77                     | 0.47              |
| 1:I:371:ASN:HB2  | 1:I:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:J:390:TYR:CE2  | 1:L:331:ALA:HB2  | 2.49                     | 0.47              |
| 1:J:409:ILE:H    | 1:J:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:M:153:ALA:HA   | 1:c:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:P:378:ARG:HD2  | 1:P:378:ARG:HA   | 1.73                     | 0.47              |
| 1:S:109:GLN:NE2  | 1:T:488:ARG:O    | 2.47                     | 0.47              |
| 1:S:488:ARG:O    | 1:T:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:U:109:GLN:NE2  | 1:V:488:ARG:O    | 2.48                     | 0.47              |
| 1:U:371:ASN:HB2  | 1:U:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:U:378:ARG:HD2  | 1:U:378:ARG:HA   | 1.73                     | 0.47              |
| 1:c:409:ILE:H    | 1:c:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:e:134:GLN:NE2  | 1:h:153:ALA:HA   | 2.30                     | 0.47              |
| 1:f:270:TYR:O    | 1:h:350:GLU:HG2  | 2.14                     | 0.47              |
| 1:g:229:LEU:HD22 | 1:g:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:i:229:LEU:HD22 | 1:i:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:i:270:TYR:O    | 1:j:350:GLU:HG2  | 2.13                     | 0.47              |
| 1:m:109:GLN:NE2  | 1:r:488:ARG:O    | 2.47                     | 0.47              |
| 1:p:488:ARG:O    | 1:s:109:GLN:NE2  | 2.48                     | 0.47              |
| 1:q:109:GLN:NE2  | 1:x:488:ARG:O    | 2.47                     | 0.47              |
| 1:s:371:ASN:HB2  | 1:s:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:t:488:ARG:O    | 1:5:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:w:371:ASN:HB2  | 1:w:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:y:78:ILE:HD12  | 1:y:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:z:357:GLN:NE2  | 1:z:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:1:270:TYR:O    | 1:2:350:GLU:HG2  | 2.13                     | 0.47              |
| 1:2:295:THR:HG23 | 1:2:380:GLN:HB3  | 1.96                     | 0.47              |
| 1:4:371:ASN:HB2  | 1:4:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:C:109:GLN:NE2  | 1:L:488:ARG:O    | 2.47                     | 0.47              |
| 1:C:409:ILE:H    | 1:C:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:D:153:ALA:HA   | 1:E:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:D:295:THR:HG23 | 1:D:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:D:488:ARG:O    | 1:M:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:G:488:ARG:O    | 1:H:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:H:295:THR:HG23 | 1:H:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:H:371:ASN:HB2  | 1:H:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:I:60:ARG:HG3   | 1:I:177:MET:HG3  | 1.95                     | 0.47              |
| 1:J:60:ARG:HG3   | 1:J:177:MET:HG3  | 1.95                     | 0.47              |
| 1:K:371:ASN:HB2  | 1:K:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:M:371:ASN:HB2  | 1:M:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:N:60:ARG:HG3   | 1:N:177:MET:HG3  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:109:GLN:NE2  | 1:O:488:ARG:O    | 2.47                     | 0.47              |
| 1:N:229:LEU:HD22 | 1:N:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:N:270:TYR:O    | 1:P:350:GLU:HG2  | 2.13                     | 0.47              |
| 1:O:134:GLN:NE2  | 1:P:153:ALA:HA   | 2.30                     | 0.47              |
| 1:O:153:ALA:HA   | 1:d:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:Q:488:ARG:O    | 1:R:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:T:409:ILE:H    | 1:T:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:Y:295:THR:HG23 | 1:Y:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:Y:371:ASN:HB2  | 1:Y:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:Z:229:LEU:HD22 | 1:Z:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:a:229:LEU:HA   | 1:a:233:GLU:OE1  | 2.12                     | 0.47              |
| 1:b:371:ASN:HB2  | 1:b:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:d:229:LEU:HD22 | 1:d:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:d:338:ASP:HA   | 1:d:339:PRO:C    | 2.38                     | 0.47              |
| 1:e:409:ILE:H    | 1:e:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:f:371:ASN:HB2  | 1:f:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:g:338:ASP:HA   | 1:g:339:PRO:C    | 2.38                     | 0.47              |
| 1:g:488:ARG:O    | 1:z:109:GLN:NE2  | 2.48                     | 0.47              |
| 1:h:109:GLN:NE2  | 1:k:488:ARG:O    | 2.47                     | 0.47              |
| 1:h:371:ASN:HB2  | 1:h:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:i:109:GLN:NE2  | 1:l:488:ARG:O    | 2.47                     | 0.47              |
| 1:j:153:ALA:HA   | 1:l:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:k:78:ILE:HD12  | 1:k:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:k:153:ALA:HA   | 1:w:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:k:295:THR:HG23 | 1:k:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:k:357:GLN:NE2  | 1:k:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:l:153:ALA:HA   | 1:n:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:m:488:ARG:O    | 1:r:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:q:134:GLN:NE2  | 1:y:153:ALA:HA   | 2.29                     | 0.47              |
| 1:u:60:ARG:HG3   | 1:u:177:MET:HG3  | 1.95                     | 0.47              |
| 1:u:371:ASN:HB2  | 1:u:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:u:488:ARG:O    | 1:1:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:w:295:THR:HG23 | 1:w:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:2:409:ILE:H    | 1:2:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:5:371:ASN:HB2  | 1:5:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:6:270:TYR:O    | 1:7:350:GLU:HG2  | 2.13                     | 0.47              |
| 1:7:371:ASN:HB2  | 1:7:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:8:60:ARG:HG3   | 1:8:177:MET:HG3  | 1.95                     | 0.47              |
| 1:A:436:ALA:C    | 1:A:437:MET:HG3  | 2.39                     | 0.47              |
| 1:B:109:GLN:NE2  | 1:I:488:ARG:O    | 2.47                     | 0.47              |
| 1:B:179:GLU:OE2  | 1:B:411:ARG:NH1  | 2.38                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:229:LEU:HD22 | 1:C:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:C:295:THR:HG23 | 1:C:380:GLN:HB3  | 1.96                     | 0.47              |
| 1:D:78:ILE:HD12  | 1:D:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:D:357:GLN:NE2  | 1:D:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:J:383:TYR:HE2  | 1:L:318:VAL:HG21 | 1.80                     | 0.47              |
| 1:J:488:ARG:O    | 1:K:109:GLN:NE2  | 2.48                     | 0.47              |
| 1:M:350:GLU:HG2  | 1:b:270:TYR:O    | 2.14                     | 0.47              |
| 1:N:371:ASN:HB2  | 1:N:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:U:409:ILE:H    | 1:U:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:X:153:ALA:HA   | 1:f:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:Y:409:ILE:H    | 1:Y:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:a:371:ASN:HB2  | 1:a:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:a:382:LEU:HD12 | 1:a:396:VAL:HG22 | 1.94                     | 0.47              |
| 1:b:134:GLN:NE2  | 1:o:153:ALA:HA   | 2.30                     | 0.47              |
| 1:d:136:LYS:NZ   | 1:d:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:e:357:GLN:NE2  | 1:e:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:g:295:THR:HG23 | 1:g:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:i:60:ARG:HG3   | 1:i:177:MET:HG3  | 1.95                     | 0.47              |
| 1:i:371:ASN:HB2  | 1:i:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:k:371:ASN:HB2  | 1:k:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:m:179:GLU:OE2  | 1:m:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:m:409:ILE:H    | 1:m:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:n:229:LEU:HD22 | 1:n:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:u:109:GLN:NE2  | 1:l:488:ARG:O    | 2.47                     | 0.47              |
| 1:v:436:ALA:C    | 1:v:437:MET:HG3  | 2.39                     | 0.47              |
| 1:z:350:GLU:HG2  | 1:2:270:TYR:O    | 2.14                     | 0.47              |
| 1:1:295:THR:HG23 | 1:1:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:3:229:LEU:HA   | 1:3:233:GLU:OE1  | 2.12                     | 0.47              |
| 1:5:179:GLU:OE2  | 1:5:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:5:295:THR:HG23 | 1:5:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:7:436:ALA:C    | 1:7:437:MET:HG3  | 2.39                     | 0.47              |
| 1:8:136:LYS:NZ   | 1:8:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:A:318:VAL:HG21 | 1:I:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:B:488:ARG:O    | 1:I:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:C:153:ALA:HA   | 1:D:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:C:338:ASP:HA   | 1:C:339:PRO:C    | 2.38                     | 0.47              |
| 1:D:371:ASN:HB2  | 1:D:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:H:436:ALA:C    | 1:H:437:MET:HG3  | 2.39                     | 0.47              |
| 1:L:451:ILE:HD12 | 1:L:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:T:78:ILE:HD12  | 1:T:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:T:153:ALA:HA   | 1:i:134:GLN:NE2  | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:295:THR:HG23 | 1:V:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:W:436:ALA:C    | 1:W:437:MET:HG3  | 2.39                     | 0.47              |
| 1:Y:338:ASP:HA   | 1:Y:339:PRO:C    | 2.38                     | 0.47              |
| 1:Y:436:ALA:C    | 1:Y:437:MET:HG3  | 2.39                     | 0.47              |
| 1:Z:60:ARG:HG3   | 1:Z:177:MET:HG3  | 1.95                     | 0.47              |
| 1:Z:136:LYS:NZ   | 1:Z:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:d:371:ASN:HB2  | 1:d:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:g:153:ALA:HA   | 1:k:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:g:409:ILE:H    | 1:g:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:h:436:ALA:C    | 1:h:437:MET:HG3  | 2.39                     | 0.47              |
| 1:m:78:ILE:HD12  | 1:m:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:n:371:ASN:HB2  | 1:n:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:p:295:THR:HG23 | 1:p:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:r:136:LYS:NZ   | 1:r:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:t:78:ILE:HD12  | 1:t:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:u:78:ILE:HD12  | 1:u:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:u:383:TYR:HE2  | 1:v:318:VAL:HG21 | 1.80                     | 0.47              |
| 1:z:153:ALA:HA   | 1:4:134:GLN:NE2  | 2.29                     | 0.47              |
| 1:z:318:VAL:HG21 | 1:2:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:2:60:ARG:HG3   | 1:2:177:MET:HG3  | 1.95                     | 0.47              |
| 1:2:179:GLU:OE2  | 1:2:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:3:229:LEU:HD22 | 1:3:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:3:371:ASN:HB2  | 1:3:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:5:270:TYR:O    | 1:6:350:GLU:HG2  | 2.13                     | 0.47              |
| 1:5:409:ILE:H    | 1:5:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:5:436:ALA:C    | 1:5:437:MET:HG3  | 2.39                     | 0.47              |
| 1:7:338:ASP:HA   | 1:7:339:PRO:C    | 2.38                     | 0.47              |
| 1:7:409:ILE:H    | 1:7:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:E:51:ASP:OD1   | 1:E:481:ARG:NE   | 2.39                     | 0.47              |
| 1:F:73:ARG:HD2   | 1:R:514:LYS:O    | 2.15                     | 0.47              |
| 1:F:318:VAL:HG21 | 1:Q:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:G:78:ILE:HD12  | 1:G:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:H:270:TYR:O    | 1:W:350:GLU:HG2  | 2.13                     | 0.47              |
| 1:H:409:ILE:H    | 1:H:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:I:78:ILE:HD12  | 1:I:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:N:134:GLN:NE2  | 1:m:153:ALA:HA   | 2.30                     | 0.47              |
| 1:N:294:MET:CE   | 1:N:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:Q:179:GLU:OE2  | 1:Q:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:S:371:ASN:HB2  | 1:S:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:T:436:ALA:C    | 1:T:437:MET:HG3  | 2.39                     | 0.47              |
| 1:T:514:LYS:O    | 1:U:73:ARG:HD2   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:371:ASN:HB2  | 1:W:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:Z:451:ILE:HD12 | 1:Z:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:c:357:GLN:NE2  | 1:c:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:e:109:GLN:NE2  | 1:f:488:ARG:O    | 2.47                     | 0.47              |
| 1:f:73:ARG:HD2   | 1:z:514:LYS:O    | 2.15                     | 0.47              |
| 1:i:294:MET:CE   | 1:i:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:k:136:LYS:NZ   | 1:k:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:m:436:ALA:C    | 1:m:437:MET:HG3  | 2.39                     | 0.47              |
| 1:m:514:LYS:O    | 1:s:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:p:371:ASN:HB2  | 1:p:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:q:514:LYS:O    | 1:y:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:s:378:ARG:HD2  | 1:s:378:ARG:HA   | 1.73                     | 0.47              |
| 1:s:409:ILE:H    | 1:s:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:t:436:ALA:C    | 1:t:437:MET:HG3  | 2.39                     | 0.47              |
| 1:x:179:GLU:OE2  | 1:x:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:x:383:TYR:HE2  | 1:y:318:VAL:HG21 | 1.80                     | 0.47              |
| 1:z:270:TYR:O    | 1:l:350:GLU:HG2  | 2.15                     | 0.47              |
| 1:z:451:ILE:HD12 | 1:z:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:6:371:ASN:HB2  | 1:6:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:A:294:MET:CE   | 1:A:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:A:371:ASN:HB2  | 1:A:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:A:451:ILE:HD12 | 1:A:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:B:295:THR:HG23 | 1:B:380:GLN:HB3  | 1.96                     | 0.47              |
| 1:C:270:TYR:O    | 1:b:350:GLU:HG2  | 2.14                     | 0.47              |
| 1:C:350:GLU:HG2  | 1:M:270:TYR:O    | 2.14                     | 0.47              |
| 1:E:318:VAL:HG21 | 1:F:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:F:357:GLN:NE2  | 1:F:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:F:514:LYS:O    | 1:G:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:G:134:GLN:NE2  | 1:W:153:ALA:HA   | 2.30                     | 0.47              |
| 1:G:436:ALA:C    | 1:G:437:MET:HG3  | 2.39                     | 0.47              |
| 1:H:153:ALA:HA   | 1:Z:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:I:294:MET:CE   | 1:I:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:I:514:LYS:O    | 1:J:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:J:371:ASN:HB2  | 1:J:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:K:153:ALA:HA   | 1:7:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:M:357:GLN:NE2  | 1:M:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:M:436:ALA:C    | 1:M:437:MET:HG3  | 2.39                     | 0.47              |
| 1:O:78:ILE:HD12  | 1:O:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:Q:109:GLN:NE2  | 1:R:488:ARG:O    | 2.47                     | 0.47              |
| 1:Q:133:LEU:HD23 | 1:Q:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:R:318:VAL:HG21 | 1:U:383:TYR:HE2  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:331:ALA:HB2  | 1:U:390:TYR:CE2  | 2.50                     | 0.47              |
| 1:R:371:ASN:HB2  | 1:R:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:S:78:ILE:HD12  | 1:S:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:S:134:GLN:NE2  | 1:d:153:ALA:HA   | 2.29                     | 0.47              |
| 1:S:409:ILE:H    | 1:S:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:T:371:ASN:HB2  | 1:T:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:U:133:LEU:HD23 | 1:U:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:U:294:MET:CE   | 1:U:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:U:356:TYR:CE1  | 1:U:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:V:73:ARG:HD2   | 1:W:514:LYS:O    | 2.15                     | 0.47              |
| 1:V:234:SER:O    | 1:W:29:GLY:N     | 2.33                     | 0.47              |
| 1:V:318:VAL:HG21 | 1:X:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:V:371:ASN:HB2  | 1:V:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:W:136:LYS:NZ   | 1:W:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:Y:134:GLN:NE2  | 1:4:153:ALA:HA   | 2.30                     | 0.47              |
| 1:Y:136:LYS:NZ   | 1:Y:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:Z:356:TYR:CE1  | 1:Z:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:a:109:GLN:NE2  | 1:3:488:ARG:O    | 2.47                     | 0.47              |
| 1:a:294:MET:CE   | 1:a:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:a:488:ARG:O    | 1:3:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:b:294:MET:CE   | 1:b:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:b:488:ARG:O    | 1:c:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:d:294:MET:CE   | 1:d:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:f:294:MET:CE   | 1:f:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:f:350:GLU:HG2  | 1:g:270:TYR:O    | 2.14                     | 0.47              |
| 1:l:78:ILE:HD12  | 1:l:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:l:133:LEU:HD23 | 1:l:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:l:294:MET:CE   | 1:l:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:n:136:LYS:NZ   | 1:n:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:n:153:ALA:HA   | 1:r:134:GLN:NE2  | 2.29                     | 0.47              |
| 1:n:294:MET:CE   | 1:n:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:o:383:TYR:HE2  | 1:p:318:VAL:HG21 | 1.80                     | 0.47              |
| 1:p:73:ARG:HD2   | 1:6:514:LYS:O    | 2.15                     | 0.47              |
| 1:p:134:GLN:NE2  | 1:q:153:ALA:HA   | 2.30                     | 0.47              |
| 1:p:153:ALA:HA   | 1:6:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:q:318:VAL:HG21 | 1:s:383:TYR:HE2  | 1.79                     | 0.47              |
| 1:q:331:ALA:HB2  | 1:s:390:TYR:CE2  | 2.50                     | 0.47              |
| 1:q:371:ASN:HB2  | 1:q:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:q:488:ARG:O    | 1:x:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:r:371:ASN:HB2  | 1:r:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:r:451:ILE:HD12 | 1:r:465:ILE:HD13 | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:133:LEU:HD23 | 1:s:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:s:294:MET:CE   | 1:s:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:s:356:TYR:CE1  | 1:s:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:t:73:ARG:HD2   | 1:y:514:LYS:O    | 2.15                     | 0.47              |
| 1:t:134:GLN:NE2  | 1:6:153:ALA:HA   | 2.30                     | 0.47              |
| 1:u:134:GLN:NE2  | 1:2:153:ALA:HA   | 2.30                     | 0.47              |
| 1:v:294:MET:CE   | 1:v:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:v:371:ASN:HB2  | 1:v:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:w:294:MET:CE   | 1:w:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:w:318:VAL:HG21 | 1:y:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:x:133:LEU:HD23 | 1:x:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:y:357:GLN:NE2  | 1:y:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:1:179:GLU:OE2  | 1:1:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:2:371:ASN:HB2  | 1:2:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:3:294:MET:CE   | 1:3:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:3:382:LEU:HD12 | 1:3:396:VAL:HG22 | 1.95                     | 0.47              |
| 1:4:295:THR:HG23 | 1:4:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:5:153:ALA:HA   | 1:8:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:6:436:ALA:C    | 1:6:437:MET:HG3  | 2.39                     | 0.47              |
| 1:7:136:LYS:NZ   | 1:7:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:8:294:MET:CE   | 1:8:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:8:356:TYR:CE1  | 1:8:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:8:451:ILE:HD12 | 1:8:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:A:73:ARG:HD2   | 1:B:514:LYS:O    | 2.15                     | 0.47              |
| 1:D:229:LEU:HD22 | 1:D:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:E:109:GLN:NE2  | 1:P:488:ARG:O    | 2.48                     | 0.47              |
| 1:E:294:MET:CE   | 1:E:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:G:109:GLN:NE2  | 1:H:488:ARG:O    | 2.48                     | 0.47              |
| 1:G:514:LYS:O    | 1:W:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:H:234:SER:O    | 1:Z:29:GLY:N     | 2.32                     | 0.47              |
| 1:I:356:TYR:CE1  | 1:I:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:J:179:GLU:OE2  | 1:J:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:K:295:THR:HG23 | 1:K:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:K:409:ILE:H    | 1:K:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:M:134:GLN:NE2  | 1:N:153:ALA:HA   | 2.30                     | 0.47              |
| 1:N:136:LYS:NZ   | 1:N:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:O:133:LEU:HD23 | 1:O:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:O:294:MET:CE   | 1:O:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:R:153:ALA:HA   | 1:V:134:GLN:NE2  | 2.30                     | 0.47              |
| 1:S:451:ILE:HD12 | 1:S:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:V:153:ALA:HA   | 1:W:134:GLN:NE2  | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:356:TYR:CE1  | 1:Y:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:Z:294:MET:CE   | 1:Z:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:Z:295:THR:HG23 | 1:Z:380:GLN:HB3  | 1.96                     | 0.47              |
| 1:b:356:TYR:CE1  | 1:b:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:f:356:TYR:CE1  | 1:f:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:f:357:GLN:NE2  | 1:f:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:g:294:MET:CE   | 1:g:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:g:371:ASN:HB2  | 1:g:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:m:371:ASN:HB2  | 1:m:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:p:234:SER:O    | 1:6:29:GLY:N     | 2.33                     | 0.47              |
| 1:q:356:TYR:CE1  | 1:q:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:r:78:ILE:HD12  | 1:r:79:PRO:HD2   | 1.95                     | 0.47              |
| 1:r:409:ILE:H    | 1:r:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:t:109:GLN:NE2  | 1:5:488:ARG:O    | 2.48                     | 0.47              |
| 1:t:514:LYS:O    | 1:6:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:u:294:MET:CE   | 1:u:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:u:356:TYR:CE1  | 1:u:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:v:451:ILE:HD12 | 1:v:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:w:51:ASP:OD1   | 1:w:481:ARG:NE   | 2.39                     | 0.47              |
| 1:w:356:TYR:CE1  | 1:w:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:w:409:ILE:H    | 1:w:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:2:229:LEU:HD11 | 1:2:235:THR:HG23 | 1.97                     | 0.47              |
| 1:3:436:ALA:C    | 1:3:437:MET:HG3  | 2.39                     | 0.47              |
| 1:6:356:TYR:CE1  | 1:6:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:8:295:THR:HG23 | 1:8:380:GLN:HB3  | 1.96                     | 0.47              |
| 1:A:153:ALA:HA   | 1:B:134:GLN:NE2  | 2.29                     | 0.47              |
| 1:C:294:MET:CE   | 1:C:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:C:371:ASN:HB2  | 1:C:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:E:356:TYR:CE1  | 1:E:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:F:356:TYR:CE1  | 1:F:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:I:134:GLN:NE2  | 1:J:153:ALA:HA   | 2.30                     | 0.47              |
| 1:K:451:ILE:HD12 | 1:K:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:N:488:ARG:O    | 1:O:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:O:73:ARG:HD2   | 1:d:514:LYS:O    | 2.15                     | 0.47              |
| 1:O:318:VAL:HG21 | 1:n:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:O:514:LYS:O    | 1:P:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:P:133:LEU:HD23 | 1:P:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:P:356:TYR:CE1  | 1:P:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:R:356:TYR:CE1  | 1:R:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:V:229:LEU:HD11 | 1:V:235:THR:HG23 | 1.97                     | 0.47              |
| 1:V:229:LEU:HD22 | 1:V:233:GLU:HB3  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:451:ILE:HD12 | 1:V:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:W:356:TYR:CE1  | 1:W:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:a:229:LEU:HD11 | 1:a:235:THR:HG23 | 1.97                     | 0.47              |
| 1:b:357:GLN:NE2  | 1:b:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:b:451:ILE:HD12 | 1:b:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:c:133:LEU:HD23 | 1:c:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:d:383:TYR:HE2  | 1:l:318:VAL:HG21 | 1.80                     | 0.47              |
| 1:f:451:ILE:HD12 | 1:f:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:g:350:GLU:HG2  | 1:h:270:TYR:O    | 2.14                     | 0.47              |
| 1:h:357:GLN:NE2  | 1:h:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:h:451:ILE:HD12 | 1:h:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:i:136:LYS:NZ   | 1:i:149:ASN:OD1  | 2.37                     | 0.47              |
| 1:j:73:ARG:HD2   | 1:l:514:LYS:O    | 2.15                     | 0.47              |
| 1:j:109:GLN:NE2  | 1:w:488:ARG:O    | 2.47                     | 0.47              |
| 1:j:133:LEU:HD23 | 1:j:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:j:356:TYR:CE1  | 1:j:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:k:229:LEU:HD22 | 1:k:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:l:73:ARG:HD2   | 1:n:514:LYS:O    | 2.15                     | 0.47              |
| 1:l:371:ASN:HB2  | 1:l:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:p:229:LEU:HD22 | 1:p:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:p:229:LEU:HD11 | 1:p:235:THR:HG23 | 1.97                     | 0.47              |
| 1:s:179:GLU:OE2  | 1:s:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:t:179:GLU:OE2  | 1:t:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:t:331:ALA:HB2  | 1:v:390:TYR:CE2  | 2.50                     | 0.47              |
| 1:v:73:ARG:HD2   | 1:l:514:LYS:O    | 2.15                     | 0.47              |
| 1:y:356:TYR:CE1  | 1:y:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:2:356:TYR:CE1  | 1:2:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:3:229:LEU:HD11 | 1:3:235:THR:HG23 | 1.97                     | 0.47              |
| 1:3:295:THR:HG23 | 1:3:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:4:409:ILE:H    | 1:4:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:6:229:LEU:HD22 | 1:6:233:GLU:HB3  | 1.95                     | 0.47              |
| 1:7:356:TYR:CE1  | 1:7:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:8:371:ASN:HB2  | 1:8:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:A:390:TYR:CE2  | 1:G:331:ALA:HB2  | 2.50                     | 0.47              |
| 1:B:371:ASN:HB2  | 1:B:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:D:73:ARG:HD2   | 1:E:514:LYS:O    | 2.15                     | 0.47              |
| 1:D:294:MET:CE   | 1:D:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:E:229:LEU:HD11 | 1:E:235:THR:HG23 | 1.97                     | 0.47              |
| 1:E:409:ILE:H    | 1:E:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:E:488:ARG:O    | 1:P:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:H:134:GLN:NE2  | 1:I:153:ALA:HA   | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:514:LYS:O    | 1:I:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:I:338:ASP:HA   | 1:I:339:PRO:C    | 2.38                     | 0.47              |
| 1:J:229:LEU:HD11 | 1:J:235:THR:HG23 | 1.97                     | 0.47              |
| 1:J:356:TYR:CE1  | 1:J:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:L:356:TYR:CE1  | 1:L:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:M:294:MET:CE   | 1:M:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:M:451:ILE:HD12 | 1:M:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:O:309:GLY:O    | 1:n:287:TYR:OH   | 2.28                     | 0.47              |
| 1:O:371:ASN:HB2  | 1:O:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:P:294:MET:CE   | 1:P:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:P:436:ALA:C    | 1:P:437:MET:HG3  | 2.39                     | 0.47              |
| 1:Q:356:TYR:CE1  | 1:Q:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:Q:409:ILE:H    | 1:Q:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:S:294:MET:CE   | 1:S:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:T:294:MET:CE   | 1:T:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:V:436:ALA:C    | 1:V:437:MET:HG3  | 2.39                     | 0.47              |
| 1:Z:85:LYS:CG    | 1:Z:332:GLY:HA3  | 2.45                     | 0.47              |
| 1:Z:371:ASN:HB2  | 1:Z:524:TRP:CE3  | 2.50                     | 0.47              |
| 1:a:85:LYS:CG    | 1:a:332:GLY:HA3  | 2.46                     | 0.47              |
| 1:a:295:THR:HG23 | 1:a:380:GLN:HB3  | 1.95                     | 0.47              |
| 1:a:436:ALA:C    | 1:a:437:MET:HG3  | 2.39                     | 0.47              |
| 1:c:318:VAL:HG21 | 1:p:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:e:133:LEU:HD23 | 1:e:469:GLY:HA3  | 1.95                     | 0.47              |
| 1:h:134:GLN:NE2  | 1:i:153:ALA:HA   | 2.30                     | 0.47              |
| 1:h:294:MET:CE   | 1:h:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:j:488:ARG:O    | 1:w:109:GLN:NE2  | 2.47                     | 0.47              |
| 1:k:294:MET:CE   | 1:k:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:m:294:MET:CE   | 1:m:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:o:356:TYR:CE1  | 1:o:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:o:390:TYR:CE2  | 1:p:331:ALA:HB2  | 2.50                     | 0.47              |
| 1:p:451:ILE:HD12 | 1:p:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:q:357:GLN:NE2  | 1:q:368:ILE:HD12 | 2.29                     | 0.47              |
| 1:r:294:MET:CE   | 1:r:382:LEU:HD11 | 2.45                     | 0.47              |
| 1:t:318:VAL:HG21 | 1:v:383:TYR:HE2  | 1.80                     | 0.47              |
| 1:u:73:ARG:HD2   | 1:5:514:LYS:O    | 2.15                     | 0.47              |
| 1:v:153:ALA:HA   | 1:1:134:GLN:NE2  | 2.29                     | 0.47              |
| 1:v:514:LYS:O    | 1:w:73:ARG:HD2   | 2.15                     | 0.47              |
| 1:w:179:GLU:OE2  | 1:w:411:ARG:NH1  | 2.38                     | 0.47              |
| 1:w:229:LEU:HD11 | 1:w:235:THR:HG23 | 1.97                     | 0.47              |
| 1:x:356:TYR:CE1  | 1:x:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:x:409:ILE:H    | 1:x:530:ILE:HG12 | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:y:409:ILE:H    | 1:y:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:z:356:TYR:CE1  | 1:z:367:ASN:HB3  | 2.50                     | 0.47              |
| 1:2:134:GLN:NE2  | 1:3:153:ALA:HA   | 2.29                     | 0.47              |
| 1:3:85:LYS:CG    | 1:3:332:GLY:HA3  | 2.45                     | 0.47              |
| 1:3:134:GLN:NE2  | 1:8:153:ALA:HA   | 2.30                     | 0.47              |
| 1:4:451:ILE:HD12 | 1:4:465:ILE:HD13 | 1.97                     | 0.47              |
| 1:8:85:LYS:CG    | 1:8:332:GLY:HA3  | 2.45                     | 0.47              |
| 1:8:409:ILE:H    | 1:8:530:ILE:HG12 | 1.79                     | 0.47              |
| 1:A:514:LYS:O    | 1:E:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:B:387:GLN:HA   | 1:J:305:VAL:HG22 | 1.95                     | 0.46              |
| 1:B:451:ILE:HD12 | 1:B:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:C:85:LYS:CG    | 1:C:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:E:179:GLU:OE2  | 1:E:411:ARG:NH1  | 2.38                     | 0.46              |
| 1:F:85:LYS:CG    | 1:F:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:F:409:ILE:H    | 1:F:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:K:85:LYS:CG    | 1:K:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:L:134:GLN:NE2  | 1:b:153:ALA:HA   | 2.29                     | 0.46              |
| 1:L:514:LYS:O    | 1:b:73:ARG:HD2   | 2.16                     | 0.46              |
| 1:O:85:LYS:CG    | 1:O:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:P:179:GLU:OE2  | 1:P:411:ARG:NH1  | 2.38                     | 0.46              |
| 1:Q:85:LYS:CG    | 1:Q:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:R:294:MET:CE   | 1:R:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:R:357:GLN:NE2  | 1:R:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:S:357:GLN:NE2  | 1:S:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:V:331:ALA:HB2  | 1:X:390:TYR:CE2  | 2.50                     | 0.46              |
| 1:V:383:TYR:HE2  | 1:e:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:W:229:LEU:HD22 | 1:W:233:GLU:HB3  | 1.95                     | 0.46              |
| 1:X:134:GLN:NE2  | 1:Y:153:ALA:HA   | 2.30                     | 0.46              |
| 1:X:356:TYR:CE1  | 1:X:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:Y:229:LEU:HD11 | 1:Y:235:THR:HG23 | 1.97                     | 0.46              |
| 1:Z:153:ALA:HA   | 1:a:134:GLN:NE2  | 2.30                     | 0.46              |
| 1:g:85:LYS:CG    | 1:g:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:h:514:LYS:O    | 1:i:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:i:488:ARG:O    | 1:l:109:GLN:NE2  | 2.47                     | 0.46              |
| 1:j:294:MET:CE   | 1:j:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:k:73:ARG:HD2   | 1:w:514:LYS:O    | 2.15                     | 0.46              |
| 1:l:85:LYS:CG    | 1:l:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:n:229:LEU:HD11 | 1:n:235:THR:HG23 | 1.97                     | 0.46              |
| 1:r:229:LEU:HD11 | 1:r:235:THR:HG23 | 1.97                     | 0.46              |
| 1:r:383:TYR:HE2  | 1:s:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:u:153:ALA:HA   | 1:5:134:GLN:NE2  | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:338:ASP:HA   | 1:u:339:PRO:C    | 2.38                     | 0.46              |
| 1:v:229:LEU:HD11 | 1:v:235:THR:HG23 | 1.97                     | 0.46              |
| 1:x:85:LYS:CG    | 1:x:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:y:85:LYS:CG    | 1:y:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:z:371:ASN:HB2  | 1:z:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:1:451:ILE:HD12 | 1:1:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:4:85:LYS:CG    | 1:4:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:6:136:LYS:NZ   | 1:6:149:ASN:OD1  | 2.37                     | 0.46              |
| 1:7:229:LEU:HD11 | 1:7:235:THR:HG23 | 1.97                     | 0.46              |
| 1:7:451:ILE:HD12 | 1:7:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:229:LEU:HD11 | 1:A:235:THR:HG23 | 1.97                     | 0.46              |
| 1:A:383:TYR:HE2  | 1:G:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:F:371:ASN:HB2  | 1:F:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:K:134:GLN:NE2  | 1:L:153:ALA:HA   | 2.30                     | 0.46              |
| 1:K:406:ARG:HB2  | 1:K:531:LYS:HZ1  | 1.80                     | 0.46              |
| 1:M:514:LYS:O    | 1:N:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:Q:371:ASN:HB2  | 1:Q:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:Q:451:ILE:HD12 | 1:Q:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:Q:514:LYS:O    | 1:S:73:ARG:HD2   | 2.16                     | 0.46              |
| 1:T:318:VAL:HG21 | 1:l:383:TYR:HE2  | 1.80                     | 0.46              |
| 1:T:383:TYR:HE2  | 1:d:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:U:451:ILE:HD12 | 1:U:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:V:356:TYR:CE1  | 1:V:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:X:318:VAL:HG21 | 1:e:383:TYR:HE2  | 1.80                     | 0.46              |
| 1:X:451:ILE:HD12 | 1:X:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:X:514:LYS:O    | 1:Y:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:Y:451:ILE:HD12 | 1:Y:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:Z:51:ASP:OD1   | 1:Z:481:ARG:NE   | 2.39                     | 0.46              |
| 1:Z:409:ILE:H    | 1:Z:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:c:383:TYR:HE2  | 1:o:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:c:436:ALA:C    | 1:c:437:MET:HG3  | 2.39                     | 0.46              |
| 1:d:229:LEU:HD11 | 1:d:235:THR:HG23 | 1.97                     | 0.46              |
| 1:e:436:ALA:C    | 1:e:437:MET:HG3  | 2.39                     | 0.46              |
| 1:f:295:THR:HG23 | 1:f:380:GLN:HB3  | 1.95                     | 0.46              |
| 1:j:436:ALA:C    | 1:j:437:MET:HG3  | 2.39                     | 0.46              |
| 1:o:451:ILE:HD12 | 1:o:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:o:514:LYS:O    | 1:7:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:q:294:MET:CE   | 1:q:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:r:73:ARG:HD2   | 1:x:514:LYS:O    | 2.16                     | 0.46              |
| 1:r:357:GLN:NE2  | 1:r:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:s:451:ILE:HD12 | 1:s:465:ILE:HD13 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:294:MET:CE   | 1:t:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:t:371:ASN:HB2  | 1:t:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:x:371:ASN:HB2  | 1:x:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:y:371:ASN:HB2  | 1:y:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:z:73:ARG:HD2   | 1:4:514:LYS:O    | 2.15                     | 0.46              |
| 1:z:331:ALA:HB2  | 1:2:390:TYR:CE2  | 2.50                     | 0.46              |
| 1:z:390:TYR:CE2  | 1:1:331:ALA:HB2  | 2.50                     | 0.46              |
| 1:1:371:ASN:HB2  | 1:1:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:2:514:LYS:O    | 1:3:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:5:294:MET:CE   | 1:5:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:B:357:GLN:NE2  | 1:B:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:E:383:TYR:HE2  | 1:Q:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:F:134:GLN:NE2  | 1:G:153:ALA:HA   | 2.30                     | 0.46              |
| 1:G:179:GLU:OE2  | 1:G:411:ARG:NH1  | 2.38                     | 0.46              |
| 1:H:229:LEU:HD11 | 1:H:235:THR:HG23 | 1.97                     | 0.46              |
| 1:J:85:LYS:CG    | 1:J:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:L:229:LEU:HD11 | 1:L:235:THR:HG23 | 1.97                     | 0.46              |
| 1:L:371:ASN:HB2  | 1:L:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:O:383:TYR:HE2  | 1:m:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:P:134:GLN:NE2  | 1:Q:153:ALA:HA   | 2.30                     | 0.46              |
| 1:R:436:ALA:C    | 1:R:437:MET:HG3  | 2.39                     | 0.46              |
| 1:S:51:ASP:OD1   | 1:S:481:ARG:NE   | 2.38                     | 0.46              |
| 1:S:229:LEU:HD11 | 1:S:235:THR:HG23 | 1.97                     | 0.46              |
| 1:S:383:TYR:HE2  | 1:U:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:T:85:LYS:CG    | 1:T:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:W:51:ASP:OD1   | 1:W:481:ARG:NE   | 2.38                     | 0.46              |
| 1:b:85:LYS:CG    | 1:b:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:d:85:LYS:CG    | 1:d:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:e:85:LYS:CG    | 1:e:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:e:514:LYS:O    | 1:h:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:f:85:LYS:CG    | 1:f:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:i:51:ASP:OD1   | 1:i:481:ARG:NE   | 2.38                     | 0.46              |
| 1:i:318:VAL:HG21 | 1:k:383:TYR:HE2  | 1.80                     | 0.46              |
| 1:m:383:TYR:HE2  | 1:n:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:n:409:ILE:H    | 1:n:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:o:134:GLN:NE2  | 1:7:153:ALA:HA   | 2.30                     | 0.46              |
| 1:p:356:TYR:CE1  | 1:p:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:q:85:LYS:CG    | 1:q:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:t:153:ALA:HA   | 1:y:134:GLN:NE2  | 2.30                     | 0.46              |
| 1:t:409:ILE:H    | 1:t:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:w:383:TYR:HE2  | 1:x:318:VAL:HG21 | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:451:ILE:HD12 | 1:x:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:1:357:GLN:NE2  | 1:1:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:5:229:LEU:HD11 | 1:5:235:THR:HG23 | 1.97                     | 0.46              |
| 1:8:357:GLN:NE2  | 1:8:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:D:383:TYR:HE2  | 1:N:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:G:294:MET:CE   | 1:G:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:G:371:ASN:HB2  | 1:G:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:H:294:MET:CE   | 1:H:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:K:356:TYR:CE1  | 1:K:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:M:73:ARG:HD2   | 1:c:514:LYS:O    | 2.15                     | 0.46              |
| 1:N:51:ASP:OD1   | 1:N:481:ARG:NE   | 2.38                     | 0.46              |
| 1:R:85:LYS:CG    | 1:R:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:S:85:LYS:CG    | 1:S:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:X:85:LYS:CG    | 1:X:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:X:357:GLN:NE2  | 1:X:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:Z:127:HIS:HD2  | 1:Z:238:THR:HG22 | 1.81                     | 0.46              |
| 1:b:295:THR:HG23 | 1:b:380:GLN:HB3  | 1.95                     | 0.46              |
| 1:c:85:LYS:CG    | 1:c:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:f:383:TYR:HE2  | 1:h:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:m:68:ASN:HB2   | 1:m:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:m:85:LYS:CG    | 1:m:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:n:85:LYS:CG    | 1:n:332:GLY:HA3  | 2.45                     | 0.46              |
| 1:o:229:LEU:HD11 | 1:o:235:THR:HG23 | 1.97                     | 0.46              |
| 1:p:294:MET:CE   | 1:p:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:q:350:GLU:HG2  | 1:s:270:TYR:O    | 2.15                     | 0.46              |
| 1:r:85:LYS:CG    | 1:r:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:v:357:GLN:NE2  | 1:v:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:w:85:LYS:CG    | 1:w:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:1:229:LEU:HD11 | 1:1:235:THR:HG23 | 1.97                     | 0.46              |
| 1:4:51:ASP:OD1   | 1:4:481:ARG:NE   | 2.38                     | 0.46              |
| 1:5:234:SER:O    | 1:8:29:GLY:N     | 2.32                     | 0.46              |
| 1:6:294:MET:CE   | 1:6:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:6:451:ILE:HD12 | 1:6:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:8:51:ASP:OD1   | 1:8:481:ARG:NE   | 2.38                     | 0.46              |
| 1:8:127:HIS:HD2  | 1:8:238:THR:HG22 | 1.81                     | 0.46              |
| 1:B:229:LEU:HD11 | 1:B:235:THR:HG23 | 1.97                     | 0.46              |
| 1:B:294:MET:CE   | 1:B:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:D:390:TYR:CE2  | 1:N:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:E:85:LYS:CG    | 1:E:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:E:136:LYS:NZ   | 1:E:149:ASN:OD1  | 2.37                     | 0.46              |
| 1:E:451:ILE:HD12 | 1:E:465:ILE:HD13 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:85:LYS:CG    | 1:G:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:G:412:GLU:OE1  | 1:G:412:GLU:N    | 2.49                     | 0.46              |
| 1:J:412:GLU:OE1  | 1:J:412:GLU:N    | 2.49                     | 0.46              |
| 1:K:294:MET:CE   | 1:K:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:K:412:GLU:N    | 1:K:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:M:85:LYS:CG    | 1:M:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:M:229:LEU:HD11 | 1:M:235:THR:HG23 | 1.97                     | 0.46              |
| 1:M:318:VAL:HG21 | 1:b:383:TYR:HE2  | 1.80                     | 0.46              |
| 1:N:357:GLN:NE2  | 1:N:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:N:390:TYR:CE2  | 1:P:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:O:356:TYR:CE1  | 1:O:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:P:371:ASN:HB2  | 1:P:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:Q:134:GLN:NE2  | 1:S:153:ALA:HA   | 2.30                     | 0.46              |
| 1:R:350:GLU:HG2  | 1:U:270:TYR:O    | 2.15                     | 0.46              |
| 1:S:127:HIS:HD2  | 1:S:238:THR:HG22 | 1.81                     | 0.46              |
| 1:T:451:ILE:HD12 | 1:T:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:V:294:MET:CE   | 1:V:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:W:451:ILE:HD12 | 1:W:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:X:73:ARG:HD2   | 1:f:514:LYS:O    | 2.15                     | 0.46              |
| 1:X:229:LEU:HD11 | 1:X:235:THR:HG23 | 1.97                     | 0.46              |
| 1:Y:68:ASN:HB2   | 1:Y:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:Z:357:GLN:NE2  | 1:Z:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:a:390:TYR:CE2  | 1:8:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:c:371:ASN:HB2  | 1:c:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:d:409:ILE:H    | 1:d:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:e:371:ASN:HB2  | 1:e:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:f:390:TYR:CE2  | 1:h:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:h:229:LEU:HD11 | 1:h:235:THR:HG23 | 1.97                     | 0.46              |
| 1:j:134:GLN:NE2  | 1:x:153:ALA:HA   | 2.30                     | 0.46              |
| 1:j:179:GLU:OE2  | 1:j:411:ARG:NH1  | 2.38                     | 0.46              |
| 1:k:156:HIS:N    | 1:k:447:LYS:O    | 2.43                     | 0.46              |
| 1:m:451:ILE:HD12 | 1:m:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:o:85:LYS:CG    | 1:o:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:p:91:SER:HB2   | 1:p:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:r:51:ASP:OD1   | 1:r:481:ARG:NE   | 2.38                     | 0.46              |
| 1:r:127:HIS:HD2  | 1:r:238:THR:HG22 | 1.81                     | 0.46              |
| 1:t:85:LYS:CG    | 1:t:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:t:383:TYR:HE2  | 1:u:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:t:412:GLU:OE1  | 1:t:412:GLU:N    | 2.49                     | 0.46              |
| 1:x:51:ASP:OD1   | 1:x:481:ARG:NE   | 2.38                     | 0.46              |
| 1:z:229:LEU:HD11 | 1:z:235:THR:HG23 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:412:GLU:OE1  | 1:1:412:GLU:N    | 2.49                     | 0.46              |
| 1:2:85:LYS:CG    | 1:2:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:2:412:GLU:OE1  | 1:2:412:GLU:N    | 2.49                     | 0.46              |
| 1:4:356:TYR:CE1  | 1:4:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:4:412:GLU:OE1  | 1:4:412:GLU:N    | 2.49                     | 0.46              |
| 1:5:73:ARG:HD2   | 1:8:514:LYS:O    | 2.15                     | 0.46              |
| 1:7:85:LYS:CG    | 1:7:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:7:294:MET:CE   | 1:7:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:A:357:GLN:NE2  | 1:A:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:B:73:ARG:HD2   | 1:C:514:LYS:O    | 2.16                     | 0.46              |
| 1:B:318:VAL:HG21 | 1:L:383:TYR:HE2  | 1.81                     | 0.46              |
| 1:B:383:TYR:HE2  | 1:J:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:B:412:GLU:OE1  | 1:B:412:GLU:N    | 2.49                     | 0.46              |
| 1:C:73:ARG:HD2   | 1:D:514:LYS:O    | 2.15                     | 0.46              |
| 1:G:383:TYR:HE2  | 1:I:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:G:409:ILE:H    | 1:G:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:H:73:ARG:HD2   | 1:Z:514:LYS:O    | 2.15                     | 0.46              |
| 1:I:85:LYS:CG    | 1:I:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:K:331:ALA:HB2  | 1:8:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:M:331:ALA:HB2  | 1:b:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:N:85:LYS:CG    | 1:N:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:N:356:TYR:CE1  | 1:N:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:O:331:ALA:HB2  | 1:n:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:P:409:ILE:H    | 1:P:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:Q:412:GLU:OE1  | 1:Q:412:GLU:N    | 2.49                     | 0.46              |
| 1:R:91:SER:HB2   | 1:R:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:R:390:TYR:CE2  | 1:S:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:R:409:ILE:H    | 1:R:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:T:29:GLY:N     | 1:U:234:SER:O    | 2.33                     | 0.46              |
| 1:T:68:ASN:HB2   | 1:T:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:U:127:HIS:HD2  | 1:U:238:THR:HG22 | 1.81                     | 0.46              |
| 1:U:134:GLN:NE2  | 1:e:153:ALA:HA   | 2.30                     | 0.46              |
| 1:V:91:SER:HB2   | 1:V:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:W:229:LEU:HD11 | 1:W:235:THR:HG23 | 1.98                     | 0.46              |
| 1:W:294:MET:CE   | 1:W:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:X:294:MET:CE   | 1:X:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:Y:85:LYS:CG    | 1:Y:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:Y:294:MET:CE   | 1:Y:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:Y:514:LYS:O    | 1:4:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:Z:331:ALA:HB2  | 1:3:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:Z:390:TYR:CE2  | 1:4:331:ALA:HB2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:412:GLU:N    | 1:a:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:b:514:LYS:O    | 1:o:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:c:153:ALA:HA   | 1:s:134:GLN:NE2  | 2.30                     | 0.46              |
| 1:c:412:GLU:N    | 1:c:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:d:390:TYR:CE2  | 1:l:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:e:412:GLU:OE1  | 1:e:412:GLU:N    | 2.49                     | 0.46              |
| 1:g:73:ARG:HD2   | 1:k:514:LYS:O    | 2.15                     | 0.46              |
| 1:g:514:LYS:O    | 1:l:73:ARG:HD2   | 2.16                     | 0.46              |
| 1:h:85:LYS:CG    | 1:h:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:i:85:LYS:CG    | 1:i:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:i:331:ALA:HB2  | 1:k:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:i:357:GLN:NE2  | 1:i:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:i:390:TYR:CE2  | 1:j:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:j:371:ASN:HB2  | 1:j:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:l:356:TYR:CE1  | 1:l:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:n:73:ARG:HD2   | 1:r:514:LYS:O    | 2.15                     | 0.46              |
| 1:o:357:GLN:NE2  | 1:o:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:o:412:GLU:OE1  | 1:o:412:GLU:N    | 2.49                     | 0.46              |
| 1:q:91:SER:HB2   | 1:q:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:q:390:TYR:CE2  | 1:r:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:q:436:ALA:C    | 1:q:437:MET:HG3  | 2.39                     | 0.46              |
| 1:s:85:LYS:CG    | 1:s:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:u:85:LYS:CG    | 1:u:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:v:91:SER:HB2   | 1:v:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:w:451:ILE:HD12 | 1:w:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:x:68:ASN:HB2   | 1:x:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:x:412:GLU:OE1  | 1:x:412:GLU:N    | 2.49                     | 0.46              |
| 1:1:294:MET:CE   | 1:1:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:3:412:GLU:N    | 1:3:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:6:85:LYS:CG    | 1:6:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:6:229:LEU:HD11 | 1:6:235:THR:HG23 | 1.98                     | 0.46              |
| 1:8:91:SER:HB2   | 1:8:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:A:85:LYS:CG    | 1:A:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:A:91:SER:HB2   | 1:A:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:A:412:GLU:OE1  | 1:A:412:GLU:N    | 2.49                     | 0.46              |
| 1:B:356:TYR:CE1  | 1:B:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:B:381:ALA:HB3  | 1:J:318:VAL:HG22 | 1.98                     | 0.46              |
| 1:C:356:TYR:CE1  | 1:C:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:D:68:ASN:HB2   | 1:D:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:D:91:SER:HB2   | 1:D:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:D:331:ALA:HB2  | 1:P:390:TYR:CE2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:451:ILE:HD12 | 1:F:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:G:451:ILE:HD12 | 1:G:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:K:51:ASP:OD1   | 1:K:481:ARG:NE   | 2.38                     | 0.46              |
| 1:K:73:ARG:HD2   | 1:7:514:LYS:O    | 2.15                     | 0.46              |
| 1:K:229:LEU:HD11 | 1:K:235:THR:HG23 | 1.97                     | 0.46              |
| 1:L:68:ASN:HB2   | 1:L:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:M:356:TYR:CE1  | 1:M:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:O:451:ILE:HD12 | 1:O:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:Q:51:ASP:OD1   | 1:Q:481:ARG:NE   | 2.38                     | 0.46              |
| 1:Q:68:ASN:HB2   | 1:Q:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:S:412:GLU:N    | 1:S:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:S:514:LYS:O    | 1:d:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:T:229:LEU:HD11 | 1:T:235:THR:HG23 | 1.97                     | 0.46              |
| 1:U:85:LYS:CG    | 1:U:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:V:68:ASN:HB2   | 1:V:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:W:85:LYS:CG    | 1:W:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:X:371:ASN:HB2  | 1:X:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:X:412:GLU:OE1  | 1:X:412:GLU:N    | 2.49                     | 0.46              |
| 1:Z:73:ARG:HD2   | 1:a:514:LYS:O    | 2.15                     | 0.46              |
| 1:Z:91:SER:HB2   | 1:Z:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:a:356:TYR:CE1  | 1:a:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:b:91:SER:HB2   | 1:b:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:d:68:ASN:HB2   | 1:d:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:i:91:SER:HB2   | 1:i:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:i:356:TYR:CE1  | 1:i:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:j:409:ILE:H    | 1:j:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:k:91:SER:HB2   | 1:k:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:l:156:HIS:N    | 1:l:447:LYS:O    | 2.43                     | 0.46              |
| 1:m:29:GLY:N     | 1:s:234:SER:O    | 2.33                     | 0.46              |
| 1:m:229:LEU:HD11 | 1:m:235:THR:HG23 | 1.97                     | 0.46              |
| 1:n:68:ASN:HB2   | 1:n:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:n:451:ILE:HD12 | 1:n:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:o:294:MET:CE   | 1:o:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:p:68:ASN:HB2   | 1:p:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:q:156:HIS:N    | 1:q:447:LYS:O    | 2.43                     | 0.46              |
| 1:q:409:ILE:H    | 1:q:530:ILE:HG12 | 1.79                     | 0.46              |
| 1:r:153:ALA:HA   | 1:x:134:GLN:NE2  | 2.30                     | 0.46              |
| 1:r:412:GLU:OE1  | 1:r:412:GLU:N    | 2.49                     | 0.46              |
| 1:s:127:HIS:HD2  | 1:s:238:THR:HG22 | 1.81                     | 0.46              |
| 1:t:451:ILE:HD12 | 1:t:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:v:85:LYS:CG    | 1:v:332:GLY:HA3  | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:294:MET:CE   | 1:x:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:x:436:ALA:C    | 1:x:437:MET:HG3  | 2.39                     | 0.46              |
| 1:z:68:ASN:HB2   | 1:z:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:z:127:HIS:HD2  | 1:z:238:THR:HG22 | 1.81                     | 0.46              |
| 1:1:127:HIS:HD2  | 1:1:238:THR:HG22 | 1.81                     | 0.46              |
| 1:1:180:LEU:HD21 | 1:1:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:4:294:MET:CE   | 1:4:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:5:356:TYR:CE1  | 1:5:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:6:51:ASP:OD1   | 1:6:481:ARG:NE   | 2.38                     | 0.46              |
| 1:6:127:HIS:HD2  | 1:6:238:THR:HG22 | 1.81                     | 0.46              |
| 1:7:68:ASN:HB2   | 1:7:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:8:229:LEU:HD11 | 1:8:235:THR:HG23 | 1.97                     | 0.46              |
| 1:B:127:HIS:HD2  | 1:B:238:THR:HG22 | 1.81                     | 0.46              |
| 1:C:91:SER:HB2   | 1:C:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:E:390:TYR:CE2  | 1:Q:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:H:356:TYR:CE1  | 1:H:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:K:318:VAL:HG21 | 1:8:383:TYR:HE2  | 1.80                     | 0.46              |
| 1:L:127:HIS:HD2  | 1:L:238:THR:HG22 | 1.81                     | 0.46              |
| 1:N:91:SER:HB2   | 1:N:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:N:156:HIS:N    | 1:N:447:LYS:O    | 2.43                     | 0.46              |
| 1:P:68:ASN:HB2   | 1:P:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:Q:436:ALA:C    | 1:Q:437:MET:HG3  | 2.39                     | 0.46              |
| 1:R:180:LEU:HD21 | 1:R:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:S:356:TYR:CE1  | 1:S:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:V:179:GLU:OE2  | 1:V:411:ARG:NH1  | 2.38                     | 0.46              |
| 1:V:390:TYR:CE2  | 1:e:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:V:412:GLU:N    | 1:V:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:W:127:HIS:HD2  | 1:W:238:THR:HG22 | 1.81                     | 0.46              |
| 1:Z:229:LEU:HD11 | 1:Z:235:THR:HG23 | 1.97                     | 0.46              |
| 1:c:127:HIS:HD2  | 1:c:238:THR:HG22 | 1.81                     | 0.46              |
| 1:c:331:ALA:HB2  | 1:p:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:d:180:LEU:HD21 | 1:d:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:d:356:TYR:CE1  | 1:d:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:d:412:GLU:OE1  | 1:d:412:GLU:N    | 2.49                     | 0.46              |
| 1:d:451:ILE:HD12 | 1:d:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:f:91:SER:HB2   | 1:f:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:g:91:SER:HB2   | 1:g:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:h:356:TYR:CE1  | 1:h:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:j:68:ASN:HB2   | 1:j:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:j:229:LEU:HD11 | 1:j:235:THR:HG23 | 1.97                     | 0.46              |
| 1:j:390:TYR:CE2  | 1:k:331:ALA:HB2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:68:ASN:HB2   | 1:k:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:l:91:SER:HB2   | 1:l:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:m:356:TYR:CE1  | 1:m:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:m:390:TYR:CE2  | 1:n:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:n:91:SER:HB2   | 1:n:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:n:180:LEU:HD21 | 1:n:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:o:371:ASN:HB2  | 1:o:524:TRP:CE3  | 2.50                     | 0.46              |
| 1:p:179:GLU:OE2  | 1:p:411:ARG:NH1  | 2.38                     | 0.46              |
| 1:q:68:ASN:HB2   | 1:q:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:v:412:GLU:N    | 1:v:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:y:91:SER:HB2   | 1:y:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:y:127:HIS:HD2  | 1:y:238:THR:HG22 | 1.81                     | 0.46              |
| 1:3:356:TYR:CE1  | 1:3:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:4:229:LEU:HD11 | 1:4:235:THR:HG23 | 1.97                     | 0.46              |
| 1:A:180:LEU:HD21 | 1:A:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:A:331:ALA:HB2  | 1:I:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:B:180:LEU:HD21 | 1:B:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:D:356:TYR:CE1  | 1:D:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:E:68:ASN:HB2   | 1:E:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:F:91:SER:HB2   | 1:F:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:F:127:HIS:HD2  | 1:F:238:THR:HG22 | 1.81                     | 0.46              |
| 1:I:68:ASN:HB2   | 1:I:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:I:451:ILE:HD12 | 1:I:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:M:68:ASN:HB2   | 1:M:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:O:91:SER:HB2   | 1:O:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:O:229:LEU:HD11 | 1:O:235:THR:HG23 | 1.97                     | 0.46              |
| 1:O:390:TYR:CE2  | 1:m:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:P:127:HIS:HD2  | 1:P:238:THR:HG22 | 1.81                     | 0.46              |
| 1:Q:180:LEU:HD21 | 1:Q:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:Q:294:MET:CE   | 1:Q:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:R:68:ASN:HB2   | 1:R:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:S:68:ASN:HB2   | 1:S:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:S:180:LEU:HD21 | 1:S:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:T:356:TYR:CE1  | 1:T:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:T:390:TYR:CE2  | 1:d:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:T:412:GLU:OE1  | 1:T:412:GLU:N    | 2.49                     | 0.46              |
| 1:U:136:LYS:NZ   | 1:U:149:ASN:OD1  | 2.37                     | 0.46              |
| 1:U:514:LYS:O    | 1:e:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:V:180:LEU:HD21 | 1:V:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:W:91:SER:HB2   | 1:W:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:b:136:LYS:NZ   | 1:b:149:ASN:OD1  | 2.37                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:73:ARG:HD2   | 1:s:514:LYS:O    | 2.15                     | 0.46              |
| 1:c:294:MET:CE   | 1:c:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:d:91:SER:HB2   | 1:d:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:e:127:HIS:HD2  | 1:e:238:THR:HG22 | 1.81                     | 0.46              |
| 1:g:356:TYR:CE1  | 1:g:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:h:68:ASN:HB2   | 1:h:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:k:356:TYR:CE1  | 1:k:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:k:451:ILE:HD12 | 1:k:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:l:451:ILE:HD12 | 1:l:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:m:412:GLU:OE1  | 1:m:412:GLU:N    | 2.49                     | 0.46              |
| 1:n:356:TYR:CE1  | 1:n:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:n:412:GLU:N    | 1:n:412:GLU:OE1  | 2.49                     | 0.46              |
| 1:p:180:LEU:HD21 | 1:p:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:p:412:GLU:OE1  | 1:p:412:GLU:N    | 2.49                     | 0.46              |
| 1:q:180:LEU:HD21 | 1:q:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:r:68:ASN:HB2   | 1:r:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:r:356:TYR:CE1  | 1:r:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:r:406:ARG:HB2  | 1:r:531:LYS:HZ1  | 1.80                     | 0.46              |
| 1:s:136:LYS:NZ   | 1:s:149:ASN:OD1  | 2.37                     | 0.46              |
| 1:u:68:ASN:HB2   | 1:u:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:u:357:GLN:NE2  | 1:u:368:ILE:HD12 | 2.29                     | 0.46              |
| 1:u:390:TYR:CE2  | 1:v:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:u:514:LYS:O    | 1:2:73:ARG:HD2   | 2.16                     | 0.46              |
| 1:v:180:LEU:HD21 | 1:v:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:w:68:ASN:HB2   | 1:w:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:w:136:LYS:NZ   | 1:w:149:ASN:OD1  | 2.37                     | 0.46              |
| 1:w:390:TYR:CE2  | 1:x:331:ALA:HB2  | 2.51                     | 0.46              |
| 1:x:180:LEU:HD21 | 1:x:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:y:68:ASN:HB2   | 1:y:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:y:451:ILE:HD12 | 1:y:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:z:51:ASP:OD1   | 1:z:481:ARG:NE   | 2.38                     | 0.46              |
| 1:z:294:MET:CE   | 1:z:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:1:91:SER:HB2   | 1:1:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:1:356:TYR:CE1  | 1:1:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:1:383:TYR:HE2  | 1:2:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:3:514:LYS:O    | 1:8:73:ARG:HD2   | 2.15                     | 0.46              |
| 1:4:406:ARG:HB2  | 1:4:531:LYS:HZ1  | 1.81                     | 0.46              |
| 1:6:91:SER:HB2   | 1:6:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:6:412:GLU:OE1  | 1:6:412:GLU:N    | 2.49                     | 0.46              |
| 1:A:51:ASP:OD1   | 1:A:481:ARG:NE   | 2.38                     | 0.46              |
| 1:B:68:ASN:HB2   | 1:B:189:GLN:NE2  | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:91:SER:HB2   | 1:B:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:C:180:LEU:HD21 | 1:C:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:C:451:ILE:HD12 | 1:C:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:D:85:LYS:CG    | 1:D:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:D:127:HIS:HD2  | 1:D:238:THR:HG22 | 1.81                     | 0.46              |
| 1:D:451:ILE:HD12 | 1:D:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:F:68:ASN:HB2   | 1:F:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:G:356:TYR:CE1  | 1:G:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:H:136:LYS:NZ   | 1:H:149:ASN:OD1  | 2.37                     | 0.46              |
| 1:H:451:ILE:HD12 | 1:H:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:J:51:ASP:OD1   | 1:J:481:ARG:NE   | 2.38                     | 0.46              |
| 1:K:68:ASN:HB2   | 1:K:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:K:180:LEU:HD21 | 1:K:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:L:85:LYS:CG    | 1:L:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:L:294:MET:CE   | 1:L:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:N:229:LEU:HD21 | 1:N:235:THR:HG23 | 1.98                     | 0.46              |
| 1:P:229:LEU:HD11 | 1:P:235:THR:HG23 | 1.97                     | 0.46              |
| 1:R:73:ARG:HD2   | 1:V:514:LYS:O    | 2.16                     | 0.46              |
| 1:R:156:HIS:N    | 1:R:447:LYS:O    | 2.43                     | 0.46              |
| 1:S:91:SER:HB2   | 1:S:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:T:331:ALA:HB2  | 1:l:390:TYR:CE2  | 2.51                     | 0.46              |
| 1:W:412:GLU:OE1  | 1:W:412:GLU:N    | 2.49                     | 0.46              |
| 1:X:180:LEU:HD21 | 1:X:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:Z:383:TYR:HE2  | 1:4:318:VAL:HG21 | 1.80                     | 0.46              |
| 1:a:180:LEU:HD21 | 1:a:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:b:180:LEU:HD21 | 1:b:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:c:451:ILE:HD12 | 1:c:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:e:294:MET:CE   | 1:e:382:LEU:HD11 | 2.45                     | 0.46              |
| 1:f:180:LEU:HD21 | 1:f:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:f:229:LEU:HD11 | 1:f:235:THR:HG23 | 1.97                     | 0.46              |
| 1:g:127:HIS:HD2  | 1:g:238:THR:HG22 | 1.81                     | 0.46              |
| 1:g:180:LEU:HD21 | 1:g:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:g:451:ILE:HD12 | 1:g:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:i:229:LEU:HD21 | 1:i:235:THR:HG23 | 1.98                     | 0.46              |
| 1:k:179:GLU:OE2  | 1:k:411:ARG:NH1  | 2.38                     | 0.46              |
| 1:k:378:ARG:HD2  | 1:k:378:ARG:HA   | 1.73                     | 0.46              |
| 1:l:68:ASN:HB2   | 1:l:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:l:229:LEU:HD11 | 1:l:235:THR:HG23 | 1.97                     | 0.46              |
| 1:p:85:LYS:CG    | 1:p:332:GLY:HA3  | 2.46                     | 0.46              |
| 1:p:514:LYS:O    | 1:q:73:ARG:HD2   | 2.16                     | 0.46              |
| 1:q:127:HIS:HD2  | 1:q:238:THR:HG22 | 1.81                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:180:LEU:HD21 | 1:r:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:t:356:TYR:CE1  | 1:t:367:ASN:HB3  | 2.50                     | 0.46              |
| 1:u:451:ILE:HD12 | 1:u:465:ILE:HD13 | 1.97                     | 0.46              |
| 1:z:412:GLU:OE1  | 1:z:412:GLU:N    | 2.49                     | 0.46              |
| 1:3:180:LEU:HD21 | 1:3:518:TYR:CD1  | 2.51                     | 0.46              |
| 1:4:68:ASN:HB2   | 1:4:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:4:91:SER:HB2   | 1:4:189:GLN:NE2  | 2.31                     | 0.46              |
| 1:C:127:HIS:HD2  | 1:C:238:THR:HG22 | 1.81                     | 0.45              |
| 1:G:68:ASN:HB2   | 1:G:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:H:85:LYS:CG    | 1:H:332:GLY:HA3  | 2.46                     | 0.45              |
| 1:H:318:VAL:HG21 | 1:Y:383:TYR:HE2  | 1.80                     | 0.45              |
| 1:I:357:GLN:NE2  | 1:I:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:I:378:ARG:HA   | 1:I:378:ARG:HD2  | 1.73                     | 0.45              |
| 1:I:412:GLU:OE1  | 1:I:412:GLU:N    | 2.49                     | 0.45              |
| 1:J:294:MET:CE   | 1:J:382:LEU:HD11 | 2.45                     | 0.45              |
| 1:L:156:HIS:N    | 1:L:447:LYS:O    | 2.43                     | 0.45              |
| 1:L:180:LEU:HD21 | 1:L:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:L:412:GLU:OE1  | 1:L:412:GLU:N    | 2.49                     | 0.45              |
| 1:M:91:SER:HB2   | 1:M:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:M:412:GLU:OE1  | 1:M:412:GLU:N    | 2.49                     | 0.45              |
| 1:O:68:ASN:HB2   | 1:O:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:O:156:HIS:N    | 1:O:447:LYS:O    | 2.43                     | 0.45              |
| 1:P:91:SER:HB2   | 1:P:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:R:451:ILE:HD12 | 1:R:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:V:85:LYS:CG    | 1:V:332:GLY:HA3  | 2.46                     | 0.45              |
| 1:W:180:LEU:HD21 | 1:W:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:Z:180:LEU:HD21 | 1:Z:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:c:229:LEU:HD11 | 1:c:235:THR:HG23 | 1.97                     | 0.45              |
| 1:c:356:TYR:CE1  | 1:c:367:ASN:HB3  | 2.50                     | 0.45              |
| 1:e:356:TYR:CE1  | 1:e:367:ASN:HB3  | 2.50                     | 0.45              |
| 1:f:331:ALA:HB2  | 1:g:390:TYR:CE2  | 2.51                     | 0.45              |
| 1:g:318:VAL:HG21 | 1:h:383:TYR:HE2  | 1.80                     | 0.45              |
| 1:h:91:SER:HB2   | 1:h:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:h:412:GLU:OE1  | 1:h:412:GLU:N    | 2.49                     | 0.45              |
| 1:i:156:HIS:N    | 1:i:447:LYS:O    | 2.43                     | 0.45              |
| 1:i:383:TYR:HE2  | 1:j:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:i:451:ILE:HD12 | 1:i:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:j:127:HIS:HD2  | 1:j:238:THR:HG22 | 1.81                     | 0.45              |
| 1:k:85:LYS:CG    | 1:k:332:GLY:HA3  | 2.46                     | 0.45              |
| 1:k:127:HIS:HD2  | 1:k:238:THR:HG22 | 1.81                     | 0.45              |
| 1:k:180:LEU:HD21 | 1:k:518:TYR:CD1  | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:180:LEU:HD21 | 1:o:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:q:451:ILE:HD12 | 1:q:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:r:91:SER:HB2   | 1:r:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:w:357:GLN:NE2  | 1:w:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:x:91:SER:HB2   | 1:x:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:z:85:LYS:CG    | 1:z:332:GLY:HA3  | 2.46                     | 0.45              |
| 1:1:68:ASN:HB2   | 1:1:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:2:294:MET:CE   | 1:2:382:LEU:HD11 | 2.45                     | 0.45              |
| 1:4:180:LEU:HD21 | 1:4:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:5:85:LYS:CG    | 1:5:332:GLY:HA3  | 2.46                     | 0.45              |
| 1:A:356:TYR:CE1  | 1:A:367:ASN:HB3  | 2.50                     | 0.45              |
| 1:C:390:TYR:CE2  | 1:b:331:ALA:HB2  | 2.51                     | 0.45              |
| 1:D:180:LEU:HD21 | 1:D:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:F:294:MET:CE   | 1:F:382:LEU:HD11 | 2.45                     | 0.45              |
| 1:J:68:ASN:HB2   | 1:J:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:J:514:LYS:O    | 1:a:73:ARG:HD2   | 2.16                     | 0.45              |
| 1:K:91:SER:HB2   | 1:K:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:K:179:GLU:OE2  | 1:K:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:K:514:LYS:O    | 1:L:73:ARG:HD2   | 2.16                     | 0.45              |
| 1:L:91:SER:HB2   | 1:L:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:N:383:TYR:HE2  | 1:P:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:O:127:HIS:HD2  | 1:O:238:THR:HG22 | 1.81                     | 0.45              |
| 1:O:229:LEU:HD21 | 1:O:235:THR:HG23 | 1.98                     | 0.45              |
| 1:Q:91:SER:HB2   | 1:Q:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:R:127:HIS:HD2  | 1:R:238:THR:HG22 | 1.81                     | 0.45              |
| 1:T:73:ARG:HD2   | 1:i:514:LYS:O    | 2.15                     | 0.45              |
| 1:U:91:SER:HB2   | 1:U:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:Z:68:ASN:HB2   | 1:Z:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:b:229:LEU:HD11 | 1:b:235:THR:HG23 | 1.97                     | 0.45              |
| 1:e:229:LEU:HD11 | 1:e:235:THR:HG23 | 1.97                     | 0.45              |
| 1:e:451:ILE:HD12 | 1:e:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:f:153:ALA:HA   | 1:z:134:GLN:NE2  | 2.30                     | 0.45              |
| 1:j:85:LYS:CG    | 1:j:332:GLY:HA3  | 2.46                     | 0.45              |
| 1:j:91:SER:HB2   | 1:j:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:j:451:ILE:HD12 | 1:j:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:q:383:TYR:HE2  | 1:r:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:r:229:LEU:HD21 | 1:r:235:THR:HG23 | 1.98                     | 0.45              |
| 1:t:91:SER:HB2   | 1:t:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:u:127:HIS:HD2  | 1:u:238:THR:HG22 | 1.81                     | 0.45              |
| 1:u:412:GLU:OE1  | 1:u:412:GLU:N    | 2.49                     | 0.45              |
| 1:v:356:TYR:CE1  | 1:v:367:ASN:HB3  | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:412:GLU:OE1  | 1:w:412:GLU:N    | 2.49                     | 0.45              |
| 1:x:156:HIS:N    | 1:x:447:LYS:O    | 2.43                     | 0.45              |
| 1:x:229:LEU:HD11 | 1:x:235:THR:HG23 | 1.97                     | 0.45              |
| 1:y:294:MET:CE   | 1:y:382:LEU:HD11 | 2.45                     | 0.45              |
| 1:z:180:LEU:HD21 | 1:z:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:3:68:ASN:HB2   | 1:3:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:5:68:ASN:HB2   | 1:5:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:5:318:VAL:HG21 | 1:7:383:TYR:HE2  | 1.80                     | 0.45              |
| 1:5:451:ILE:HD12 | 1:5:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:6:180:LEU:HD21 | 1:6:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:6:229:LEU:HD21 | 1:6:235:THR:HG23 | 1.98                     | 0.45              |
| 1:7:357:GLN:NE2  | 1:7:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:8:68:ASN:HB2   | 1:8:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:8:180:LEU:HD21 | 1:8:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:A:136:LYS:NZ   | 1:A:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:B:270:TYR:O    | 1:J:350:GLU:HG2  | 2.16                     | 0.45              |
| 1:C:318:VAL:HG21 | 1:M:383:TYR:HE2  | 1.80                     | 0.45              |
| 1:E:229:LEU:HD21 | 1:E:235:THR:HG23 | 1.98                     | 0.45              |
| 1:E:357:GLN:NE2  | 1:E:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:E:412:GLU:OE1  | 1:E:412:GLU:N    | 2.49                     | 0.45              |
| 1:G:91:SER:HB2   | 1:G:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:G:127:HIS:HD2  | 1:G:238:THR:HG22 | 1.81                     | 0.45              |
| 1:H:68:ASN:HB2   | 1:H:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:H:390:TYR:CE2  | 1:W:331:ALA:HB2  | 2.51                     | 0.45              |
| 1:J:270:TYR:O    | 1:L:350:GLU:HG2  | 2.16                     | 0.45              |
| 1:K:127:HIS:HD2  | 1:K:238:THR:HG22 | 1.81                     | 0.45              |
| 1:M:180:LEU:HD21 | 1:M:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:N:451:ILE:HD12 | 1:N:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:O:234:SER:O    | 1:d:29:GLY:N     | 2.33                     | 0.45              |
| 1:P:85:LYS:CG    | 1:P:332:GLY:HA3  | 2.46                     | 0.45              |
| 1:P:451:ILE:HD12 | 1:P:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:Q:229:LEU:HD11 | 1:Q:235:THR:HG23 | 1.97                     | 0.45              |
| 1:R:229:LEU:HD21 | 1:R:235:THR:HG23 | 1.98                     | 0.45              |
| 1:R:383:TYR:HE2  | 1:S:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:S:229:LEU:HD21 | 1:S:235:THR:HG23 | 1.98                     | 0.45              |
| 1:W:229:LEU:HD21 | 1:W:235:THR:HG23 | 1.98                     | 0.45              |
| 1:Z:318:VAL:HG21 | 1:3:383:TYR:HE2  | 1.80                     | 0.45              |
| 1:a:383:TYR:HE2  | 1:8:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:a:451:ILE:HD12 | 1:a:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:b:412:GLU:OE1  | 1:b:412:GLU:N    | 2.49                     | 0.45              |
| 1:c:229:LEU:HD21 | 1:c:235:THR:HG23 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:136:LYS:NZ   | 1:f:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:f:229:LEU:HD21 | 1:f:235:THR:HG23 | 1.98                     | 0.45              |
| 1:f:378:ARG:HA   | 1:f:378:ARG:HD2  | 1.73                     | 0.45              |
| 1:h:127:HIS:HD2  | 1:h:238:THR:HG22 | 1.81                     | 0.45              |
| 1:i:127:HIS:HD2  | 1:i:238:THR:HG22 | 1.81                     | 0.45              |
| 1:l:127:HIS:HD2  | 1:l:238:THR:HG22 | 1.81                     | 0.45              |
| 1:l:229:LEU:HD21 | 1:l:235:THR:HG23 | 1.98                     | 0.45              |
| 1:q:229:LEU:HD21 | 1:q:235:THR:HG23 | 1.98                     | 0.45              |
| 1:s:91:SER:HB2   | 1:s:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:t:29:GLY:N     | 1:6:234:SER:O    | 2.33                     | 0.45              |
| 1:t:68:ASN:HB2   | 1:t:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:t:127:HIS:HD2  | 1:t:238:THR:HG22 | 1.81                     | 0.45              |
| 1:t:180:LEU:HD21 | 1:t:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:t:390:TYR:CE2  | 1:u:331:ALA:HB2  | 2.51                     | 0.45              |
| 1:v:134:GLN:NE2  | 1:w:153:ALA:HA   | 2.30                     | 0.45              |
| 1:w:229:LEU:HD21 | 1:w:235:THR:HG23 | 1.98                     | 0.45              |
| 1:z:91:SER:HB2   | 1:z:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:z:156:HIS:N    | 1:z:447:LYS:O    | 2.43                     | 0.45              |
| 1:1:85:LYS:CG    | 1:1:332:GLY:HA3  | 2.45                     | 0.45              |
| 1:2:51:ASP:OD1   | 1:2:481:ARG:NE   | 2.38                     | 0.45              |
| 1:2:68:ASN:HB2   | 1:2:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:3:451:ILE:HD12 | 1:3:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:4:127:HIS:HD2  | 1:4:238:THR:HG22 | 1.81                     | 0.45              |
| 1:5:136:LYS:NZ   | 1:5:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:5:331:ALA:HB2  | 1:7:390:TYR:CE2  | 2.51                     | 0.45              |
| 1:A:127:HIS:HD2  | 1:A:238:THR:HG22 | 1.81                     | 0.45              |
| 1:A:134:GLN:NE2  | 1:E:153:ALA:HA   | 2.30                     | 0.45              |
| 1:B:85:LYS:CG    | 1:B:332:GLY:HA3  | 2.45                     | 0.45              |
| 1:C:229:LEU:HD21 | 1:C:235:THR:HG23 | 1.98                     | 0.45              |
| 1:D:250:ARG:HD2  | 1:D:532:THR:O    | 2.17                     | 0.45              |
| 1:D:318:VAL:HG12 | 1:D:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:E:331:ALA:HB2  | 1:F:390:TYR:CE2  | 2.50                     | 0.45              |
| 1:F:229:LEU:HD11 | 1:F:235:THR:HG23 | 1.97                     | 0.45              |
| 1:F:250:ARG:HD2  | 1:F:532:THR:O    | 2.17                     | 0.45              |
| 1:G:180:LEU:HD21 | 1:G:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:G:229:LEU:HD11 | 1:G:235:THR:HG23 | 1.97                     | 0.45              |
| 1:G:390:TYR:CE2  | 1:I:331:ALA:HB2  | 2.51                     | 0.45              |
| 1:H:180:LEU:HD21 | 1:H:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:H:331:ALA:HB2  | 1:Y:390:TYR:CE2  | 2.51                     | 0.45              |
| 1:I:127:HIS:HD2  | 1:I:238:THR:HG22 | 1.81                     | 0.45              |
| 1:I:229:LEU:HD11 | 1:I:235:THR:HG23 | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:229:LEU:HD21 | 1:J:235:THR:HG23 | 1.98                     | 0.45              |
| 1:K:383:TYR:HE2  | 1:a:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:L:51:ASP:OD1   | 1:L:481:ARG:NE   | 2.38                     | 0.45              |
| 1:M:127:HIS:HD2  | 1:M:238:THR:HG22 | 1.81                     | 0.45              |
| 1:N:127:HIS:HD2  | 1:N:238:THR:HG22 | 1.81                     | 0.45              |
| 1:N:229:LEU:HD11 | 1:N:235:THR:HG23 | 1.97                     | 0.45              |
| 1:N:514:LYS:O    | 1:m:73:ARG:HD2   | 2.15                     | 0.45              |
| 1:P:180:LEU:HD21 | 1:P:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:T:127:HIS:HD2  | 1:T:238:THR:HG22 | 1.81                     | 0.45              |
| 1:U:180:LEU:HD21 | 1:U:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:Y:357:GLN:NE2  | 1:Y:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:b:229:LEU:HD21 | 1:b:235:THR:HG23 | 1.98                     | 0.45              |
| 1:c:390:TYR:CE2  | 1:o:331:ALA:HB2  | 2.51                     | 0.45              |
| 1:e:229:LEU:HD21 | 1:e:235:THR:HG23 | 1.98                     | 0.45              |
| 1:f:318:VAL:HG21 | 1:g:383:TYR:HE2  | 1.80                     | 0.45              |
| 1:f:412:GLU:N    | 1:f:412:GLU:OE1  | 2.49                     | 0.45              |
| 1:g:229:LEU:HD21 | 1:g:235:THR:HG23 | 1.98                     | 0.45              |
| 1:h:180:LEU:HD21 | 1:h:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:i:179:GLU:OE2  | 1:i:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:i:229:LEU:HD11 | 1:i:235:THR:HG23 | 1.97                     | 0.45              |
| 1:j:229:LEU:HD21 | 1:j:235:THR:HG23 | 1.98                     | 0.45              |
| 1:j:514:LYS:O    | 1:x:73:ARG:HD2   | 2.15                     | 0.45              |
| 1:k:229:LEU:HD11 | 1:k:235:THR:HG23 | 1.98                     | 0.45              |
| 1:k:250:ARG:HD2  | 1:k:532:THR:O    | 2.17                     | 0.45              |
| 1:s:180:LEU:HD21 | 1:s:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:t:234:SER:O    | 1:y:29:GLY:N     | 2.33                     | 0.45              |
| 1:u:91:SER:HB2   | 1:u:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:u:229:LEU:HD11 | 1:u:235:THR:HG23 | 1.97                     | 0.45              |
| 1:v:51:ASP:OD1   | 1:v:481:ARG:NE   | 2.38                     | 0.45              |
| 1:w:180:LEU:HD21 | 1:w:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:x:357:GLN:NE2  | 1:x:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:y:229:LEU:HD11 | 1:y:235:THR:HG23 | 1.97                     | 0.45              |
| 1:y:250:ARG:HD2  | 1:y:532:THR:O    | 2.17                     | 0.45              |
| 1:y:412:GLU:N    | 1:y:412:GLU:OE1  | 2.49                     | 0.45              |
| 1:2:229:LEU:HD21 | 1:2:235:THR:HG23 | 1.98                     | 0.45              |
| 1:3:91:SER:HB2   | 1:3:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:4:229:LEU:HD21 | 1:4:235:THR:HG23 | 1.98                     | 0.45              |
| 1:8:412:GLU:N    | 1:8:412:GLU:OE1  | 2.49                     | 0.45              |
| 1:C:331:ALA:HB2  | 1:M:390:TYR:CE2  | 2.51                     | 0.45              |
| 1:C:383:TYR:HE2  | 1:b:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:C:412:GLU:N    | 1:C:412:GLU:OE1  | 2.49                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:179:GLU:OE2  | 1:D:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:D:229:LEU:HD11 | 1:D:235:THR:HG23 | 1.97                     | 0.45              |
| 1:D:229:LEU:HD21 | 1:D:235:THR:HG23 | 1.98                     | 0.45              |
| 1:D:412:GLU:OE1  | 1:D:412:GLU:N    | 2.49                     | 0.45              |
| 1:E:91:SER:HB2   | 1:E:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:E:127:HIS:HD2  | 1:E:238:THR:HG22 | 1.81                     | 0.45              |
| 1:E:180:LEU:HD21 | 1:E:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:F:180:LEU:HD21 | 1:F:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:J:134:GLN:NE2  | 1:a:153:ALA:HA   | 2.31                     | 0.45              |
| 1:K:229:LEU:HD21 | 1:K:235:THR:HG23 | 1.98                     | 0.45              |
| 1:N:412:GLU:N    | 1:N:412:GLU:OE1  | 2.49                     | 0.45              |
| 1:O:180:LEU:HD21 | 1:O:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:P:229:LEU:HD21 | 1:P:235:THR:HG23 | 1.98                     | 0.45              |
| 1:R:136:LYS:NZ   | 1:R:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:X:91:SER:HB2   | 1:X:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:Y:127:HIS:HD2  | 1:Y:238:THR:HG22 | 1.81                     | 0.45              |
| 1:Z:412:GLU:OE1  | 1:Z:412:GLU:N    | 2.49                     | 0.45              |
| 1:a:68:ASN:HB2   | 1:a:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:a:91:SER:HB2   | 1:a:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:g:331:ALA:HB2  | 1:h:390:TYR:CE2  | 2.50                     | 0.45              |
| 1:g:412:GLU:OE1  | 1:g:412:GLU:N    | 2.49                     | 0.45              |
| 1:i:412:GLU:N    | 1:i:412:GLU:OE1  | 2.49                     | 0.45              |
| 1:j:180:LEU:HD21 | 1:j:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:k:229:LEU:HD21 | 1:k:235:THR:HG23 | 1.98                     | 0.45              |
| 1:k:318:VAL:HG12 | 1:k:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:l:180:LEU:HD21 | 1:l:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:n:127:HIS:HD2  | 1:n:238:THR:HG22 | 1.81                     | 0.45              |
| 1:o:229:LEU:HD21 | 1:o:235:THR:HG23 | 1.99                     | 0.45              |
| 1:s:412:GLU:OE1  | 1:s:412:GLU:N    | 2.49                     | 0.45              |
| 1:t:229:LEU:HD11 | 1:t:235:THR:HG23 | 1.97                     | 0.45              |
| 1:2:91:SER:HB2   | 1:2:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:2:250:ARG:HD2  | 1:2:532:THR:O    | 2.17                     | 0.45              |
| 1:2:451:ILE:HD12 | 1:2:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:3:156:HIS:N    | 1:3:447:LYS:O    | 2.43                     | 0.45              |
| 1:5:180:LEU:HD21 | 1:5:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:5:390:TYR:CE2  | 1:6:331:ALA:HB2  | 2.51                     | 0.45              |
| 1:6:383:TYR:HE2  | 1:7:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:F:412:GLU:N    | 1:F:412:GLU:OE1  | 2.49                     | 0.45              |
| 1:G:29:GLY:N     | 1:W:234:SER:O    | 2.33                     | 0.45              |
| 1:I:91:SER:HB2   | 1:I:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:I:318:VAL:HG12 | 1:I:334:GLY:HA3  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:91:SER:HB2   | 1:J:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:J:250:ARG:HD2  | 1:J:532:THR:O    | 2.17                     | 0.45              |
| 1:J:451:ILE:HD12 | 1:J:465:ILE:HD13 | 1.97                     | 0.45              |
| 1:L:250:ARG:HD2  | 1:L:532:THR:O    | 2.17                     | 0.45              |
| 1:O:250:ARG:HD2  | 1:O:532:THR:O    | 2.17                     | 0.45              |
| 1:P:514:LYS:O    | 1:Q:73:ARG:HD2   | 2.15                     | 0.45              |
| 1:Q:229:LEU:HD21 | 1:Q:235:THR:HG23 | 1.98                     | 0.45              |
| 1:Q:357:GLN:NE2  | 1:Q:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:R:234:SER:O    | 1:V:29:GLY:N     | 2.32                     | 0.45              |
| 1:S:318:VAL:HG12 | 1:S:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:U:250:ARG:HD2  | 1:U:532:THR:O    | 2.17                     | 0.45              |
| 1:W:250:ARG:HD2  | 1:W:532:THR:O    | 2.17                     | 0.45              |
| 1:W:318:VAL:HG12 | 1:W:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:W:383:TYR:HE2  | 1:Y:318:VAL:HG21 | 1.80                     | 0.45              |
| 1:X:127:HIS:HD2  | 1:X:238:THR:HG22 | 1.81                     | 0.45              |
| 1:X:179:GLU:OE2  | 1:X:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:X:229:LEU:HD21 | 1:X:235:THR:HG23 | 1.99                     | 0.45              |
| 1:X:331:ALA:HB2  | 1:e:390:TYR:CE2  | 2.51                     | 0.45              |
| 1:Z:406:ARG:HB2  | 1:Z:531:LYS:HZ1  | 1.80                     | 0.45              |
| 1:e:91:SER:HB2   | 1:e:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:f:68:ASN:HB2   | 1:f:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:g:134:GLN:NE2  | 1:1:153:ALA:HA   | 2.30                     | 0.45              |
| 1:j:357:GLN:NE2  | 1:j:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:o:91:SER:HB2   | 1:o:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:o:127:HIS:HD2  | 1:o:238:THR:HG22 | 1.81                     | 0.45              |
| 1:q:318:VAL:HG12 | 1:q:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:r:318:VAL:HG12 | 1:r:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:s:250:ARG:HD2  | 1:s:532:THR:O    | 2.17                     | 0.45              |
| 1:u:318:VAL:HG12 | 1:u:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:v:127:HIS:HD2  | 1:v:238:THR:HG22 | 1.81                     | 0.45              |
| 1:w:91:SER:HB2   | 1:w:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:w:127:HIS:HD2  | 1:w:238:THR:HG22 | 1.81                     | 0.45              |
| 1:w:331:ALA:HB2  | 1:y:390:TYR:CE2  | 2.50                     | 0.45              |
| 1:x:127:HIS:HD2  | 1:x:238:THR:HG22 | 1.81                     | 0.45              |
| 1:x:229:LEU:HD21 | 1:x:235:THR:HG23 | 1.98                     | 0.45              |
| 1:y:180:LEU:HD21 | 1:y:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:z:250:ARG:HD2  | 1:z:532:THR:O    | 2.17                     | 0.45              |
| 1:3:318:VAL:HG21 | 1:4:383:TYR:HE2  | 1.80                     | 0.45              |
| 1:6:250:ARG:HD2  | 1:6:532:THR:O    | 2.17                     | 0.45              |
| 1:6:318:VAL:HG12 | 1:6:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:A:234:SER:O    | 1:B:29:GLY:N     | 2.33                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:318:VAL:HG12 | 1:A:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:B:136:LYS:NZ   | 1:B:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:B:153:ALA:HA   | 1:C:134:GLN:NE2  | 2.30                     | 0.45              |
| 1:C:179:GLU:OE2  | 1:C:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:C:318:VAL:HG12 | 1:C:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:D:318:VAL:HG21 | 1:P:383:TYR:HE2  | 1.81                     | 0.45              |
| 1:D:378:ARG:HA   | 1:D:378:ARG:HD2  | 1.73                     | 0.45              |
| 1:E:318:VAL:HG12 | 1:E:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:F:29:GLY:N     | 1:G:234:SER:O    | 2.33                     | 0.45              |
| 1:H:412:GLU:OE1  | 1:H:412:GLU:N    | 2.49                     | 0.45              |
| 1:I:180:LEU:HD21 | 1:I:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:J:127:HIS:HD2  | 1:J:238:THR:HG22 | 1.81                     | 0.45              |
| 1:K:390:TYR:CE2  | 1:a:331:ALA:HB2  | 2.51                     | 0.45              |
| 1:O:412:GLU:OE1  | 1:O:412:GLU:N    | 2.49                     | 0.45              |
| 1:P:357:GLN:NE2  | 1:P:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:Q:127:HIS:HD2  | 1:Q:238:THR:HG22 | 1.81                     | 0.45              |
| 1:R:318:VAL:HG12 | 1:R:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:S:390:TYR:CE2  | 1:U:331:ALA:HB2  | 2.50                     | 0.45              |
| 1:U:412:GLU:OE1  | 1:U:412:GLU:N    | 2.49                     | 0.45              |
| 1:X:68:ASN:HB2   | 1:X:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:Y:180:LEU:HD21 | 1:Y:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:Z:229:LEU:HD21 | 1:Z:235:THR:HG23 | 1.98                     | 0.45              |
| 1:Z:318:VAL:HG12 | 1:Z:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:a:156:HIS:N    | 1:a:447:LYS:O    | 2.43                     | 0.45              |
| 1:a:250:ARG:HD2  | 1:a:532:THR:O    | 2.17                     | 0.45              |
| 1:b:68:ASN:HB2   | 1:b:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:c:91:SER:HB2   | 1:c:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:c:250:ARG:HD2  | 1:c:532:THR:O    | 2.17                     | 0.45              |
| 1:d:127:HIS:HD2  | 1:d:238:THR:HG22 | 1.81                     | 0.45              |
| 1:e:68:ASN:HB2   | 1:e:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:j:383:TYR:HE2  | 1:k:318:VAL:HG21 | 1.81                     | 0.45              |
| 1:k:412:GLU:OE1  | 1:k:412:GLU:N    | 2.49                     | 0.45              |
| 1:l:250:ARG:HD2  | 1:l:532:THR:O    | 2.17                     | 0.45              |
| 1:l:412:GLU:OE1  | 1:l:412:GLU:N    | 2.49                     | 0.45              |
| 1:m:127:HIS:HD2  | 1:m:238:THR:HG22 | 1.81                     | 0.45              |
| 1:m:136:LYS:NZ   | 1:m:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:o:136:LYS:NZ   | 1:o:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:v:136:LYS:NZ   | 1:v:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:v:318:VAL:HG12 | 1:v:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:v:489:PRO:HD3  | 1:y:108:PRO:HB2  | 1.99                     | 0.45              |
| 1:w:318:VAL:HG12 | 1:w:334:GLY:HA3  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:250:ARG:HD2  | 1:3:532:THR:O    | 2.17                     | 0.45              |
| 1:3:331:ALA:HB2  | 1:4:390:TYR:CE2  | 2.51                     | 0.45              |
| 1:4:179:GLU:OE2  | 1:4:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:5:412:GLU:OE1  | 1:5:412:GLU:N    | 2.49                     | 0.45              |
| 1:7:127:HIS:HD2  | 1:7:238:THR:HG22 | 1.81                     | 0.45              |
| 1:8:318:VAL:HG12 | 1:8:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:C:229:LEU:HD11 | 1:C:235:THR:HG23 | 1.97                     | 0.45              |
| 1:G:229:LEU:HD21 | 1:G:235:THR:HG23 | 1.98                     | 0.45              |
| 1:N:179:GLU:OE2  | 1:N:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:X:136:LYS:NZ   | 1:X:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:b:250:ARG:HD2  | 1:b:532:THR:O    | 2.17                     | 0.45              |
| 1:c:68:ASN:HB2   | 1:c:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:e:250:ARG:HD2  | 1:e:532:THR:O    | 2.17                     | 0.45              |
| 1:f:250:ARG:HD2  | 1:f:532:THR:O    | 2.17                     | 0.45              |
| 1:g:229:LEU:HD11 | 1:g:235:THR:HG23 | 1.97                     | 0.45              |
| 1:g:318:VAL:HG12 | 1:g:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:o:179:GLU:OE2  | 1:o:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:q:136:LYS:NZ   | 1:q:149:ASN:OD1  | 2.37                     | 0.45              |
| 1:q:229:LEU:HD11 | 1:q:235:THR:HG23 | 1.97                     | 0.45              |
| 1:q:412:GLU:N    | 1:q:412:GLU:OE1  | 2.49                     | 0.45              |
| 1:r:390:TYR:CE2  | 1:s:331:ALA:HB2  | 2.50                     | 0.45              |
| 1:t:229:LEU:HD21 | 1:t:235:THR:HG23 | 1.98                     | 0.45              |
| 1:u:180:LEU:HD21 | 1:u:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:7:91:SER:HB2   | 1:7:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:7:180:LEU:HD21 | 1:7:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:8:229:LEU:HD21 | 1:8:235:THR:HG23 | 1.98                     | 0.45              |
| 1:A:229:LEU:HD21 | 1:A:235:THR:HG23 | 1.98                     | 0.45              |
| 1:A:489:PRO:HD3  | 1:F:108:PRO:HB2  | 1.99                     | 0.45              |
| 1:B:331:ALA:HB2  | 1:L:390:TYR:CE2  | 2.51                     | 0.45              |
| 1:B:397:TRP:HB2  | 1:J:397:TRP:CD2  | 2.52                     | 0.45              |
| 1:J:180:LEU:HD21 | 1:J:518:TYR:CD1  | 2.51                     | 0.45              |
| 1:J:397:TRP:HB2  | 1:L:397:TRP:CD2  | 2.52                     | 0.45              |
| 1:N:68:ASN:HB2   | 1:N:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:P:412:GLU:OE1  | 1:P:412:GLU:N    | 2.49                     | 0.45              |
| 1:Q:250:ARG:HD2  | 1:Q:532:THR:O    | 2.17                     | 0.45              |
| 1:U:68:ASN:HB2   | 1:U:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:U:229:LEU:HD11 | 1:U:235:THR:HG23 | 1.97                     | 0.45              |
| 1:d:357:GLN:NE2  | 1:d:368:ILE:HD12 | 2.29                     | 0.45              |
| 1:i:68:ASN:HB2   | 1:i:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:l:234:SER:O    | 1:n:29:GLY:N     | 2.33                     | 0.45              |
| 1:n:357:GLN:NE2  | 1:n:368:ILE:HD12 | 2.29                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:68:ASN:HB2   | 1:o:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:p:108:PRO:HB2  | 1:s:489:PRO:HD3  | 1.99                     | 0.45              |
| 1:2:127:HIS:HD2  | 1:2:238:THR:HG22 | 1.81                     | 0.45              |
| 1:5:383:TYR:HE2  | 1:6:318:VAL:HG21 | 1.81                     | 0.45              |
| 1:B:250:ARG:HD2  | 1:B:532:THR:O    | 2.17                     | 0.45              |
| 1:F:318:VAL:HG12 | 1:F:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:G:250:ARG:HD2  | 1:G:532:THR:O    | 2.17                     | 0.45              |
| 1:R:229:LEU:HD11 | 1:R:235:THR:HG23 | 1.97                     | 0.45              |
| 1:R:412:GLU:OE1  | 1:R:412:GLU:N    | 2.49                     | 0.45              |
| 1:U:489:PRO:HD3  | 1:V:108:PRO:HB2  | 1.99                     | 0.45              |
| 1:W:68:ASN:HB2   | 1:W:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:Y:91:SER:HB2   | 1:Y:189:GLN:NE2  | 2.31                     | 0.45              |
| 1:d:51:ASP:OD1   | 1:d:481:ARG:NE   | 2.38                     | 0.45              |
| 1:f:179:GLU:OE2  | 1:f:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:g:179:GLU:OE2  | 1:g:411:ARG:NH1  | 2.38                     | 0.45              |
| 1:j:412:GLU:OE1  | 1:j:412:GLU:N    | 2.49                     | 0.45              |
| 1:p:127:HIS:HD2  | 1:p:238:THR:HG22 | 1.81                     | 0.45              |
| 1:s:229:LEU:HD11 | 1:s:235:THR:HG23 | 1.97                     | 0.45              |
| 1:t:250:ARG:HD2  | 1:t:532:THR:O    | 2.17                     | 0.45              |
| 1:v:229:LEU:HD21 | 1:v:235:THR:HG23 | 1.98                     | 0.45              |
| 1:x:250:ARG:HD2  | 1:x:532:THR:O    | 2.17                     | 0.45              |
| 1:y:318:VAL:HG12 | 1:y:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:2:318:VAL:HG12 | 1:2:334:GLY:HA3  | 1.99                     | 0.45              |
| 1:B:318:VAL:HG12 | 1:B:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:C:68:ASN:HB2   | 1:C:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:F:331:ALA:HB2  | 1:Q:390:TYR:CE2  | 2.51                     | 0.44              |
| 1:G:489:PRO:HD3  | 1:H:108:PRO:HB2  | 1.99                     | 0.44              |
| 1:H:250:ARG:HD2  | 1:H:532:THR:O    | 2.17                     | 0.44              |
| 1:H:383:TYR:HE2  | 1:W:318:VAL:HG21 | 1.81                     | 0.44              |
| 1:K:250:ARG:HD2  | 1:K:532:THR:O    | 2.17                     | 0.44              |
| 1:M:318:VAL:HG12 | 1:M:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:N:108:PRO:HB2  | 1:O:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:T:180:LEU:HD21 | 1:T:518:TYR:CD1  | 2.51                     | 0.44              |
| 1:Y:108:PRO:HB2  | 1:Z:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:Y:250:ARG:HD2  | 1:Y:532:THR:O    | 2.17                     | 0.44              |
| 1:c:180:LEU:HD21 | 1:c:518:TYR:CD1  | 2.51                     | 0.44              |
| 1:e:180:LEU:HD21 | 1:e:518:TYR:CD1  | 2.51                     | 0.44              |
| 1:g:68:ASN:HB2   | 1:g:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:h:318:VAL:HG12 | 1:h:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:m:180:LEU:HD21 | 1:m:518:TYR:CD1  | 2.51                     | 0.44              |
| 1:p:29:GLY:N     | 1:q:234:SER:O    | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:68:ASN:HB2   | 1:s:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:v:234:SER:O    | 1:1:29:GLY:N     | 2.33                     | 0.44              |
| 1:x:390:TYR:CE2  | 1:y:331:ALA:HB2  | 2.51                     | 0.44              |
| 1:1:70:HIS:CD2   | 1:1:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:1:136:LYS:NZ   | 1:1:149:ASN:OD1  | 2.37                     | 0.44              |
| 1:1:318:VAL:HG12 | 1:1:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:3:318:VAL:HG12 | 1:3:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:4:250:ARG:HD2  | 1:4:532:THR:O    | 2.17                     | 0.44              |
| 1:5:250:ARG:HD2  | 1:5:532:THR:O    | 2.17                     | 0.44              |
| 1:6:68:ASN:HB2   | 1:6:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:6:390:TYR:CE2  | 1:7:331:ALA:HB2  | 2.51                     | 0.44              |
| 1:7:108:PRO:HB2  | 1:8:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:A:68:ASN:HB2   | 1:A:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:D:399:PHE:CD1  | 1:D:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:J:108:PRO:HB2  | 1:K:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:J:318:VAL:HG12 | 1:J:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:N:489:PRO:HD3  | 1:O:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:O:318:VAL:HG12 | 1:O:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:T:91:SER:HB2   | 1:T:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:T:136:LYS:NZ   | 1:T:149:ASN:OD1  | 2.37                     | 0.44              |
| 1:U:318:VAL:HG12 | 1:U:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:V:70:HIS:CD2   | 1:V:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:V:127:HIS:HD2  | 1:V:238:THR:HG22 | 1.81                     | 0.44              |
| 1:V:250:ARG:HD2  | 1:V:532:THR:O    | 2.17                     | 0.44              |
| 1:W:390:TYR:CE2  | 1:Y:331:ALA:HB2  | 2.51                     | 0.44              |
| 1:X:250:ARG:HD2  | 1:X:532:THR:O    | 2.17                     | 0.44              |
| 1:X:399:PHE:CD1  | 1:X:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:Y:229:LEU:HD21 | 1:Y:235:THR:HG23 | 1.98                     | 0.44              |
| 1:Z:70:HIS:CD2   | 1:Z:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:a:318:VAL:HG12 | 1:a:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:f:127:HIS:HD2  | 1:f:238:THR:HG22 | 1.81                     | 0.44              |
| 1:i:108:PRO:HB2  | 1:l:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:i:489:PRO:HD3  | 1:l:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:k:399:PHE:CD1  | 1:k:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:m:91:SER:HB2   | 1:m:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:m:108:PRO:HB2  | 1:r:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:o:399:PHE:CD1  | 1:o:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:p:70:HIS:CD2   | 1:p:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:s:229:LEU:HD21 | 1:s:235:THR:HG23 | 1.98                     | 0.44              |
| 1:s:318:VAL:HG12 | 1:s:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:t:489:PRO:HD3  | 1:5:108:PRO:HB2  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:70:HIS:CD2   | 1:u:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:v:68:ASN:HB2   | 1:v:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:1:250:ARG:HD2  | 1:1:532:THR:O    | 2.17                     | 0.44              |
| 1:1:390:TYR:CE2  | 1:2:331:ALA:HB2  | 2.51                     | 0.44              |
| 1:2:180:LEU:HD21 | 1:2:518:TYR:CD1  | 2.51                     | 0.44              |
| 1:7:229:LEU:HD21 | 1:7:235:THR:HG23 | 1.98                     | 0.44              |
| 1:7:250:ARG:HD2  | 1:7:532:THR:O    | 2.17                     | 0.44              |
| 1:7:412:GLU:OE1  | 1:7:412:GLU:N    | 2.49                     | 0.44              |
| 1:8:70:HIS:CD2   | 1:8:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:B:70:HIS:CD2   | 1:B:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:D:489:PRO:HD3  | 1:M:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:I:70:HIS:CD2   | 1:I:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:I:399:PHE:CD1  | 1:I:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:K:399:PHE:CD1  | 1:K:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:O:70:HIS:CD2   | 1:O:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:O:357:GLN:NE2  | 1:O:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:P:399:PHE:CD1  | 1:P:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:S:250:ARG:HD2  | 1:S:532:THR:O    | 2.17                     | 0.44              |
| 1:S:489:PRO:HD3  | 1:T:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:T:70:HIS:CD2   | 1:T:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:V:136:LYS:NZ   | 1:V:149:ASN:OD1  | 2.37                     | 0.44              |
| 1:V:318:VAL:HG12 | 1:V:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:X:70:HIS:CD2   | 1:X:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:a:489:PRO:HD3  | 1:3:108:PRO:HB2  | 1.99                     | 0.44              |
| 1:b:108:PRO:HB2  | 1:c:489:PRO:HD3  | 1.99                     | 0.44              |
| 1:c:70:HIS:CD2   | 1:c:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:e:70:HIS:CD2   | 1:e:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:g:108:PRO:HB2  | 1:z:489:PRO:HD3  | 1.99                     | 0.44              |
| 1:h:108:PRO:HB2  | 1:k:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:i:180:LEU:HD21 | 1:i:518:TYR:CD1  | 2.51                     | 0.44              |
| 1:i:318:VAL:HG12 | 1:i:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:j:399:PHE:CD1  | 1:j:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:l:318:VAL:HG12 | 1:l:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:m:70:HIS:CD2   | 1:m:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:m:229:LEU:HD21 | 1:m:235:THR:HG23 | 1.98                     | 0.44              |
| 1:o:70:HIS:CD2   | 1:o:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:o:250:ARG:HD2  | 1:o:532:THR:O    | 2.17                     | 0.44              |
| 1:p:250:ARG:HD2  | 1:p:532:THR:O    | 2.17                     | 0.44              |
| 1:p:318:VAL:HG12 | 1:p:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:u:399:PHE:CD1  | 1:u:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:3:127:HIS:HD2  | 1:3:238:THR:HG22 | 1.81                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:357:GLN:NE2  | 1:3:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:4:399:PHE:CD1  | 1:4:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:5:91:SER:HB2   | 1:5:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:A:70:HIS:CD2   | 1:A:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:B:108:PRO:HB2  | 1:I:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:D:51:ASP:OD1   | 1:D:481:ARG:NE   | 2.38                     | 0.44              |
| 1:F:51:ASP:OD1   | 1:F:481:ARG:NE   | 2.38                     | 0.44              |
| 1:G:156:HIS:N    | 1:G:447:LYS:O    | 2.43                     | 0.44              |
| 1:H:91:SER:HB2   | 1:H:189:GLN:NE2  | 2.31                     | 0.44              |
| 1:J:381:ALA:HB3  | 1:L:318:VAL:HG22 | 1.98                     | 0.44              |
| 1:J:399:PHE:CD1  | 1:J:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:L:229:LEU:HD21 | 1:L:235:THR:HG23 | 1.98                     | 0.44              |
| 1:N:180:LEU:HD21 | 1:N:518:TYR:CD1  | 2.51                     | 0.44              |
| 1:N:318:VAL:HG12 | 1:N:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:R:70:HIS:CD2   | 1:R:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:T:229:LEU:HD21 | 1:T:235:THR:HG23 | 1.98                     | 0.44              |
| 1:U:229:LEU:HD21 | 1:U:235:THR:HG23 | 1.98                     | 0.44              |
| 1:W:357:GLN:NE2  | 1:W:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:Y:70:HIS:CD2   | 1:Y:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:Y:412:GLU:OE1  | 1:Y:412:GLU:N    | 2.49                     | 0.44              |
| 1:a:127:HIS:HD2  | 1:a:238:THR:HG22 | 1.81                     | 0.44              |
| 1:a:357:GLN:NE2  | 1:a:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:b:127:HIS:HD2  | 1:b:238:THR:HG22 | 1.81                     | 0.44              |
| 1:b:179:GLU:OE2  | 1:b:411:ARG:NH1  | 2.38                     | 0.44              |
| 1:e:489:PRO:HD3  | 1:f:108:PRO:HB2  | 1.99                     | 0.44              |
| 1:h:250:ARG:HD2  | 1:h:532:THR:O    | 2.17                     | 0.44              |
| 1:j:250:ARG:HD2  | 1:j:532:THR:O    | 2.17                     | 0.44              |
| 1:j:489:PRO:HD3  | 1:w:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:l:70:HIS:CD2   | 1:l:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:l:357:GLN:NE2  | 1:l:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:m:318:VAL:HG12 | 1:m:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:n:229:LEU:HD21 | 1:n:235:THR:HG23 | 1.98                     | 0.44              |
| 1:r:250:ARG:HD2  | 1:r:532:THR:O    | 2.17                     | 0.44              |
| 1:z:229:LEU:HD21 | 1:z:235:THR:HG23 | 1.98                     | 0.44              |
| 1:1:229:LEU:HD21 | 1:1:235:THR:HG23 | 1.98                     | 0.44              |
| 1:2:108:PRO:HB2  | 1:4:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:2:399:PHE:CD1  | 1:2:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:7:70:HIS:CD2   | 1:7:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:8:250:ARG:HD2  | 1:8:532:THR:O    | 2.17                     | 0.44              |
| 1:B:229:LEU:HD21 | 1:B:235:THR:HG23 | 1.98                     | 0.44              |
| 1:E:70:HIS:CD2   | 1:E:450:LYS:HG3  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:108:PRO:HB2  | 1:P:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:L:399:PHE:CD1  | 1:L:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:M:250:ARG:HD2  | 1:M:532:THR:O    | 2.17                     | 0.44              |
| 1:N:399:PHE:CD1  | 1:N:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:R:399:PHE:CD1  | 1:R:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:T:318:VAL:HG12 | 1:T:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:U:108:PRO:HB2  | 1:V:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:Z:250:ARG:HD2  | 1:Z:532:THR:O    | 2.17                     | 0.44              |
| 1:Z:399:PHE:CD1  | 1:Z:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:a:70:HIS:CD2   | 1:a:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:a:108:PRO:HB2  | 1:3:489:PRO:HD3  | 1.99                     | 0.44              |
| 1:g:357:GLN:NE2  | 1:g:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:i:399:PHE:CD1  | 1:i:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:k:70:HIS:CD2   | 1:k:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:n:51:ASP:OD1   | 1:n:481:ARG:NE   | 2.38                     | 0.44              |
| 1:n:250:ARG:HD2  | 1:n:532:THR:O    | 2.17                     | 0.44              |
| 1:n:318:VAL:HG12 | 1:n:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:o:489:PRO:HD3  | 1:6:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:p:489:PRO:HD3  | 1:s:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:q:70:HIS:CD2   | 1:q:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:q:399:PHE:CD1  | 1:q:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:s:70:HIS:CD2   | 1:s:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:s:399:PHE:CD1  | 1:s:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:u:108:PRO:HB2  | 1:1:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:v:70:HIS:CD2   | 1:v:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:w:70:HIS:CD2   | 1:w:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:w:399:PHE:CD1  | 1:w:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:3:70:HIS:CD2   | 1:3:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:6:179:GLU:OE2  | 1:6:411:ARG:NH1  | 2.38                     | 0.44              |
| 1:6:357:GLN:NE2  | 1:6:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:8:399:PHE:CD1  | 1:8:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:B:489:PRO:HD3  | 1:I:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:D:70:HIS:CD2   | 1:D:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:E:250:ARG:HD2  | 1:E:532:THR:O    | 2.17                     | 0.44              |
| 1:E:399:PHE:CD1  | 1:E:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:H:229:LEU:HD21 | 1:H:235:THR:HG23 | 1.98                     | 0.44              |
| 1:P:250:ARG:HD2  | 1:P:532:THR:O    | 2.17                     | 0.44              |
| 1:R:250:ARG:HD2  | 1:R:532:THR:O    | 2.17                     | 0.44              |
| 1:U:70:HIS:CD2   | 1:U:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:U:399:PHE:CD1  | 1:U:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:W:108:PRO:HB2  | 1:X:489:PRO:HD3  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:489:PRO:HD3  | 1:X:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:Y:399:PHE:CD1  | 1:Y:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:Y:406:ARG:HB2  | 1:Y:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:Z:378:ARG:HA   | 1:Z:378:ARG:HD2  | 1.73                     | 0.44              |
| 1:d:229:LEU:HD21 | 1:d:235:THR:HG23 | 1.98                     | 0.44              |
| 1:d:250:ARG:HD2  | 1:d:532:THR:O    | 2.17                     | 0.44              |
| 1:d:318:VAL:HG12 | 1:d:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:f:70:HIS:CD2   | 1:f:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:l:378:ARG:HD2  | 1:l:378:ARG:HA   | 1.73                     | 0.44              |
| 1:l:399:PHE:CD1  | 1:l:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:o:108:PRO:HB2  | 1:6:489:PRO:HD3  | 2.00                     | 0.44              |
| 1:p:136:LYS:NZ   | 1:p:149:ASN:OD1  | 2.37                     | 0.44              |
| 1:u:489:PRO:HD3  | 1:1:108:PRO:HB2  | 2.00                     | 0.44              |
| 1:z:399:PHE:CD1  | 1:z:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:5:127:HIS:HD2  | 1:5:238:THR:HG22 | 1.81                     | 0.44              |
| 1:7:406:ARG:HB2  | 1:7:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:A:108:PRO:HB2  | 1:F:489:PRO:HD3  | 1.99                     | 0.44              |
| 1:C:250:ARG:HD2  | 1:C:532:THR:O    | 2.17                     | 0.44              |
| 1:H:70:HIS:CD2   | 1:H:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:H:127:HIS:HD2  | 1:H:238:THR:HG22 | 1.81                     | 0.44              |
| 1:H:318:VAL:HG12 | 1:H:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:K:222:GLU:OE1  | 1:K:222:GLU:N    | 2.50                     | 0.44              |
| 1:K:406:ARG:HB2  | 1:K:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:M:229:LEU:HD21 | 1:M:235:THR:HG23 | 1.98                     | 0.44              |
| 1:O:399:PHE:CD1  | 1:O:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:V:229:LEU:HD21 | 1:V:235:THR:HG23 | 1.98                     | 0.44              |
| 1:Y:318:VAL:HG12 | 1:Y:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:b:70:HIS:CD2   | 1:b:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:e:378:ARG:HA   | 1:e:378:ARG:HD2  | 1.73                     | 0.44              |
| 1:p:229:LEU:HD21 | 1:p:235:THR:HG23 | 1.98                     | 0.44              |
| 1:p:399:PHE:CD1  | 1:p:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:q:250:ARG:HD2  | 1:q:532:THR:O    | 2.17                     | 0.44              |
| 1:r:70:HIS:CD2   | 1:r:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:v:108:PRO:HB2  | 1:y:489:PRO:HD3  | 1.99                     | 0.44              |
| 1:w:250:ARG:HD2  | 1:w:532:THR:O    | 2.17                     | 0.44              |
| 1:3:406:ARG:HB2  | 1:3:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:5:70:HIS:CD2   | 1:5:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:7:399:PHE:CD1  | 1:7:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:A:250:ARG:HD2  | 1:A:532:THR:O    | 2.17                     | 0.44              |
| 1:C:357:GLN:NE2  | 1:C:368:ILE:HD12 | 2.29                     | 0.44              |
| 1:C:399:PHE:CD1  | 1:C:400:PRO:HD2  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:406:ARG:HB2  | 1:D:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:F:70:HIS:CD2   | 1:F:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:F:229:LEU:HD21 | 1:F:235:THR:HG23 | 1.98                     | 0.44              |
| 1:I:229:LEU:HD21 | 1:I:235:THR:HG23 | 1.98                     | 0.44              |
| 1:I:406:ARG:HB2  | 1:I:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:J:489:PRO:HD3  | 1:K:108:PRO:HB2  | 1.99                     | 0.44              |
| 1:K:318:VAL:HG22 | 1:8:381:ALA:HB3  | 2.00                     | 0.44              |
| 1:L:70:HIS:CD2   | 1:L:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:M:179:GLU:OE2  | 1:M:411:ARG:NH1  | 2.38                     | 0.44              |
| 1:Q:70:HIS:CD2   | 1:Q:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:S:70:HIS:CD2   | 1:S:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:V:399:PHE:CD1  | 1:V:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:X:29:GLY:N     | 1:Y:234:SER:O    | 2.33                     | 0.44              |
| 1:X:234:SER:O    | 1:f:29:GLY:N     | 2.33                     | 0.44              |
| 1:Z:179:GLU:OE2  | 1:Z:411:ARG:NH1  | 2.38                     | 0.44              |
| 1:Z:381:ALA:HB3  | 1:4:318:VAL:HG22 | 2.00                     | 0.44              |
| 1:a:406:ARG:HB2  | 1:a:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:b:399:PHE:CD1  | 1:b:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:c:318:VAL:HG12 | 1:c:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:c:399:PHE:CD1  | 1:c:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:e:136:LYS:NZ   | 1:e:149:ASN:OD1  | 2.37                     | 0.44              |
| 1:e:318:VAL:HG12 | 1:e:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:f:399:PHE:CD1  | 1:f:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:g:399:PHE:CD1  | 1:g:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:h:156:HIS:N    | 1:h:447:LYS:O    | 2.43                     | 0.44              |
| 1:h:229:LEU:HD21 | 1:h:235:THR:HG23 | 1.99                     | 0.44              |
| 1:k:406:ARG:HB2  | 1:k:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:m:250:ARG:HD2  | 1:m:532:THR:O    | 2.17                     | 0.44              |
| 1:t:156:HIS:N    | 1:t:447:LYS:O    | 2.43                     | 0.44              |
| 1:u:250:ARG:HD2  | 1:u:532:THR:O    | 2.17                     | 0.44              |
| 1:y:51:ASP:OD1   | 1:y:481:ARG:NE   | 2.38                     | 0.44              |
| 1:y:229:LEU:HD21 | 1:y:235:THR:HG23 | 1.98                     | 0.44              |
| 1:1:381:ALA:HB3  | 1:2:318:VAL:HG22 | 2.00                     | 0.44              |
| 1:4:222:GLU:OE1  | 1:4:222:GLU:N    | 2.50                     | 0.44              |
| 1:5:229:LEU:HD21 | 1:5:235:THR:HG23 | 1.98                     | 0.44              |
| 1:7:318:VAL:HG12 | 1:7:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:H:222:GLU:OE1  | 1:H:222:GLU:N    | 2.50                     | 0.44              |
| 1:H:406:ARG:HB2  | 1:H:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:M:156:HIS:N    | 1:M:447:LYS:O    | 2.43                     | 0.44              |
| 1:O:378:ARG:HD2  | 1:O:378:ARG:HA   | 1.73                     | 0.44              |
| 1:P:29:GLY:N     | 1:Q:234:SER:O    | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:234:SER:O    | 1:i:29:GLY:N     | 2.32                     | 0.44              |
| 1:V:250:ARG:O    | 1:V:536:LYS:HG2  | 2.18                     | 0.44              |
| 1:a:229:LEU:HD21 | 1:a:235:THR:HG23 | 1.98                     | 0.44              |
| 1:c:378:ARG:HA   | 1:c:378:ARG:HD2  | 1.73                     | 0.44              |
| 1:e:399:PHE:CD1  | 1:e:400:PRO:HD2  | 2.53                     | 0.44              |
| 1:f:318:VAL:HG22 | 1:g:381:ALA:HB3  | 2.00                     | 0.44              |
| 1:g:250:ARG:HD2  | 1:g:532:THR:O    | 2.17                     | 0.44              |
| 1:h:29:GLY:N     | 1:i:234:SER:O    | 2.33                     | 0.44              |
| 1:h:70:HIS:CD2   | 1:h:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:i:250:ARG:HD2  | 1:i:532:THR:O    | 2.17                     | 0.44              |
| 1:i:381:ALA:HB3  | 1:j:318:VAL:HG22 | 2.00                     | 0.44              |
| 1:j:29:GLY:N     | 1:x:234:SER:O    | 2.32                     | 0.44              |
| 1:k:51:ASP:OD1   | 1:k:481:ARG:NE   | 2.38                     | 0.44              |
| 1:p:250:ARG:O    | 1:p:536:LYS:HG2  | 2.18                     | 0.44              |
| 1:t:70:HIS:CD2   | 1:t:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:u:406:ARG:HB2  | 1:u:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:v:250:ARG:HD2  | 1:v:532:THR:O    | 2.17                     | 0.44              |
| 1:x:70:HIS:CD2   | 1:x:450:LYS:HG3  | 2.53                     | 0.44              |
| 1:3:229:LEU:HD21 | 1:3:235:THR:HG23 | 1.98                     | 0.44              |
| 1:4:406:ARG:HB2  | 1:4:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:5:318:VAL:HG12 | 1:5:334:GLY:HA3  | 1.99                     | 0.44              |
| 1:5:406:ARG:HB2  | 1:5:531:LYS:NZ   | 2.33                     | 0.44              |
| 1:6:287:TYR:OH   | 1:7:309:GLY:O    | 2.27                     | 0.44              |
| 1:8:378:ARG:HA   | 1:8:378:ARG:HD2  | 1.73                     | 0.44              |
| 1:C:381:ALA:HB3  | 1:b:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:F:250:ARG:O    | 1:F:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:G:70:HIS:CD2   | 1:G:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:G:222:GLU:OE1  | 1:G:222:GLU:N    | 2.50                     | 0.43              |
| 1:G:318:VAL:HG12 | 1:G:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:I:250:ARG:HD2  | 1:I:532:THR:O    | 2.17                     | 0.43              |
| 1:I:300:LEU:HG   | 1:I:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:K:70:HIS:CD2   | 1:K:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:M:234:SER:O    | 1:c:29:GLY:N     | 2.33                     | 0.43              |
| 1:N:250:ARG:HD2  | 1:N:532:THR:O    | 2.17                     | 0.43              |
| 1:N:381:ALA:HB3  | 1:P:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:T:250:ARG:HD2  | 1:T:532:THR:O    | 2.17                     | 0.43              |
| 1:W:179:GLU:OE2  | 1:W:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:c:136:LYS:NZ   | 1:c:149:ASN:OD1  | 2.37                     | 0.43              |
| 1:d:399:PHE:CD1  | 1:d:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:d:489:PRO:HD3  | 1:n:108:PRO:HB2  | 1.99                     | 0.43              |
| 1:n:399:PHE:CD1  | 1:n:400:PRO:HD2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:51:ASP:OD1   | 1:s:481:ARG:NE   | 2.38                     | 0.43              |
| 1:s:85:LYS:HG3   | 1:s:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:t:222:GLU:OE1  | 1:t:222:GLU:N    | 2.50                     | 0.43              |
| 1:u:229:LEU:HD21 | 1:u:235:THR:HG23 | 1.98                     | 0.43              |
| 1:w:406:ARG:HB2  | 1:w:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:y:70:HIS:CD2   | 1:y:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:y:179:GLU:OE2  | 1:y:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:y:250:ARG:O    | 1:y:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:z:397:TRP:HB2  | 1:1:397:TRP:CD2  | 2.53                     | 0.43              |
| 1:1:399:PHE:CD1  | 1:1:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:7:300:LEU:HG   | 1:7:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:B:399:PHE:CD1  | 1:B:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:D:234:SER:O    | 1:E:29:GLY:N     | 2.33                     | 0.43              |
| 1:D:397:TRP:HB2  | 1:N:397:TRP:CD2  | 2.53                     | 0.43              |
| 1:E:406:ARG:HB2  | 1:E:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:F:179:GLU:OE2  | 1:F:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:F:399:PHE:CD1  | 1:F:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:G:85:LYS:HG3   | 1:G:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:K:397:TRP:CD2  | 1:8:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:M:70:HIS:CD2   | 1:M:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:Q:318:VAL:HG12 | 1:Q:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:T:399:PHE:CD1  | 1:T:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:U:85:LYS:HG3   | 1:U:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:U:300:LEU:HG   | 1:U:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:V:381:ALA:HB3  | 1:e:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:X:318:VAL:HG12 | 1:X:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:Y:300:LEU:HG   | 1:Y:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:Z:397:TRP:HB2  | 1:4:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:d:108:PRO:HB2  | 1:n:489:PRO:HD3  | 1.99                     | 0.43              |
| 1:d:406:ARG:HB2  | 1:d:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:g:300:LEU:HG   | 1:g:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:i:397:TRP:CD2  | 1:k:397:TRP:HB2  | 2.53                     | 0.43              |
| 1:o:300:LEU:HG   | 1:o:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:s:300:LEU:HG   | 1:s:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:t:85:LYS:HG3   | 1:t:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:t:108:PRO:HB2  | 1:5:489:PRO:HD3  | 2.00                     | 0.43              |
| 1:t:318:VAL:HG12 | 1:t:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:u:300:LEU:HG   | 1:u:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:x:318:VAL:HG12 | 1:x:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:y:399:PHE:CD1  | 1:y:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:z:70:HIS:CD2   | 1:z:450:LYS:HG3  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:378:ARG:HD2  | 1:3:378:ARG:HA   | 1.73                     | 0.43              |
| 1:5:222:GLU:OE1  | 1:5:222:GLU:N    | 2.50                     | 0.43              |
| 1:B:397:TRP:CD2  | 1:L:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:C:70:HIS:CD2   | 1:C:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:C:300:LEU:HG   | 1:C:344:LEU:HD23 | 2.01                     | 0.43              |
| 1:E:318:VAL:HG22 | 1:F:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:G:108:PRO:HB2  | 1:H:489:PRO:HD3  | 2.00                     | 0.43              |
| 1:G:397:TRP:HB2  | 1:I:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:H:85:LYS:HG3   | 1:H:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:H:397:TRP:CD2  | 1:Y:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:I:250:ARG:O    | 1:I:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:K:318:VAL:HG12 | 1:K:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:L:300:LEU:HG   | 1:L:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:L:318:VAL:HG12 | 1:L:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:M:85:LYS:HG3   | 1:M:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:O:51:ASP:OD1   | 1:O:481:ARG:NE   | 2.39                     | 0.43              |
| 1:O:397:TRP:HB2  | 1:m:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:P:85:LYS:HG3   | 1:P:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:Q:300:LEU:HG   | 1:Q:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:R:85:LYS:HG3   | 1:R:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:R:222:GLU:OE1  | 1:R:222:GLU:N    | 2.50                     | 0.43              |
| 1:R:318:VAL:HG22 | 1:U:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:T:397:TRP:CD2  | 1:l:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:T:406:ARG:HB2  | 1:T:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:X:300:LEU:HG   | 1:X:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:c:318:VAL:HG22 | 1:p:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:f:406:ARG:HB2  | 1:f:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:g:70:HIS:CD2   | 1:g:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:h:85:LYS:HG3   | 1:h:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:h:179:GLU:OE2  | 1:h:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:h:399:PHE:CD1  | 1:h:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:h:489:PRO:HD3  | 1:k:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:j:85:LYS:HG3   | 1:j:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:j:88:ARG:NH2   | 1:l:507:ASN:OD1  | 2.51                     | 0.43              |
| 1:j:406:ARG:HB2  | 1:j:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:k:234:SER:O    | 1:w:29:GLY:N     | 2.33                     | 0.43              |
| 1:m:399:PHE:CD1  | 1:m:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:m:406:ARG:HB2  | 1:m:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:n:406:ARG:HB2  | 1:n:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:o:318:VAL:HG12 | 1:o:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:q:85:LYS:HG3   | 1:q:332:GLY:HA3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:318:VAL:HG22 | 1:s:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:t:250:ARG:O    | 1:t:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:t:397:TRP:HB2  | 1:u:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:u:250:ARG:O    | 1:u:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:v:250:ARG:O    | 1:v:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:w:318:VAL:HG22 | 1:y:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:x:300:LEU:HG   | 1:x:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:y:85:LYS:HG3   | 1:y:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:z:126:MET:HB2  | 1:z:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:z:250:ARG:O    | 1:z:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:z:300:LEU:HG   | 1:z:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:z:318:VAL:HG12 | 1:z:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:z:406:ARG:HB2  | 1:z:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:4:70:HIS:CD2   | 1:4:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:5:397:TRP:CD2  | 1:7:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:5:399:PHE:CD1  | 1:5:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:8:179:GLU:OE2  | 1:8:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:C:250:ARG:O    | 1:C:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:D:108:PRO:HB2  | 1:M:489:PRO:HD3  | 2.00                     | 0.43              |
| 1:D:126:MET:HB2  | 1:D:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:E:397:TRP:HB2  | 1:Q:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:F:85:LYS:HG3   | 1:F:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:G:250:ARG:O    | 1:G:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:H:399:PHE:CD1  | 1:H:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:H:507:ASN:OD1  | 1:I:88:ARG:NH2   | 2.51                     | 0.43              |
| 1:I:85:LYS:HG3   | 1:I:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:L:126:MET:HB2  | 1:L:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:L:250:ARG:O    | 1:L:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:M:125:LYS:HG2  | 1:M:476:VAL:HB   | 2.01                     | 0.43              |
| 1:M:300:LEU:HG   | 1:M:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:M:399:PHE:CD1  | 1:M:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:O:507:ASN:OD1  | 1:P:88:ARG:NH2   | 2.51                     | 0.43              |
| 1:P:406:ARG:HB2  | 1:P:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:Q:250:ARG:O    | 1:Q:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:S:108:PRO:HB2  | 1:T:489:PRO:HD3  | 2.00                     | 0.43              |
| 1:S:381:ALA:HB3  | 1:U:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:U:156:HIS:N    | 1:U:447:LYS:O    | 2.43                     | 0.43              |
| 1:U:250:ARG:O    | 1:U:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:V:318:VAL:HG22 | 1:X:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:X:507:ASN:OD1  | 1:Y:88:ARG:NH2   | 2.51                     | 0.43              |
| 1:a:85:LYS:HG3   | 1:a:332:GLY:HA3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:29:GLY:N     | 1:o:234:SER:O    | 2.33                     | 0.43              |
| 1:b:406:ARG:HB2  | 1:b:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:c:250:ARG:O    | 1:c:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:e:29:GLY:N     | 1:h:234:SER:O    | 2.33                     | 0.43              |
| 1:e:250:ARG:O    | 1:e:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:h:125:LYS:HG2  | 1:h:476:VAL:HB   | 2.01                     | 0.43              |
| 1:h:300:LEU:HG   | 1:h:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:j:300:LEU:HG   | 1:j:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:k:126:MET:HB2  | 1:k:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:l:126:MET:HB2  | 1:l:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:n:300:LEU:HG   | 1:n:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:s:156:HIS:N    | 1:s:447:LYS:O    | 2.43                     | 0.43              |
| 1:s:250:ARG:O    | 1:s:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:u:85:LYS:HG3   | 1:u:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:w:397:TRP:HB2  | 1:x:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:3:85:LYS:HG3   | 1:3:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:4:318:VAL:HG12 | 1:4:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:5:85:LYS:HG3   | 1:5:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:A:250:ARG:O    | 1:A:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:B:125:LYS:HG2  | 1:B:476:VAL:HB   | 2.01                     | 0.43              |
| 1:B:300:LEU:HG   | 1:B:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:C:136:LYS:NZ   | 1:C:149:ASN:OD1  | 2.37                     | 0.43              |
| 1:J:70:HIS:CD2   | 1:J:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:L:406:ARG:HB2  | 1:L:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:M:29:GLY:N     | 1:N:234:SER:O    | 2.33                     | 0.43              |
| 1:M:126:MET:HB2  | 1:M:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:M:250:ARG:O    | 1:M:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:N:250:ARG:O    | 1:N:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:N:397:TRP:HB2  | 1:P:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:O:126:MET:HB2  | 1:O:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:O:250:ARG:O    | 1:O:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:P:300:LEU:HG   | 1:P:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:P:318:VAL:HG12 | 1:P:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:Q:378:ARG:HA   | 1:Q:378:ARG:HD2  | 1.73                     | 0.43              |
| 1:Y:489:PRO:HD3  | 1:Z:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:Z:250:ARG:O    | 1:Z:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:c:126:MET:HB2  | 1:c:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:d:250:ARG:O    | 1:d:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:d:300:LEU:HG   | 1:d:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:e:126:MET:HB2  | 1:e:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:g:88:ARG:NH2   | 1:k:507:ASN:OD1  | 2.51                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:g:250:ARG:O   | 1:g:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:h:126:MET:HB2 | 1:h:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:h:250:ARG:O   | 1:h:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:i:250:ARG:O   | 1:i:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:i:397:TRP:HB2 | 1:j:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:j:108:PRO:HB2 | 1:w:489:PRO:HD3  | 1.99                     | 0.43              |
| 1:k:300:LEU:HG  | 1:k:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:m:489:PRO:HD3 | 1:r:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:n:250:ARG:O   | 1:n:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:o:381:ALA:HB3 | 1:p:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:o:507:ASN:OD1 | 1:7:88:ARG:NH2   | 2.51                     | 0.43              |
| 1:p:378:ARG:HD2 | 1:p:378:ARG:HA   | 1.73                     | 0.43              |
| 1:q:222:GLU:OE1 | 1:q:222:GLU:N    | 2.50                     | 0.43              |
| 1:u:88:ARG:NH2  | 1:5:507:ASN:OD1  | 2.51                     | 0.43              |
| 1:v:399:PHE:CD1 | 1:v:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:w:250:ARG:O   | 1:w:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:x:126:MET:HB2 | 1:x:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:x:250:ARG:O   | 1:x:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:1:125:LYS:HG2 | 1:1:476:VAL:HB   | 2.01                     | 0.43              |
| 1:7:489:PRO:HD3 | 1:8:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:A:125:LYS:HG2 | 1:A:476:VAL:HB   | 2.01                     | 0.43              |
| 1:A:399:PHE:CD1 | 1:A:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:B:287:TYR:OH  | 1:J:309:GLY:O    | 2.29                     | 0.43              |
| 1:B:320:ASN:ND2 | 1:B:324:THR:OG1  | 2.52                     | 0.43              |
| 1:C:72:TYR:OH   | 1:C:222:GLU:OE1  | 2.36                     | 0.43              |
| 1:C:320:ASN:ND2 | 1:C:324:THR:OG1  | 2.52                     | 0.43              |
| 1:C:397:TRP:HB2 | 1:b:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:D:125:LYS:HG2 | 1:D:476:VAL:HB   | 2.01                     | 0.43              |
| 1:D:300:LEU:HG  | 1:D:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:D:320:ASN:ND2 | 1:D:324:THR:OG1  | 2.52                     | 0.43              |
| 1:E:250:ARG:O   | 1:E:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:G:399:PHE:CD1 | 1:G:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:H:381:ALA:HB3 | 1:W:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:K:125:LYS:HG2 | 1:K:476:VAL:HB   | 2.01                     | 0.43              |
| 1:M:406:ARG:HB2 | 1:M:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:M:507:ASN:OD1 | 1:N:88:ARG:NH2   | 2.51                     | 0.43              |
| 1:N:29:GLY:N    | 1:m:234:SER:O    | 2.32                     | 0.43              |
| 1:N:126:MET:HB2 | 1:N:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:N:222:GLU:OE1 | 1:N:222:GLU:N    | 2.50                     | 0.43              |
| 1:P:70:HIS:CD2  | 1:P:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:Q:125:LYS:HG2 | 1:Q:476:VAL:HB   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:126:MET:HB2  | 1:Q:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:S:250:ARG:O    | 1:S:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:U:51:ASP:OD1   | 1:U:481:ARG:NE   | 2.38                     | 0.43              |
| 1:U:125:LYS:HG2  | 1:U:476:VAL:HB   | 2.01                     | 0.43              |
| 1:W:70:HIS:CD2   | 1:W:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:Z:125:LYS:HG2  | 1:Z:476:VAL:HB   | 2.01                     | 0.43              |
| 1:Z:397:TRP:CD2  | 1:3:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:a:397:TRP:HB2  | 1:8:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:b:318:VAL:HG12 | 1:b:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:b:489:PRO:HD3  | 1:c:108:PRO:HB2  | 1.99                     | 0.43              |
| 1:c:125:LYS:HG2  | 1:c:476:VAL:HB   | 2.01                     | 0.43              |
| 1:c:300:LEU:HG   | 1:c:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:e:108:PRO:HB2  | 1:f:489:PRO:HD3  | 1.99                     | 0.43              |
| 1:e:300:LEU:HG   | 1:e:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:f:397:TRP:CD2  | 1:g:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:g:320:ASN:ND2  | 1:g:324:THR:OG1  | 2.52                     | 0.43              |
| 1:k:320:ASN:ND2  | 1:k:324:THR:OG1  | 2.52                     | 0.43              |
| 1:l:51:ASP:OD1   | 1:l:481:ARG:NE   | 2.39                     | 0.43              |
| 1:n:126:MET:HB2  | 1:n:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:o:250:ARG:O    | 1:o:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:r:250:ARG:O    | 1:r:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:r:381:ALA:HB3  | 1:s:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:r:406:ARG:HB2  | 1:r:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:t:399:PHE:CD1  | 1:t:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:u:179:GLU:OE2  | 1:u:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:v:125:LYS:HG2  | 1:v:476:VAL:HB   | 2.01                     | 0.43              |
| 1:w:126:MET:HB2  | 1:w:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:x:125:LYS:HG2  | 1:x:476:VAL:HB   | 2.01                     | 0.43              |
| 1:x:320:ASN:ND2  | 1:x:324:THR:OG1  | 2.52                     | 0.43              |
| 1:z:85:LYS:HG3   | 1:z:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:1:250:ARG:O    | 1:1:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:1:300:LEU:HG   | 1:1:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:2:70:HIS:CD2   | 1:2:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:3:179:GLU:OE2  | 1:3:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:4:125:LYS:HG2  | 1:4:476:VAL:HB   | 2.01                     | 0.43              |
| 1:4:378:ARG:HA   | 1:4:378:ARG:HD2  | 1.73                     | 0.43              |
| 1:5:126:MET:HB2  | 1:5:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:5:381:ALA:HB3  | 1:6:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:6:250:ARG:O    | 1:6:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:8:125:LYS:HG2  | 1:8:476:VAL:HB   | 2.01                     | 0.43              |
| 1:8:250:ARG:O    | 1:8:536:LYS:HG2  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:85:LYS:HG3   | 1:B:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:B:250:ARG:O    | 1:B:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:C:88:ARG:NH2   | 1:D:507:ASN:OD1  | 2.51                     | 0.43              |
| 1:C:489:PRO:HD3  | 1:L:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:D:250:ARG:O    | 1:D:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:D:397:TRP:CD2  | 1:P:397:TRP:HB2  | 2.53                     | 0.43              |
| 1:E:126:MET:HB2  | 1:E:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:E:381:ALA:HB3  | 1:Q:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:E:489:PRO:HD3  | 1:P:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:H:126:MET:HB2  | 1:H:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:H:300:LEU:HG   | 1:H:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:J:156:HIS:N    | 1:J:447:LYS:O    | 2.43                     | 0.43              |
| 1:L:85:LYS:HG3   | 1:L:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:N:70:HIS:CD2   | 1:N:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:O:125:LYS:HG2  | 1:O:476:VAL:HB   | 2.01                     | 0.43              |
| 1:O:397:TRP:CD2  | 1:n:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:P:320:ASN:ND2  | 1:P:324:THR:OG1  | 2.52                     | 0.43              |
| 1:Q:85:LYS:HG3   | 1:Q:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:Q:320:ASN:ND2  | 1:Q:324:THR:OG1  | 2.52                     | 0.43              |
| 1:T:300:LEU:HG   | 1:T:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:U:320:ASN:ND2  | 1:U:324:THR:OG1  | 2.52                     | 0.43              |
| 1:V:126:MET:HB2  | 1:V:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:W:250:ARG:O    | 1:W:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:X:250:ARG:O    | 1:X:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:a:300:LEU:HG   | 1:a:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:b:85:LYS:HG3   | 1:b:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:b:126:MET:HB2  | 1:b:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:d:126:MET:HB2  | 1:d:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:e:125:LYS:HG2  | 1:e:476:VAL:HB   | 2.01                     | 0.43              |
| 1:f:126:MET:HB2  | 1:f:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:h:406:ARG:HB2  | 1:h:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:h:507:ASN:OD1  | 1:i:88:ARG:NH2   | 2.51                     | 0.43              |
| 1:i:126:MET:HB2  | 1:i:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:i:222:GLU:OE1  | 1:i:222:GLU:N    | 2.50                     | 0.43              |
| 1:j:70:HIS:CD2   | 1:j:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:j:318:VAL:HG12 | 1:j:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:j:320:ASN:ND2  | 1:j:324:THR:OG1  | 2.52                     | 0.43              |
| 1:k:125:LYS:HG2  | 1:k:476:VAL:HB   | 2.01                     | 0.43              |
| 1:l:125:LYS:HG2  | 1:l:476:VAL:HB   | 2.01                     | 0.43              |
| 1:l:250:ARG:O    | 1:l:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:m:300:LEU:HG   | 1:m:344:LEU:HD23 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:125:LYS:HG2  | 1:s:476:VAL:HB   | 2.01                     | 0.43              |
| 1:s:320:ASN:ND2  | 1:s:324:THR:OG1  | 2.52                     | 0.43              |
| 1:t:300:LEU:HG   | 1:t:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:t:406:ARG:HB2  | 1:t:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:w:381:ALA:HB3  | 1:x:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:x:85:LYS:HG3   | 1:x:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:x:406:ARG:HB2  | 1:x:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:z:125:LYS:HG2  | 1:z:476:VAL:HB   | 2.01                     | 0.43              |
| 1:1:85:LYS:HG3   | 1:1:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:1:320:ASN:ND2  | 1:1:324:THR:OG1  | 2.52                     | 0.43              |
| 1:1:397:TRP:HB2  | 1:2:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:2:320:ASN:ND2  | 1:2:324:THR:OG1  | 2.52                     | 0.43              |
| 1:2:489:PRO:HD3  | 1:4:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:4:85:LYS:HG3   | 1:4:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:5:300:LEU:HG   | 1:5:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:252:TYR:CD1  | 1:A:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:B:88:ARG:NH2   | 1:C:507:ASN:OD1  | 2.51                     | 0.43              |
| 1:B:252:TYR:CD1  | 1:B:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:C:108:PRO:HB2  | 1:L:489:PRO:HD3  | 2.00                     | 0.43              |
| 1:C:252:TYR:CD1  | 1:C:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:E:397:TRP:CD2  | 1:F:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:G:406:ARG:HB2  | 1:G:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:H:29:GLY:N     | 1:I:234:SER:O    | 2.32                     | 0.43              |
| 1:J:320:ASN:ND2  | 1:J:324:THR:OG1  | 2.52                     | 0.43              |
| 1:K:85:LYS:HG3   | 1:K:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:K:261:PRO:HG3  | 1:a:193:ILE:HD11 | 2.01                     | 0.43              |
| 1:M:397:TRP:CD2  | 1:b:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:P:125:LYS:HG2  | 1:P:476:VAL:HB   | 2.01                     | 0.43              |
| 1:Q:406:ARG:HB2  | 1:Q:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:R:51:ASP:OD1   | 1:R:481:ARG:NE   | 2.38                     | 0.43              |
| 1:S:397:TRP:HB2  | 1:U:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:U:126:MET:HB2  | 1:U:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:U:252:TYR:CD1  | 1:U:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:V:125:LYS:HG2  | 1:V:476:VAL:HB   | 2.01                     | 0.43              |
| 1:W:397:TRP:HB2  | 1:Y:397:TRP:CD2  | 2.53                     | 0.43              |
| 1:X:125:LYS:HG2  | 1:X:476:VAL:HB   | 2.01                     | 0.43              |
| 1:Y:250:ARG:O    | 1:Y:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:d:397:TRP:HB2  | 1:l:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:f:85:LYS:HG3   | 1:f:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:f:318:VAL:HG12 | 1:f:334:GLY:HA3  | 1.99                     | 0.43              |
| 1:g:72:TYR:OH    | 1:g:222:GLU:OE1  | 2.37                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:252:TYR:CD1  | 1:g:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:i:70:HIS:CD2   | 1:i:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:j:125:LYS:HG2  | 1:j:476:VAL:HB   | 2.01                     | 0.43              |
| 1:j:250:ARG:O    | 1:j:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:j:397:TRP:HB2  | 1:k:397:TRP:CD2  | 2.53                     | 0.43              |
| 1:k:250:ARG:O    | 1:k:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:o:85:LYS:HG3   | 1:o:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:o:125:LYS:HG2  | 1:o:476:VAL:HB   | 2.01                     | 0.43              |
| 1:o:406:ARG:HB2  | 1:o:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:q:179:GLU:OE2  | 1:q:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:r:397:TRP:HB2  | 1:s:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:r:399:PHE:CD1  | 1:r:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:s:252:TYR:CD1  | 1:s:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:z:252:TYR:CD1  | 1:z:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:1:252:TYR:CD1  | 1:1:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:3:193:ILE:HD11 | 1:4:261:PRO:HG3  | 2.01                     | 0.43              |
| 1:6:70:HIS:CD2   | 1:6:450:LYS:HG3  | 2.53                     | 0.43              |
| 1:6:399:PHE:CD1  | 1:6:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:7:250:ARG:O    | 1:7:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:C:397:TRP:CD2  | 1:M:397:TRP:HB2  | 2.53                     | 0.43              |
| 1:G:300:LEU:HG   | 1:G:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:G:320:ASN:ND2  | 1:G:324:THR:OG1  | 2.52                     | 0.43              |
| 1:I:179:GLU:OE2  | 1:I:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:J:252:TYR:CD1  | 1:J:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:L:125:LYS:HG2  | 1:L:476:VAL:HB   | 2.01                     | 0.43              |
| 1:L:252:TYR:CD1  | 1:L:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:O:85:LYS:HG3   | 1:O:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:P:250:ARG:O    | 1:P:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:Q:399:PHE:CD1  | 1:Q:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:R:179:GLU:OE2  | 1:R:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:R:250:ARG:O    | 1:R:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:R:300:LEU:HG   | 1:R:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:S:85:LYS:HG3   | 1:S:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:S:399:PHE:CD1  | 1:S:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:T:320:ASN:ND2  | 1:T:324:THR:OG1  | 2.52                     | 0.43              |
| 1:W:399:PHE:CD1  | 1:W:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:X:85:LYS:HG3   | 1:X:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:Y:252:TYR:CD1  | 1:Y:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:Z:252:TYR:CD1  | 1:Z:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:Z:300:LEU:HG   | 1:Z:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:a:125:LYS:HG2  | 1:a:476:VAL:HB   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:378:ARG:HD2  | 1:a:378:ARG:HA   | 1.73                     | 0.43              |
| 1:b:250:ARG:O    | 1:b:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:b:320:ASN:ND2  | 1:b:324:THR:OG1  | 2.52                     | 0.43              |
| 1:f:320:ASN:ND2  | 1:f:324:THR:OG1  | 2.52                     | 0.43              |
| 1:f:397:TRP:HB2  | 1:h:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:g:507:ASN:OD1  | 1:l:88:ARG:NH2   | 2.51                     | 0.43              |
| 1:k:85:LYS:HG3   | 1:k:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:m:250:ARG:O    | 1:m:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:m:320:ASN:ND2  | 1:m:324:THR:OG1  | 2.52                     | 0.43              |
| 1:n:85:LYS:HG3   | 1:n:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:o:320:ASN:ND2  | 1:o:324:THR:OG1  | 2.52                     | 0.43              |
| 1:p:125:LYS:HG2  | 1:p:476:VAL:HB   | 2.01                     | 0.43              |
| 1:p:126:MET:HB2  | 1:p:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:r:85:LYS:HG3   | 1:r:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:r:126:MET:HB2  | 1:r:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:s:126:MET:HB2  | 1:s:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:t:320:ASN:ND2  | 1:t:324:THR:OG1  | 2.52                     | 0.43              |
| 1:v:252:TYR:CD1  | 1:v:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:w:397:TRP:CD2  | 1:y:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:y:406:ARG:HB2  | 1:y:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:3:300:LEU:HG   | 1:3:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:4:126:MET:HB2  | 1:4:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:6:397:TRP:HB2  | 1:7:397:TRP:CD2  | 2.53                     | 0.43              |
| 1:8:406:ARG:HB2  | 1:8:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:D:85:LYS:HG3   | 1:D:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:D:261:PRO:HG3  | 1:N:193:ILE:HD11 | 2.01                     | 0.43              |
| 1:F:252:TYR:CD1  | 1:F:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:F:397:TRP:CD2  | 1:Q:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:H:318:VAL:HG22 | 1:Y:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:K:193:ILE:HD11 | 1:8:261:PRO:HG3  | 2.01                     | 0.43              |
| 1:K:378:ARG:HA   | 1:K:378:ARG:HD2  | 1.73                     | 0.43              |
| 1:O:193:ILE:HD11 | 1:n:261:PRO:HG3  | 2.01                     | 0.43              |
| 1:Q:108:PRO:HB2  | 1:R:489:PRO:HD3  | 2.00                     | 0.43              |
| 1:R:406:ARG:HB2  | 1:R:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:S:126:MET:HB2  | 1:S:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:W:381:ALA:HB3  | 1:Y:318:VAL:HG22 | 2.00                     | 0.43              |
| 1:X:126:MET:HB2  | 1:X:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:X:320:ASN:ND2  | 1:X:324:THR:OG1  | 2.52                     | 0.43              |
| 1:X:397:TRP:CD2  | 1:e:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:X:406:ARG:HB2  | 1:X:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:Z:406:ARG:HB2  | 1:Z:531:LYS:NZ   | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:179:GLU:OE2  | 1:a:411:ARG:NH1  | 2.38                     | 0.43              |
| 1:a:399:PHE:CD1  | 1:a:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:c:397:TRP:HB2  | 1:o:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:d:85:LYS:HG3   | 1:d:332:GLY:HA3  | 2.01                     | 0.43              |
| 1:f:250:ARG:O    | 1:f:536:LYS:HG2  | 2.18                     | 0.43              |
| 1:g:126:MET:HB2  | 1:g:241:PHE:HE2  | 1.84                     | 0.43              |
| 1:g:136:LYS:NZ   | 1:g:149:ASN:OD1  | 2.37                     | 0.43              |
| 1:g:318:VAL:HG22 | 1:h:381:ALA:HB3  | 2.00                     | 0.43              |
| 1:g:397:TRP:CD2  | 1:h:397:TRP:HB2  | 2.53                     | 0.43              |
| 1:g:489:PRO:HD3  | 1:z:108:PRO:HB2  | 2.00                     | 0.43              |
| 1:i:193:ILE:HD11 | 1:k:261:PRO:HG3  | 2.01                     | 0.43              |
| 1:i:320:ASN:ND2  | 1:i:324:THR:OG1  | 2.52                     | 0.43              |
| 1:i:406:ARG:HB2  | 1:i:531:LYS:NZ   | 2.33                     | 0.43              |
| 1:l:85:LYS:HG3   | 1:l:332:GLY:HA3  | 2.00                     | 0.43              |
| 1:l:252:TYR:CD1  | 1:l:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:q:51:ASP:OD1   | 1:q:481:ARG:NE   | 2.38                     | 0.43              |
| 1:q:300:LEU:HG   | 1:q:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:t:397:TRP:CD2  | 1:v:397:TRP:HB2  | 2.54                     | 0.43              |
| 1:u:234:SER:O    | 1:5:29:GLY:N     | 2.33                     | 0.43              |
| 1:v:29:GLY:N     | 1:w:234:SER:O    | 2.33                     | 0.43              |
| 1:x:378:ARG:HA   | 1:x:378:ARG:HD2  | 1.73                     | 0.43              |
| 1:x:397:TRP:HB2  | 1:y:397:TRP:CD2  | 2.54                     | 0.43              |
| 1:x:399:PHE:CD1  | 1:x:400:PRO:HD2  | 2.53                     | 0.43              |
| 1:y:252:TYR:CD1  | 1:y:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:2:252:TYR:CD1  | 1:2:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:4:300:LEU:HG   | 1:4:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:7:252:TYR:CD1  | 1:7:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:8:252:TYR:CD1  | 1:8:253:ILE:HG23 | 2.54                     | 0.43              |
| 1:8:300:LEU:HG   | 1:8:344:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:320:ASN:ND2  | 1:A:324:THR:OG1  | 2.52                     | 0.42              |
| 1:C:261:PRO:HG3  | 1:b:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:C:318:VAL:HG22 | 1:M:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:D:252:TYR:CD1  | 1:D:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:D:318:VAL:HG22 | 1:P:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:E:261:PRO:HG3  | 1:Q:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:F:300:LEU:HG   | 1:F:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:F:406:ARG:HB2  | 1:F:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:G:126:MET:HB2  | 1:G:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:H:51:ASP:OD1   | 1:H:481:ARG:NE   | 2.38                     | 0.42              |
| 1:I:252:TYR:CD1  | 1:I:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:K:126:MET:HB2  | 1:K:241:PHE:HE2  | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:250:ARG:O    | 1:K:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:K:300:LEU:HG   | 1:K:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:N:320:ASN:ND2  | 1:N:324:THR:OG1  | 2.52                     | 0.42              |
| 1:O:252:TYR:CD1  | 1:O:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:O:381:ALA:HB3  | 1:m:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:P:126:MET:HB2  | 1:P:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:R:261:PRO:HG3  | 1:S:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:T:250:ARG:O    | 1:T:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:T:318:VAL:HG22 | 1:l:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:V:397:TRP:HB2  | 1:e:397:TRP:CD2  | 2.54                     | 0.42              |
| 1:X:318:VAL:HG22 | 1:e:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:Y:126:MET:HB2  | 1:Y:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:Z:261:PRO:HG3  | 1:4:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:Z:320:ASN:ND2  | 1:Z:324:THR:OG1  | 2.52                     | 0.42              |
| 1:c:381:ALA:HB3  | 1:o:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:d:252:TYR:CD1  | 1:d:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:d:261:PRO:HG3  | 1:l:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:f:193:ILE:HD11 | 1:g:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:h:252:TYR:CD1  | 1:h:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:j:126:MET:HB2  | 1:j:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:k:252:TYR:CD1  | 1:k:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:m:381:ALA:HB3  | 1:n:318:VAL:HG22 | 2.01                     | 0.42              |
| 1:n:252:TYR:CD1  | 1:n:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:n:320:ASN:ND2  | 1:n:324:THR:OG1  | 2.52                     | 0.42              |
| 1:o:126:MET:HB2  | 1:o:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:q:250:ARG:O    | 1:q:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:q:261:PRO:HG3  | 1:r:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:q:397:TRP:HB2  | 1:r:397:TRP:CD2  | 2.54                     | 0.42              |
| 1:q:489:PRO:HD3  | 1:x:108:PRO:HB2  | 2.00                     | 0.42              |
| 1:r:252:TYR:CD1  | 1:r:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:w:252:TYR:CD1  | 1:w:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:w:261:PRO:HG3  | 1:x:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:2:126:MET:HB2  | 1:2:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:2:156:HIS:N    | 1:2:447:LYS:O    | 2.43                     | 0.42              |
| 1:2:250:ARG:O    | 1:2:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:2:507:ASN:OD1  | 1:3:88:ARG:NH2   | 2.51                     | 0.42              |
| 1:3:125:LYS:HG2  | 1:3:476:VAL:HB   | 2.01                     | 0.42              |
| 1:3:250:ARG:O    | 1:3:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:3:399:PHE:CD1  | 1:3:400:PRO:HD2  | 2.53                     | 0.42              |
| 1:4:250:ARG:O    | 1:4:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:5:250:ARG:O    | 1:5:536:LYS:HG2  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:5:318:VAL:HG22 | 1:7:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:6:300:LEU:HG   | 1:6:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:6:381:ALA:HB3  | 1:7:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:7:126:MET:HB2  | 1:7:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:8:320:ASN:ND2  | 1:8:324:THR:OG1  | 2.52                     | 0.42              |
| 1:A:29:GLY:N     | 1:E:234:SER:O    | 2.33                     | 0.42              |
| 1:A:397:TRP:HB2  | 1:G:397:TRP:CD2  | 2.54                     | 0.42              |
| 1:B:193:ILE:HD11 | 1:L:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:E:252:TYR:CD1  | 1:E:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:F:193:ILE:HD11 | 1:Q:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:F:318:VAL:HG22 | 1:Q:381:ALA:HB3  | 2.01                     | 0.42              |
| 1:H:252:TYR:CD1  | 1:H:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:J:126:MET:HB2  | 1:J:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:K:234:SER:O    | 1:7:29:GLY:N     | 2.32                     | 0.42              |
| 1:K:397:TRP:HB2  | 1:a:397:TRP:CD2  | 2.54                     | 0.42              |
| 1:M:252:TYR:CD1  | 1:M:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:N:406:ARG:HB2  | 1:N:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:O:136:LYS:NZ   | 1:O:149:ASN:OD1  | 2.37                     | 0.42              |
| 1:O:261:PRO:HG3  | 1:m:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:P:252:TYR:CD1  | 1:P:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:R:125:LYS:HG2  | 1:R:476:VAL:HB   | 2.01                     | 0.42              |
| 1:R:381:ALA:HB3  | 1:S:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:R:397:TRP:HB2  | 1:S:397:TRP:CD2  | 2.54                     | 0.42              |
| 1:S:252:TYR:CD1  | 1:S:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:T:381:ALA:HB3  | 1:d:318:VAL:HG22 | 2.01                     | 0.42              |
| 1:U:194:PRO:HB2  | 1:U:216:ILE:HG23 | 2.01                     | 0.42              |
| 1:V:193:ILE:HD11 | 1:X:261:PRO:HG3  | 2.02                     | 0.42              |
| 1:V:261:PRO:HG3  | 1:e:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:V:378:ARG:HD2  | 1:V:378:ARG:HA   | 1.73                     | 0.42              |
| 1:V:397:TRP:CD2  | 1:X:397:TRP:HB2  | 2.53                     | 0.42              |
| 1:W:300:LEU:HG   | 1:W:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:a:250:ARG:O    | 1:a:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:c:193:ILE:HD11 | 1:p:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:c:397:TRP:CD2  | 1:p:397:TRP:HB2  | 2.54                     | 0.42              |
| 1:d:70:HIS:CD2   | 1:d:450:LYS:HG3  | 2.53                     | 0.42              |
| 1:j:252:TYR:CD1  | 1:j:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:j:381:ALA:HB3  | 1:k:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:l:406:ARG:HB2  | 1:l:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:m:85:LYS:HG3   | 1:m:332:GLY:HA3  | 2.00                     | 0.42              |
| 1:o:261:PRO:HG3  | 1:p:193:ILE:HD11 | 2.02                     | 0.42              |
| 1:q:381:ALA:HB3  | 1:r:318:VAL:HG22 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:406:ARG:HB2  | 1:q:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:s:194:PRO:HB2  | 1:s:216:ILE:HG23 | 2.01                     | 0.42              |
| 1:t:126:MET:HB2  | 1:t:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:u:252:TYR:CD1  | 1:u:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:v:320:ASN:ND2  | 1:v:324:THR:OG1  | 2.52                     | 0.42              |
| 1:v:406:ARG:HB2  | 1:v:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:x:261:PRO:HG3  | 1:y:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:x:381:ALA:HB3  | 1:y:318:VAL:HG22 | 2.01                     | 0.42              |
| 1:y:300:LEU:HG   | 1:y:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:3:397:TRP:CD2  | 1:4:397:TRP:HB2  | 2.54                     | 0.42              |
| 1:5:51:ASP:OD1   | 1:5:481:ARG:NE   | 2.38                     | 0.42              |
| 1:5:252:TYR:CD1  | 1:5:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:5:320:ASN:ND2  | 1:5:324:THR:OG1  | 2.52                     | 0.42              |
| 1:5:397:TRP:HB2  | 1:6:397:TRP:CD2  | 2.53                     | 0.42              |
| 1:C:126:MET:HB2  | 1:C:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:G:252:TYR:CD1  | 1:G:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:G:261:PRO:HG3  | 1:I:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:H:125:LYS:HG2  | 1:H:476:VAL:HB   | 2.01                     | 0.42              |
| 1:H:250:ARG:O    | 1:H:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:H:320:ASN:ND2  | 1:H:324:THR:OG1  | 2.52                     | 0.42              |
| 1:I:125:LYS:HG2  | 1:I:476:VAL:HB   | 2.01                     | 0.42              |
| 1:I:194:PRO:HB2  | 1:I:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:N:252:TYR:CD1  | 1:N:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:N:507:ASN:OD1  | 1:m:88:ARG:NH2   | 2.51                     | 0.42              |
| 1:O:406:ARG:HB2  | 1:O:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:Q:489:PRO:HD3  | 1:R:108:PRO:HB2  | 2.00                     | 0.42              |
| 1:S:320:ASN:ND2  | 1:S:324:THR:OG1  | 2.52                     | 0.42              |
| 1:S:378:ARG:HA   | 1:S:378:ARG:HD2  | 1.73                     | 0.42              |
| 1:T:193:ILE:HD11 | 1:l:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:Y:320:ASN:ND2  | 1:Y:324:THR:OG1  | 2.52                     | 0.42              |
| 1:b:125:LYS:HG2  | 1:b:476:VAL:HB   | 2.01                     | 0.42              |
| 1:c:72:TYR:OH    | 1:c:222:GLU:OE1  | 2.37                     | 0.42              |
| 1:d:320:ASN:ND2  | 1:d:324:THR:OG1  | 2.52                     | 0.42              |
| 1:f:125:LYS:HG2  | 1:f:476:VAL:HB   | 2.01                     | 0.42              |
| 1:n:70:HIS:CD2   | 1:n:450:LYS:HG3  | 2.53                     | 0.42              |
| 1:n:194:PRO:HB2  | 1:n:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:n:222:GLU:OE1  | 1:n:222:GLU:N    | 2.50                     | 0.42              |
| 1:p:85:LYS:HG3   | 1:p:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:q:108:PRO:HB2  | 1:x:489:PRO:HD3  | 2.00                     | 0.42              |
| 1:q:125:LYS:HG2  | 1:q:476:VAL:HB   | 2.01                     | 0.42              |
| 1:r:320:ASN:ND2  | 1:r:324:THR:OG1  | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:252:TYR:CD1  | 1:t:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:t:261:PRO:HG3  | 1:u:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:t:318:VAL:HG22 | 1:v:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:u:194:PRO:HB2  | 1:u:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:u:378:ARG:HD2  | 1:u:378:ARG:HA   | 1.73                     | 0.42              |
| 1:5:125:LYS:HG2  | 1:5:476:VAL:HB   | 2.01                     | 0.42              |
| 1:6:320:ASN:ND2  | 1:6:324:THR:OG1  | 2.52                     | 0.42              |
| 1:7:320:ASN:ND2  | 1:7:324:THR:OG1  | 2.52                     | 0.42              |
| 1:A:354:GLN:HG3  | 1:I:268:ALA:HB3  | 2.01                     | 0.42              |
| 1:A:381:ALA:HB3  | 1:G:318:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:397:TRP:CD2  | 1:I:397:TRP:HB2  | 2.54                     | 0.42              |
| 1:A:406:ARG:HB2  | 1:A:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:B:406:ARG:HB2  | 1:B:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:B:508:PRO:HB2  | 1:I:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:E:320:ASN:ND2  | 1:E:324:THR:OG1  | 2.52                     | 0.42              |
| 1:F:125:LYS:HG2  | 1:F:476:VAL:HB   | 2.01                     | 0.42              |
| 1:F:378:ARG:HA   | 1:F:378:ARG:HD2  | 1.73                     | 0.42              |
| 1:H:397:TRP:HB2  | 1:W:397:TRP:CD2  | 2.53                     | 0.42              |
| 1:I:222:GLU:OE1  | 1:I:222:GLU:N    | 2.50                     | 0.42              |
| 1:J:250:ARG:O    | 1:J:536:LYS:HG2  | 2.18                     | 0.42              |
| 1:J:501:GLY:O    | 1:J:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:L:320:ASN:ND2  | 1:L:324:THR:OG1  | 2.52                     | 0.42              |
| 1:N:194:PRO:HB2  | 1:N:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:N:300:LEU:HG   | 1:N:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:Q:488:ARG:NH2  | 1:R:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:R:193:ILE:HD11 | 1:U:261:PRO:HG3  | 2.02                     | 0.42              |
| 1:R:501:GLY:O    | 1:R:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:T:85:LYS:HG3   | 1:T:332:GLY:HA3  | 2.00                     | 0.42              |
| 1:T:261:PRO:HG3  | 1:d:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:V:85:LYS:HG3   | 1:V:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:W:320:ASN:ND2  | 1:W:324:THR:OG1  | 2.52                     | 0.42              |
| 1:X:501:GLY:O    | 1:X:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:Y:85:LYS:HG3   | 1:Y:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:Z:318:VAL:HG22 | 1:3:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:b:300:LEU:HG   | 1:b:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:d:194:PRO:HB2  | 1:d:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:i:252:TYR:CD1  | 1:i:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:j:261:PRO:HG3  | 1:k:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:m:125:LYS:HG2  | 1:m:476:VAL:HB   | 2.01                     | 0.42              |
| 1:m:252:TYR:CD1  | 1:m:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:m:261:PRO:HG3  | 1:n:193:ILE:HD11 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:397:TRP:HB2  | 1:p:397:TRP:CD2  | 2.53                     | 0.42              |
| 1:q:193:ILE:HD11 | 1:s:261:PRO:HG3  | 2.02                     | 0.42              |
| 1:q:397:TRP:CD2  | 1:s:397:TRP:HB2  | 2.53                     | 0.42              |
| 1:q:501:GLY:O    | 1:q:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:s:72:TYR:OH    | 1:s:222:GLU:OE1  | 2.37                     | 0.42              |
| 1:t:125:LYS:HG2  | 1:t:476:VAL:HB   | 2.01                     | 0.42              |
| 1:u:125:LYS:HG2  | 1:u:476:VAL:HB   | 2.01                     | 0.42              |
| 1:u:397:TRP:HB2  | 1:v:397:TRP:CD2  | 2.54                     | 0.42              |
| 1:u:501:GLY:O    | 1:u:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:w:300:LEU:HG   | 1:w:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:w:320:ASN:ND2  | 1:w:324:THR:OG1  | 2.52                     | 0.42              |
| 1:z:179:GLU:OE2  | 1:z:411:ARG:NH1  | 2.38                     | 0.42              |
| 1:1:194:PRO:HB2  | 1:1:216:ILE:HG23 | 2.01                     | 0.42              |
| 1:2:300:LEU:HG   | 1:2:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:2:501:GLY:O    | 1:2:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:3:126:MET:HB2  | 1:3:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:A:193:ILE:HD11 | 1:I:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:C:125:LYS:HG2  | 1:C:476:VAL:HB   | 2.01                     | 0.42              |
| 1:D:193:ILE:HD11 | 1:P:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:E:300:LEU:HG   | 1:E:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:G:194:PRO:HB2  | 1:G:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:G:501:GLY:O    | 1:G:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:I:501:GLY:O    | 1:I:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:J:300:LEU:HG   | 1:J:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:K:320:ASN:ND2  | 1:K:324:THR:OG1  | 2.52                     | 0.42              |
| 1:N:378:ARG:HD2  | 1:N:378:ARG:HA   | 1.73                     | 0.42              |
| 1:O:194:PRO:HB2  | 1:O:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:O:300:LEU:HG   | 1:O:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:T:88:ARG:NH2   | 1:i:507:ASN:OD1  | 2.51                     | 0.42              |
| 1:T:125:LYS:HG2  | 1:T:476:VAL:HB   | 2.01                     | 0.42              |
| 1:T:252:TYR:CD1  | 1:T:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:U:507:ASN:OD1  | 1:e:88:ARG:NH2   | 2.51                     | 0.42              |
| 1:W:85:LYS:HG3   | 1:W:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:W:126:MET:HB2  | 1:W:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:Y:194:PRO:HB2  | 1:Y:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:a:136:LYS:NZ   | 1:a:149:ASN:OD1  | 2.37                     | 0.42              |
| 1:a:381:ALA:HB3  | 1:8:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:d:222:GLU:OE1  | 1:d:222:GLU:N    | 2.50                     | 0.42              |
| 1:e:72:TYR:OH    | 1:e:222:GLU:OE1  | 2.37                     | 0.42              |
| 1:f:300:LEU:HG   | 1:f:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:g:488:ARG:NH2  | 1:z:508:PRO:HB2  | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:194:PRO:HB2  | 1:h:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:i:194:PRO:HB2  | 1:i:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:i:300:LEU:HG   | 1:i:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:l:194:PRO:HB2  | 1:l:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:l:300:LEU:HG   | 1:l:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:o:501:GLY:O    | 1:o:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:q:194:PRO:HB2  | 1:q:216:ILE:HG23 | 2.01                     | 0.42              |
| 1:q:508:PRO:HB2  | 1:x:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:t:501:GLY:O    | 1:t:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:u:320:ASN:ND2  | 1:u:324:THR:OG1  | 2.52                     | 0.42              |
| 1:u:488:ARG:NH2  | 1:1:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:y:125:LYS:HG2  | 1:y:476:VAL:HB   | 2.01                     | 0.42              |
| 1:z:318:VAL:HG22 | 1:2:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:z:397:TRP:CD2  | 1:2:397:TRP:HB2  | 2.54                     | 0.42              |
| 1:2:406:ARG:HB2  | 1:2:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:6:252:TYR:CD1  | 1:6:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:7:194:PRO:HB2  | 1:7:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:A:126:MET:HB2  | 1:A:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:A:318:VAL:HG22 | 1:I:381:ALA:HB3  | 2.01                     | 0.42              |
| 1:F:354:GLN:HG3  | 1:Q:268:ALA:HB3  | 2.02                     | 0.42              |
| 1:G:125:LYS:HG2  | 1:G:476:VAL:HB   | 2.01                     | 0.42              |
| 1:L:134:GLN:HE22 | 1:b:153:ALA:HA   | 1.85                     | 0.42              |
| 1:L:179:GLU:OE2  | 1:L:411:ARG:NH1  | 2.38                     | 0.42              |
| 1:M:194:PRO:HB2  | 1:M:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:R:194:PRO:HB2  | 1:R:216:ILE:HG23 | 2.01                     | 0.42              |
| 1:R:397:TRP:CD2  | 1:U:397:TRP:HB2  | 2.53                     | 0.42              |
| 1:W:252:TYR:CD1  | 1:W:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:W:501:GLY:O    | 1:W:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:X:193:ILE:HD11 | 1:e:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:Z:126:MET:HB2  | 1:Z:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:a:126:MET:HB2  | 1:a:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:c:88:ARG:NH2   | 1:s:507:ASN:OD1  | 2.51                     | 0.42              |
| 1:c:406:ARG:HB2  | 1:c:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:e:252:TYR:CD1  | 1:e:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:f:194:PRO:HB2  | 1:f:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:o:252:TYR:CD1  | 1:o:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:r:125:LYS:HG2  | 1:r:476:VAL:HB   | 2.01                     | 0.42              |
| 1:t:194:PRO:HB2  | 1:t:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:t:508:PRO:HB2  | 1:5:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:u:381:ALA:HB3  | 1:v:318:VAL:HG22 | 2.01                     | 0.42              |
| 1:z:381:ALA:HB3  | 1:1:318:VAL:HG22 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:156:HIS:N    | 1:1:447:LYS:O    | 2.43                     | 0.42              |
| 1:2:378:ARG:HD2  | 1:2:378:ARG:HA   | 1.73                     | 0.42              |
| 1:3:320:ASN:ND2  | 1:3:324:THR:OG1  | 2.52                     | 0.42              |
| 1:4:320:ASN:ND2  | 1:4:324:THR:OG1  | 2.52                     | 0.42              |
| 1:6:85:LYS:HG3   | 1:6:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:6:501:GLY:O    | 1:6:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:8:126:MET:HB2  | 1:8:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:A:153:ALA:HA   | 1:B:134:GLN:HE22 | 1.84                     | 0.42              |
| 1:A:501:GLY:O    | 1:A:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:B:180:LEU:HD11 | 1:B:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:B:194:PRO:HB2  | 1:B:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:D:488:ARG:NH2  | 1:M:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:E:85:LYS:HG3   | 1:E:332:GLY:HA3  | 2.00                     | 0.42              |
| 1:E:194:PRO:HB2  | 1:E:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:E:501:GLY:O    | 1:E:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:F:501:GLY:O    | 1:F:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:G:508:PRO:HB2  | 1:H:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:K:501:GLY:O    | 1:K:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:N:261:PRO:HG3  | 1:P:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:P:501:GLY:O    | 1:P:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:R:252:TYR:CD1  | 1:R:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:S:261:PRO:HG3  | 1:U:193:ILE:HD11 | 2.02                     | 0.42              |
| 1:T:134:GLN:HE22 | 1:U:153:ALA:HA   | 1.85                     | 0.42              |
| 1:T:501:GLY:O    | 1:T:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:W:261:PRO:HG3  | 1:Y:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:W:406:ARG:HB2  | 1:W:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:Y:180:LEU:HD11 | 1:Y:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:a:252:TYR:CD1  | 1:a:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:a:320:ASN:ND2  | 1:a:324:THR:OG1  | 2.52                     | 0.42              |
| 1:b:399:PHE:CG   | 1:b:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:c:252:TYR:CD1  | 1:c:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:c:261:PRO:HG3  | 1:o:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:e:85:LYS:HG3   | 1:e:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:f:252:TYR:CD1  | 1:f:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:f:381:ALA:HB3  | 1:h:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:g:125:LYS:HG2  | 1:g:476:VAL:HB   | 2.01                     | 0.42              |
| 1:h:508:PRO:HB2  | 1:k:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:j:501:GLY:O    | 1:j:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:k:501:GLY:O    | 1:k:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:l:136:LYS:NZ   | 1:l:149:ASN:OD1  | 2.37                     | 0.42              |
| 1:l:320:ASN:ND2  | 1:l:324:THR:OG1  | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:399:PHE:CG   | 1:m:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:m:501:GLY:O    | 1:m:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:n:501:GLY:O    | 1:n:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:q:252:TYR:CD1  | 1:q:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:r:261:PRO:HG3  | 1:s:193:ILE:HD11 | 2.02                     | 0.42              |
| 1:r:300:LEU:HG   | 1:r:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:u:126:MET:HB2  | 1:u:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:u:222:GLU:OE1  | 1:u:222:GLU:N    | 2.50                     | 0.42              |
| 1:u:268:ALA:HB3  | 1:v:354:GLN:HG3  | 2.02                     | 0.42              |
| 1:v:501:GLY:O    | 1:v:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:w:193:ILE:HD11 | 1:y:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:x:268:ALA:HB3  | 1:y:354:GLN:HG3  | 2.02                     | 0.42              |
| 1:y:501:GLY:O    | 1:y:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:1:180:LEU:HD11 | 1:1:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:2:508:PRO:HB2  | 1:4:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:6:126:MET:HB2  | 1:6:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:6:261:PRO:HG3  | 1:7:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:7:180:LEU:HD11 | 1:7:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:A:85:LYS:HG3   | 1:A:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:A:507:ASN:OD1  | 1:E:88:ARG:NH2   | 2.51                     | 0.42              |
| 1:B:126:MET:HB2  | 1:B:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:C:488:ARG:NH2  | 1:L:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:D:501:GLY:O    | 1:D:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:E:399:PHE:CG   | 1:E:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:F:399:PHE:CG   | 1:F:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:G:378:ARG:HD2  | 1:G:378:ARG:HA   | 1.73                     | 0.42              |
| 1:H:88:ARG:NH2   | 1:Z:507:ASN:OD1  | 2.51                     | 0.42              |
| 1:H:501:GLY:O    | 1:H:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:I:40:THR:HG1   | 1:I:132:ASN:H    | 1.68                     | 0.42              |
| 1:J:29:GLY:N     | 1:a:234:SER:O    | 2.31                     | 0.42              |
| 1:J:85:LYS:HG3   | 1:J:332:GLY:HA3  | 2.00                     | 0.42              |
| 1:J:399:PHE:CG   | 1:J:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:J:406:ARG:HB2  | 1:J:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:K:180:LEU:HD11 | 1:K:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:M:318:VAL:HG22 | 1:b:381:ALA:HB3  | 2.00                     | 0.42              |
| 1:M:320:ASN:ND2  | 1:M:324:THR:OG1  | 2.52                     | 0.42              |
| 1:R:180:LEU:HD11 | 1:R:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:S:125:LYS:HG2  | 1:S:476:VAL:HB   | 2.01                     | 0.42              |
| 1:S:134:GLN:HE22 | 1:d:153:ALA:HA   | 1.85                     | 0.42              |
| 1:S:300:LEU:HG   | 1:S:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:T:399:PHE:CG   | 1:T:400:PRO:HD2  | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:180:LEU:HD11 | 1:V:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:W:488:ARG:NH2  | 1:X:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:X:180:LEU:HD11 | 1:X:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:X:252:TYR:CD1  | 1:X:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:Y:29:GLY:N     | 1:4:234:SER:O    | 2.32                     | 0.42              |
| 1:Y:125:LYS:HG2  | 1:Y:476:VAL:HB   | 2.01                     | 0.42              |
| 1:Z:399:PHE:CG   | 1:Z:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:b:194:PRO:HB2  | 1:b:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:b:252:TYR:CD1  | 1:b:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:b:488:ARG:NH2  | 1:c:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:c:85:LYS:HG3   | 1:c:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:d:488:ARG:NH2  | 1:n:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:d:501:GLY:O    | 1:d:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:d:508:PRO:HB2  | 1:n:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:e:406:ARG:HB2  | 1:e:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:f:399:PHE:CG   | 1:f:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:g:501:GLY:O    | 1:g:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:i:261:PRO:HG3  | 1:j:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:m:134:GLN:HE22 | 1:s:153:ALA:HA   | 1.85                     | 0.42              |
| 1:m:488:ARG:NH2  | 1:r:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:n:153:ALA:HA   | 1:r:134:GLN:HE22 | 1.85                     | 0.42              |
| 1:o:180:LEU:HD11 | 1:o:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:o:194:PRO:HB2  | 1:o:216:ILE:HG23 | 2.01                     | 0.42              |
| 1:o:508:PRO:HB2  | 1:6:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:p:180:LEU:HD11 | 1:p:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:q:180:LEU:HD11 | 1:q:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:r:399:PHE:CG   | 1:r:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:u:261:PRO:HG3  | 1:v:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:v:85:LYS:HG3   | 1:v:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:v:126:MET:HB2  | 1:v:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:w:85:LYS:HG3   | 1:w:332:GLY:HA3  | 2.00                     | 0.42              |
| 1:w:194:PRO:HB2  | 1:w:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:w:399:PHE:CG   | 1:w:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:w:501:GLY:O    | 1:w:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:y:156:HIS:N    | 1:y:447:LYS:O    | 2.43                     | 0.42              |
| 1:y:399:PHE:CG   | 1:y:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:z:261:PRO:HG3  | 1:1:193:ILE:HD11 | 2.02                     | 0.42              |
| 1:1:126:MET:HB2  | 1:1:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:1:261:PRO:HG3  | 1:2:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:2:85:LYS:HG3   | 1:2:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:2:399:PHE:CG   | 1:2:400:PRO:HD2  | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:252:TYR:CD1  | 1:3:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:3:501:GLY:O    | 1:3:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:4:252:TYR:CD1  | 1:4:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:4:501:GLY:O    | 1:4:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:5:88:ARG:NH2   | 1:8:507:ASN:OD1  | 2.51                     | 0.42              |
| 1:5:501:GLY:O    | 1:5:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:6:406:ARG:HB2  | 1:6:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:7:51:ASP:OD1   | 1:7:481:ARG:NE   | 2.38                     | 0.42              |
| 1:7:85:LYS:HG3   | 1:7:332:GLY:HA3  | 2.01                     | 0.42              |
| 1:8:85:LYS:HG3   | 1:8:332:GLY:HA3  | 2.00                     | 0.42              |
| 1:8:399:PHE:CG   | 1:8:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:A:180:LEU:HD11 | 1:A:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:A:222:GLU:OE1  | 1:A:222:GLU:N    | 2.50                     | 0.42              |
| 1:C:153:ALA:HA   | 1:D:134:GLN:HE22 | 1.85                     | 0.42              |
| 1:C:501:GLY:O    | 1:C:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:D:354:GLN:HG3  | 1:P:268:ALA:HB3  | 2.02                     | 0.42              |
| 1:E:193:ILE:HD11 | 1:F:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:F:126:MET:HB2  | 1:F:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:F:180:LEU:HD11 | 1:F:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:H:193:ILE:HD11 | 1:Y:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:N:399:PHE:CG   | 1:N:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:N:501:GLY:O    | 1:N:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:O:180:LEU:HD11 | 1:O:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:O:320:ASN:ND2  | 1:O:324:THR:OG1  | 2.52                     | 0.42              |
| 1:P:222:GLU:OE1  | 1:P:222:GLU:N    | 2.50                     | 0.42              |
| 1:S:399:PHE:CG   | 1:S:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:S:406:ARG:HB2  | 1:S:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:S:508:PRO:HB2  | 1:T:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:V:320:ASN:ND2  | 1:V:324:THR:OG1  | 2.52                     | 0.42              |
| 1:X:194:PRO:HB2  | 1:X:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:Y:51:ASP:OD1   | 1:Y:481:ARG:NE   | 2.38                     | 0.42              |
| 1:Z:85:LYS:HG3   | 1:Z:332:GLY:HA3  | 2.00                     | 0.42              |
| 1:a:399:PHE:CG   | 1:a:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:b:508:PRO:HB2  | 1:c:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:c:320:ASN:ND2  | 1:c:324:THR:OG1  | 2.52                     | 0.42              |
| 1:d:125:LYS:HG2  | 1:d:476:VAL:HB   | 2.01                     | 0.42              |
| 1:e:488:ARG:NH2  | 1:f:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:e:508:PRO:HB2  | 1:f:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:f:180:LEU:HD11 | 1:f:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:g:153:ALA:HA   | 1:k:134:GLN:HE22 | 1.85                     | 0.42              |
| 1:h:320:ASN:ND2  | 1:h:324:THR:OG1  | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:399:PHE:CG   | 1:i:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:i:501:GLY:O    | 1:i:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:m:397:TRP:HB2  | 1:n:397:TRP:CD2  | 2.54                     | 0.42              |
| 1:p:320:ASN:ND2  | 1:p:324:THR:OG1  | 2.52                     | 0.42              |
| 1:q:320:ASN:ND2  | 1:q:324:THR:OG1  | 2.52                     | 0.42              |
| 1:u:40:THR:HG1   | 1:u:132:ASN:H    | 1.68                     | 0.42              |
| 1:y:126:MET:HB2  | 1:y:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:y:180:LEU:HD11 | 1:y:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:y:320:ASN:ND2  | 1:y:324:THR:OG1  | 2.52                     | 0.42              |
| 1:y:378:ARG:HA   | 1:y:378:ARG:HD2  | 1.73                     | 0.42              |
| 1:z:193:ILE:HD11 | 1:2:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:3:507:ASN:OD1  | 1:8:88:ARG:NH2   | 2.51                     | 0.42              |
| 1:4:180:LEU:HD11 | 1:4:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:7:125:LYS:HG2  | 1:7:476:VAL:HB   | 2.01                     | 0.42              |
| 1:A:300:LEU:HG   | 1:A:344:LEU:HD23 | 2.00                     | 0.42              |
| 1:C:193:ILE:HD11 | 1:M:261:PRO:HG3  | 2.02                     | 0.42              |
| 1:D:381:ALA:HB3  | 1:N:318:VAL:HG22 | 2.00                     | 0.42              |
| 1:F:320:ASN:ND2  | 1:F:324:THR:OG1  | 2.52                     | 0.42              |
| 1:G:507:ASN:OD1  | 1:W:88:ARG:NH2   | 2.51                     | 0.42              |
| 1:H:180:LEU:HD11 | 1:H:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:I:126:MET:HB2  | 1:I:241:PHE:HE2  | 1.84                     | 0.42              |
| 1:J:508:PRO:HB2  | 1:K:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:K:252:TYR:CD1  | 1:K:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:L:378:ARG:HD2  | 1:L:378:ARG:HA   | 1.73                     | 0.42              |
| 1:L:507:ASN:OD1  | 1:b:88:ARG:NH2   | 2.51                     | 0.42              |
| 1:M:193:ILE:HD11 | 1:b:261:PRO:HG3  | 2.01                     | 0.42              |
| 1:M:501:GLY:O    | 1:M:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:N:125:LYS:HG2  | 1:N:476:VAL:HB   | 2.01                     | 0.42              |
| 1:O:399:PHE:CG   | 1:O:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:R:320:ASN:ND2  | 1:R:324:THR:OG1  | 2.52                     | 0.42              |
| 1:S:488:ARG:NH2  | 1:T:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:T:194:PRO:HB2  | 1:T:216:ILE:HG23 | 2.02                     | 0.42              |
| 1:U:222:GLU:OE1  | 1:U:222:GLU:N    | 2.50                     | 0.42              |
| 1:V:252:TYR:CD1  | 1:V:253:ILE:HG23 | 2.54                     | 0.42              |
| 1:W:180:LEU:HD11 | 1:W:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:Z:88:ARG:NH2   | 1:a:507:ASN:OD1  | 2.51                     | 0.42              |
| 1:a:488:ARG:NH2  | 1:3:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:a:501:GLY:O    | 1:a:507:ASN:HB2  | 2.20                     | 0.42              |
| 1:c:51:ASP:OD1   | 1:c:481:ARG:NE   | 2.38                     | 0.42              |
| 1:e:320:ASN:ND2  | 1:e:324:THR:OG1  | 2.52                     | 0.42              |
| 1:f:88:ARG:NH2   | 1:z:507:ASN:OD1  | 2.51                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:180:LEU:HD11 | 1:g:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:g:193:ILE:HD11 | 1:h:261:PRO:HG3  | 2.02                     | 0.42              |
| 1:g:222:GLU:OE1  | 1:g:222:GLU:N    | 2.50                     | 0.42              |
| 1:i:508:PRO:HB2  | 1:l:488:ARG:NH2  | 2.35                     | 0.42              |
| 1:j:268:ALA:HB3  | 1:k:354:GLN:HG3  | 2.02                     | 0.42              |
| 1:l:180:LEU:HD11 | 1:l:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:l:399:PHE:CG   | 1:l:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:n:180:LEU:HD11 | 1:n:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:s:406:ARG:HB2  | 1:s:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:v:180:LEU:HD11 | 1:v:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:z:194:PRO:HB2  | 1:z:216:ILE:HG23 | 2.01                     | 0.42              |
| 1:1:399:PHE:CG   | 1:1:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:1:406:ARG:HB2  | 1:1:531:LYS:NZ   | 2.33                     | 0.42              |
| 1:2:134:GLN:HE22 | 1:3:153:ALA:HA   | 1.85                     | 0.42              |
| 1:3:399:PHE:CG   | 1:3:400:PRO:HD2  | 2.55                     | 0.42              |
| 1:5:180:LEU:HD11 | 1:5:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:6:180:LEU:HD11 | 1:6:518:TYR:CE2  | 2.55                     | 0.42              |
| 1:7:488:ARG:NH2  | 1:8:508:PRO:HB2  | 2.35                     | 0.42              |
| 1:B:354:GLN:HG3  | 1:L:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:B:399:PHE:CG   | 1:B:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:B:488:ARG:NH2  | 1:I:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:C:180:LEU:HD11 | 1:C:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:F:156:HIS:N    | 1:F:447:LYS:O    | 2.43                     | 0.41              |
| 1:G:381:ALA:HB3  | 1:I:318:VAL:HG22 | 2.00                     | 0.41              |
| 1:H:268:ALA:HB3  | 1:W:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:J:136:LYS:NZ   | 1:J:149:ASN:OD1  | 2.37                     | 0.41              |
| 1:J:194:PRO:HB2  | 1:J:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:L:194:PRO:HB2  | 1:L:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:L:399:PHE:CG   | 1:L:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:M:88:ARG:NH2   | 1:c:507:ASN:OD1  | 2.51                     | 0.41              |
| 1:M:153:ALA:HA   | 1:c:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:M:399:PHE:CG   | 1:M:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:N:508:PRO:HB2  | 1:O:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:O:318:VAL:HG22 | 1:n:381:ALA:HB3  | 2.00                     | 0.41              |
| 1:P:507:ASN:OD1  | 1:Q:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:Q:194:PRO:HB2  | 1:Q:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:T:126:MET:HB2  | 1:T:241:PHE:HE2  | 1.84                     | 0.41              |
| 1:T:397:TRP:HB2  | 1:d:397:TRP:CD2  | 2.54                     | 0.41              |
| 1:U:180:LEU:HD11 | 1:U:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:Y:488:ARG:NH2  | 1:Z:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:Y:501:GLY:O    | 1:Y:507:ASN:HB2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:508:PRO:HB2  | 1:3:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:b:180:LEU:HD11 | 1:b:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:d:180:LEU:HD11 | 1:d:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:e:51:ASP:OD1   | 1:e:481:ARG:NE   | 2.38                     | 0.41              |
| 1:e:507:ASN:OD1  | 1:h:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:f:501:GLY:O    | 1:f:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:g:406:ARG:HB2  | 1:g:531:LYS:NZ   | 2.33                     | 0.41              |
| 1:h:399:PHE:CG   | 1:h:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:h:501:GLY:O    | 1:h:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:i:125:LYS:HG2  | 1:i:476:VAL:HB   | 2.01                     | 0.41              |
| 1:i:378:ARG:HD2  | 1:i:378:ARG:HA   | 1.73                     | 0.41              |
| 1:n:125:LYS:HG2  | 1:n:476:VAL:HB   | 2.01                     | 0.41              |
| 1:r:378:ARG:HA   | 1:r:378:ARG:HD2  | 1.73                     | 0.41              |
| 1:t:507:ASN:OD1  | 1:6:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:u:180:LEU:HD11 | 1:u:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:v:153:ALA:HA   | 1:1:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:v:300:LEU:HG   | 1:v:344:LEU:HD23 | 2.00                     | 0.41              |
| 1:v:507:ASN:OD1  | 1:w:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:z:320:ASN:ND2  | 1:z:324:THR:OG1  | 2.52                     | 0.41              |
| 1:2:180:LEU:HD11 | 1:2:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:2:194:PRO:HB2  | 1:2:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:2:222:GLU:OE1  | 1:2:222:GLU:N    | 2.50                     | 0.41              |
| 1:4:156:HIS:N    | 1:4:447:LYS:O    | 2.43                     | 0.41              |
| 1:5:193:ILE:HD11 | 1:7:261:PRO:HG3  | 2.01                     | 0.41              |
| 1:5:268:ALA:HB3  | 1:6:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:7:508:PRO:HB2  | 1:8:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:8:501:GLY:O    | 1:8:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:194:PRO:HB2  | 1:A:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:C:406:ARG:HB2  | 1:C:531:LYS:NZ   | 2.33                     | 0.41              |
| 1:E:508:PRO:HB2  | 1:P:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:H:153:ALA:HA   | 1:Z:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:I:320:ASN:ND2  | 1:I:324:THR:OG1  | 2.52                     | 0.41              |
| 1:J:180:LEU:HD11 | 1:J:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:J:222:GLU:OE1  | 1:J:222:GLU:N    | 2.50                     | 0.41              |
| 1:J:378:ARG:HD2  | 1:J:378:ARG:HA   | 1.73                     | 0.41              |
| 1:N:134:GLN:HE22 | 1:m:153:ALA:HA   | 1.85                     | 0.41              |
| 1:N:488:ARG:NH2  | 1:O:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:O:134:GLN:HE22 | 1:P:153:ALA:HA   | 1.85                     | 0.41              |
| 1:O:153:ALA:HA   | 1:d:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:P:134:GLN:HE22 | 1:Q:153:ALA:HA   | 1.85                     | 0.41              |
| 1:T:222:GLU:OE1  | 1:T:222:GLU:N    | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:406:ARG:HB2  | 1:U:531:LYS:NZ   | 2.33                     | 0.41              |
| 1:V:300:LEU:HG   | 1:V:344:LEU:HD23 | 2.00                     | 0.41              |
| 1:V:399:PHE:CG   | 1:V:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:W:399:PHE:CG   | 1:W:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:X:153:ALA:HA   | 1:f:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:Y:508:PRO:HB2  | 1:Z:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:Z:194:PRO:HB2  | 1:Z:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:Z:501:GLY:O    | 1:Z:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:b:134:GLN:HE22 | 1:o:153:ALA:HA   | 1.85                     | 0.41              |
| 1:b:501:GLY:O    | 1:b:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:e:134:GLN:HE22 | 1:h:153:ALA:HA   | 1.85                     | 0.41              |
| 1:e:501:GLY:O    | 1:e:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:f:261:PRO:HG3  | 1:h:193:ILE:HD11 | 2.01                     | 0.41              |
| 1:i:318:VAL:HG22 | 1:k:381:ALA:HB3  | 2.00                     | 0.41              |
| 1:i:488:ARG:NH2  | 1:l:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:j:134:GLN:HE22 | 1:x:153:ALA:HA   | 1.85                     | 0.41              |
| 1:j:153:ALA:HA   | 1:l:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:j:180:LEU:HD11 | 1:j:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:j:222:GLU:OE1  | 1:j:222:GLU:N    | 2.50                     | 0.41              |
| 1:j:488:ARG:NH2  | 1:w:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:l:153:ALA:HA   | 1:n:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:l:501:GLY:O    | 1:l:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:m:194:PRO:HB2  | 1:m:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:m:508:PRO:HB2  | 1:r:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:p:153:ALA:HA   | 1:6:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:p:252:TYR:CD1  | 1:p:253:ILE:HG23 | 2.54                     | 0.41              |
| 1:p:399:PHE:CG   | 1:p:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:s:222:GLU:OE1  | 1:s:222:GLU:N    | 2.50                     | 0.41              |
| 1:s:501:GLY:O    | 1:s:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:u:508:PRO:HB2  | 1:1:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:v:194:PRO:HB2  | 1:v:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:v:222:GLU:OE1  | 1:v:222:GLU:N    | 2.50                     | 0.41              |
| 1:x:194:PRO:HB2  | 1:x:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:z:180:LEU:HD11 | 1:z:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:8:156:HIS:N    | 1:8:447:LYS:O    | 2.43                     | 0.41              |
| 1:8:194:PRO:HB2  | 1:8:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:B:156:HIS:N    | 1:B:447:LYS:O    | 2.43                     | 0.41              |
| 1:C:85:LYS:HG3   | 1:C:332:GLY:HA3  | 2.01                     | 0.41              |
| 1:C:222:GLU:OE1  | 1:C:222:GLU:N    | 2.50                     | 0.41              |
| 1:C:508:PRO:HB2  | 1:L:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:D:156:HIS:N    | 1:D:447:LYS:O    | 2.43                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:180:LEU:HD11 | 1:I:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:I:399:PHE:CG   | 1:I:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:I:507:ASN:OD1  | 1:J:88:ARG:NH2   | 2.50                     | 0.41              |
| 1:J:125:LYS:HG2  | 1:J:476:VAL:HB   | 2.01                     | 0.41              |
| 1:L:180:LEU:HD11 | 1:L:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:N:85:LYS:HG3   | 1:N:332:GLY:HA3  | 2.01                     | 0.41              |
| 1:O:268:ALA:HB3  | 1:m:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:O:354:GLN:HG3  | 1:n:268:ALA:HB3  | 2.03                     | 0.41              |
| 1:O:370:SER:HA   | 1:O:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:O:501:GLY:O    | 1:O:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:P:180:LEU:HD11 | 1:P:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:Q:507:ASN:OD1  | 1:S:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:R:268:ALA:HB3  | 1:S:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:R:399:PHE:CG   | 1:R:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:S:501:GLY:O    | 1:S:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:T:153:ALA:HA   | 1:i:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:T:354:GLN:HG3  | 1:l:268:ALA:HB3  | 2.03                     | 0.41              |
| 1:U:399:PHE:CG   | 1:U:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:V:153:ALA:HA   | 1:W:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:V:501:GLY:O    | 1:V:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:W:125:LYS:HG2  | 1:W:476:VAL:HB   | 2.01                     | 0.41              |
| 1:W:194:PRO:HB2  | 1:W:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:Z:180:LEU:HD11 | 1:Z:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:c:501:GLY:O    | 1:c:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:d:268:ALA:HB3  | 1:l:354:GLN:HG3  | 2.03                     | 0.41              |
| 1:d:381:ALA:HB3  | 1:l:318:VAL:HG22 | 2.00                     | 0.41              |
| 1:f:40:THR:HG1   | 1:f:132:ASN:H    | 1.68                     | 0.41              |
| 1:f:234:SER:O    | 1:z:29:GLY:N     | 2.33                     | 0.41              |
| 1:h:134:GLN:HE22 | 1:i:153:ALA:HA   | 1.85                     | 0.41              |
| 1:j:507:ASN:OD1  | 1:x:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:l:370:SER:HA   | 1:l:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:m:126:MET:HB2  | 1:m:241:PHE:HE2  | 1.84                     | 0.41              |
| 1:m:222:GLU:OE1  | 1:m:222:GLU:N    | 2.50                     | 0.41              |
| 1:o:488:ARG:NH2  | 1:6:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:p:300:LEU:HG   | 1:p:344:LEU:HD23 | 2.00                     | 0.41              |
| 1:p:501:GLY:O    | 1:p:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:q:268:ALA:HB3  | 1:r:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:q:488:ARG:NH2  | 1:x:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:s:180:LEU:HD11 | 1:s:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:s:399:PHE:CG   | 1:s:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:t:381:ALA:HB3  | 1:u:318:VAL:HG22 | 2.00                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:252:TYR:CD1  | 1:x:253:ILE:HG23 | 2.54                     | 0.41              |
| 1:z:399:PHE:CG   | 1:z:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:1:501:GLY:O    | 1:1:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:3:318:VAL:HG22 | 1:4:381:ALA:HB3  | 2.01                     | 0.41              |
| 1:5:153:ALA:HA   | 1:8:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:6:125:LYS:HG2  | 1:6:476:VAL:HB   | 2.01                     | 0.41              |
| 1:6:194:PRO:HB2  | 1:6:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:6:399:PHE:CG   | 1:6:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:7:399:PHE:CG   | 1:7:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:7:501:GLY:O    | 1:7:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:C:399:PHE:CG   | 1:C:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:I:136:LYS:NZ   | 1:I:149:ASN:OD1  | 2.37                     | 0.41              |
| 1:J:507:ASN:OD1  | 1:a:88:ARG:NH2   | 2.52                     | 0.41              |
| 1:K:156:HIS:N    | 1:K:447:LYS:O    | 2.43                     | 0.41              |
| 1:K:381:ALA:HB3  | 1:a:318:VAL:HG22 | 2.00                     | 0.41              |
| 1:L:501:GLY:O    | 1:L:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:M:180:LEU:HD11 | 1:M:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:U:501:GLY:O    | 1:U:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:Y:370:SER:HA   | 1:Y:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:b:156:HIS:N    | 1:b:447:LYS:O    | 2.43                     | 0.41              |
| 1:g:85:LYS:HG3   | 1:g:332:GLY:HA3  | 2.01                     | 0.41              |
| 1:g:399:PHE:CG   | 1:g:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:h:180:LEU:HD11 | 1:h:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:i:180:LEU:HD11 | 1:i:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:p:406:ARG:HB2  | 1:p:531:LYS:NZ   | 2.33                     | 0.41              |
| 1:q:126:MET:HB2  | 1:q:241:PHE:HE2  | 1.84                     | 0.41              |
| 1:r:88:ARG:NH2   | 1:x:507:ASN:OD1  | 2.51                     | 0.41              |
| 1:r:501:GLY:O    | 1:r:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:u:136:LYS:NZ   | 1:u:149:ASN:OD1  | 2.37                     | 0.41              |
| 1:u:399:PHE:CG   | 1:u:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:y:40:THR:HG1   | 1:y:132:ASN:H    | 1.68                     | 0.41              |
| 1:z:378:ARG:HD2  | 1:z:378:ARG:HA   | 1.73                     | 0.41              |
| 1:5:194:PRO:HB2  | 1:5:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:5:399:PHE:CG   | 1:5:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:7:370:SER:HA   | 1:7:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:8:180:LEU:HD11 | 1:8:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:B:501:GLY:O    | 1:B:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:E:488:ARG:NH2  | 1:P:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:F:194:PRO:HB2  | 1:F:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:F:370:SER:HA   | 1:F:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:H:399:PHE:CG   | 1:H:400:PRO:HD2  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:370:SER:HA   | 1:J:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:M:134:GLN:HE22 | 1:N:153:ALA:HA   | 1.85                     | 0.41              |
| 1:N:180:LEU:HD11 | 1:N:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:Q:180:LEU:HD11 | 1:Q:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:Q:252:TYR:CD1  | 1:Q:253:ILE:HG23 | 2.54                     | 0.41              |
| 1:Q:508:PRO:HB2  | 1:R:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:V:406:ARG:HB2  | 1:V:531:LYS:NZ   | 2.33                     | 0.41              |
| 1:W:508:PRO:HB2  | 1:X:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:X:399:PHE:CG   | 1:X:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:Y:399:PHE:CG   | 1:Y:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:c:399:PHE:CG   | 1:c:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:i:72:TYR:OH    | 1:i:222:GLU:OE1  | 2.37                     | 0.41              |
| 1:j:508:PRO:HB2  | 1:w:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:n:156:HIS:N    | 1:n:447:LYS:O    | 2.43                     | 0.41              |
| 1:q:399:PHE:CG   | 1:q:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:r:268:ALA:HB3  | 1:s:354:GLN:HG3  | 2.03                     | 0.41              |
| 1:t:399:PHE:CG   | 1:t:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:v:399:PHE:CG   | 1:v:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:x:180:LEU:HD11 | 1:x:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:x:399:PHE:CG   | 1:x:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:y:370:SER:HA   | 1:y:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:z:501:GLY:O    | 1:z:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:399:PHE:CG   | 1:A:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:B:318:VAL:HG22 | 1:L:381:ALA:HB3  | 2.00                     | 0.41              |
| 1:C:40:THR:OG1   | 1:C:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:D:261:PRO:O    | 1:D:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:E:261:PRO:O    | 1:E:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:G:399:PHE:CG   | 1:G:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:H:194:PRO:HB2  | 1:H:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:H:261:PRO:HG3  | 1:W:193:ILE:HD11 | 2.01                     | 0.41              |
| 1:K:399:PHE:CG   | 1:K:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:Q:261:PRO:O    | 1:Q:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:Q:399:PHE:CG   | 1:Q:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:R:126:MET:HB2  | 1:R:241:PHE:HE2  | 1.84                     | 0.41              |
| 1:S:268:ALA:HB3  | 1:U:354:GLN:HG3  | 2.03                     | 0.41              |
| 1:Z:268:ALA:HB3  | 1:4:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:Z:370:SER:HA   | 1:Z:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:b:261:PRO:O    | 1:b:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:d:261:PRO:O    | 1:d:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:d:370:SER:HA   | 1:d:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:e:180:LEU:HD11 | 1:e:518:TYR:CE2  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:399:PHE:CG   | 1:e:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:i:85:LYS:HG3   | 1:i:332:GLY:HA3  | 2.01                     | 0.41              |
| 1:j:194:PRO:HB2  | 1:j:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:n:261:PRO:O    | 1:n:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:n:370:SER:HA   | 1:n:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:o:40:THR:HG1   | 1:o:132:ASN:H    | 1.67                     | 0.41              |
| 1:o:399:PHE:CG   | 1:o:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:r:370:SER:HA   | 1:r:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:t:193:ILE:HD11 | 1:v:261:PRO:HG3  | 2.01                     | 0.41              |
| 1:t:378:ARG:HA   | 1:t:378:ARG:HD2  | 1.73                     | 0.41              |
| 1:u:51:ASP:OD1   | 1:u:481:ARG:NE   | 2.38                     | 0.41              |
| 1:w:125:LYS:HG2  | 1:w:476:VAL:HB   | 2.01                     | 0.41              |
| 1:w:261:PRO:O    | 1:w:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:w:354:GLN:HG3  | 1:y:268:ALA:HB3  | 2.03                     | 0.41              |
| 1:x:261:PRO:O    | 1:x:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:y:194:PRO:HB2  | 1:y:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:z:153:ALA:HA   | 1:4:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:2:125:LYS:HG2  | 1:2:476:VAL:HB   | 2.01                     | 0.41              |
| 1:2:370:SER:HA   | 1:2:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:4:399:PHE:CG   | 1:4:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:A:261:PRO:HG3  | 1:G:193:ILE:HD11 | 2.01                     | 0.41              |
| 1:C:40:THR:HG1   | 1:C:132:ASN:H    | 1.67                     | 0.41              |
| 1:C:370:SER:HA   | 1:C:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:E:354:GLN:HG3  | 1:F:268:ALA:HB3  | 2.03                     | 0.41              |
| 1:G:180:LEU:HD11 | 1:G:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:I:51:ASP:OD1   | 1:I:481:ARG:NE   | 2.39                     | 0.41              |
| 1:K:261:PRO:O    | 1:K:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:K:354:GLN:HG3  | 1:8:268:ALA:HB3  | 2.03                     | 0.41              |
| 1:L:40:THR:OG1   | 1:L:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:S:156:HIS:N    | 1:S:447:LYS:O    | 2.43                     | 0.41              |
| 1:S:370:SER:HA   | 1:S:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:T:370:SER:HA   | 1:T:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:Z:156:HIS:N    | 1:Z:447:LYS:O    | 2.43                     | 0.41              |
| 1:Z:354:GLN:HG3  | 1:3:268:ALA:HB3  | 2.03                     | 0.41              |
| 1:a:40:THR:OG1   | 1:a:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:a:180:LEU:HD11 | 1:a:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:a:406:ARG:O    | 1:a:531:LYS:NZ   | 2.54                     | 0.41              |
| 1:c:40:THR:OG1   | 1:c:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:c:180:LEU:HD11 | 1:c:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:c:222:GLU:OE1  | 1:c:222:GLU:N    | 2.50                     | 0.41              |
| 1:f:153:ALA:HA   | 1:z:134:GLN:HE22 | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:261:PRO:O    | 1:f:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:g:40:THR:OG1   | 1:g:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:g:40:THR:HG1   | 1:g:132:ASN:H    | 1.67                     | 0.41              |
| 1:g:194:PRO:HB2  | 1:g:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:g:370:SER:HA   | 1:g:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:k:180:LEU:HD11 | 1:k:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:k:261:PRO:O    | 1:k:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:m:370:SER:HA   | 1:m:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:t:180:LEU:HD11 | 1:t:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:v:370:SER:HA   | 1:v:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:v:488:ARG:NH2  | 1:y:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:z:40:THR:OG1   | 1:z:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:z:354:GLN:HG3  | 1:2:268:ALA:HB3  | 2.03                     | 0.41              |
| 1:2:136:LYS:NZ   | 1:2:149:ASN:OD1  | 2.37                     | 0.41              |
| 1:2:488:ARG:NH2  | 1:4:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:3:406:ARG:O    | 1:3:531:LYS:NZ   | 2.54                     | 0.41              |
| 1:4:261:PRO:O    | 1:4:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:8:370:SER:HA   | 1:8:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:A:370:SER:HA   | 1:A:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:A:488:ARG:NH2  | 1:F:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:D:268:ALA:HB3  | 1:N:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:E:125:LYS:HG2  | 1:E:476:VAL:HB   | 2.01                     | 0.41              |
| 1:F:261:PRO:O    | 1:F:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:K:153:ALA:HA   | 1:7:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:K:194:PRO:HB2  | 1:K:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:L:261:PRO:O    | 1:L:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:O:88:ARG:NH2   | 1:d:507:ASN:OD1  | 2.51                     | 0.41              |
| 1:P:194:PRO:HB2  | 1:P:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:Q:501:GLY:O    | 1:Q:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:S:222:GLU:OE1  | 1:S:222:GLU:N    | 2.50                     | 0.41              |
| 1:T:180:LEU:HD11 | 1:T:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:T:507:ASN:OD1  | 1:U:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:W:295:THR:O    | 1:W:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:a:268:ALA:HB3  | 1:8:354:GLN:HG3  | 2.03                     | 0.41              |
| 1:e:40:THR:OG1   | 1:e:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:e:222:GLU:OE1  | 1:e:222:GLU:N    | 2.50                     | 0.41              |
| 1:e:370:SER:HA   | 1:e:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:f:156:HIS:N    | 1:f:447:LYS:O    | 2.43                     | 0.41              |
| 1:h:370:SER:HA   | 1:h:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:l:88:ARG:NH2   | 1:n:507:ASN:OD1  | 2.51                     | 0.41              |
| 1:p:194:PRO:HB2  | 1:p:216:ILE:HG23 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:261:PRO:O    | 1:r:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:t:153:ALA:HA   | 1:y:134:GLN:HE22 | 1.85                     | 0.41              |
| 1:t:488:ARG:NH2  | 1:5:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:v:508:PRO:HB2  | 1:y:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:x:501:GLY:O    | 1:x:507:ASN:HB2  | 2.20                     | 0.41              |
| 1:y:261:PRO:O    | 1:y:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:z:261:PRO:O    | 1:z:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:1:370:SER:HA   | 1:1:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:3:40:THR:OG1   | 1:3:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:4:194:PRO:HB2  | 1:4:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:5:261:PRO:HG3  | 1:6:193:ILE:HD11 | 2.01                     | 0.41              |
| 1:6:295:THR:O    | 1:6:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:A:261:PRO:O    | 1:A:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:B:370:SER:HA   | 1:B:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:C:354:GLN:HG3  | 1:M:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:C:378:ARG:HA   | 1:C:378:ARG:HD2  | 1.73                     | 0.41              |
| 1:D:180:LEU:HD11 | 1:D:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:D:399:PHE:CG   | 1:D:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:F:40:THR:OG1   | 1:F:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:F:134:GLN:HE22 | 1:G:153:ALA:HA   | 1.85                     | 0.41              |
| 1:G:51:ASP:OD1   | 1:G:481:ARG:NE   | 2.39                     | 0.41              |
| 1:G:295:THR:O    | 1:G:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:G:488:ARG:NH2  | 1:H:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:H:40:THR:OG1   | 1:H:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:H:295:THR:O    | 1:H:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:H:354:GLN:HG3  | 1:Y:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:H:370:SER:HA   | 1:H:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:I:84:GLY:O     | 1:I:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:I:134:GLN:HE22 | 1:J:153:ALA:HA   | 1.86                     | 0.41              |
| 1:I:406:ARG:O    | 1:I:531:LYS:NZ   | 2.54                     | 0.41              |
| 1:J:488:ARG:NH2  | 1:K:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:L:295:THR:O    | 1:L:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:M:370:SER:HA   | 1:M:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:O:84:GLY:O     | 1:O:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:O:179:GLU:OE2  | 1:O:411:ARG:NH1  | 2.38                     | 0.41              |
| 1:P:399:PHE:CG   | 1:P:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:R:88:ARG:NH2   | 1:V:507:ASN:OD1  | 2.51                     | 0.41              |
| 1:S:194:PRO:HB2  | 1:S:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:S:261:PRO:O    | 1:S:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:T:268:ALA:HB3  | 1:d:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:U:370:SER:HA   | 1:U:524:TRP:CD1  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:194:PRO:HB2  | 1:V:216:ILE:HG23 | 2.01                     | 0.41              |
| 1:V:261:PRO:O    | 1:V:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:X:40:THR:OG1   | 1:X:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:X:354:GLN:HG3  | 1:e:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:Y:84:GLY:O     | 1:Y:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:Z:40:THR:OG1   | 1:Z:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:b:295:THR:O    | 1:b:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:c:194:PRO:HB2  | 1:c:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:c:268:ALA:HB3  | 1:o:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:c:370:SER:HA   | 1:c:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:d:156:HIS:N    | 1:d:447:LYS:O    | 2.43                     | 0.41              |
| 1:f:295:THR:O    | 1:f:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:g:354:GLN:HG3  | 1:h:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:i:354:GLN:HG3  | 1:k:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:k:399:PHE:CG   | 1:k:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:l:84:GLY:O     | 1:l:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:m:40:THR:OG1   | 1:m:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:m:180:LEU:HD11 | 1:m:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:m:261:PRO:O    | 1:m:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:m:507:ASN:OD1  | 1:s:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:o:29:GLY:N     | 1:7:234:SER:O    | 2.33                     | 0.41              |
| 1:o:40:THR:OG1   | 1:o:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:p:261:PRO:O    | 1:p:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:p:507:ASN:OD1  | 1:q:88:ARG:NH2   | 2.51                     | 0.41              |
| 1:q:378:ARG:HD2  | 1:q:378:ARG:HA   | 1.73                     | 0.41              |
| 1:r:153:ALA:HA   | 1:x:134:GLN:HE22 | 1.86                     | 0.41              |
| 1:r:194:PRO:HB2  | 1:r:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:r:222:GLU:OE1  | 1:r:222:GLU:N    | 2.50                     | 0.41              |
| 1:r:406:ARG:O    | 1:r:531:LYS:NZ   | 2.54                     | 0.41              |
| 1:s:370:SER:HA   | 1:s:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:t:295:THR:O    | 1:t:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:u:84:GLY:O     | 1:u:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:u:261:PRO:O    | 1:u:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:u:406:ARG:O    | 1:u:531:LYS:NZ   | 2.54                     | 0.41              |
| 1:v:261:PRO:O    | 1:v:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:x:295:THR:O    | 1:x:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:x:370:SER:HA   | 1:x:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:y:40:THR:OG1   | 1:y:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:y:72:TYR:OH    | 1:y:222:GLU:OE1  | 2.37                     | 0.41              |
| 1:z:84:GLY:O     | 1:z:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:z:295:THR:O    | 1:z:402:GLN:HG2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:180:LEU:HD11 | 1:3:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:3:194:PRO:HB2  | 1:3:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:3:345:ARG:HB2  | 1:3:379:ASP:HB3  | 2.03                     | 0.41              |
| 1:3:354:GLN:HG3  | 1:4:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:4:370:SER:HA   | 1:4:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:4:406:ARG:O    | 1:4:531:LYS:NZ   | 2.54                     | 0.41              |
| 1:5:40:THR:OG1   | 1:5:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:5:354:GLN:HG3  | 1:7:268:ALA:HB3  | 2.02                     | 0.41              |
| 1:5:370:SER:HA   | 1:5:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:7:84:GLY:O     | 1:7:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:7:158:PHE:O    | 1:7:445:PHE:N    | 2.44                     | 0.41              |
| 1:8:40:THR:OG1   | 1:8:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:C:194:PRO:HB2  | 1:C:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:D:84:GLY:O     | 1:D:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:D:194:PRO:HB2  | 1:D:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:D:508:PRO:HB2  | 1:M:488:ARG:NH2  | 2.35                     | 0.41              |
| 1:G:84:GLY:O     | 1:G:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:I:261:PRO:O    | 1:I:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:K:268:ALA:HB3  | 1:a:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:K:295:THR:O    | 1:K:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:K:370:SER:HA   | 1:K:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:K:531:LYS:NZ   | 1:a:423:ASP:OD2  | 2.44                     | 0.41              |
| 1:L:84:GLY:O     | 1:L:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:L:222:GLU:OE1  | 1:L:222:GLU:N    | 2.50                     | 0.41              |
| 1:Q:134:GLN:HE22 | 1:S:153:ALA:HA   | 1.86                     | 0.41              |
| 1:Q:295:THR:O    | 1:Q:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:Q:370:SER:HA   | 1:Q:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:S:180:LEU:HD11 | 1:S:518:TYR:CE2  | 2.55                     | 0.41              |
| 1:T:40:THR:OG1   | 1:T:131:TYR:HB2  | 2.21                     | 0.41              |
| 1:T:245:TRP:HH2  | 1:T:478:GLU:HG2  | 1.86                     | 0.41              |
| 1:T:261:PRO:O    | 1:T:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:X:261:PRO:O    | 1:X:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:Y:134:GLN:HE22 | 1:4:153:ALA:HA   | 1.86                     | 0.41              |
| 1:Y:261:PRO:O    | 1:Y:286:PRO:HB2  | 2.21                     | 0.41              |
| 1:Z:193:ILE:HD11 | 1:3:261:PRO:HG3  | 2.01                     | 0.41              |
| 1:a:194:PRO:HB2  | 1:a:216:ILE:HG23 | 2.02                     | 0.41              |
| 1:a:345:ARG:HB2  | 1:a:379:ASP:HB3  | 2.03                     | 0.41              |
| 1:b:345:ARG:HB2  | 1:b:379:ASP:HB3  | 2.03                     | 0.41              |
| 1:d:399:PHE:CG   | 1:d:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:h:488:ARG:NH2  | 1:k:508:PRO:HB2  | 2.35                     | 0.41              |
| 1:j:399:PHE:CG   | 1:j:400:PRO:HD2  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:84:GLY:O     | 1:k:85:LYS:HD2   | 2.21                     | 0.41              |
| 1:m:245:TRP:HH2  | 1:m:478:GLU:HG2  | 1.86                     | 0.41              |
| 1:m:268:ALA:HB3  | 1:n:354:GLN:HG3  | 2.02                     | 0.41              |
| 1:n:399:PHE:CG   | 1:n:400:PRO:HD2  | 2.55                     | 0.41              |
| 1:q:370:SER:HA   | 1:q:524:TRP:CD1  | 2.56                     | 0.41              |
| 1:u:134:GLN:HE22 | 1:2:153:ALA:HA   | 1.86                     | 0.41              |
| 1:3:222:GLU:OE1  | 1:3:222:GLU:N    | 2.50                     | 0.41              |
| 1:3:423:ASP:OD2  | 1:4:531:LYS:NZ   | 2.44                     | 0.41              |
| 1:4:295:THR:O    | 1:4:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:5:295:THR:O    | 1:5:402:GLN:HG2  | 2.21                     | 0.41              |
| 1:A:245:TRP:HH2  | 1:A:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:A:508:PRO:HB2  | 1:F:488:ARG:NH2  | 2.35                     | 0.40              |
| 1:D:153:ALA:HA   | 1:E:134:GLN:HE22 | 1.85                     | 0.40              |
| 1:E:370:SER:HA   | 1:E:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:H:345:ARG:HB2  | 1:H:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:J:40:THR:OG1   | 1:J:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:J:245:TRP:HH2  | 1:J:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:J:261:PRO:HG3  | 1:L:193:ILE:HD11 | 2.03                     | 0.40              |
| 1:M:245:TRP:HH2  | 1:M:478:GLU:HG2  | 1.86                     | 0.40              |
| 1:M:345:ARG:HB2  | 1:M:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:O:40:THR:OG1   | 1:O:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:P:245:TRP:HH2  | 1:P:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:R:295:THR:O    | 1:R:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:R:370:SER:HA   | 1:R:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:X:134:GLN:HE22 | 1:Y:153:ALA:HA   | 1.85                     | 0.40              |
| 1:Y:158:PHE:O    | 1:Y:445:PHE:N    | 2.44                     | 0.40              |
| 1:Z:245:TRP:HH2  | 1:Z:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:e:194:PRO:HB2  | 1:e:216:ILE:HG23 | 2.02                     | 0.40              |
| 1:f:345:ARG:HB2  | 1:f:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:g:84:GLY:O     | 1:g:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:j:245:TRP:HH2  | 1:j:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:j:261:PRO:O    | 1:j:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:j:370:SER:HA   | 1:j:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:k:40:THR:OG1   | 1:k:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:l:261:PRO:O    | 1:l:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:o:134:GLN:HE22 | 1:7:153:ALA:HA   | 1.85                     | 0.40              |
| 1:o:261:PRO:O    | 1:o:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:p:40:THR:OG1   | 1:p:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:q:295:THR:O    | 1:q:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:r:156:HIS:N    | 1:r:447:LYS:O    | 2.43                     | 0.40              |
| 1:r:180:LEU:HD11 | 1:r:518:TYR:CE2  | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:261:PRO:O    | 1:s:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:t:84:GLY:O     | 1:t:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:t:370:SER:HA   | 1:t:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:v:245:TRP:HH2  | 1:v:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:v:378:ARG:HD2  | 1:v:378:ARG:HA   | 1.73                     | 0.40              |
| 1:w:370:SER:HA   | 1:w:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:2:40:THR:OG1   | 1:2:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:2:245:TRP:HH2  | 1:2:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:6:261:PRO:O    | 1:6:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:7:261:PRO:O    | 1:7:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:8:245:TRP:HH2  | 1:8:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:A:179:GLU:OE2  | 1:A:411:ARG:NH1  | 2.38                     | 0.40              |
| 1:B:261:PRO:O    | 1:B:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:C:84:GLY:O     | 1:C:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:C:158:PHE:O    | 1:C:445:PHE:N    | 2.44                     | 0.40              |
| 1:D:40:THR:OG1   | 1:D:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:D:406:ARG:O    | 1:D:531:LYS:NZ   | 2.54                     | 0.40              |
| 1:E:180:LEU:HD11 | 1:E:518:TYR:CE2  | 2.55                     | 0.40              |
| 1:G:370:SER:HA   | 1:G:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:K:40:THR:OG1   | 1:K:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:M:378:ARG:HD2  | 1:M:378:ARG:HA   | 1.73                     | 0.40              |
| 1:O:261:PRO:O    | 1:O:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:P:84:GLY:O     | 1:P:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:P:261:PRO:O    | 1:P:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:Q:40:THR:OG1   | 1:Q:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:R:40:THR:OG1   | 1:R:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:T:345:ARG:HB2  | 1:T:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:W:261:PRO:O    | 1:W:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:W:268:ALA:HB3  | 1:Y:354:GLN:HG3  | 2.02                     | 0.40              |
| 1:X:295:THR:O    | 1:X:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:Y:245:TRP:HH2  | 1:Y:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:Z:531:LYS:NZ   | 1:4:423:ASP:OD2  | 2.44                     | 0.40              |
| 1:h:245:TRP:HH2  | 1:h:478:GLU:HG2  | 1.86                     | 0.40              |
| 1:h:345:ARG:HB2  | 1:h:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:h:406:ARG:O    | 1:h:531:LYS:NZ   | 2.54                     | 0.40              |
| 1:k:153:ALA:HA   | 1:w:134:GLN:HE22 | 1.85                     | 0.40              |
| 1:k:194:PRO:HB2  | 1:k:216:ILE:HG23 | 2.02                     | 0.40              |
| 1:l:40:THR:OG1   | 1:l:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:u:507:ASN:OD1  | 1:2:88:ARG:NH2   | 2.51                     | 0.40              |
| 1:w:40:THR:OG1   | 1:w:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:z:370:SER:HA   | 1:z:524:TRP:CD1  | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:261:PRO:O    | 1:1:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:2:29:GLY:N     | 1:3:234:SER:O    | 2.33                     | 0.40              |
| 1:3:370:SER:HA   | 1:3:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:5:345:ARG:HB2  | 1:5:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:7:179:GLU:OE2  | 1:7:411:ARG:NH1  | 2.38                     | 0.40              |
| 1:A:84:GLY:O     | 1:A:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:A:134:GLN:HE22 | 1:E:153:ALA:HA   | 1.86                     | 0.40              |
| 1:D:370:SER:HA   | 1:D:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:E:40:THR:OG1   | 1:E:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:M:406:ARG:O    | 1:M:531:LYS:NZ   | 2.54                     | 0.40              |
| 1:O:29:GLY:N     | 1:P:234:SER:O    | 2.32                     | 0.40              |
| 1:P:370:SER:HA   | 1:P:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:R:345:ARG:HB2  | 1:R:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:R:378:ARG:HD2  | 1:R:378:ARG:HA   | 1.73                     | 0.40              |
| 1:U:261:PRO:O    | 1:U:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:V:40:THR:OG1   | 1:V:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:W:84:GLY:O     | 1:W:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:X:84:GLY:O     | 1:X:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:X:370:SER:HA   | 1:X:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:Y:40:THR:OG1   | 1:Y:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:Z:406:ARG:O    | 1:Z:531:LYS:NZ   | 2.54                     | 0.40              |
| 1:a:84:GLY:O     | 1:a:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:a:222:GLU:OE1  | 1:a:222:GLU:N    | 2.50                     | 0.40              |
| 1:a:261:PRO:HG3  | 1:8:193:ILE:HD11 | 2.01                     | 0.40              |
| 1:b:40:THR:OG1   | 1:b:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:d:345:ARG:HB2  | 1:d:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:f:40:THR:OG1   | 1:f:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:g:378:ARG:HA   | 1:g:378:ARG:HD2  | 1.73                     | 0.40              |
| 1:i:268:ALA:HB3  | 1:j:354:GLN:HG3  | 2.02                     | 0.40              |
| 1:i:370:SER:HA   | 1:i:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:j:84:GLY:O     | 1:j:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:k:370:SER:HA   | 1:k:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:k:406:ARG:O    | 1:k:531:LYS:NZ   | 2.54                     | 0.40              |
| 1:l:295:THR:O    | 1:l:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:m:345:ARG:HB2  | 1:m:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:n:179:GLU:OE2  | 1:n:411:ARG:NH1  | 2.38                     | 0.40              |
| 1:n:345:ARG:HB2  | 1:n:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:o:295:THR:O    | 1:o:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:o:370:SER:HA   | 1:o:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:p:488:ARG:NH2  | 1:s:508:PRO:HB2  | 2.35                     | 0.40              |
| 1:q:40:THR:OG1   | 1:q:131:TYR:HB2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:r:295:THR:O    | 1:r:402:GLN:HG2 | 2.21                     | 0.40              |
| 1:u:40:THR:OG1   | 1:u:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:v:84:GLY:O     | 1:v:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:v:134:GLN:HE22 | 1:w:153:ALA:HA  | 1.85                     | 0.40              |
| 1:v:156:HIS:N    | 1:v:447:LYS:O   | 2.43                     | 0.40              |
| 1:x:40:THR:OG1   | 1:x:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:z:222:GLU:OE1  | 1:z:222:GLU:N   | 2.50                     | 0.40              |
| 1:z:268:ALA:HB3  | 1:1:354:GLN:HG3 | 2.03                     | 0.40              |
| 1:2:84:GLY:O     | 1:2:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:7:40:THR:OG1   | 1:7:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:7:245:TRP:HH2  | 1:7:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:B:245:TRP:HH2  | 1:B:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:G:40:THR:OG1   | 1:G:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:G:268:ALA:HB3  | 1:I:354:GLN:HG3 | 2.02                     | 0.40              |
| 1:H:84:GLY:O     | 1:H:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:H:261:PRO:O    | 1:H:286:PRO:HB2 | 2.21                     | 0.40              |
| 1:I:40:THR:OG1   | 1:I:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:J:84:GLY:O     | 1:J:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:J:134:GLN:HE22 | 1:a:153:ALA:HA  | 1.86                     | 0.40              |
| 1:K:84:GLY:O     | 1:K:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:K:134:GLN:HE22 | 1:L:153:ALA:HA  | 1.86                     | 0.40              |
| 1:K:345:ARG:HB2  | 1:K:379:ASP:HB3 | 2.03                     | 0.40              |
| 1:L:370:SER:HA   | 1:L:524:TRP:CD1 | 2.56                     | 0.40              |
| 1:N:268:ALA:HB3  | 1:P:354:GLN:HG3 | 2.02                     | 0.40              |
| 1:N:370:SER:HA   | 1:N:524:TRP:CD1 | 2.56                     | 0.40              |
| 1:S:40:THR:OG1   | 1:S:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:S:295:THR:O    | 1:S:402:GLN:HG2 | 2.21                     | 0.40              |
| 1:U:488:ARG:NH2  | 1:V:508:PRO:HB2 | 2.36                     | 0.40              |
| 1:V:245:TRP:HH2  | 1:V:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:X:345:ARG:HB2  | 1:X:379:ASP:HB3 | 2.03                     | 0.40              |
| 1:c:245:TRP:HH2  | 1:c:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:c:295:THR:O    | 1:c:402:GLN:HG2 | 2.21                     | 0.40              |
| 1:d:179:GLU:OE2  | 1:d:411:ARG:NH1 | 2.38                     | 0.40              |
| 1:d:245:TRP:HH2  | 1:d:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:e:295:THR:O    | 1:e:402:GLN:HG2 | 2.21                     | 0.40              |
| 1:f:51:ASP:OD1   | 1:f:481:ARG:NE  | 2.38                     | 0.40              |
| 1:l:179:GLU:OE2  | 1:l:411:ARG:NH1 | 2.38                     | 0.40              |
| 1:m:51:ASP:OD1   | 1:m:481:ARG:NE  | 2.38                     | 0.40              |
| 1:n:40:THR:OG1   | 1:n:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:o:84:GLY:O     | 1:o:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:p:134:GLN:HE22 | 1:q:153:ALA:HA  | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:p:222:GLU:OE1  | 1:p:222:GLU:N    | 2.50                     | 0.40              |
| 1:p:370:SER:HA   | 1:p:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:q:177:MET:HA   | 1:q:178:PRO:HD3  | 1.99                     | 0.40              |
| 1:r:40:THR:OG1   | 1:r:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:s:84:GLY:O     | 1:s:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:t:51:ASP:OD1   | 1:t:481:ARG:NE   | 2.39                     | 0.40              |
| 1:t:245:TRP:HH2  | 1:t:478:GLU:HG2  | 1.86                     | 0.40              |
| 1:u:370:SER:HA   | 1:u:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:w:180:LEU:HD11 | 1:w:518:TYR:CE2  | 2.55                     | 0.40              |
| 1:3:84:GLY:O     | 1:3:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:4:40:THR:OG1   | 1:4:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:4:84:GLY:O     | 1:4:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:6:40:THR:OG1   | 1:6:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:6:84:GLY:O     | 1:6:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:6:268:ALA:HB3  | 1:7:354:GLN:HG3  | 2.02                     | 0.40              |
| 1:6:370:SER:HA   | 1:6:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:7:345:ARG:HB2  | 1:7:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:B:51:ASP:OD1   | 1:B:481:ARG:NE   | 2.38                     | 0.40              |
| 1:B:374:LEU:HD22 | 1:J:212:ILE:HD11 | 2.04                     | 0.40              |
| 1:C:245:TRP:HH2  | 1:C:478:GLU:HG2  | 1.87                     | 0.40              |
| 1:D:295:THR:O    | 1:D:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:F:295:THR:O    | 1:F:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:G:245:TRP:HH2  | 1:G:478:GLU:HG2  | 1.86                     | 0.40              |
| 1:I:370:SER:HA   | 1:I:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:J:261:PRO:O    | 1:J:286:PRO:HB2  | 2.21                     | 0.40              |
| 1:J:295:THR:O    | 1:J:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:O:295:THR:O    | 1:O:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:R:84:GLY:O     | 1:R:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:R:177:MET:HA   | 1:R:178:PRO:HD3  | 1.99                     | 0.40              |
| 1:S:345:ARG:HB2  | 1:S:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:T:84:GLY:O     | 1:T:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:T:156:HIS:CD2  | 1:T:226:HIS:CD2  | 3.10                     | 0.40              |
| 1:U:508:PRO:HB2  | 1:V:488:ARG:NH2  | 2.35                     | 0.40              |
| 1:V:370:SER:HA   | 1:V:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:W:370:SER:HA   | 1:W:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:Y:295:THR:O    | 1:Y:402:GLN:HG2  | 2.21                     | 0.40              |
| 1:Y:345:ARG:HB2  | 1:Y:379:ASP:HB3  | 2.03                     | 0.40              |
| 1:a:370:SER:HA   | 1:a:524:TRP:CD1  | 2.56                     | 0.40              |
| 1:b:84:GLY:O     | 1:b:85:LYS:HD2   | 2.21                     | 0.40              |
| 1:d:40:THR:OG1   | 1:d:131:TYR:HB2  | 2.21                     | 0.40              |
| 1:e:245:TRP:HH2  | 1:e:478:GLU:HG2  | 1.87                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:f:84:GLY:O     | 1:f:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:g:245:TRP:HH2  | 1:g:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:g:508:PRO:HB2  | 1:z:488:ARG:NH2 | 2.36                     | 0.40              |
| 1:i:245:TRP:HH2  | 1:i:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:j:51:ASP:OD1   | 1:j:481:ARG:NE  | 2.38                     | 0.40              |
| 1:m:156:HIS:CD2  | 1:m:226:HIS:CD2 | 3.10                     | 0.40              |
| 1:n:245:TRP:HH2  | 1:n:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:o:345:ARG:HB2  | 1:o:379:ASP:HB3 | 2.03                     | 0.40              |
| 1:p:245:TRP:HH2  | 1:p:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:p:508:PRO:HB2  | 1:s:488:ARG:NH2 | 2.36                     | 0.40              |
| 1:q:84:GLY:O     | 1:q:85:LYS:HD2  | 2.21                     | 0.40              |
| 1:q:345:ARG:HB2  | 1:q:379:ASP:HB3 | 2.03                     | 0.40              |
| 1:t:40:THR:OG1   | 1:t:131:TYR:HB2 | 2.21                     | 0.40              |
| 1:t:268:ALA:HB3  | 1:u:354:GLN:HG3 | 2.02                     | 0.40              |
| 1:y:345:ARG:HB2  | 1:y:379:ASP:HB3 | 2.03                     | 0.40              |
| 1:1:245:TRP:HH2  | 1:1:478:GLU:HG2 | 1.87                     | 0.40              |
| 1:3:134:GLN:HE22 | 1:8:153:ALA:HA  | 1.85                     | 0.40              |
| 1:4:345:ARG:HB2  | 1:4:379:ASP:HB3 | 2.03                     | 0.40              |
| 1:5:261:PRO:O    | 1:5:286:PRO:HB2 | 2.21                     | 0.40              |
| 1:6:222:GLU:OE1  | 1:6:222:GLU:N   | 2.50                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | 1     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 2     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 3     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 4     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | 5     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 6     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 7     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | 8     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | A     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | B     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | C     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | D     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | E     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | F     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | G     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | H     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | I     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | J     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | K     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | L     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | M     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | N     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | O     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | P     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | Q     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | R     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | S     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | T     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | U     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | V     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | W     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | X     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | Y     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | Z     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | a     | 514/516 (100%) | 498 (97%) | 16 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed           | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|--------------------|-------------|----------|----------|-------------|-----|
| 1   | b     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | c     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | d     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | e     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | f     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | g     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | h     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | i     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | j     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | k     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | l     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | m     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | n     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | o     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | p     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | q     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | r     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | s     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | t     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | u     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | v     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | w     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | x     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | y     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | z     | 514/516 (100%)     | 498 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| All | All   | 30840/30960 (100%) | 29880 (97%) | 960 (3%) | 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   | 1     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | 2     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | 3     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | 4     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | 5     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | 6     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | 7     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | 8     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | A     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | B     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | C     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | D     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | E     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | F     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | G     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | H     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | I     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | J     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | K     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | L     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | M     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | N     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | O     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | P     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | Q     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | R     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | S     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | T     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | U     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |    |
|-----|-------|----------------|------------|----------|-------------|----|
| 1   | V     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | W     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | X     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | Y     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | Z     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | a     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | b     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | c     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | d     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | e     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | f     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | g     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | h     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | i     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | j     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | k     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | l     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | m     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | n     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | o     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | p     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | q     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | r     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | s     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | t     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | u     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | v     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | w     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | x     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | y     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |
| 1   | z     | 447/448 (100%) | 446 (100%) | 1 (0%)   | 87          | 95 |

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| Mol | Chain | Analysed           | Rotameric    | Outliers | Percentiles |    |
|-----|-------|--------------------|--------------|----------|-------------|----|
| All | All   | 26820/26880 (100%) | 26760 (100%) | 60 (0%)  | 85          | 95 |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 183 | GLU  |
| 1   | B     | 183 | GLU  |
| 1   | C     | 183 | GLU  |
| 1   | D     | 183 | GLU  |
| 1   | E     | 183 | GLU  |
| 1   | F     | 183 | GLU  |
| 1   | G     | 183 | GLU  |
| 1   | H     | 183 | GLU  |
| 1   | I     | 183 | GLU  |
| 1   | J     | 183 | GLU  |
| 1   | K     | 183 | GLU  |
| 1   | L     | 183 | GLU  |
| 1   | M     | 183 | GLU  |
| 1   | N     | 183 | GLU  |
| 1   | O     | 183 | GLU  |
| 1   | P     | 183 | GLU  |
| 1   | Q     | 183 | GLU  |
| 1   | R     | 183 | GLU  |
| 1   | S     | 183 | GLU  |
| 1   | T     | 183 | GLU  |
| 1   | U     | 183 | GLU  |
| 1   | V     | 183 | GLU  |
| 1   | W     | 183 | GLU  |
| 1   | X     | 183 | GLU  |
| 1   | Y     | 183 | GLU  |
| 1   | Z     | 183 | GLU  |
| 1   | a     | 183 | GLU  |
| 1   | b     | 183 | GLU  |
| 1   | c     | 183 | GLU  |
| 1   | d     | 183 | GLU  |
| 1   | e     | 183 | GLU  |
| 1   | f     | 183 | GLU  |
| 1   | g     | 183 | GLU  |
| 1   | h     | 183 | GLU  |
| 1   | i     | 183 | GLU  |
| 1   | j     | 183 | GLU  |
| 1   | k     | 183 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | l     | 183 | GLU  |
| 1   | m     | 183 | GLU  |
| 1   | n     | 183 | GLU  |
| 1   | o     | 183 | GLU  |
| 1   | p     | 183 | GLU  |
| 1   | q     | 183 | GLU  |
| 1   | r     | 183 | GLU  |
| 1   | s     | 183 | GLU  |
| 1   | t     | 183 | GLU  |
| 1   | u     | 183 | GLU  |
| 1   | v     | 183 | GLU  |
| 1   | w     | 183 | GLU  |
| 1   | x     | 183 | GLU  |
| 1   | y     | 183 | GLU  |
| 1   | z     | 183 | GLU  |
| 1   | 1     | 183 | GLU  |
| 1   | 2     | 183 | GLU  |
| 1   | 3     | 183 | GLU  |
| 1   | 4     | 183 | GLU  |
| 1   | 5     | 183 | GLU  |
| 1   | 6     | 183 | GLU  |
| 1   | 7     | 183 | GLU  |
| 1   | 8     | 183 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1052) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 61  | GLN  |
| 1   | A     | 67  | GLN  |
| 1   | A     | 70  | HIS  |
| 1   | A     | 87  | GLN  |
| 1   | A     | 109 | GLN  |
| 1   | A     | 127 | HIS  |
| 1   | A     | 134 | GLN  |
| 1   | A     | 156 | HIS  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 170 | HIS  |
| 1   | A     | 206 | ASN  |
| 1   | A     | 226 | HIS  |
| 1   | A     | 357 | GLN  |
| 1   | A     | 391 | ASN  |
| 1   | A     | 401 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 413 | ASN  |
| 1   | A     | 533 | ASN  |
| 1   | B     | 61  | GLN  |
| 1   | B     | 67  | GLN  |
| 1   | B     | 70  | HIS  |
| 1   | B     | 87  | GLN  |
| 1   | B     | 109 | GLN  |
| 1   | B     | 127 | HIS  |
| 1   | B     | 134 | GLN  |
| 1   | B     | 156 | HIS  |
| 1   | B     | 167 | ASN  |
| 1   | B     | 170 | HIS  |
| 1   | B     | 189 | GLN  |
| 1   | B     | 206 | ASN  |
| 1   | B     | 226 | HIS  |
| 1   | B     | 357 | GLN  |
| 1   | B     | 391 | ASN  |
| 1   | B     | 401 | ASN  |
| 1   | B     | 413 | ASN  |
| 1   | B     | 533 | ASN  |
| 1   | C     | 61  | GLN  |
| 1   | C     | 67  | GLN  |
| 1   | C     | 70  | HIS  |
| 1   | C     | 87  | GLN  |
| 1   | C     | 109 | GLN  |
| 1   | C     | 127 | HIS  |
| 1   | C     | 134 | GLN  |
| 1   | C     | 156 | HIS  |
| 1   | C     | 167 | ASN  |
| 1   | C     | 170 | HIS  |
| 1   | C     | 189 | GLN  |
| 1   | C     | 206 | ASN  |
| 1   | C     | 226 | HIS  |
| 1   | C     | 357 | GLN  |
| 1   | C     | 391 | ASN  |
| 1   | C     | 401 | ASN  |
| 1   | C     | 413 | ASN  |
| 1   | C     | 533 | ASN  |
| 1   | D     | 61  | GLN  |
| 1   | D     | 67  | GLN  |
| 1   | D     | 70  | HIS  |
| 1   | D     | 87  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 109 | GLN  |
| 1   | D     | 127 | HIS  |
| 1   | D     | 134 | GLN  |
| 1   | D     | 156 | HIS  |
| 1   | D     | 167 | ASN  |
| 1   | D     | 170 | HIS  |
| 1   | D     | 189 | GLN  |
| 1   | D     | 206 | ASN  |
| 1   | D     | 226 | HIS  |
| 1   | D     | 357 | GLN  |
| 1   | D     | 391 | ASN  |
| 1   | D     | 401 | ASN  |
| 1   | D     | 413 | ASN  |
| 1   | D     | 533 | ASN  |
| 1   | E     | 61  | GLN  |
| 1   | E     | 67  | GLN  |
| 1   | E     | 70  | HIS  |
| 1   | E     | 87  | GLN  |
| 1   | E     | 109 | GLN  |
| 1   | E     | 127 | HIS  |
| 1   | E     | 134 | GLN  |
| 1   | E     | 156 | HIS  |
| 1   | E     | 167 | ASN  |
| 1   | E     | 170 | HIS  |
| 1   | E     | 189 | GLN  |
| 1   | E     | 226 | HIS  |
| 1   | E     | 357 | GLN  |
| 1   | E     | 391 | ASN  |
| 1   | E     | 401 | ASN  |
| 1   | E     | 413 | ASN  |
| 1   | E     | 533 | ASN  |
| 1   | F     | 61  | GLN  |
| 1   | F     | 67  | GLN  |
| 1   | F     | 70  | HIS  |
| 1   | F     | 87  | GLN  |
| 1   | F     | 109 | GLN  |
| 1   | F     | 127 | HIS  |
| 1   | F     | 134 | GLN  |
| 1   | F     | 156 | HIS  |
| 1   | F     | 167 | ASN  |
| 1   | F     | 170 | HIS  |
| 1   | F     | 189 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 206 | ASN  |
| 1   | F     | 226 | HIS  |
| 1   | F     | 357 | GLN  |
| 1   | F     | 391 | ASN  |
| 1   | F     | 401 | ASN  |
| 1   | F     | 413 | ASN  |
| 1   | F     | 493 | HIS  |
| 1   | F     | 533 | ASN  |
| 1   | G     | 61  | GLN  |
| 1   | G     | 67  | GLN  |
| 1   | G     | 70  | HIS  |
| 1   | G     | 87  | GLN  |
| 1   | G     | 109 | GLN  |
| 1   | G     | 127 | HIS  |
| 1   | G     | 134 | GLN  |
| 1   | G     | 156 | HIS  |
| 1   | G     | 167 | ASN  |
| 1   | G     | 170 | HIS  |
| 1   | G     | 189 | GLN  |
| 1   | G     | 226 | HIS  |
| 1   | G     | 357 | GLN  |
| 1   | G     | 391 | ASN  |
| 1   | G     | 401 | ASN  |
| 1   | G     | 413 | ASN  |
| 1   | G     | 533 | ASN  |
| 1   | H     | 61  | GLN  |
| 1   | H     | 67  | GLN  |
| 1   | H     | 70  | HIS  |
| 1   | H     | 87  | GLN  |
| 1   | H     | 109 | GLN  |
| 1   | H     | 127 | HIS  |
| 1   | H     | 134 | GLN  |
| 1   | H     | 156 | HIS  |
| 1   | H     | 167 | ASN  |
| 1   | H     | 170 | HIS  |
| 1   | H     | 189 | GLN  |
| 1   | H     | 206 | ASN  |
| 1   | H     | 226 | HIS  |
| 1   | H     | 357 | GLN  |
| 1   | H     | 391 | ASN  |
| 1   | H     | 401 | ASN  |
| 1   | H     | 413 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 470 | GLN  |
| 1   | H     | 533 | ASN  |
| 1   | I     | 61  | GLN  |
| 1   | I     | 67  | GLN  |
| 1   | I     | 70  | HIS  |
| 1   | I     | 87  | GLN  |
| 1   | I     | 109 | GLN  |
| 1   | I     | 127 | HIS  |
| 1   | I     | 134 | GLN  |
| 1   | I     | 156 | HIS  |
| 1   | I     | 167 | ASN  |
| 1   | I     | 170 | HIS  |
| 1   | I     | 189 | GLN  |
| 1   | I     | 206 | ASN  |
| 1   | I     | 226 | HIS  |
| 1   | I     | 357 | GLN  |
| 1   | I     | 391 | ASN  |
| 1   | I     | 401 | ASN  |
| 1   | I     | 413 | ASN  |
| 1   | I     | 533 | ASN  |
| 1   | J     | 61  | GLN  |
| 1   | J     | 67  | GLN  |
| 1   | J     | 70  | HIS  |
| 1   | J     | 87  | GLN  |
| 1   | J     | 109 | GLN  |
| 1   | J     | 127 | HIS  |
| 1   | J     | 134 | GLN  |
| 1   | J     | 156 | HIS  |
| 1   | J     | 167 | ASN  |
| 1   | J     | 170 | HIS  |
| 1   | J     | 189 | GLN  |
| 1   | J     | 226 | HIS  |
| 1   | J     | 357 | GLN  |
| 1   | J     | 391 | ASN  |
| 1   | J     | 401 | ASN  |
| 1   | J     | 413 | ASN  |
| 1   | J     | 470 | GLN  |
| 1   | J     | 533 | ASN  |
| 1   | K     | 61  | GLN  |
| 1   | K     | 67  | GLN  |
| 1   | K     | 70  | HIS  |
| 1   | K     | 87  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 109 | GLN  |
| 1   | K     | 127 | HIS  |
| 1   | K     | 134 | GLN  |
| 1   | K     | 156 | HIS  |
| 1   | K     | 167 | ASN  |
| 1   | K     | 170 | HIS  |
| 1   | K     | 206 | ASN  |
| 1   | K     | 226 | HIS  |
| 1   | K     | 357 | GLN  |
| 1   | K     | 391 | ASN  |
| 1   | K     | 401 | ASN  |
| 1   | K     | 413 | ASN  |
| 1   | K     | 470 | GLN  |
| 1   | K     | 533 | ASN  |
| 1   | L     | 61  | GLN  |
| 1   | L     | 67  | GLN  |
| 1   | L     | 70  | HIS  |
| 1   | L     | 87  | GLN  |
| 1   | L     | 109 | GLN  |
| 1   | L     | 127 | HIS  |
| 1   | L     | 134 | GLN  |
| 1   | L     | 156 | HIS  |
| 1   | L     | 167 | ASN  |
| 1   | L     | 170 | HIS  |
| 1   | L     | 226 | HIS  |
| 1   | L     | 357 | GLN  |
| 1   | L     | 391 | ASN  |
| 1   | L     | 401 | ASN  |
| 1   | L     | 413 | ASN  |
| 1   | L     | 533 | ASN  |
| 1   | M     | 61  | GLN  |
| 1   | M     | 67  | GLN  |
| 1   | M     | 70  | HIS  |
| 1   | M     | 87  | GLN  |
| 1   | M     | 109 | GLN  |
| 1   | M     | 127 | HIS  |
| 1   | M     | 134 | GLN  |
| 1   | M     | 156 | HIS  |
| 1   | M     | 167 | ASN  |
| 1   | M     | 170 | HIS  |
| 1   | M     | 189 | GLN  |
| 1   | M     | 206 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 226 | HIS  |
| 1   | M     | 357 | GLN  |
| 1   | M     | 391 | ASN  |
| 1   | M     | 401 | ASN  |
| 1   | M     | 413 | ASN  |
| 1   | M     | 533 | ASN  |
| 1   | N     | 61  | GLN  |
| 1   | N     | 67  | GLN  |
| 1   | N     | 70  | HIS  |
| 1   | N     | 87  | GLN  |
| 1   | N     | 109 | GLN  |
| 1   | N     | 127 | HIS  |
| 1   | N     | 134 | GLN  |
| 1   | N     | 156 | HIS  |
| 1   | N     | 167 | ASN  |
| 1   | N     | 170 | HIS  |
| 1   | N     | 189 | GLN  |
| 1   | N     | 226 | HIS  |
| 1   | N     | 357 | GLN  |
| 1   | N     | 391 | ASN  |
| 1   | N     | 401 | ASN  |
| 1   | N     | 413 | ASN  |
| 1   | N     | 533 | ASN  |
| 1   | O     | 61  | GLN  |
| 1   | O     | 67  | GLN  |
| 1   | O     | 70  | HIS  |
| 1   | O     | 87  | GLN  |
| 1   | O     | 109 | GLN  |
| 1   | O     | 127 | HIS  |
| 1   | O     | 134 | GLN  |
| 1   | O     | 156 | HIS  |
| 1   | O     | 167 | ASN  |
| 1   | O     | 170 | HIS  |
| 1   | O     | 189 | GLN  |
| 1   | O     | 226 | HIS  |
| 1   | O     | 357 | GLN  |
| 1   | O     | 391 | ASN  |
| 1   | O     | 401 | ASN  |
| 1   | O     | 413 | ASN  |
| 1   | O     | 464 | ASN  |
| 1   | O     | 533 | ASN  |
| 1   | P     | 61  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 67  | GLN  |
| 1   | P     | 70  | HIS  |
| 1   | P     | 87  | GLN  |
| 1   | P     | 109 | GLN  |
| 1   | P     | 127 | HIS  |
| 1   | P     | 134 | GLN  |
| 1   | P     | 156 | HIS  |
| 1   | P     | 167 | ASN  |
| 1   | P     | 170 | HIS  |
| 1   | P     | 189 | GLN  |
| 1   | P     | 206 | ASN  |
| 1   | P     | 226 | HIS  |
| 1   | P     | 357 | GLN  |
| 1   | P     | 391 | ASN  |
| 1   | P     | 401 | ASN  |
| 1   | P     | 413 | ASN  |
| 1   | P     | 533 | ASN  |
| 1   | Q     | 61  | GLN  |
| 1   | Q     | 67  | GLN  |
| 1   | Q     | 70  | HIS  |
| 1   | Q     | 87  | GLN  |
| 1   | Q     | 109 | GLN  |
| 1   | Q     | 127 | HIS  |
| 1   | Q     | 134 | GLN  |
| 1   | Q     | 156 | HIS  |
| 1   | Q     | 167 | ASN  |
| 1   | Q     | 170 | HIS  |
| 1   | Q     | 189 | GLN  |
| 1   | Q     | 206 | ASN  |
| 1   | Q     | 226 | HIS  |
| 1   | Q     | 357 | GLN  |
| 1   | Q     | 391 | ASN  |
| 1   | Q     | 401 | ASN  |
| 1   | Q     | 413 | ASN  |
| 1   | Q     | 533 | ASN  |
| 1   | R     | 61  | GLN  |
| 1   | R     | 67  | GLN  |
| 1   | R     | 70  | HIS  |
| 1   | R     | 87  | GLN  |
| 1   | R     | 109 | GLN  |
| 1   | R     | 127 | HIS  |
| 1   | R     | 134 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 156 | HIS  |
| 1   | R     | 167 | ASN  |
| 1   | R     | 170 | HIS  |
| 1   | R     | 226 | HIS  |
| 1   | R     | 357 | GLN  |
| 1   | R     | 391 | ASN  |
| 1   | R     | 401 | ASN  |
| 1   | R     | 413 | ASN  |
| 1   | R     | 533 | ASN  |
| 1   | S     | 61  | GLN  |
| 1   | S     | 67  | GLN  |
| 1   | S     | 70  | HIS  |
| 1   | S     | 87  | GLN  |
| 1   | S     | 109 | GLN  |
| 1   | S     | 127 | HIS  |
| 1   | S     | 134 | GLN  |
| 1   | S     | 156 | HIS  |
| 1   | S     | 167 | ASN  |
| 1   | S     | 170 | HIS  |
| 1   | S     | 189 | GLN  |
| 1   | S     | 226 | HIS  |
| 1   | S     | 357 | GLN  |
| 1   | S     | 391 | ASN  |
| 1   | S     | 401 | ASN  |
| 1   | S     | 413 | ASN  |
| 1   | S     | 533 | ASN  |
| 1   | T     | 61  | GLN  |
| 1   | T     | 67  | GLN  |
| 1   | T     | 70  | HIS  |
| 1   | T     | 87  | GLN  |
| 1   | T     | 109 | GLN  |
| 1   | T     | 127 | HIS  |
| 1   | T     | 134 | GLN  |
| 1   | T     | 156 | HIS  |
| 1   | T     | 167 | ASN  |
| 1   | T     | 170 | HIS  |
| 1   | T     | 189 | GLN  |
| 1   | T     | 206 | ASN  |
| 1   | T     | 226 | HIS  |
| 1   | T     | 357 | GLN  |
| 1   | T     | 391 | ASN  |
| 1   | T     | 401 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 413 | ASN  |
| 1   | T     | 533 | ASN  |
| 1   | U     | 61  | GLN  |
| 1   | U     | 67  | GLN  |
| 1   | U     | 70  | HIS  |
| 1   | U     | 87  | GLN  |
| 1   | U     | 109 | GLN  |
| 1   | U     | 127 | HIS  |
| 1   | U     | 134 | GLN  |
| 1   | U     | 156 | HIS  |
| 1   | U     | 167 | ASN  |
| 1   | U     | 170 | HIS  |
| 1   | U     | 189 | GLN  |
| 1   | U     | 226 | HIS  |
| 1   | U     | 357 | GLN  |
| 1   | U     | 391 | ASN  |
| 1   | U     | 401 | ASN  |
| 1   | U     | 413 | ASN  |
| 1   | U     | 533 | ASN  |
| 1   | V     | 61  | GLN  |
| 1   | V     | 67  | GLN  |
| 1   | V     | 70  | HIS  |
| 1   | V     | 87  | GLN  |
| 1   | V     | 109 | GLN  |
| 1   | V     | 127 | HIS  |
| 1   | V     | 134 | GLN  |
| 1   | V     | 156 | HIS  |
| 1   | V     | 167 | ASN  |
| 1   | V     | 170 | HIS  |
| 1   | V     | 189 | GLN  |
| 1   | V     | 226 | HIS  |
| 1   | V     | 357 | GLN  |
| 1   | V     | 391 | ASN  |
| 1   | V     | 401 | ASN  |
| 1   | V     | 413 | ASN  |
| 1   | V     | 533 | ASN  |
| 1   | W     | 61  | GLN  |
| 1   | W     | 67  | GLN  |
| 1   | W     | 70  | HIS  |
| 1   | W     | 87  | GLN  |
| 1   | W     | 109 | GLN  |
| 1   | W     | 127 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 134 | GLN  |
| 1   | W     | 156 | HIS  |
| 1   | W     | 167 | ASN  |
| 1   | W     | 170 | HIS  |
| 1   | W     | 206 | ASN  |
| 1   | W     | 226 | HIS  |
| 1   | W     | 357 | GLN  |
| 1   | W     | 391 | ASN  |
| 1   | W     | 401 | ASN  |
| 1   | W     | 413 | ASN  |
| 1   | W     | 493 | HIS  |
| 1   | W     | 533 | ASN  |
| 1   | X     | 61  | GLN  |
| 1   | X     | 67  | GLN  |
| 1   | X     | 70  | HIS  |
| 1   | X     | 87  | GLN  |
| 1   | X     | 109 | GLN  |
| 1   | X     | 127 | HIS  |
| 1   | X     | 134 | GLN  |
| 1   | X     | 156 | HIS  |
| 1   | X     | 167 | ASN  |
| 1   | X     | 170 | HIS  |
| 1   | X     | 189 | GLN  |
| 1   | X     | 226 | HIS  |
| 1   | X     | 357 | GLN  |
| 1   | X     | 391 | ASN  |
| 1   | X     | 401 | ASN  |
| 1   | X     | 413 | ASN  |
| 1   | X     | 470 | GLN  |
| 1   | X     | 533 | ASN  |
| 1   | Y     | 61  | GLN  |
| 1   | Y     | 67  | GLN  |
| 1   | Y     | 70  | HIS  |
| 1   | Y     | 87  | GLN  |
| 1   | Y     | 109 | GLN  |
| 1   | Y     | 127 | HIS  |
| 1   | Y     | 134 | GLN  |
| 1   | Y     | 156 | HIS  |
| 1   | Y     | 167 | ASN  |
| 1   | Y     | 170 | HIS  |
| 1   | Y     | 189 | GLN  |
| 1   | Y     | 206 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 226 | HIS  |
| 1   | Y     | 357 | GLN  |
| 1   | Y     | 391 | ASN  |
| 1   | Y     | 401 | ASN  |
| 1   | Y     | 413 | ASN  |
| 1   | Y     | 533 | ASN  |
| 1   | Z     | 61  | GLN  |
| 1   | Z     | 67  | GLN  |
| 1   | Z     | 70  | HIS  |
| 1   | Z     | 87  | GLN  |
| 1   | Z     | 109 | GLN  |
| 1   | Z     | 127 | HIS  |
| 1   | Z     | 134 | GLN  |
| 1   | Z     | 156 | HIS  |
| 1   | Z     | 167 | ASN  |
| 1   | Z     | 170 | HIS  |
| 1   | Z     | 189 | GLN  |
| 1   | Z     | 226 | HIS  |
| 1   | Z     | 357 | GLN  |
| 1   | Z     | 391 | ASN  |
| 1   | Z     | 401 | ASN  |
| 1   | Z     | 413 | ASN  |
| 1   | Z     | 470 | GLN  |
| 1   | Z     | 533 | ASN  |
| 1   | a     | 61  | GLN  |
| 1   | a     | 67  | GLN  |
| 1   | a     | 70  | HIS  |
| 1   | a     | 87  | GLN  |
| 1   | a     | 109 | GLN  |
| 1   | a     | 127 | HIS  |
| 1   | a     | 134 | GLN  |
| 1   | a     | 156 | HIS  |
| 1   | a     | 167 | ASN  |
| 1   | a     | 170 | HIS  |
| 1   | a     | 189 | GLN  |
| 1   | a     | 206 | ASN  |
| 1   | a     | 226 | HIS  |
| 1   | a     | 357 | GLN  |
| 1   | a     | 391 | ASN  |
| 1   | a     | 401 | ASN  |
| 1   | a     | 413 | ASN  |
| 1   | a     | 533 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 61  | GLN  |
| 1   | b     | 67  | GLN  |
| 1   | b     | 70  | HIS  |
| 1   | b     | 87  | GLN  |
| 1   | b     | 109 | GLN  |
| 1   | b     | 127 | HIS  |
| 1   | b     | 134 | GLN  |
| 1   | b     | 156 | HIS  |
| 1   | b     | 167 | ASN  |
| 1   | b     | 170 | HIS  |
| 1   | b     | 189 | GLN  |
| 1   | b     | 226 | HIS  |
| 1   | b     | 357 | GLN  |
| 1   | b     | 391 | ASN  |
| 1   | b     | 401 | ASN  |
| 1   | b     | 413 | ASN  |
| 1   | b     | 533 | ASN  |
| 1   | c     | 61  | GLN  |
| 1   | c     | 67  | GLN  |
| 1   | c     | 70  | HIS  |
| 1   | c     | 87  | GLN  |
| 1   | c     | 109 | GLN  |
| 1   | c     | 127 | HIS  |
| 1   | c     | 134 | GLN  |
| 1   | c     | 156 | HIS  |
| 1   | c     | 167 | ASN  |
| 1   | c     | 170 | HIS  |
| 1   | c     | 189 | GLN  |
| 1   | c     | 226 | HIS  |
| 1   | c     | 357 | GLN  |
| 1   | c     | 391 | ASN  |
| 1   | c     | 401 | ASN  |
| 1   | c     | 413 | ASN  |
| 1   | c     | 533 | ASN  |
| 1   | d     | 61  | GLN  |
| 1   | d     | 67  | GLN  |
| 1   | d     | 70  | HIS  |
| 1   | d     | 87  | GLN  |
| 1   | d     | 109 | GLN  |
| 1   | d     | 127 | HIS  |
| 1   | d     | 134 | GLN  |
| 1   | d     | 156 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | d     | 167 | ASN  |
| 1   | d     | 170 | HIS  |
| 1   | d     | 189 | GLN  |
| 1   | d     | 226 | HIS  |
| 1   | d     | 357 | GLN  |
| 1   | d     | 391 | ASN  |
| 1   | d     | 401 | ASN  |
| 1   | d     | 413 | ASN  |
| 1   | d     | 533 | ASN  |
| 1   | e     | 61  | GLN  |
| 1   | e     | 67  | GLN  |
| 1   | e     | 70  | HIS  |
| 1   | e     | 87  | GLN  |
| 1   | e     | 109 | GLN  |
| 1   | e     | 127 | HIS  |
| 1   | e     | 134 | GLN  |
| 1   | e     | 156 | HIS  |
| 1   | e     | 167 | ASN  |
| 1   | e     | 170 | HIS  |
| 1   | e     | 189 | GLN  |
| 1   | e     | 206 | ASN  |
| 1   | e     | 226 | HIS  |
| 1   | e     | 357 | GLN  |
| 1   | e     | 391 | ASN  |
| 1   | e     | 401 | ASN  |
| 1   | e     | 413 | ASN  |
| 1   | e     | 533 | ASN  |
| 1   | f     | 61  | GLN  |
| 1   | f     | 67  | GLN  |
| 1   | f     | 70  | HIS  |
| 1   | f     | 87  | GLN  |
| 1   | f     | 109 | GLN  |
| 1   | f     | 127 | HIS  |
| 1   | f     | 134 | GLN  |
| 1   | f     | 156 | HIS  |
| 1   | f     | 167 | ASN  |
| 1   | f     | 170 | HIS  |
| 1   | f     | 189 | GLN  |
| 1   | f     | 226 | HIS  |
| 1   | f     | 357 | GLN  |
| 1   | f     | 391 | ASN  |
| 1   | f     | 401 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | f     | 413 | ASN  |
| 1   | f     | 533 | ASN  |
| 1   | g     | 61  | GLN  |
| 1   | g     | 67  | GLN  |
| 1   | g     | 70  | HIS  |
| 1   | g     | 87  | GLN  |
| 1   | g     | 109 | GLN  |
| 1   | g     | 127 | HIS  |
| 1   | g     | 134 | GLN  |
| 1   | g     | 156 | HIS  |
| 1   | g     | 170 | HIS  |
| 1   | g     | 189 | GLN  |
| 1   | g     | 206 | ASN  |
| 1   | g     | 226 | HIS  |
| 1   | g     | 357 | GLN  |
| 1   | g     | 391 | ASN  |
| 1   | g     | 401 | ASN  |
| 1   | g     | 413 | ASN  |
| 1   | g     | 533 | ASN  |
| 1   | h     | 61  | GLN  |
| 1   | h     | 67  | GLN  |
| 1   | h     | 70  | HIS  |
| 1   | h     | 87  | GLN  |
| 1   | h     | 109 | GLN  |
| 1   | h     | 127 | HIS  |
| 1   | h     | 134 | GLN  |
| 1   | h     | 156 | HIS  |
| 1   | h     | 167 | ASN  |
| 1   | h     | 170 | HIS  |
| 1   | h     | 189 | GLN  |
| 1   | h     | 226 | HIS  |
| 1   | h     | 357 | GLN  |
| 1   | h     | 391 | ASN  |
| 1   | h     | 401 | ASN  |
| 1   | h     | 413 | ASN  |
| 1   | h     | 533 | ASN  |
| 1   | i     | 61  | GLN  |
| 1   | i     | 67  | GLN  |
| 1   | i     | 70  | HIS  |
| 1   | i     | 87  | GLN  |
| 1   | i     | 109 | GLN  |
| 1   | i     | 127 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | i     | 134 | GLN  |
| 1   | i     | 156 | HIS  |
| 1   | i     | 167 | ASN  |
| 1   | i     | 170 | HIS  |
| 1   | i     | 189 | GLN  |
| 1   | i     | 226 | HIS  |
| 1   | i     | 357 | GLN  |
| 1   | i     | 391 | ASN  |
| 1   | i     | 401 | ASN  |
| 1   | i     | 413 | ASN  |
| 1   | i     | 533 | ASN  |
| 1   | j     | 61  | GLN  |
| 1   | j     | 67  | GLN  |
| 1   | j     | 70  | HIS  |
| 1   | j     | 87  | GLN  |
| 1   | j     | 109 | GLN  |
| 1   | j     | 127 | HIS  |
| 1   | j     | 134 | GLN  |
| 1   | j     | 156 | HIS  |
| 1   | j     | 167 | ASN  |
| 1   | j     | 170 | HIS  |
| 1   | j     | 189 | GLN  |
| 1   | j     | 206 | ASN  |
| 1   | j     | 226 | HIS  |
| 1   | j     | 357 | GLN  |
| 1   | j     | 391 | ASN  |
| 1   | j     | 401 | ASN  |
| 1   | j     | 413 | ASN  |
| 1   | j     | 533 | ASN  |
| 1   | k     | 61  | GLN  |
| 1   | k     | 67  | GLN  |
| 1   | k     | 70  | HIS  |
| 1   | k     | 87  | GLN  |
| 1   | k     | 109 | GLN  |
| 1   | k     | 127 | HIS  |
| 1   | k     | 134 | GLN  |
| 1   | k     | 156 | HIS  |
| 1   | k     | 167 | ASN  |
| 1   | k     | 170 | HIS  |
| 1   | k     | 189 | GLN  |
| 1   | k     | 206 | ASN  |
| 1   | k     | 226 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | k     | 357 | GLN  |
| 1   | k     | 391 | ASN  |
| 1   | k     | 401 | ASN  |
| 1   | k     | 413 | ASN  |
| 1   | k     | 533 | ASN  |
| 1   | l     | 61  | GLN  |
| 1   | l     | 67  | GLN  |
| 1   | l     | 70  | HIS  |
| 1   | l     | 87  | GLN  |
| 1   | l     | 109 | GLN  |
| 1   | l     | 127 | HIS  |
| 1   | l     | 134 | GLN  |
| 1   | l     | 156 | HIS  |
| 1   | l     | 167 | ASN  |
| 1   | l     | 170 | HIS  |
| 1   | l     | 189 | GLN  |
| 1   | l     | 226 | HIS  |
| 1   | l     | 357 | GLN  |
| 1   | l     | 391 | ASN  |
| 1   | l     | 401 | ASN  |
| 1   | l     | 413 | ASN  |
| 1   | l     | 464 | ASN  |
| 1   | l     | 533 | ASN  |
| 1   | m     | 61  | GLN  |
| 1   | m     | 67  | GLN  |
| 1   | m     | 70  | HIS  |
| 1   | m     | 87  | GLN  |
| 1   | m     | 109 | GLN  |
| 1   | m     | 127 | HIS  |
| 1   | m     | 134 | GLN  |
| 1   | m     | 156 | HIS  |
| 1   | m     | 167 | ASN  |
| 1   | m     | 170 | HIS  |
| 1   | m     | 189 | GLN  |
| 1   | m     | 206 | ASN  |
| 1   | m     | 226 | HIS  |
| 1   | m     | 357 | GLN  |
| 1   | m     | 391 | ASN  |
| 1   | m     | 401 | ASN  |
| 1   | m     | 413 | ASN  |
| 1   | m     | 533 | ASN  |
| 1   | n     | 61  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | n     | 67  | GLN  |
| 1   | n     | 70  | HIS  |
| 1   | n     | 87  | GLN  |
| 1   | n     | 109 | GLN  |
| 1   | n     | 127 | HIS  |
| 1   | n     | 134 | GLN  |
| 1   | n     | 156 | HIS  |
| 1   | n     | 167 | ASN  |
| 1   | n     | 170 | HIS  |
| 1   | n     | 189 | GLN  |
| 1   | n     | 206 | ASN  |
| 1   | n     | 226 | HIS  |
| 1   | n     | 357 | GLN  |
| 1   | n     | 391 | ASN  |
| 1   | n     | 401 | ASN  |
| 1   | n     | 413 | ASN  |
| 1   | n     | 533 | ASN  |
| 1   | o     | 61  | GLN  |
| 1   | o     | 67  | GLN  |
| 1   | o     | 70  | HIS  |
| 1   | o     | 87  | GLN  |
| 1   | o     | 109 | GLN  |
| 1   | o     | 127 | HIS  |
| 1   | o     | 134 | GLN  |
| 1   | o     | 156 | HIS  |
| 1   | o     | 167 | ASN  |
| 1   | o     | 170 | HIS  |
| 1   | o     | 189 | GLN  |
| 1   | o     | 226 | HIS  |
| 1   | o     | 357 | GLN  |
| 1   | o     | 391 | ASN  |
| 1   | o     | 401 | ASN  |
| 1   | o     | 413 | ASN  |
| 1   | o     | 470 | GLN  |
| 1   | o     | 533 | ASN  |
| 1   | p     | 61  | GLN  |
| 1   | p     | 67  | GLN  |
| 1   | p     | 70  | HIS  |
| 1   | p     | 87  | GLN  |
| 1   | p     | 109 | GLN  |
| 1   | p     | 127 | HIS  |
| 1   | p     | 134 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | p     | 156 | HIS  |
| 1   | p     | 167 | ASN  |
| 1   | p     | 170 | HIS  |
| 1   | p     | 189 | GLN  |
| 1   | p     | 226 | HIS  |
| 1   | p     | 357 | GLN  |
| 1   | p     | 391 | ASN  |
| 1   | p     | 401 | ASN  |
| 1   | p     | 413 | ASN  |
| 1   | p     | 533 | ASN  |
| 1   | q     | 61  | GLN  |
| 1   | q     | 67  | GLN  |
| 1   | q     | 70  | HIS  |
| 1   | q     | 87  | GLN  |
| 1   | q     | 109 | GLN  |
| 1   | q     | 127 | HIS  |
| 1   | q     | 134 | GLN  |
| 1   | q     | 156 | HIS  |
| 1   | q     | 167 | ASN  |
| 1   | q     | 170 | HIS  |
| 1   | q     | 226 | HIS  |
| 1   | q     | 357 | GLN  |
| 1   | q     | 391 | ASN  |
| 1   | q     | 401 | ASN  |
| 1   | q     | 413 | ASN  |
| 1   | q     | 533 | ASN  |
| 1   | r     | 61  | GLN  |
| 1   | r     | 67  | GLN  |
| 1   | r     | 70  | HIS  |
| 1   | r     | 87  | GLN  |
| 1   | r     | 109 | GLN  |
| 1   | r     | 127 | HIS  |
| 1   | r     | 134 | GLN  |
| 1   | r     | 156 | HIS  |
| 1   | r     | 167 | ASN  |
| 1   | r     | 170 | HIS  |
| 1   | r     | 189 | GLN  |
| 1   | r     | 226 | HIS  |
| 1   | r     | 357 | GLN  |
| 1   | r     | 391 | ASN  |
| 1   | r     | 401 | ASN  |
| 1   | r     | 413 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | r     | 533 | ASN  |
| 1   | s     | 61  | GLN  |
| 1   | s     | 67  | GLN  |
| 1   | s     | 70  | HIS  |
| 1   | s     | 87  | GLN  |
| 1   | s     | 109 | GLN  |
| 1   | s     | 127 | HIS  |
| 1   | s     | 134 | GLN  |
| 1   | s     | 156 | HIS  |
| 1   | s     | 170 | HIS  |
| 1   | s     | 189 | GLN  |
| 1   | s     | 226 | HIS  |
| 1   | s     | 357 | GLN  |
| 1   | s     | 391 | ASN  |
| 1   | s     | 401 | ASN  |
| 1   | s     | 413 | ASN  |
| 1   | s     | 533 | ASN  |
| 1   | t     | 61  | GLN  |
| 1   | t     | 67  | GLN  |
| 1   | t     | 70  | HIS  |
| 1   | t     | 87  | GLN  |
| 1   | t     | 109 | GLN  |
| 1   | t     | 127 | HIS  |
| 1   | t     | 134 | GLN  |
| 1   | t     | 156 | HIS  |
| 1   | t     | 170 | HIS  |
| 1   | t     | 189 | GLN  |
| 1   | t     | 206 | ASN  |
| 1   | t     | 226 | HIS  |
| 1   | t     | 357 | GLN  |
| 1   | t     | 391 | ASN  |
| 1   | t     | 401 | ASN  |
| 1   | t     | 413 | ASN  |
| 1   | t     | 533 | ASN  |
| 1   | u     | 61  | GLN  |
| 1   | u     | 67  | GLN  |
| 1   | u     | 70  | HIS  |
| 1   | u     | 87  | GLN  |
| 1   | u     | 109 | GLN  |
| 1   | u     | 127 | HIS  |
| 1   | u     | 134 | GLN  |
| 1   | u     | 156 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | u     | 167 | ASN  |
| 1   | u     | 170 | HIS  |
| 1   | u     | 189 | GLN  |
| 1   | u     | 206 | ASN  |
| 1   | u     | 226 | HIS  |
| 1   | u     | 357 | GLN  |
| 1   | u     | 391 | ASN  |
| 1   | u     | 401 | ASN  |
| 1   | u     | 413 | ASN  |
| 1   | u     | 533 | ASN  |
| 1   | v     | 61  | GLN  |
| 1   | v     | 67  | GLN  |
| 1   | v     | 70  | HIS  |
| 1   | v     | 87  | GLN  |
| 1   | v     | 109 | GLN  |
| 1   | v     | 127 | HIS  |
| 1   | v     | 134 | GLN  |
| 1   | v     | 156 | HIS  |
| 1   | v     | 167 | ASN  |
| 1   | v     | 170 | HIS  |
| 1   | v     | 206 | ASN  |
| 1   | v     | 226 | HIS  |
| 1   | v     | 357 | GLN  |
| 1   | v     | 391 | ASN  |
| 1   | v     | 401 | ASN  |
| 1   | v     | 413 | ASN  |
| 1   | v     | 533 | ASN  |
| 1   | w     | 61  | GLN  |
| 1   | w     | 67  | GLN  |
| 1   | w     | 70  | HIS  |
| 1   | w     | 87  | GLN  |
| 1   | w     | 109 | GLN  |
| 1   | w     | 127 | HIS  |
| 1   | w     | 134 | GLN  |
| 1   | w     | 156 | HIS  |
| 1   | w     | 167 | ASN  |
| 1   | w     | 170 | HIS  |
| 1   | w     | 189 | GLN  |
| 1   | w     | 226 | HIS  |
| 1   | w     | 357 | GLN  |
| 1   | w     | 391 | ASN  |
| 1   | w     | 401 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | w     | 413 | ASN  |
| 1   | w     | 493 | HIS  |
| 1   | w     | 533 | ASN  |
| 1   | x     | 61  | GLN  |
| 1   | x     | 67  | GLN  |
| 1   | x     | 70  | HIS  |
| 1   | x     | 87  | GLN  |
| 1   | x     | 109 | GLN  |
| 1   | x     | 127 | HIS  |
| 1   | x     | 134 | GLN  |
| 1   | x     | 156 | HIS  |
| 1   | x     | 167 | ASN  |
| 1   | x     | 170 | HIS  |
| 1   | x     | 189 | GLN  |
| 1   | x     | 206 | ASN  |
| 1   | x     | 226 | HIS  |
| 1   | x     | 357 | GLN  |
| 1   | x     | 391 | ASN  |
| 1   | x     | 401 | ASN  |
| 1   | x     | 413 | ASN  |
| 1   | x     | 533 | ASN  |
| 1   | y     | 61  | GLN  |
| 1   | y     | 67  | GLN  |
| 1   | y     | 70  | HIS  |
| 1   | y     | 87  | GLN  |
| 1   | y     | 109 | GLN  |
| 1   | y     | 127 | HIS  |
| 1   | y     | 134 | GLN  |
| 1   | y     | 156 | HIS  |
| 1   | y     | 167 | ASN  |
| 1   | y     | 170 | HIS  |
| 1   | y     | 189 | GLN  |
| 1   | y     | 206 | ASN  |
| 1   | y     | 226 | HIS  |
| 1   | y     | 357 | GLN  |
| 1   | y     | 391 | ASN  |
| 1   | y     | 401 | ASN  |
| 1   | y     | 413 | ASN  |
| 1   | y     | 533 | ASN  |
| 1   | z     | 61  | GLN  |
| 1   | z     | 67  | GLN  |
| 1   | z     | 70  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | z     | 87  | GLN  |
| 1   | z     | 109 | GLN  |
| 1   | z     | 127 | HIS  |
| 1   | z     | 134 | GLN  |
| 1   | z     | 156 | HIS  |
| 1   | z     | 167 | ASN  |
| 1   | z     | 170 | HIS  |
| 1   | z     | 226 | HIS  |
| 1   | z     | 357 | GLN  |
| 1   | z     | 391 | ASN  |
| 1   | z     | 401 | ASN  |
| 1   | z     | 413 | ASN  |
| 1   | z     | 533 | ASN  |
| 1   | 1     | 61  | GLN  |
| 1   | 1     | 67  | GLN  |
| 1   | 1     | 70  | HIS  |
| 1   | 1     | 87  | GLN  |
| 1   | 1     | 109 | GLN  |
| 1   | 1     | 127 | HIS  |
| 1   | 1     | 134 | GLN  |
| 1   | 1     | 156 | HIS  |
| 1   | 1     | 167 | ASN  |
| 1   | 1     | 170 | HIS  |
| 1   | 1     | 189 | GLN  |
| 1   | 1     | 206 | ASN  |
| 1   | 1     | 226 | HIS  |
| 1   | 1     | 357 | GLN  |
| 1   | 1     | 391 | ASN  |
| 1   | 1     | 401 | ASN  |
| 1   | 1     | 413 | ASN  |
| 1   | 1     | 533 | ASN  |
| 1   | 2     | 61  | GLN  |
| 1   | 2     | 67  | GLN  |
| 1   | 2     | 70  | HIS  |
| 1   | 2     | 87  | GLN  |
| 1   | 2     | 109 | GLN  |
| 1   | 2     | 127 | HIS  |
| 1   | 2     | 134 | GLN  |
| 1   | 2     | 156 | HIS  |
| 1   | 2     | 167 | ASN  |
| 1   | 2     | 170 | HIS  |
| 1   | 2     | 189 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 226 | HIS  |
| 1   | 2     | 357 | GLN  |
| 1   | 2     | 391 | ASN  |
| 1   | 2     | 401 | ASN  |
| 1   | 2     | 413 | ASN  |
| 1   | 2     | 533 | ASN  |
| 1   | 3     | 61  | GLN  |
| 1   | 3     | 67  | GLN  |
| 1   | 3     | 70  | HIS  |
| 1   | 3     | 87  | GLN  |
| 1   | 3     | 109 | GLN  |
| 1   | 3     | 127 | HIS  |
| 1   | 3     | 134 | GLN  |
| 1   | 3     | 156 | HIS  |
| 1   | 3     | 167 | ASN  |
| 1   | 3     | 170 | HIS  |
| 1   | 3     | 189 | GLN  |
| 1   | 3     | 206 | ASN  |
| 1   | 3     | 226 | HIS  |
| 1   | 3     | 357 | GLN  |
| 1   | 3     | 391 | ASN  |
| 1   | 3     | 401 | ASN  |
| 1   | 3     | 413 | ASN  |
| 1   | 3     | 533 | ASN  |
| 1   | 4     | 61  | GLN  |
| 1   | 4     | 67  | GLN  |
| 1   | 4     | 70  | HIS  |
| 1   | 4     | 87  | GLN  |
| 1   | 4     | 109 | GLN  |
| 1   | 4     | 127 | HIS  |
| 1   | 4     | 134 | GLN  |
| 1   | 4     | 156 | HIS  |
| 1   | 4     | 167 | ASN  |
| 1   | 4     | 170 | HIS  |
| 1   | 4     | 206 | ASN  |
| 1   | 4     | 226 | HIS  |
| 1   | 4     | 357 | GLN  |
| 1   | 4     | 391 | ASN  |
| 1   | 4     | 401 | ASN  |
| 1   | 4     | 413 | ASN  |
| 1   | 4     | 533 | ASN  |
| 1   | 5     | 61  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 67  | GLN  |
| 1   | 5     | 70  | HIS  |
| 1   | 5     | 87  | GLN  |
| 1   | 5     | 109 | GLN  |
| 1   | 5     | 127 | HIS  |
| 1   | 5     | 134 | GLN  |
| 1   | 5     | 156 | HIS  |
| 1   | 5     | 167 | ASN  |
| 1   | 5     | 170 | HIS  |
| 1   | 5     | 189 | GLN  |
| 1   | 5     | 206 | ASN  |
| 1   | 5     | 226 | HIS  |
| 1   | 5     | 357 | GLN  |
| 1   | 5     | 391 | ASN  |
| 1   | 5     | 401 | ASN  |
| 1   | 5     | 413 | ASN  |
| 1   | 5     | 470 | GLN  |
| 1   | 5     | 533 | ASN  |
| 1   | 6     | 61  | GLN  |
| 1   | 6     | 67  | GLN  |
| 1   | 6     | 70  | HIS  |
| 1   | 6     | 87  | GLN  |
| 1   | 6     | 109 | GLN  |
| 1   | 6     | 127 | HIS  |
| 1   | 6     | 134 | GLN  |
| 1   | 6     | 156 | HIS  |
| 1   | 6     | 167 | ASN  |
| 1   | 6     | 170 | HIS  |
| 1   | 6     | 206 | ASN  |
| 1   | 6     | 226 | HIS  |
| 1   | 6     | 357 | GLN  |
| 1   | 6     | 391 | ASN  |
| 1   | 6     | 401 | ASN  |
| 1   | 6     | 413 | ASN  |
| 1   | 6     | 493 | HIS  |
| 1   | 6     | 533 | ASN  |
| 1   | 7     | 61  | GLN  |
| 1   | 7     | 67  | GLN  |
| 1   | 7     | 70  | HIS  |
| 1   | 7     | 87  | GLN  |
| 1   | 7     | 109 | GLN  |
| 1   | 7     | 127 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7     | 134 | GLN  |
| 1   | 7     | 156 | HIS  |
| 1   | 7     | 167 | ASN  |
| 1   | 7     | 170 | HIS  |
| 1   | 7     | 189 | GLN  |
| 1   | 7     | 206 | ASN  |
| 1   | 7     | 226 | HIS  |
| 1   | 7     | 357 | GLN  |
| 1   | 7     | 391 | ASN  |
| 1   | 7     | 401 | ASN  |
| 1   | 7     | 413 | ASN  |
| 1   | 7     | 533 | ASN  |
| 1   | 8     | 61  | GLN  |
| 1   | 8     | 67  | GLN  |
| 1   | 8     | 70  | HIS  |
| 1   | 8     | 87  | GLN  |
| 1   | 8     | 109 | GLN  |
| 1   | 8     | 127 | HIS  |
| 1   | 8     | 134 | GLN  |
| 1   | 8     | 156 | HIS  |
| 1   | 8     | 167 | ASN  |
| 1   | 8     | 170 | HIS  |
| 1   | 8     | 189 | GLN  |
| 1   | 8     | 226 | HIS  |
| 1   | 8     | 357 | GLN  |
| 1   | 8     | 391 | ASN  |
| 1   | 8     | 401 | ASN  |
| 1   | 8     | 413 | ASN  |
| 1   | 8     | 533 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

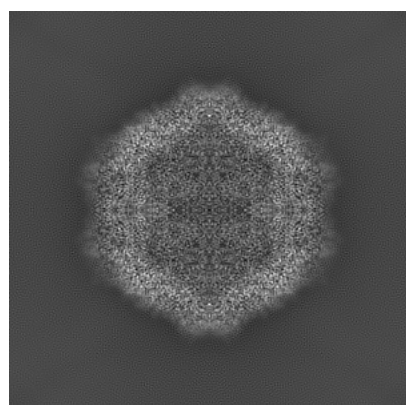
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23107. These allow visual inspection of the internal detail of the map and identification of artifacts.

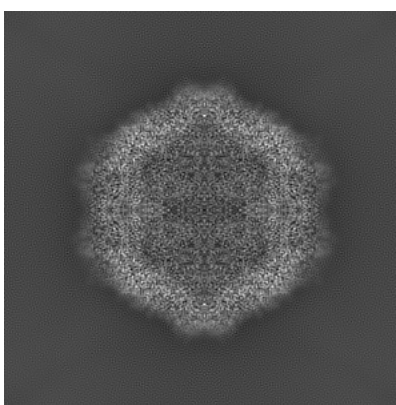
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

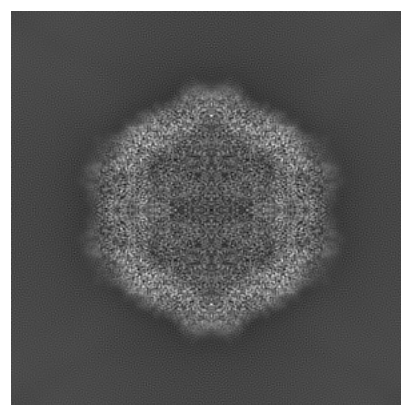
#### 6.1.1 Primary map



X



Y

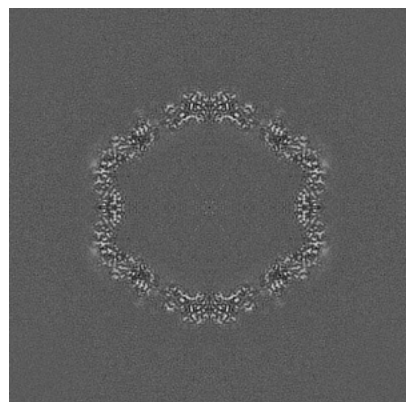


Z

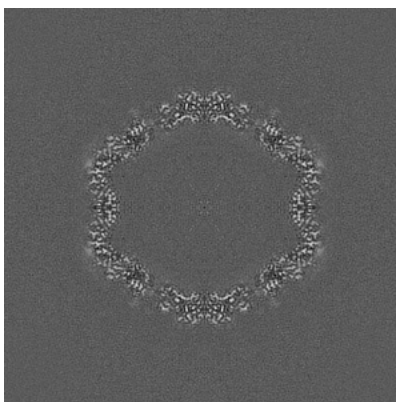
The images above show the map projected in three orthogonal directions.

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

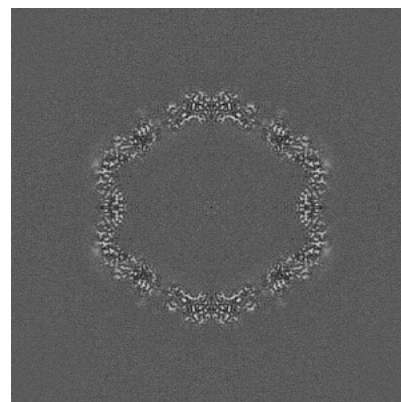
#### 6.2.1 Primary map



X Index: 225



Y Index: 225

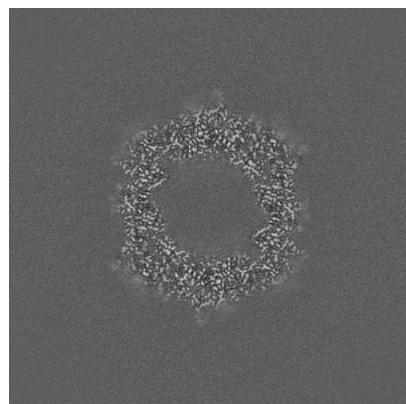


Z Index: 225

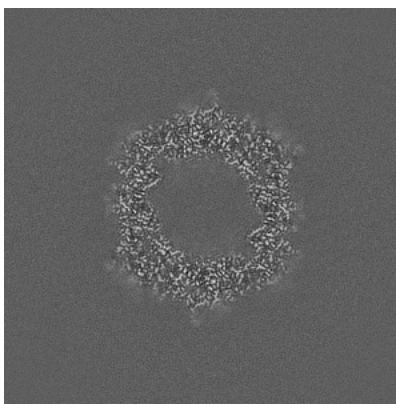
The images above show central slices of the map in three orthogonal directions.

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

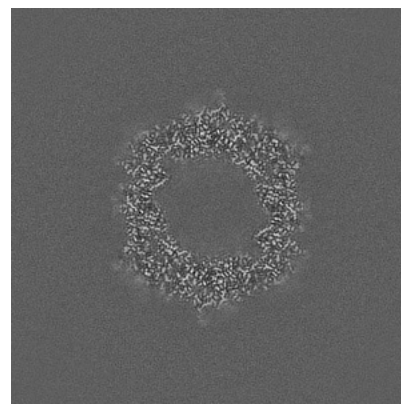
### 6.3.1 Primary map



X Index: 302



Y Index: 302

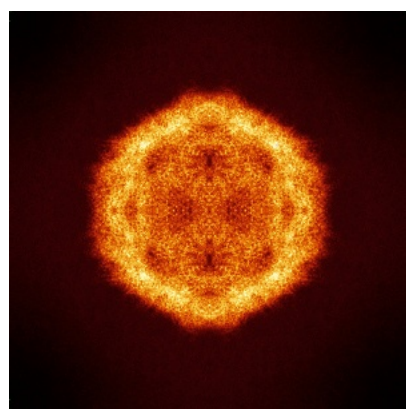


Z Index: 302

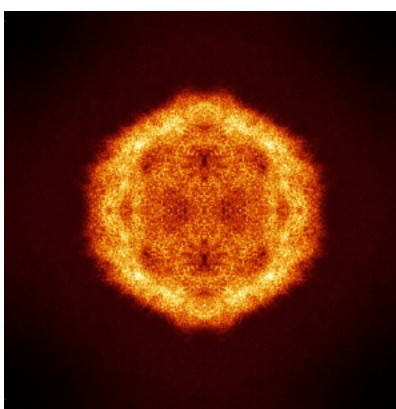
The images above show the largest variance slices of the map in three orthogonal directions.

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

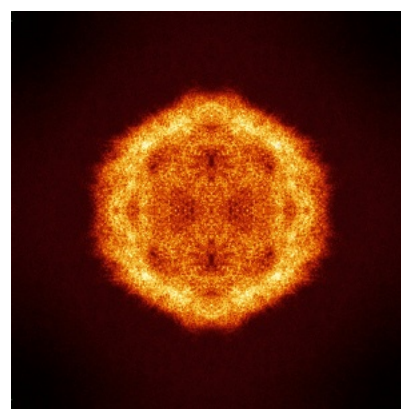
### 6.4.1 Primary map



X



Y

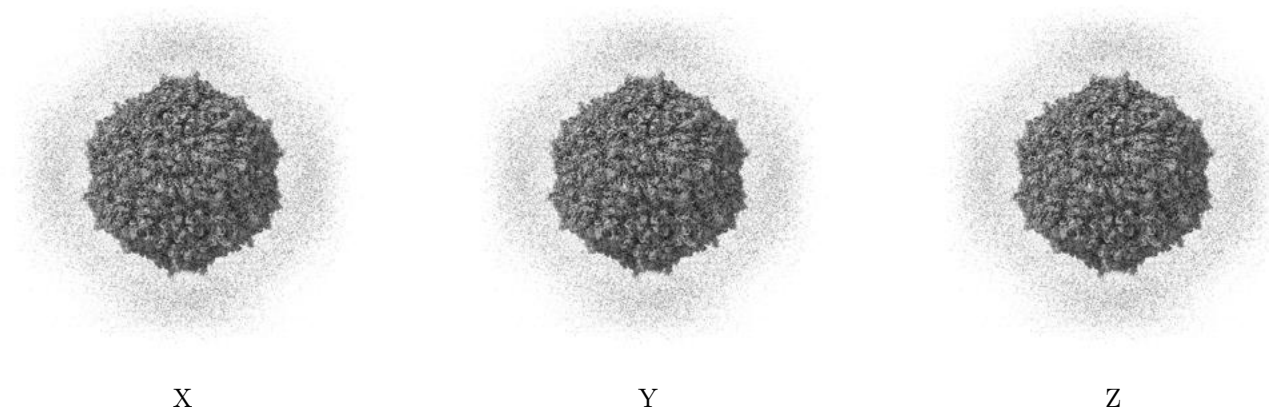


Z

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 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

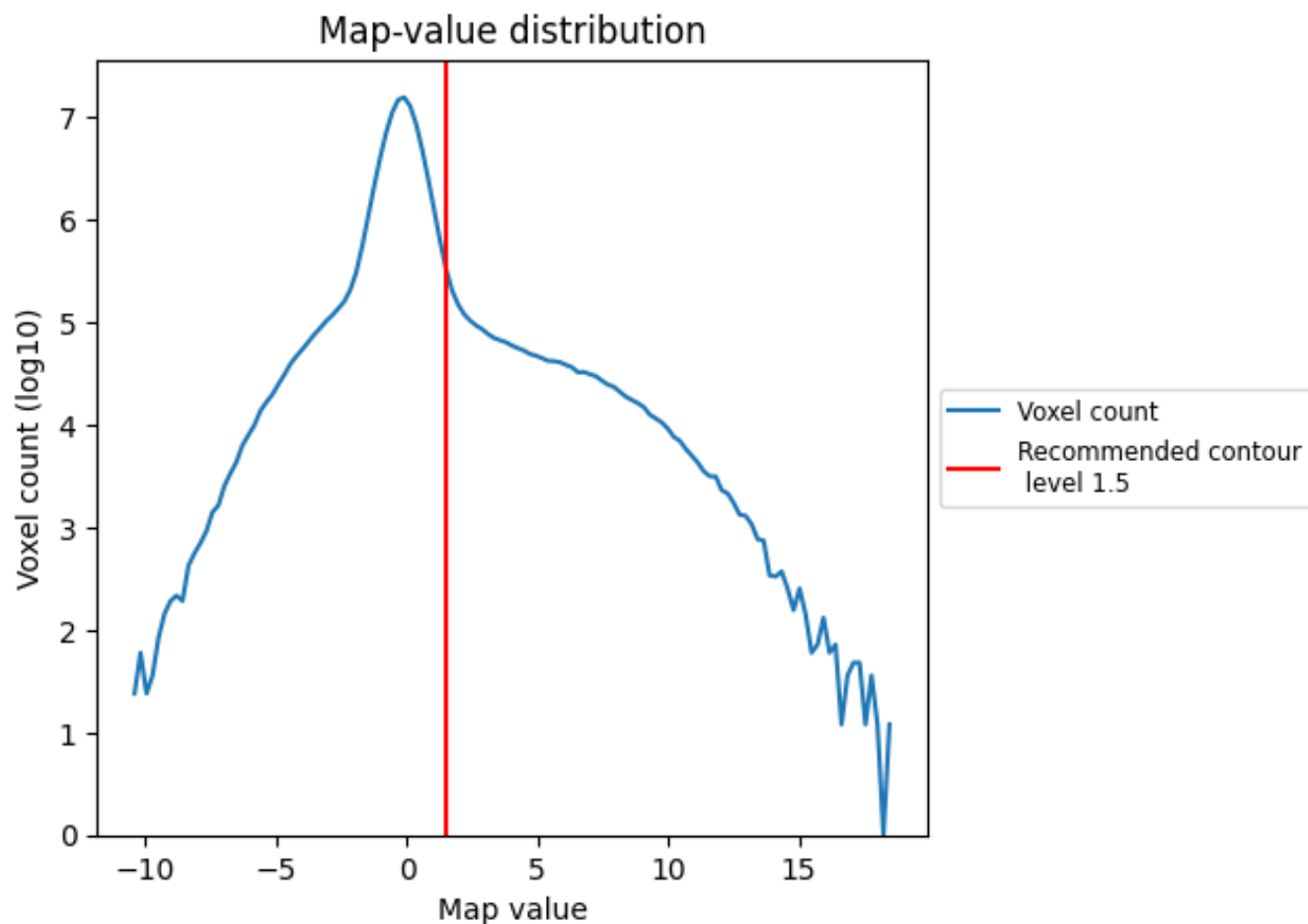
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

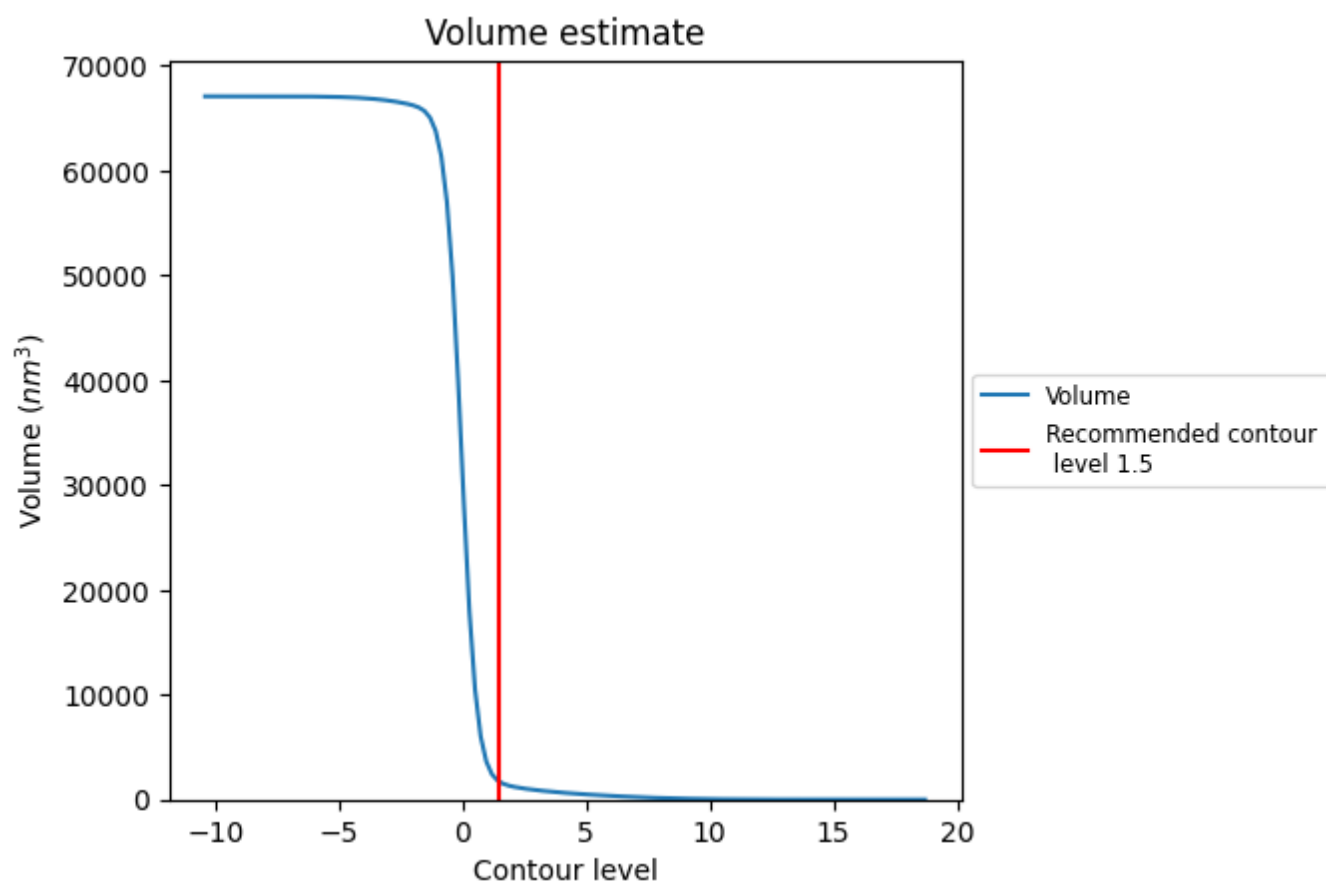
This section contains the results of statistical analysis of the map.

### 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.

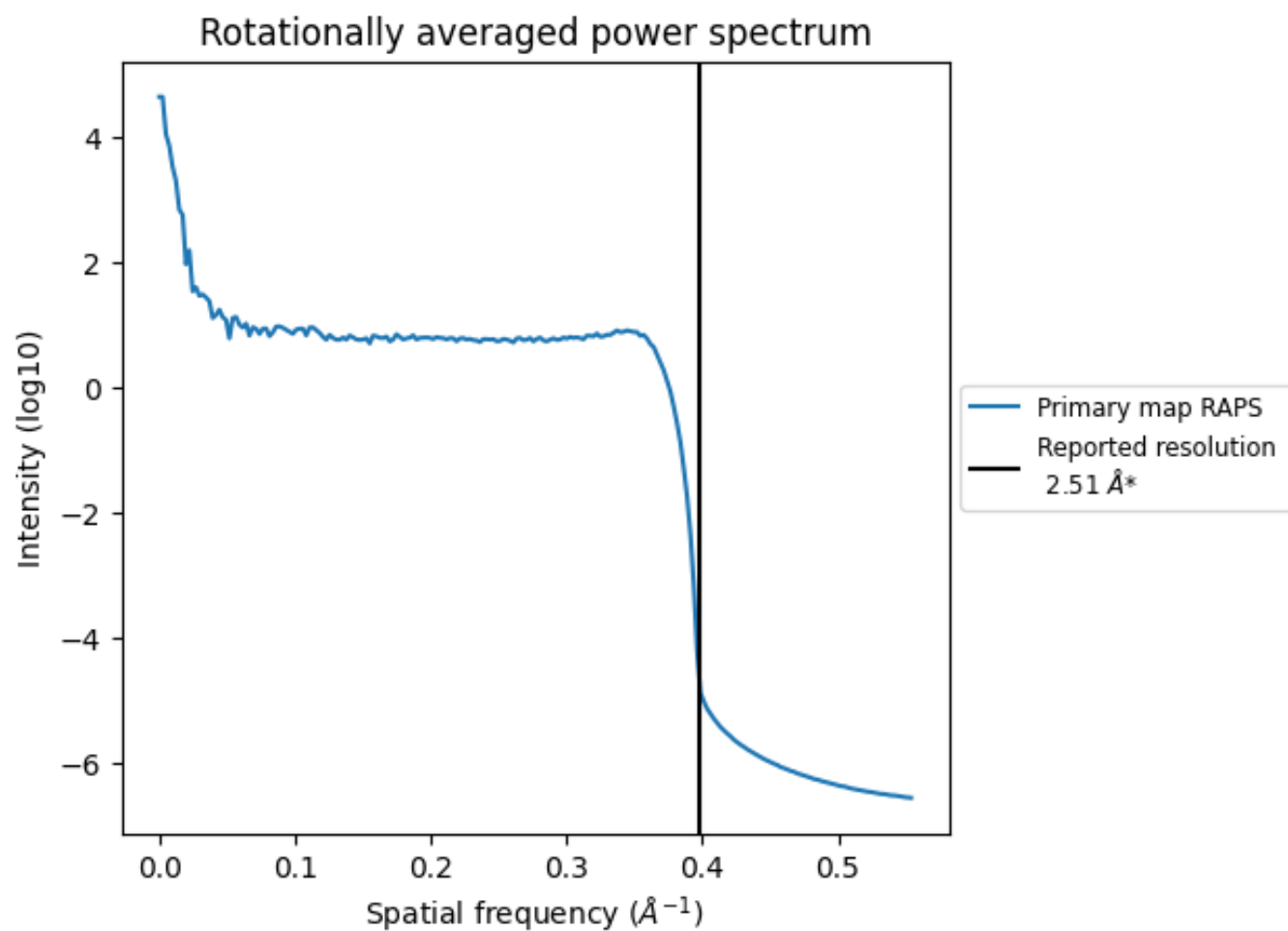
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1711 nm<sup>3</sup>; this corresponds to an approximate mass of 1546 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 0.398 Å<sup>-1</sup>

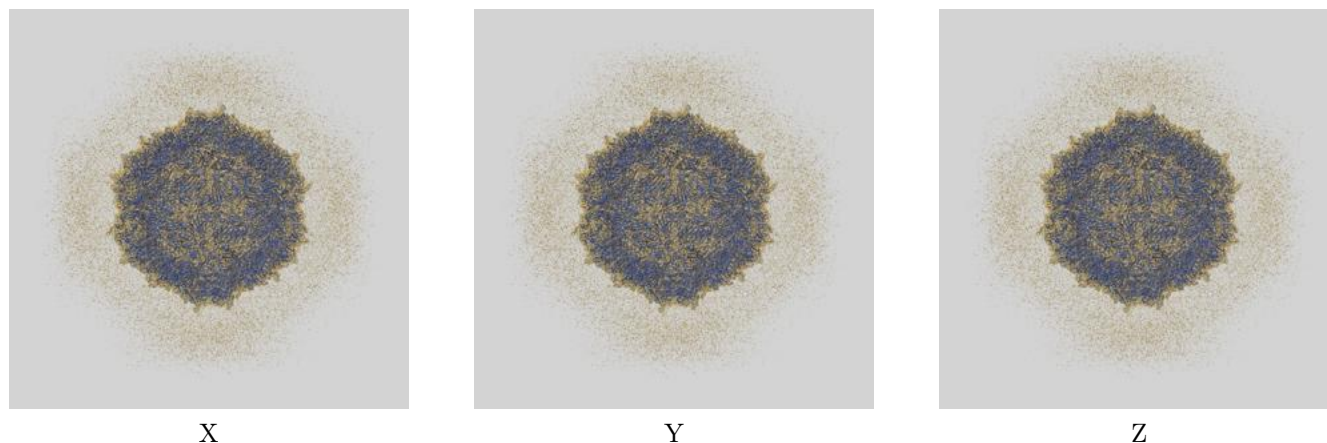
## 8 Fourier-Shell correlation

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

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

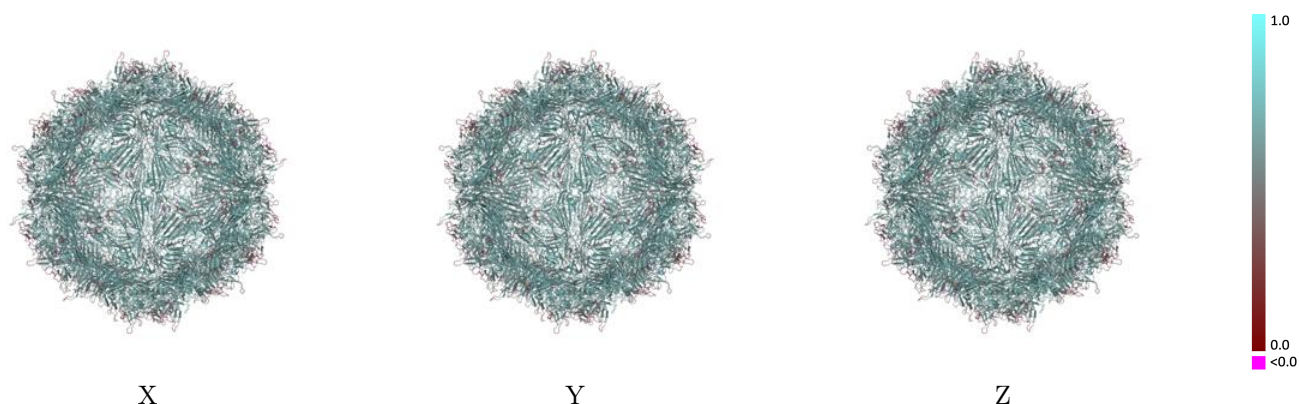
This section contains information regarding the fit between EMDB map EMD-23107 and PDB model 7L0X. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



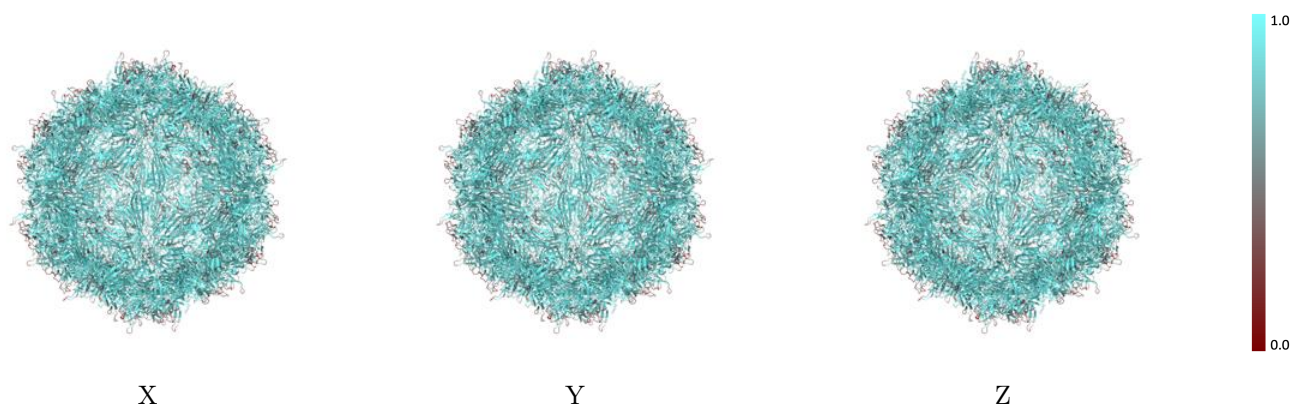
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



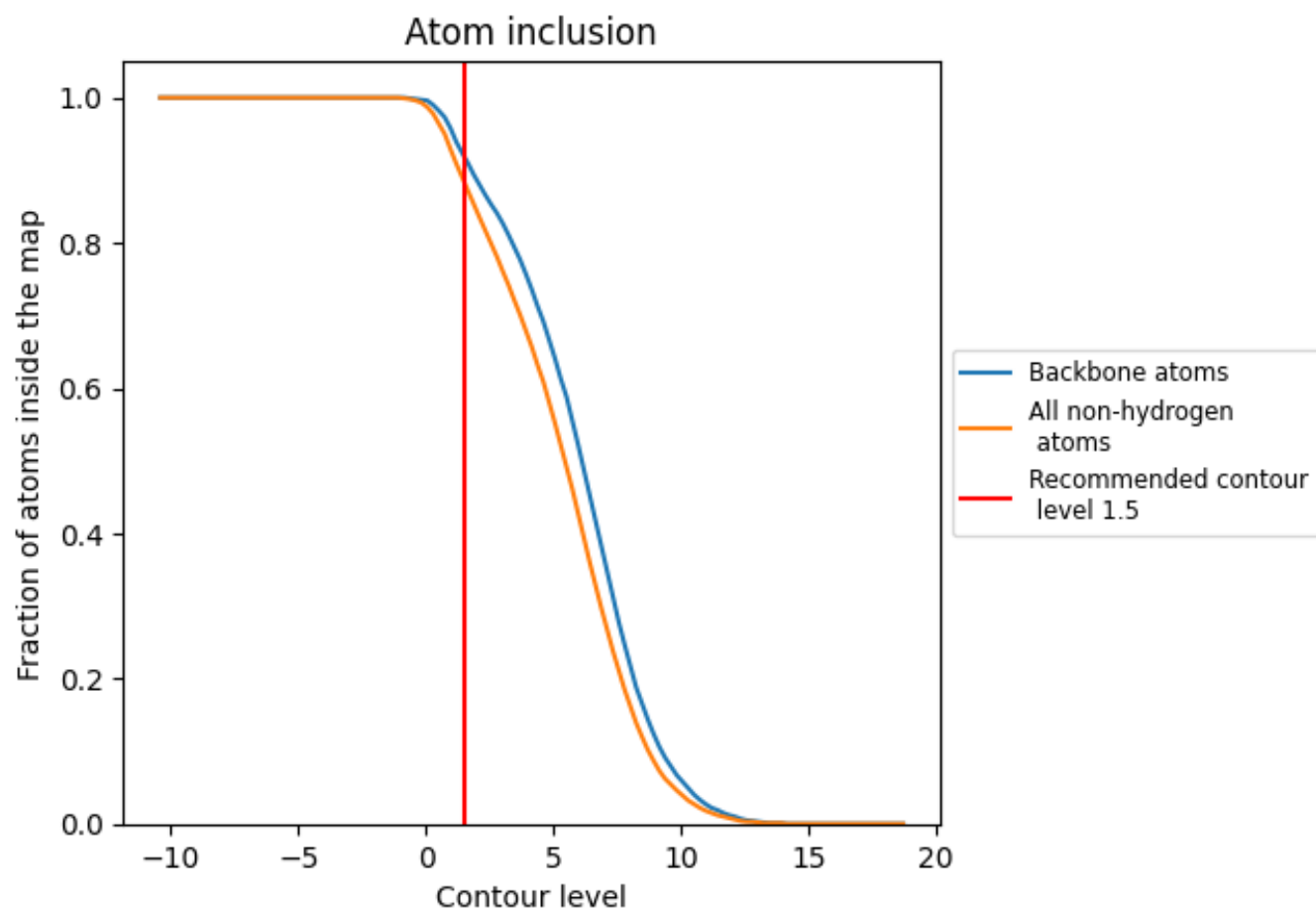
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (1.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8840   |  0.6160   |
| 1     |  0.8840   |  0.6170   |
| 2     |  0.8840   |  0.6160   |
| 3     |  0.8830   |  0.6150   |
| 4     |  0.8830   |  0.6160   |
| 5     |  0.8850   |  0.6160   |
| 6     |  0.8850   |  0.6160   |
| 7     |  0.8850   |  0.6160   |
| 8     |  0.8850   |  0.6170   |
| A     |  0.8830   |  0.6150   |
| B     |  0.8840   |  0.6180   |
| C     |  0.8830   |  0.6160   |
| D     |  0.8850   |  0.6160   |
| E     |  0.8850   |  0.6160   |
| F     |  0.8830  |  0.6150  |
| G     |  0.8850 |  0.6170 |
| H     |  0.8850 |  0.6160 |
| I     |  0.8830 |  0.6160 |
| J     |  0.8850 |  0.6170 |
| K     |  0.8830 |  0.6170 |
| L     |  0.8840 |  0.6160 |
| M     |  0.8850 |  0.6170 |
| N     |  0.8850 |  0.6170 |
| O     |  0.8850 |  0.6160 |
| P     |  0.8850 |  0.6170 |
| Q     |  0.8830 |  0.6170 |
| R     |  0.8840 |  0.6170 |
| S     |  0.8840 |  0.6160 |
| T     |  0.8830 |  0.6160 |
| U     |  0.8840 |  0.6170 |
| V     |  0.8830 |  0.6160 |
| W     |  0.8850 |  0.6170 |
| X     |  0.8850 |  0.6170 |
| Y     |  0.8850 |  0.6170 |
| Z     |  0.8850 |  0.6170 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.8830   |  0.6150   |
| b     |  0.8830   |  0.6150   |
| c     |  0.8830   |  0.6150   |
| d     |  0.8830   |  0.6160   |
| e     |  0.8830   |  0.6150   |
| f     |  0.8830   |  0.6150   |
| g     |  0.8830   |  0.6150   |
| h     |  0.8850   |  0.6170   |
| i     |  0.8850   |  0.6170   |
| j     |  0.8850   |  0.6170   |
| k     |  0.8850   |  0.6160   |
| l     |  0.8850   |  0.6160   |
| m     |  0.8830   |  0.6170   |
| n     |  0.8830   |  0.6150   |
| o     |  0.8850   |  0.6170   |
| p     |  0.8830   |  0.6160   |
| q     |  0.8840   |  0.6170   |
| r     |  0.8840   |  0.6170   |
| s     |  0.8840   |  0.6160   |
| t     |  0.8850  |  0.6160  |
| u     |  0.8830 |  0.6160 |
| v     |  0.8830 |  0.6160 |
| w     |  0.8850 |  0.6160 |
| x     |  0.8830 |  0.6150 |
| y     |  0.8830 |  0.6140 |
| z     |  0.8840 |  0.6170 |